The Heat Equation and Periodic Boundary Conditions

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Abstract

In this paper, we will explore the properties of the Heat Equation on discrete networks, in particular how a network reacts to changing boundary conditions that are periodic. In the process we hope to eventually formulate an applicable inverse problem.

Contents

1 Introduction: The Discrete Heat Equation

The first thing that we will look at is discretizing the Heat equation. The continuous Heat Equation is:

$$v_t = k\ \Delta v = \nabla(\gamma \nabla v) \tag{1}$$

In the discrete case, we will form a Δ_γ that discretizes Δv on a graph; that is, we will form a matrix that operates on a vector $v(t)$ that represents the temperature at each of the nodes that satisfies this equation:

$$v_t = \Delta_\gamma v = -Kv \tag{2}$$

The discrete analog to Laplacian, Δ_γ, is defined as:

$$\Delta_\gamma v_i = \sum_{v_j \in N(v_i)} \gamma_{ij}(v_i - v_j) \tag{3}$$

where γ_{ij} is a kind of diffusivity constant from v_i to v_j. One important difference between this 'Kirchhoff Matrix' and the one we are familiar with in the Electrical Conductivity equation is that these γ_{ij}'s are normalized, in other words, $\sum\limits_{v_j \in N(v_i)} \gamma_{ij} = -1$. This means that the K is *not* symmetric. It also means that these γ_{ij}'s can be interpreted as transition probabilities.

For self-loops,

$$\gamma_{ii} = -\sum_{v_j \in N(v_i)} \gamma_{ij}$$

Because of this, the sum of any row of K is zero.

2 Discrete Time

The following is a version of our equation with time as a discrete variable. It's important to note that this is a mere analog to the continuous Heat Equation for the $\lim\limits_{\Delta t \to 0}$ of this equation does *not* give us the continuous version.

$$(\vec{v}_t)_{int} = (\vec{v}_{n+1} - \vec{v}_n)_{int} = (-K\ \vec{v}_n)_{int} \tag{4}$$

Note that this equation only refers to the interior of the graph. Rearranging the terms we get:

$$(\vec{v}_{n+1})_{int} = [(I - K)\ \vec{v}_n]_{int} \tag{5}$$

3 Introducing Our Problem: The Periodic Boundary Problem

Jim Morrow suggested the following problem: Take any network with boundary and interior nodes. Give some arbitrary boundary condition on the boundary nodes. Then find the temperature of each interior node by taking the average of the connected neighboring nodes at that time, i.e. multiplying the $\vec{v_n}$ by the transition matrix. Then rotate the boundary values, so that each boundary node takes the temperature of its neighbor boundary node. This is one time step. Repeat this process: average, rotate boundary values, average, rotate boundary values, etc.

4 Forming Notation

Typically for a network with m interior nodes and k exterior nodes we form a $k+m$ by $k+m$ transition matrix, P, that will act on the $(k+m)\times 1$ vector of nodes $\vec{v_n}$. Let's group the set of boundary nodes into a $k \times 1$ vector we'll call $\vec{f_n}$, where n denotes the time step, and the set of interior nodes into a $m \times 1$ vector we'll call $\vec{u_n}$.

$$\vec{v}_{n+1} = P.\vec{v}_n, \text{ where } \vec{v}_n = \begin{bmatrix} \vec{f}_n \\ \vec{u}_n \end{bmatrix}$$

We can partition this transition matrix, P, into four sub-matrices as follows:

$$P = \begin{bmatrix} Q & 0 \\ -C & (I-D) \end{bmatrix}$$

We set the upper right hand sub-matrix to zero because the boundary conditions do not depend on the interior temperatures.

$$\begin{bmatrix} Q & 0 \\ -C & (I-D) \end{bmatrix} \begin{bmatrix} \vec{f}_n \\ \vec{u}_n \end{bmatrix} = \begin{bmatrix} \vec{f}_{n+1} \\ \vec{u}_{n+1} \end{bmatrix}$$

