UNIVERSITY OF CALIFORNIA, BERKELEY
MATH 127 PROJECT 2, GROUP 5

Protein Structure Determination

Will Sumfest, Noreen Wauford, Benjamin Chu, and Jonathan Boyle

May 8, 2016

1 INTRODUCTION

2 MATHEMATICAL MODEL

3 METHOD: THREE ALGORITHMS

4 RESULTS

5 EXTRA DELIVERABLE: THE HEAT EQUATION

5.1 INTRODUCTION AND MOTIVATION

So far our entire project relied heavily on concepts such as convolution and fourier series. These are crucial concepts under the field of Fourier Analysis, which arose during the early 19th century due to the mathematician Joseph Fourier's development of a solution to the famous **Heat Equation**. It has many diverse applications not only in engineering and industry, but also in biology. For instance, understanding bioheat transfer phenomena relies on constructing solutions to the heat equation for a variety of different scenarios. Due to its appearance in so many problems, our group was interested in the following motivating problem: *how do we model the transfer of heat through a system*? We will be looking at the 1D heat equation from 2 angles: the 1D-homogeneous and n-D inhomogeneous heat equation.

The analytical solution to the 1D Heat Equation with constant boundary conditions which we derive and the numerical simulation of the same problem which we implement (see 5.2 and

5.3) account for a very narrow subset of possible conditions which the Heat Equation is intended to model. In particular, the **homogeneous** equation assumes no introduction of heat to the system from external sources. Furthermore, the single dimensional constant boundary conditions further limits the applicability of the methods described in sections 5.2 and 5.3. We attemp to mitigate these problems by considering the **inhomogeneous** equations in $\mathbb{R}^n$, representing the introduction of heat to the system in question from an outside source. For this kind of equation, we appeal to the use of the fundamental solution, a general solution to the heat operator. We conclude the study with a discussion of the philosophical implications of the fundamental solution.

5.2 DERIVATION OF 1D SOLUTION

The 1D Heat Equation describes a deceptively simple physical problem with a number of assumptions. We consider a straight metal rod of homogenous composition and shape with unequal distribution of heat, insulated such that heat can only flow along the bar in the horizontal direction. After some time t has passed, what is the heat at position x? The Heat Equation is a partial differential equation (PDE) that gives the solution to this question as a function in x and t. We denote this solution as $u(x,t)$.

In one dimension, the heat equation is written $u_t = \alpha^2 u_{xx}$. This equation relates the first partial derivative of $u(x,t)$ with respect to time to the second partial derivative of the same function with respect to position. The latter differential is proportional with respect to the former by a factor of α^2, a constant representing the temperature gradient of the rod. Fourier's Law of Thermal Conductivity, a physical principle invoked to solve The Heat Equation, states that the rate of temperature change with respect to position is inversely proportional by a factor of to the heat transferred over time. In more simple terms, this implies heat is transferred from areas of high temperature to areas of low temperature, a relatively intuitive concept.

Certain conditions must be taken into account in the process of solving the Heat Equation. For a more straightforward derivation of the solution, we first consider the initial condition $u(x,0) = f(x)$, and boundary value conditions $u(0,t) = u(L,t) = 0$, where L is the length of the rod.

The initial condition describes the initial temperature as a function of x. We consider partial differentiation of $u(x,t)$ with respect to time as a linear operator A which transforms $u(x,t)$. By the statement of The Heat Equation, this is:

$$ut = Au, \qquad A = \alpha^2 \partial_x^2$$

The vector space we are concerned with is the infinite-dimensional vector space of continuous periodic functions (which we denote as V), the elements of which Fourier determined could be written as a linear combination of sine and cosine basis functions. The Fourier Decomposition of a function is just such a linear combination. Given a function $f : \mathbb{R} \to \mathbb{R}$ with period T, we write

$$f(x) = a_0 + \sum_{n=1}^{\infty} a_n \sin(\frac{2\pi n x}{T}) + \sum_{n=1}^{\infty} b_n \cos(\frac{2\pi n x}{T}),$$

