The parametrix construction of the heat kernel on a finite graph in different timescales

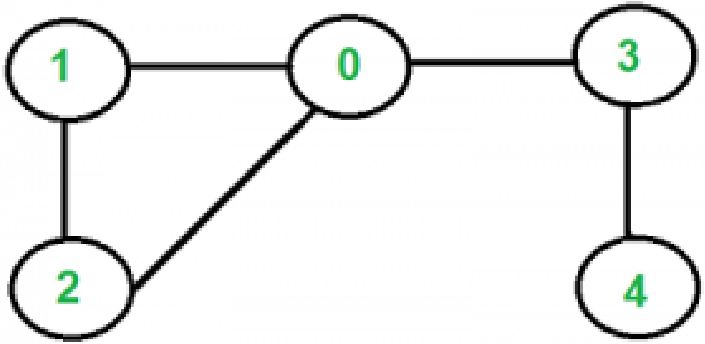
Yang Chen, Luis Lopez, Fangfang Lyu

July 20, 2023

Introduction to the problem

Have you ever wondered how to find the the heat energy at a specific point of a spoon 5 minutes later?

Now think of websites with links to other sites.



If there are 100 people entered the website through the main page 0, can we find out the number of people at website 4 after 5 minutes? 10 minutes? This is analogous to the transfer of heat, which we can also model such diffusion with an heat kernel.

Heat Kernel

Definition

The heat kernel $H_G(v_1, v_2; t)$ in $VG \times VG \times \mathbb{T}$ is a fundamental mathematical concept used to describe the diffusion of heat or other quantities over time. It is a fundamental solution to the heat equation.

Definition

Let G be the graph G, VG is the set of all vertices, and w_{xy} is the weight of the edge between x and y. The graph Laplace operator Δ_{G,v_1} is defined in as $f : VG \to \mathbb{C}$:

$$\Delta_{G,v_1} f = \sum_{y \in VG} (f(v_1) - f(y)) w_{v_1 y}$$

where we say Δ_{G,v_1} is the graph Laplacian on G acting on the first variable v_1 of f.

Definition

The heat kernel on real timescale $\mathbb{R}$ is defined as the following:

$$\left(\Delta_{G,v_1} + \frac{\partial}{\partial t}\right) H_G(v_1, v_2; t) = 0$$

with initial condition such that

$$\lim_{t \to t_0} H_G(v_1, v_2; t) = \begin{cases} 1 & \text{if } v_1 = v_2 \\ 0 & \text{if } v_1 \neq v_2 \end{cases}$$

Definition

For function $f(v_1, v_2; t) : VG \times VG \times \mathbb{T} \to \mathbb{R}$ that is differentiable as a function of t for any choice of $(v_1, v_2) \in VG \times VG$, the heat operator L_{v_1} is defined as such:

$$L_{v_1} := (\Delta_{G,v_1} + \Delta_t) f(v_1, v_2; t) \tag{1}$$

Motivation in different timescales

Why do we want to generalize the heat kernel equation for various of timescales? Time can be modeled as either continuous or discrete, depending on the context and the level of detail required in the analysis.

Example

In stock market, the meaning of day from Monday to Tuesday is different from Friday to Monday is different. So one could have a nonstandard timescale to accommodate the need.

Example

Population growth varies yearround. In certain month, one can have continuous growth at an interval of time, combined with a discrete growth on a set of time. Combine them together, we will end up with another nonstandard timescale.

Basic definitions

Time scale $\mathbb{T}$ is any non-empty closed subset of $\mathbb{R}$.

Examples

$\mathbb{Z}$, Cantor set, Quantum time scale: $q^{\mathbb{N}_0} = \{1, q, q^2, q^3, ...\}$ with $q > 1$.

Definition

For $t \in \mathbb{T}$ and $\sigma, \mu : \mathbb{T} \to \mathbb{T}$.

1. The *forward operator* σ is defined as $\sigma(t) := \inf\{s \in \mathbb{T} : s > t\}$.
2. The *graininess function* μ is defined as $\mu(t) := \sigma(t) - t$.