Q is a permutation matrix that takes $\vec{f}_{n+1}$ to $\vec{f}_n$. Thus after one iteration,

$$\vec{f}_{n+1} = Q\ \vec{f}_n$$

$$\vec{u}_{n+1} = -C\vec{f}_n + (I-D)\vec{u}_n$$

Conjecture 4.1. *For any finite boundary period of order k, the sequence of vectors $u_1, u_2, \cdots, u_k$ corresponding to the interior nodes converge as the number of iterations goes to ∞.*

To illustrate the problem, let's look at the following example:

5 Examples: The H-graph

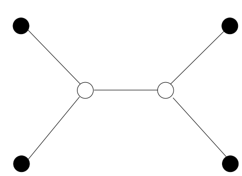

Figure 1: The H-Graph

The first example problem is the H graph. It has four boundary nodes and two interior nodes. A transition matrix might have the following form:

$$P = \begin{bmatrix} 0 & 0 & 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 \\ 1/3 & 0 & 0 & 1/3 & 0 & 1/3 \\ 0 & 1/3 & 1/3 & 0 & 1/3 & 0 \end{bmatrix}$$

The boundary function is defined as follows, $f_n = e_n$ where e_n is the unit vector in the nth dimension.

After many ($n > 30$) iterations, the vectors $\vec{v}_1$ through $\vec{v}_4$ converge to the following:

$$\vec{v}_1 = \begin{bmatrix} 1 \\ 0 \\ 0 \\ 0 \\ 7/20 \\ 3/20 \end{bmatrix}, \vec{v}_2 = \begin{bmatrix} 0 \\ 1 \\ 0 \\ 0 \\ 1/20 \\ 9/20 \end{bmatrix}, \vec{v}_3 = \begin{bmatrix} 0 \\ 0 \\ 1 \\ 0 \\ 3/20 \\ 7/20 \end{bmatrix}, \vec{v}_4 = \begin{bmatrix} 0 \\ 0 \\ 0 \\ 1 \\ 9/20 \\ 1/20 \end{bmatrix}$$

Two observations are made:

1. The sequence of vectors $\vec{v}_1$ through $\vec{v}_4$ reach steady states,
2. The values of the steady state vectors corresponding to a certain node, if summed, are equal to one.

The first observation agrees with conjecture, thus, so far our assumptions seem warranted. The second observation led us to the following further analysis.

6 A Solution to the Dirichlet Problem

Theorem 6.1. *The vector sum of these sequence of vectors is a solution to the Dirichlet problem.*

Proof. Using the definition of this problem's iteration we can write out the u_n's:

$$\begin{aligned} u_2 &= -C\vec{f}_1 + (I - D)\vec{u}_1 \\ u_3 &= -C\vec{f}_2 + (I - D)\vec{u}_2 \\ u_4 &= -C\vec{f}_3 + (I - D)\vec{u}_3 \\ &\vdots \\ u_k &= -C\vec{f}_{k-1} + (I - D)\vec{u}_{k-1} \\ u_1 &= -C\vec{f}_k + (I - D)\vec{u}_k \\ \sum_{i=1}^{k} \vec{u}_i &= -C\sum_{i=1}^{k} \vec{f}_i + (I - D)\sum_{i=1}^{k} \vec{u}_i \end{aligned}$$

$$\Rightarrow C\sum_{i=1}^{k} \vec{f}_i + D\sum_{i=1}^{k} \vec{u}_i = 0 \tag{6}$$

By observation this is the Dirichlet problem, $(K.\vec{u})_{interior} = 0$, written out in sub-matrix form. □

7 Proof of Convergence of the Sequence of Temperature Vectors

Theorem 7.1. *The temperature of interior nodes act independently of their initial temperature as the number of iterations goes to ∞.*

Proof.

$$
\begin{aligned}
u_1 &= u_{initial} \\
u_2 &= -Cf_1 + (I-D)u_1 \\
u_3 &= -Cf_2 + (I-D)(-B^T f_1 + (I-D)u_1) \\
u_4 &= -Cf_3 + (I-D)[-B^T f_2 + (I-D)(-B^T f_1 + (I-D)u_1)] \\
&\ \vdots \\
u_n &= (I-D)^{n-1}u_1 + \sum_{i=0}^{n-2}[-Cf_{n-i}(I-D)^i]
\end{aligned}
$$

We want to show that $\lim\limits_{n\to\infty}(I-D)^{n-1}u_1 = 0$.