where a_i, b_i are known as "Fourier Coefficients", which can be computed as inner products on V:

$$a_0 = \langle f(x), \frac{1}{T} \rangle = \frac{1}{T} - \int_{\frac{1}{T}}^{\frac{-1}{T}} f(x) dx$$

$$a_n = \langle f(x), \frac{2}{T} \sin(\frac{2\pi n x}{T}) \rangle = \frac{2}{T} \int_{\frac{1}{T}}^{\frac{-1}{T}} f(x) \sin(\frac{2\pi n x}{T}) dx$$

$$b_n = \langle f(x), \frac{2}{T} \cos(\frac{2\pi n x}{T}) \rangle = \frac{2}{T} \int_{\frac{1}{T}}^{\frac{-1}{T}} f(x) \cos(\frac{2\pi n x}{T}) dx$$

Eigenvalues of this linear operator are of the form $\lambda_n = \frac{-n^2\pi^2\alpha^2}{L^2}$, with corresponding eigenvectors $v_n = \sin(\frac{n\pi x}{L})$, as the function $u(x,t)$ is 0 on the bounds of its period as are sine functions. This yields a general solution of the form:

$$u(t) = \sum_{n=1}^{\infty} c_n v_n \exp(\lambda_n t)$$

Furthermore, if we are to represent our basis for V with a basis consisting of A's eigenvectors, $u(x,t) = \sum_{n=1}^{\infty} c_n \exp(\frac{-n^2\pi^2\alpha^2}{L^2})$, thus $u(x,0) = \sum_{n=1}^{\infty} c_n \sin(\frac{n\pi x}{L})$. To finally solve for the constant terms of the linear combination with which we represent $u(x,t)$, we employ a Fourier Transform of $f(x)$, the initial condition.

$$c_n = \frac{2}{L} \int_0^{\infty} f(x) \sin(\frac{n\pi x}{L}) dx$$

Let us now consider the case where our boundary values do not dictate that the ends of the rod remain constant, but rather the rate of change of their temperature. Hence, $u_t(0,t) = u_t(L,t) = 0$. A's eigenvalues are once again $\lambda_n = \frac{-n^2\pi^2\alpha^2}{L^2}$, but now that boundary values are not constant, its eigenvectors are of the form $v_n = a \in \mathbb{R} and v_n = \cos(\frac{n\pi x}{L})$, as boundary temperatures need not equal 0. Taking the eigenvectors of A as a basis for V, we now represent the general solution as a linear combination of the form

$$u(x,t) = a_0 + \sum_{n=1}^{\infty} d_n \exp(-\frac{n^2\pi^2\alpha^2}{L^2} t) \cos(\frac{n\pi x}{L})$$

For this form of the general solution, we compute our coefficients as follows:

$$a_0 = \frac{1}{L} \int_0^{\infty} f(x) dx$$

$$d_n = \frac{2}{L} f(x) \cos(\frac{n\pi x}{L}) dx$$

5.3 Numerical Simulation Problem Statement

5.3.1 Approximation Scheme: Forward Transfer Centered Space

In order to visualize the implications of the 1D Heat Equation for a given time t, it is useful to implement programming tools to produce a graphical representation of the function $u(x,t)$.

The object of this algorithm, known as "Forward Transfer Centered Space", and the implemented MATLAB function ZeroBoundsHeatFTCS.m, outlined in the paper Finite Difference Approximations to the Heat Equation, by G. Recktenwald. The plots output by ZeroBoundsHeatFTCS.m have the x-axis representing the horizontal space coordinate along the rod, and the y-axis representing the magnitude of heat u, where the graph itself is fixed at a given time t.

Approximating a differential equation numerically hinges on the the simple definition of tangent line slope as the "rise over run" of a function. In this context: $\partial u \approx \frac{u_{i+1}-u_i}{\Delta x}$, where u is evaluated for a set of discrete x-values.