Examples

$\mathbb{T} = \mathbb{R}$: $\sigma(t) = t$, and $\mu(t) = 0$.
$\mathbb{T} = \mathbb{Z}$: $\sigma(t) = t + 1$, and $\mu(t) = 1$.

Classification of points and Continuity in $\mathbb{T}$

Definition

Let $t \in \mathbb{T}$. The point t is called a *dense* point, if there exist some sequences $\{x_n\}$ and $\{y_n\}$ approaching t from the left and the right respectively, such that each x_n and y_n are not equal to t.

The point t is called a *scattered* or *isolated* point otherwise.

Examples

$\mathbb{T} = \mathbb{R}$: every point is dense. $\mathbb{T} = \mathbb{Z}$: every point is scattered.

Definition (Continuity)

Let $f : [a, b]_{\mathbb{T}} \to \mathbb{R}$ and $x \in [a, b]_{\mathbb{T}}$. f is continuous at x_0 if for every $\epsilon > 0$ there exists a $\delta > 0$ such that $|x - x_0| < \delta$ implies $|f(x) - f(x_0)| < \epsilon$.

$[a, b]_{\mathbb{T}} = [a, b] \cap \mathbb{T}$.

Examples

$\mathbb{T} = \mathbb{Z}$: every function is continuous.

Differentiation in $\mathbb{T}$

Definition (Delta-Derivative)

We define the derivative $f^{\Delta}(t)$ as the number with the property that given any $\epsilon > 0$, there is a neighborhood of U of t such that
$|f(s) - f(\sigma(t)) + f^{\Delta}(t)(s - \sigma(t))| \leq \epsilon|s - \sigma(t)|\ \forall s \in U$.

Examples

$\mathbb{T} = \mathbb{R}$: $f^{\Delta}(t) = f'(t)$
$\mathbb{T} = \mathbb{Z}$: $f^{\Delta}(t) = f(t+1) - f(t)$ (Forward difference).

Some properties of derivatives in $\mathbb{T}$

Let $f, g : \mathbb{T} \to \mathbb{R}$ be differentiable functions and $t \in \mathbb{T}^\kappa$. Then we have the following:

1. If f is differentiable at t, then f is continuous at t.
2. The sum $f + g$ is differentiable at t with $(f+g)^\Delta(t) = f^\Delta(t) + g^\Delta(t)$
3. For any constant c, the function (cf) is differentiable at t with $(cf)^\Delta(t) = cf^\Delta(t)$
4. The product fg is differentiable at t with $(fg)^\Delta(t) = f^\Delta(t)g(t) + f(\sigma(t))g^\Delta(t)$
5. The quotient $\left(\frac{f}{g}\right)$ is differentiable at t with $\left(\frac{f}{g}\right)^\Delta = \frac{f^\Delta(t)g(t) - f(t)g^\Delta(t)}{g(t)g(\sigma(t))}$ provided $g(t) \neq 0$ and $g(\sigma(t)) \neq 0$.

Integration in $\mathbb{T}$

Similar to integration in $\mathbb{R}$, We define integration in any time scale $\mathbb{T}$ as the "inverse operation" of differentiation.

Definition

For $F : \mathbb{T} \to \mathbb{R}$ is an antiderivative of $f : \mathbb{T} \to \mathbb{R}$ if

$$F^{\Delta}(t) = f(t), \text{ for all } t \in \mathbb{T}^{\kappa}$$

$$F(t) := \int_{t_0}^{t} f(\tau)\Delta\tau, t \in \mathbb{T}$$

The indefinite delta-integral of $f(t)$ is defined as

$$\int f(t)\Delta t = F(t) + C, \text{ where C is an arbitrary constant}$$

The definite delta-integral of $f(t)$ is defined as

$$\int_{r}^{s} f(t)\Delta t = F(s) - F(r) \text{ for all } r, s \in \mathbb{T}$$

Examples and properties of integral

Example

$\mathbb{T} = \mathbb{R}$: $\int_r^s f(t)\Delta t = \int_r^s f(t)dt$ (Area under the curve)
$\mathbb{T} = \mathbb{Z}$: $\int_r^s f(t)\Delta t = \sum_{n=r}^{s-1} f(n)$. (Sum of area of rectangles with height= f(n) and width =1)

