DISCRETIZATION OF THE SCHRÖDINGER EQUATION

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1. Abstract

This paper describes the discretization of the time-independent Schrödinger equation. We discuss the formulation of the forward problem, as well as the recoverability of interior data in certain graphs when dealing with the inverse problem. Since this particular problem has not been worked on much, and there is not a lot of extant background theory, this paper's results are primarily exploratory.

2. Introduction

Construct a connected graph with boundary $G = (V, \partial V, E)$, where V is the set of all vertices v_i, $\partial V \subseteq V$ is the set of all boundary vertices, and E is the set of all edges e_{ij} connecting the i^{th} vertex to the j^{th} vertex. For our purposes, we will not distinguish between e_{ij} and e_{ji}, and we will allow loops such that an edge can start at a vertex and terminate at that same vertex.

A Schrödinger network is a graph G with boundary with two real-valued functions q and u defined on V. In this paper, q will be referred to as the potential and u will be referred to as the probability distribution.

In the continuous case, the Schrödinger equation is given by the formula

$$S_q u = \Delta u - qu = 0$$

.

However, since we are dealing with an analog of the Schrödinger equation for a graph, a discretized version is required, which is given by

$$S_{q_d} u(i) = \Delta_d u(i) - q(i)u(i) = \left(\sum_{j \in \mathcal{N}(i)} u(i) - u(j) \right) + q(i)u(i),$$

where $q(i)$ and $u(i)$ are the values of q and u on the i^{th} vertex, and $\mathcal{N}(i)$ is the set of the vertices that are connected to i by an edge.

3. The Forward Problem

To guarantee that the inverse problem exists, we must first solve the forward problem. To do this, we need to show that, given any boundary data, there exists exactly one set of interior data that satisfies the conditions of a Schrödinger network. The construction of the Schrödinger problem involves an $n \times n$ Kirchoff matrix K of the following form:

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$$K = \left[\begin{array}{c|c} A & B \\ \hline B^t & C \end{array}\right]$$

where the boundary-to-boundary connections are in the upper-left partition, the interior-to-boundary connections are in the upper-right and lower-left partitions, and the interior-to-interior connections are in the lower-right partition. For the construction of a Kirchoff matrix, the sum of the entries of any row (or column) is zero, and any non-zero entry at K_{ij}, when $i \neq j$, represents an edge joining vertex i to vertex j.

From here, we consider transforming the diagonal entries of K by adding to it another $n \times n$ matrix Q, which has the values of the Schrödinger potentials q_i on its main diagonal. It is of the form

$$Q = \begin{bmatrix} q_1 & 0 & \cdots & 0 \\ 0 & q_2 & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & q_n \end{bmatrix}$$

To complete the set-up of the forward problem, we will consider an $n \times 1$ vector U that contains each of the probability distributions u_i

$$U = \begin{bmatrix} u_1 \\ u_2 \\ \vdots \\ u_n \end{bmatrix}$$

such that when U is multiplied by $K + Q$ a corresponding vector Φ of the form

$$\Phi = \left[\begin{array}{c} \phi \\ \hline 0 \end{array}\right]$$

will be created, where the lower partition contains entries that are all zero, so as to show that each ϕ_i on the interior is zero. Also, each of the ϕ_i in the upper partition are the boundary readings. The data associated with a Schrödinger network can be summarized as follows:

$$(K + Q)U = \Phi.$$

Lemma 3.1. *The matrix $K + Q$ is symmetric.*

Proof. The addition of Q changes only the diagonal rows of K, so all other entries are preserved, and thus, by construction, K is symmetric, which implies that $K + Q$ is also symmetric. □

At this point, if we make certain restrictions on q, we have the following theorem:

Theorem 3.2. *If $\forall i \in int(V), q_i \geq 0$, the forward Schrödinger problem has exactly one solution.*