In Tim Devries paper regarding random networks, it is shown that if the sum of the entries of every row of a matrix are ≤ 1 and the all the entries are ≥ 0, then $\lim\limits_{n\to\infty} M^n = 0$. The matrix $(I-D)$ has these properties, therefore $\lim\limits_{n\to\infty}(I-D)^{n-1} = 0$ and since by assumption u_1 is finite, their product also goes to 0. $\square$

Theorem 7.2. *For any finite boundary period of order k, the temperature vectors corresponding to the interior nodes converge as the number of iterations goes to ∞.*

To begin a proof of this theorem we must first introduce some new notation. Let's begin by forming a huge matrix, H, which contains all the boundary period data in one array.

$$
H.\vec{v} = \left[\begin{array}{cccc|cccc}
 & & I & & & & 0 & \\
\hline
0 & \cdots & 0 & -C & 0 & \cdots & 0 & I-D \\
-C & & & 0 & I-D & & 0 & \vdots \\
 & \ddots & 0 & \vdots & & \ddots & & \\
0 & & -C & 0 & 0 & & I-D & 0
\end{array}\right] \cdot \left[\begin{array}{c}
\vec{f}_1 \\ \vdots \\ \vec{f}_k \\ \hline \vec{u}_1 \\ \vdots \\ \vec{u}_k
\end{array}\right] \tag{7}
$$

One can check and see that this matrix is equivalent to

$$
\begin{aligned}
u_2 &= -C\vec{f}_1 + (I - D)\vec{u}_1 \\
u_3 &= -C\vec{f}_2 + (I - D)\vec{u}_2 \\
u_4 &= -C\vec{f}_3 + (I - D)\vec{u}_3 \\
&\vdots \\
u_k &= -C\vec{f}_{k-1} + (I - D)\vec{u}_{k-1} \\
u_1 &= -C\vec{f}_k + (I - D)\vec{u}_k
\end{aligned}
$$

Let's rename the sub-matrices of H for convenience. The lower left sub-matrix consisting of C's on the diagonal we will call E. The lower right matrix consisting of the $(I - D)$'s we will call F. The above equation can then be rewritten as follows:

$$
\left[\frac{\vec{f}}{\vec{u}}\right]_{iterated} = H.\left[\frac{\vec{f}}{\vec{u}}\right] = \begin{bmatrix} I & 0 \\ E & F \end{bmatrix} . \left[\frac{\vec{f}}{\vec{u}}\right] \tag{8}
$$

where

$$
\vec{f} = \begin{bmatrix} f_i \\ \vdots \\ f_k \end{bmatrix}, \vec{u} = \begin{bmatrix} u_i \\ \vdots \\ u_k \end{bmatrix}
$$

We need to find the fixed point of this equation. For the lower half of the vector we get $E.\vec{f} + F.\vec{u} = \vec{u}$. Manipulating this equation we can get

$$
(I - F).\vec{u} = E.\vec{f} \tag{9}
$$

$$
\vec{u} = (I - F)^{-1}E.\vec{f} \tag{10}
$$

Here, finally, we near a closed form for $\vec{u}$. The solution for $\vec{u}$ depends directly on the invertibility of the matrix $(I - F)$. We'll prove that this matrix, $(I - F)$, is invertible by proving that the series $I + F + F^2 + F^3 + ...$ is convergent.

Theorem 7.3. *If every entry is ≥ 0 and the sum of the entries of every row of M are ≤ 1, Then:*

$$
\sum_{n=1}^{\infty} M^n \ \textit{converges}
$$

Proof. Referring to Tim Devries proof in his paper Recoverability of Random Walk Networks we see that these are the conditions to make his proof work. □

8 Conclusions

1. We have found a generalized solution to the Dirichlet problem for networks.
2. We have proved that for any graph with rotating boundary conditions the sequence of temperature vectors converge as the number of iterations goes to ∞.

References

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