Let $f, g : \mathbb{T} \to \mathbb{R}$ be integrable functions on $[a, b]_{\mathbb{T}}$, then we have the following:

1. Continuity of f implies delta-integrability.
2. $\int_a^b \alpha f(t) + \beta g(t)\Delta t = \int_a^b \alpha f(t)\Delta t + \int_a^b \beta g(t)\Delta t$ for any constants α, β.
3. $\int_a^b f(t)\Delta t = -\int_b^a f(t)\Delta t$.
4. (FTC) Every rd-continuous function has an antiderivative. In particular if $t_0 \in \mathbb{T}$, then F defined by

$$F(t) := \int_{t_0}^{t} f(\tau)\Delta\tau \qquad \textit{for} \;\; t \in \mathbb{T}$$

is an antiderivative of f ($F(t)$ is differentiable at t).

Convolution when $\mathbb{T} = \mathbb{R}$

When $\mathbb{T} = \mathbb{R}$, the convolution of two functions f and g is defined as:

$$(f * g)(t) = \int_{t_0}^{t} f(t - s + t_0) g(s) \, \mathrm{d}s$$

usually set $t_0 = 0$.
We called the function $f(t - s + t_0)$ the *shift* of f in $\mathbb{R}$ and denote it by $\hat{f}$.

A natural question to ask is:
What is the shift of f in any time scale $\mathbb{T}$? is it $f(t - s + t_0)$?

Consider Quantum time-scale: $q^{\mathbb{N}_0} = \{1, 2, 4, 8, 16, \ldots\}$ where $q = 2$.
Observe that the value $t - s + t_0 \notin 2^{\mathbb{N}_0}$, if we let
$t_0 = 1, t = 8, s = 4 => 8 - 4 + 1 = 5 \notin 2^{\mathbb{N}_0}$.

The shifting problem

For a given $f : [t_0, \infty) \to \mathbb{C}$ the solution of the shifting problem

$$u^{\Delta_t}(t, \sigma(s)) = -u^{\Delta_s}(t, s) \qquad t \in \mathbb{T},\ t \geq s \geq t_0$$

$$u(t, t_0) = f(t) \quad ,\ t \geq t_0,$$

is denoted by $\hat{f}$ and is called the *shift* of f .

Examples

When $\mathbb{T} = \mathbb{R}$, the unique solution to this shifting problem is $\hat{f}(t, s) = f(t - s + t_0)$.
Since $\frac{\partial \hat{f}}{\partial t} = f^{'}(t - s + t_0) = -\frac{\partial \hat{f}}{\partial s}$ and $\hat{f}(t, t_0) = f(t)$.
When $\mathbb{T} = \mathbb{Z}$, the unique solution is $\hat{f}(t, s) = f(t - s + t_0)$.
When $\mathbb{T} = q^{\mathbb{N}_0}$, the shift of f is $\sum_{\nu=r}^{k} \binom{k}{\nu}(1 - t)_q^{k-\nu} f(q^{\nu})$.

Convolution in $\mathbb{T}$

Definition

We define the *time convolution* in $\mathbb{T}$ to be:

$$(f * g)(t) = \int_{t_0}^{t} \hat{f}(t, \sigma(s)) g(s) \Delta s, \text{ for } t \in \mathbb{T}$$

This operation is associative and distributive but not commutative in general (Although, it is commutative in $\mathbb{R}$).