Proof. By the construction of the forward problem, there will be exactly one solution if the sub-matrix containing the interior-to-interior information of $K + Q$ is invertible. Now, if we view $K + Q$ as the partition

$$K + Q = \left[\begin{array}{c|c} A + Q_1 & B \\ \hline B^t & C + Q_2 \end{array}\right],$$

where Q_1 and Q_2 are the boundary and interior q_i, respectively, and take the Schur complement of $K+Q$, we have $A-B(C+Q_2)^{-1}B^T$. This is a legal operation as long as the matrix $C+Q_2$ is invertible. To establish that it is invertible, we note that because every q_i in the interior of G is non-negative, adding Q_2 to C (an already positive definite matrix) results in a non-negative number being added to each of the entries of the main diagonal of C, and so the matrix $C+Q_2$ is positive definite, and thus invertible. Hence, there is a unique solution to the forward Schrödinger problem. □

Since this theorem places restrictions on the interior q_i only, we can still have any values for the q_i on the boundary. Now that we have shown that the forward problem exists, we can consider the inverse problem.

4. The Inverse Problem

Given the response map Φ, as well as the u_i and the q_i on ∂V, the goal of the inverse problem is to determine q_i on each $i \in int(G)$. Before we work on recovering any q_i on the interior, we will establish a ratio of boundary to interior vertices that must be satisfied if there is any hope of recovering all of the interior q_i.

Theorem 4.1. *Given a graph with m boundary vertices and n interior vertices, it is impossible to recover all q_i if $\frac{m(m+1)}{2} < n$.*

Proof. We are given the map from the q_i to the response matrix $\Lambda = (A+Q)-B(C+Q_2)^-1B^T$. Our goal is show that this mapping is injective only if $\frac{m(m+1)}{2} \geq n$. Suppose that the q_i form a subset of $\Re^n_+$. Decomposing the matrix $K+Q$ as before, we know the information contained in $A+Q_1$, B, B^T and $A-B(C+Q_2)^-1B^T$. Because the only known information that is dependent on Q_2 is contained in $A-B(C+Q_2)^-1B^T$, the above statement is equivalent to saying that the mapping from $\Re^n_+$ to Λ is injective only if $\frac{m(m+1)}{2} \geq n$. We can view the set of all Λ as being a subspace of $\Re^{\frac{m(m+1)}{2}}$ because there are $\frac{m(m+1)}{2}$ potentially independent entries in the response matrix, with each of these entries being located above the main diagonal. Thus, we will consider the map from $\Re^n_+$ to $\Re^{\frac{m(m+1)}{2}}$. For this to be an injective mapping, by the invariance of domain, it is necessary to require that $\frac{m(m+1)}{2} \geq n$.

□

The above theorem provides an absolute minimum that must be satisfied to find the q_i. However, if there exist relationships between any of the known data, then, even if this restriction is satisfied, we still might not be able to determine the q_i on the interior of the graph.

If we avoid graphs that do not have enough independent information or structures in which the q_i are shown to not be recoverable, there are still many remaining graphs in which we can recover the q_i. One method is to write out the matrices symbolically and solve by using matrix algebra. We have the following theorem that demonstrates this tactic:

Theorem 4.2. *If we are given a graph that has an equal number of interior and boundary vertices such that each interior vertex is connected to exactly one boundary vertex, and vice versa, we can always determine the q_i on the interior.*

Proof. After partitioning $K+Q$ in the usual way and taking its Schur complement, we have the equation

$$(A+Q_1) - B(C+Q_2)^{-1}B^T = \Lambda.$$

Since there are an equal number of boundary and interior vertices, B and B^T are necessarily square matrices. Further, because every vertex $i \in \partial V$ is connected to one interior node only, the entries in B, and by extension B^T, will be permutations of the identity. Hence their columns will be linearly independent, and thus the matrices are invertible. From here, we can use matrix multiplication to solve for Q_2 as follows:

$$(A-Q_1) - B(C+Q_2)^{-1}B^T = \Lambda$$

$$\iff B(C+Q_2)^{-1}B^T = (A+Q_1) - \Lambda$$

$$\iff (C+Q_2)^{-1}B^T = B^{-1}[(A+Q_1) - \Lambda$$

$$\iff (C+Q_2)^{-1} = B^{-1}[(A+Q_1) - \Lambda](B^T)^{-1}$$

$$\iff Q_2 = [B^{-1}[(A+Q_1) - \Lambda](B^T)^{-1}]^{-1}.$$

This last expression for Q_2 determines exactly the values for the q_i on the interior for this entire class of graphs. □

The theorem above deals with a very special case of graphs, since B and B^T are frequently non-invertible. Another special case is the triangle-in-triangle graph shown below.

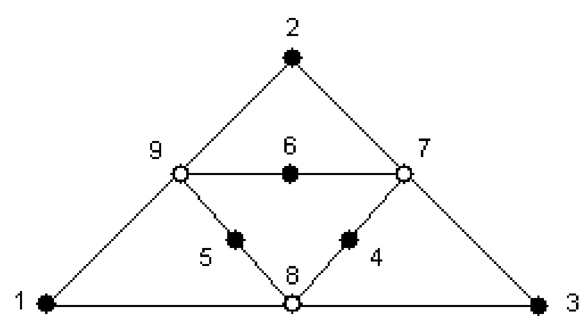

FIGURE 1. The triangle-in-triangle graph

This graph is constructed in such a way that it is almost a trivial practice to recover the q_i, since they can be read off nearly immediately.

Example 4.3. *We can recover the q_i on the interior in the triangle-in-triangle graph.*

Proof. If we write out the matrix $K+Q$, we have

$$K+Q = \begin{bmatrix} 2+q_1 & 0 & 0 & 0 & 0 & 0 & -1 & 0 & -1 \\ 0 & 2+q_2 & 0 & 0 & 0 & 0 & -1 & -1 & 0 \\ 0 & 0 & 2+q_3 & 0 & 0 & 0 & 0 & -1 & -1 \\ 0 & 0 & 0 & 2+q_4 & 0 & 0 & -1 & 0 & -1 \\ 0 & 0 & 0 & 0 & 2+q_5 & 0 & -1 & -1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 2+q_6 & 0 & -1 & -1 \\ -1 & -1 & 0 & -1 & -1 & 0 & 4+q_7 & 0 & 0 \\ 0 & -1 & -1 & 0 & -1 & -1 & 0 & 4+q_8 & 0 \\ -1 & 0 & -1 & -1 & 0 & -1 & 0 & 0 & 4+q_9 \end{bmatrix}$$

.

□

In addition to the restriction on the ratio of interior to boundary vertices, there are also certain graph structures in which we cannot recover the q_i on the interior. One such structure, pictured below, will be referred to as an "in-series connection", and is infinite-one.

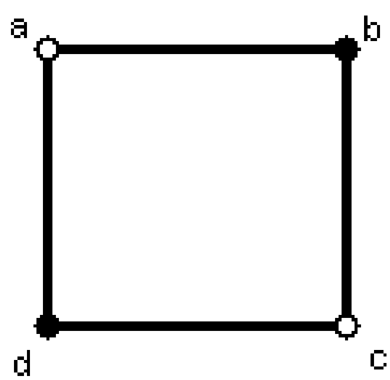

FIGURE 2. In-series connection. An example of an infinite-one graph

Theorem 4.4. *There are infinitely many values of possible q_i on the interior vertices of an in-series connection.*

Proof. Writing out $K+Q$ gives us

$$K+Q = \begin{bmatrix} 2+q_1 & 0 & -1 & -1 \\ 0 & 2+q_2 & -1 & -1 \\ -1 & -1 & 2+q_3 & 0 \\ -1 & -1 & 0 & 2+q_4 \end{bmatrix}$$

. Taking the Schur complement gives us

$$\Lambda = \begin{bmatrix} 2+q_1 & 0 \\ 0 & 2+q_2 \end{bmatrix} - \begin{bmatrix} -1 & -1 \\ -1 & -1 \end{bmatrix} \begin{bmatrix} \frac{1}{2+q_3} & 0 \\ 0 & \frac{1}{2+q_4} \end{bmatrix} \begin{bmatrix} -1 & -1 \\ -1 & -1 \end{bmatrix},$$

from which we get

$$\begin{bmatrix} 1 & 1 \\ 1 & 1 \end{bmatrix} \begin{bmatrix} \frac{1}{2+q_3} & \frac{1}{2+q_3} \\ \frac{1}{2+q_4} & \frac{1}{2+q_4} \end{bmatrix} = \begin{bmatrix} \frac{1}{2+q_3} + \frac{1}{2+q_4} & \frac{1}{2+q_3} + \frac{1}{2+q_4} \\ \frac{1}{2+q_3} + \frac{1}{2+q_4} & \frac{1}{2+q_3} + \frac{1}{2+q_4} \end{bmatrix} = \Lambda$$