Graph Convolution

Definition

Let $F_1, F_2 : VG \times VG \times \mathbb{T} \to \mathbb{R}$. The *graph convolution* of functions F_1 and F_2 is defined to be

$$(F_1 *_G F_2)(v_1, v_2; t) := \sum_{v \in VG} \int_{t_0}^{t} \hat{F}_1(v_1, v, t, \sigma(s)) F_2(v, v_2; s) \Delta s$$

Parametric I

Definition

A parametrix for the heat operator on G is any function $f : VG \times VG \times \mathbb{T}$ such that:

1. For all $v_1, v_2 \in VG$, the function $f(v_1, v_2, t)$ is continuous in the variable t on $[t_0, \infty)_{\mathbb{T}}$ and continuously differentiable in the variable t on $(t_0, \infty)_{\mathbb{T}}$ such that $f^{\Delta t}(v_1, v_2, t)$ extends to a continuous function on $[t_0, \infty)_{\mathbb{T}}$.
2. For all $v_1, v_2 \in VG$,
   1. (i) $\hat{f}(v_1, v_2, t, s)$ is a continuous function in the variables t and s on $[t_0, \infty)_{\mathbb{T}}$ and differentiable in t and s on $(t_0, \infty)_{\mathbb{T}}$ such that $\hat{f}^{\Delta t}(v_1, v_2, t, s)$ and $\hat{f}^{\Delta s}(v_1, v_2, t, s)$ have continuous extensions on $[t_0, \infty)_{\mathbb{T}}$.
   2. (ii) $\hat{f}^{\Delta t}(v_1, v_2, t, s)$ and $\hat{f}^{\Delta s}(v_1, v_2, t, s)$ are Δs and Δt differentiable on $(t_0, \infty)_{\mathbb{T}}$, respectively, such that $\hat{f}^{\Delta t \Delta s}(v_1, v_2, t, s) = \hat{f}^{\Delta s \Delta t}(v_1, v_2, t, s)$ when extended to functions on $[t_0, \infty)_{\mathbb{T}} \times [t_0, \infty)_{\mathbb{T}}$.

Parametric (Cont.) I

3. (Dirac Delta condition)

If t_0 is right-dense, then for all $v_1, v_2 \in VG$,

$$\lim_{t \to t_0^+} f(v_1, v_2, t) = \begin{cases} 1 & \text{if } v_1 = v_2 \\ 0 & \text{if } v_1 \neq v_2 \end{cases}$$

If t_0 is right-scattered, then for all $v_1, v_2 \in VG$,

$$f(v_1, v_2, t) = \begin{cases} 1 & \text{if } v_1 = v_2 \\ 0 & \text{if } v_1 \neq v_2 \end{cases}$$

The parametrix construction of the heat kernel on G

Theorem (Parametrix Construction)

Let $f : VG \times VG \times \mathbb{T}$ *be a parametrix. Then, the function*

$$H_G(v_1, v_2; t) = f(v_1, v_2; t) + (f *_G F)(v_1, v_2; t)$$

is a heat kernel on G *in timescale* $\mathbb{T}$*, where*
$F(v_1, v_2; t) = \sum_{\ell=1}^{\infty} (-1)^{\ell} (L_{v_1} f)^{*_G \ell}(v_1, v_2; t)$.

Lemma 1

Lemma

Let $f(v_1, v_2; t)$ be a parametrix function on graph G in any timescale $\mathbb{T}$, and let g be any continuous function in $VG \times VG \times [t_0, \infty)_{\mathbb{T}}$. Then,

$$L_{v_1}(f *_G g)(v_1, v_2; t) = (L_{v_1} f *_G g)(v_1, v_2; t) + g(v_1, v_2; t)$$

Lemma 2

Lemma

Let $f : VG \times VG \times \mathbb{T} \to \mathbb{R}$ such that $\hat{f}$ exists. If one of the following statements holds true:
For (i), assume further that for any fixed $T, t_0 \in \mathbb{T}$ with $T \geq t_0$ and any $v_1, v_2, v \in VG$, the function $\hat{f}(v_1, v; t, \sigma(s))f(v, v_1, s)$ is integrable on $[t_0, t]_{\mathbb{T}}$ for any $t \leq T$.