The matrix above has only one meaningful entry, $\frac{1}{2+q_3} + \frac{1}{2+q_4}$, and it is an expression involving the sum of fractions containing q_3 and q_4, respectively. Since there are infinitely many choices for q_3 and q_4 that can be used to satisfy the above equation, this graph is necessarily infinite-one. □

Another method of determining the q_i is to read off information from a given graph and to form a system of equations from which q can be determined on the interior. This is done by writing out the conditions for a Schrödinger network that a given vertex must satisfy. To provide an example of this method, consider the familiar "top-hat" graph. It is one such graph that lends itself easily to determining the q_i on its interior in this fashion.

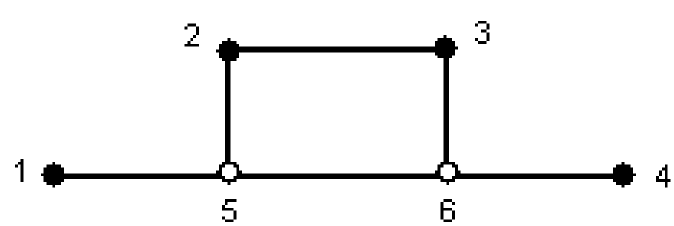

FIGURE 3. The top-hat graph

Example 4.5. *We can recover the interior q_i of a top-hat graph.*

Proof. If we write out the conditions of the Schrödinger equation on vertex 1, we get the equation

$$u_1 q_1 + (u_1 - u_5) = \phi_1,$$

where ϕ_1 is the boundary reading on the 1^{st} vertex. From here, since we are given u_1, q_1 and ϕ_1, we can determine u_5. In a symmetric argument, we can determine u_6. At this point, we can write out the Schrödinger equation for the 5^{th} vertex:

$$u_5 q_5 + (u_5 - u_1) + (u_5 - u_2) + (u_5 - u_6) = 0,$$

in which q_5 is the only unknown. If we can guarantee that u_5 is non-zero for some choice of boundary data, q_5 can be solved for using this expression. Since we are able to choose our boundary information, we will be able to construct a scenario in which $u_5 \neq 0$. Again, using a symmetric argument, q_6 can be found as well. □

This method can suffice for similar, small graphs, but the system of equations becomes intractable quickly as the number of vertices is increased. Another method is to use the connection-determinant formula, which is described in detail in [P-M], but will be only summarized here.

Theorem 4.6. *The connection-determinant formula. Suppose we are given a $k \times k$ matrix S containing all information contained in a Schrödinger network. Also, partition the matrix as before so that*

$$S = \left[\begin{array}{c|c} A + Q_1 & B \\ \hline B^t & C + Q_2 \end{array}\right].$$

Now, suppose that $S(P + C + Q_2; T + C + Q_2)$ is a sub-matrix of S, with P being a set of row indices in $A + Q_1$ and T being a set of column indices in $A + Q_1$, and $|P| = |T| = k$, for some $k \in \natural$. Then,

$$det[S(P + C + Q_2; T + C + Q_2)] = (-1)^k \Sigma$$

Corollary 4.7. *If we can form a unique connection between source and target vertices that uses all interior vertices, then $det\Lambda(S;T) = \frac{1}{det(C+Q_2)}$.*

Corollary 4.8. *If we can form a unique connection between source and target vertices that uses all but one interior vertex i, then $det\Lambda(S;T) = \frac{a+q_i}{det(C+Q_2)}$, where a is the number of vertices that i is connected to by an edge.*

This second corollary implies that under the right conditions, we can determine the value of q_i, because

$$q_i = det\Lambda(S;T)det(C + Q_2).$$

To provide an example of when the connection-determinant formula allows us to easily recover the interior q_i, consider the graph in Figure 3.