(i) *There exist $C, \hat{C} \geq 0$ such that $|f(v_1, v_2; t)| \leq C$ and $|\hat{f}(v_1, v_2; t, s)| \leq \hat{C}$ for all $v_1, v_2 \in VG$, $t, s \in \mathbb{T}$ with $s \geq t_0$.*

Then the series

$$\sum_{\ell=1}^{\infty} (-1)^{\ell} (f)^{*_G \ell}(v_1, v_2; t) \tag{2}$$

converges absolutely and uniformly on every compact subset of $VG \times VG \times \mathbb{T}$.

Proof of Main Theorem

Proof.

We want to show that $L_{v_1} H_G(v_1, v_2; t) = 0$ for all $v_1, v_2 \in VG$ and $t \in [t_0, \infty)$. We start with the equation:

$$L_{v_1} H_G(v_1, v_2; t) = L_{v_1} f(v_1, v_2; t) + L_{v_1}(f *_G F)(v_1, v_2, t).$$

Using Lemma 1, we have:

$$= L_{v_1} f(v_1, v_2; t) + (L_{v_1} *_G F)(v_1, v_2; t) + F(v_1, v_2; t).$$

Expanding the series, we have a telescoping series:

$$= L_{v_1} f(v_1, v_2; t) + \sum_{\ell=1}^{\infty} (-1)^{\ell} (L_{v_1} f)^{*_G \ell+1}(v_1, v_2; t) + \sum_{\ell=1}^{\infty} (-1)^{\ell} (L_{v_1} f)^{*_G \ell}(v_1, v_2; t).$$

Notice that the telescoping series cancels out, resulting in:

$$L_{v_1} H_G(v_1, v_2; t) = 0.$$

Family of Functions

We will define a class of functions $f : VG \times VG \times \mathbb{T} \to \mathbb{R}$ analogous to functions in class F in The Convolution on Time Scales.

Definition

Assume that $\sup \mathbb{T} = \infty$ and $t_0 \in \mathbb{T}$ is fixed. We define functions in class F from $VG \times VG \times \mathbb{T} \to \mathbb{R}$ as a series of the form

$$f(v_1, v_2; t) = \sum_{k=1}^{\infty} a_k(v_1, v_2) h_k(t, t_0), \quad v_1, v_2 \in VG, t \in (t_0, \infty], \tag{3}$$

where for each coefficient $a_k(v_1, v_2)$ satisfies the following:

$$|a_k(v_1, v_2)| \leq M(v_1, v_2) R(v_1, v_2)^k$$

We have the following property:

1. $\hat{f}(v_1, v_2; t, s) = \sum_{k=1}^{\infty} a_k(v_1, v_2) h_k(t, s), \quad v_1, v_2 \in VG, t \in (t_0, \infty]$

Example of a Function in Class F

An example of a function in class F is the I-Bessel function in any arbitrary timescale $\mathbb{T}$:

$$I_n(t) := \sum_{k=1}^{\infty} \binom{n+2k}{k} \frac{1}{2^{2k}} h_{n+2k}(t, t_0).$$

Since $\binom{n+2k}{k} \frac{1}{2^{2k}} \leq \frac{2^{n+2k}}{2^{2k}} = 2^n$ for all $k \in \mathbb{N}_0$,

by $\sum_{l=0}^{m} \binom{m}{l} = 2^m$.

Behavior of $I_n(t)$ as $t \downarrow t_0$

$$I_n(t) = \begin{cases} 1 & \text{if } n = 0 : v_1 = v_2, \\ 0 & \text{otherwise.} \end{cases}$$

A Glimpse Into the Future

In the future, our project aims to explore the following aspects:

1. Determining the uniqueness of the heat kernel in different time scales.
2. Spectral Expansion of the Heat Kernel.
3. Constructing Numerical Examples.
4. Determining the behavior of our solution in different time scales.

The end

Thank you for your attention!