Example 4.9. *We can recover the interior q_i on the graph in Figure 3.*

Proof. We can form a set of connections, for example $(5, 4; 2, 3)$, such that each interior vertex is involved in exactly one of the connections. This allows us to determine the value of $det(C+Q_2)$. Now, if we can find a unique set of connections that uses all but one interior vertex i, we will have an equation in which q_i appears as the only unknown, since we know $det(C+Q_2$, which would allow us to determine its value. Consider the source and target vertices $(1, 5; 2, 3)$. There is only one way to make this connection, but it does not use the 7^{th} vertex. Using the formula in the second lemma above for this vertex gives us

$$q_7 = det\Lambda(S;T)det(C + Q_2),$$

from which we can determine the value of q_7. Use of a symmetric argument allows for the determination q_8. We cannot, however, use symmetry to find the values of the other q_i. However, we can find other unique connections to determine the other vertices. □

5. Special Cases

In the previous section, we showed methods to recover q on some graphs that did not contain in-series connections or that did not have a ratio of interior to boundary vertices that was too high. These methods made use of a great deal of boundary information, since the u, q and ϕ_i were given on the boundary. However,

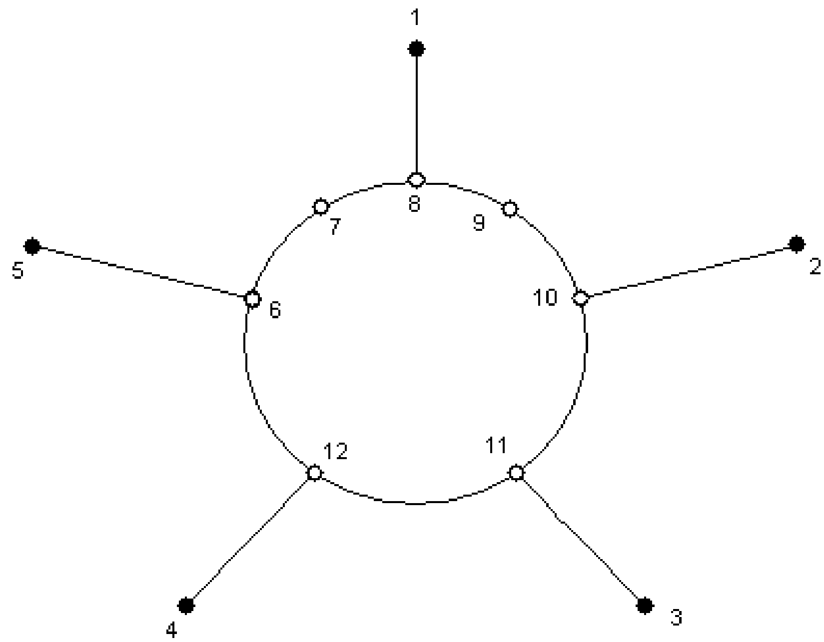

FIGURE 4. Circular graph with boundary spikes.

there are certain classes of graphs whose q_i can be recovered with somewhat relaxed conditions, such as having q_i known only on a proper subset of the boundary vertices.

For instance, Richard Oberlin described extensively the case of square lattices ([R-O]) with information about q known on only one face of the boundary. Another case is the top hat graph. With this graph, we never used the q_i appearing in vertices three and four. Because of this, we could have determined the interior q_i without any knowledge of those particular boundary q_i.

6. Future Research

There has been virtually no previous work done on Schrödinger networks, and thus there remains a large number of open questions. One class of these questions is: what similarities are there between Schrödinger networks and electrical networks? Is there an analog of the maximum/minimum principle? Is there such a structure that is "Schrödinger equivalent" in an analogous way to $Y - \Delta$ equivalence in the electrical network case? More generally, what would it mean for two graphs to be Schrödinger equivalent? What trivial modifications, if any, can be made to alter a Schrödinger network so its properties remain the same?

Also, in the case of the forward problem, we required that the q_i on the interior be nonnegative. However, since the matrix $C + Q_2$ needed only to be invertible, are there weaker conditions we can place on the q_i and retain the invertability of

$C + Q_2$? Is there also a way to form a weaker statement of the problem where we are given far less information on the boundary?

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