A forward difference approximation of a differential equation evaluates the derivative at the ith point with computations involving the function value at the ith x-coordinate and (i+1)th x-coordinate. A central difference approximation uses the values at the $(i-1)^{th}$, i^{th}, and $(i+1)^{th}$ coordinates. Using a central difference approximation at time m, the second partial derivative of u with respect to x is as follows:

$$\partial^2 u \approx \frac{u_{i-1}^m - 2u_i^m + u_{i+1}^m}{\Delta x^2}$$

Substituting a forward difference approximation of the first partial derivative of u with respect to t and the above equation into the 1D Heat Equation, we arrive at:

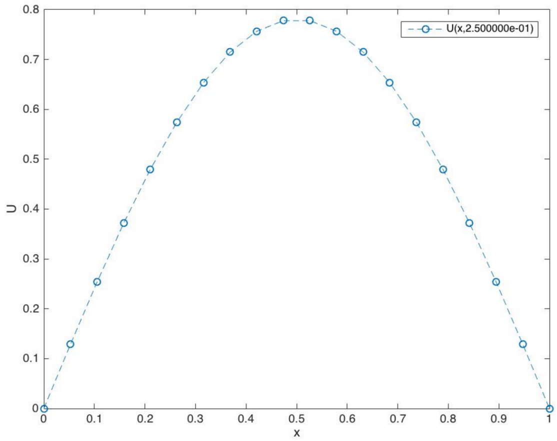
$$\frac{u_i^{m+1} - u_i^m}{\Delta t} = \alpha \frac{u_{i-1}^m - 2u_i^m + u_{i+1}^m}{\Delta x} + \mathcal{O}(\Delta t) + \mathcal{O}(\Delta x^2)$$

Big-O notation is used to represent the truncation error of the approximations. This refers to the higher-order terms of the Taylor Series Expansion for u which are not considered in the estimates. Ignoring these and solving for u_i^{m+1} gives:

$$u_i^{m+1} = u_i^m + \frac{\alpha \Delta t}{\Delta x^2}(u_{i+1}^m - 2u_i^m + u_{i-1}^m)$$

5.3.2 Stability of Approximation

5.3.3 Plots



Example plot for t=0.25, more plots with detailed explanation will be added later

5.4 Inhomogeneous Heat Equation

5.4.1 Fundamental Solution

We have introduced homogeneous heat equations and numerical methods of solving them above. In the real world, however, there are physical reasons why that is insufficient. In particular, if heat is added to a system, we encounter an inhomogeneous equations of the form $(\partial_t - \partial_{xx})u = f(x)$, where $f(x)$ represents some none zero heat added.

Simulating an inhomogeneous equation with methods introduced above is difficult. Thus we attemp to give an analytical solution - one that involves the use of what is known as a **fundamental solution**.

The heat equation $\partial_t - \partial_{xx} = 0$ is a *(constant coefficient partial)* linear differential operator. For any such linear operator P, a fundamental solution for P is a *distribution* K such that

$$PK = \delta.$$

Recall from lecture that δ is a "function" defined on the entire real line such that $\delta(x) = \infty$ if $x = 0$, and 0 otherwise. A *distribution* on $\mathbb{R}^n$ is generalization of a continuous function. Since this is not a PDE or analysis class, we will just roughly think of them as some irregular functions. For an example, the delta function is a distribution, and it satisfies the identity $\int_{-\infty}^{\infty} \delta(x)dx = 1$. This integral wouldn't make sense at the origin if we used the classical definition.

The **significance of a fundamental solution** is that it allows us to solve the inhomogeneous problem

$$(\partial_t - \partial_{xx})u = f$$

by a convolution (see theorem below). Here $f \neq 0$, and u is a function we're solving for.

5.4.2 Solving Inhomogeneous Equations by Convolution

In short, u as above is given by $K * f$. To figure out how, we need two lemmas.

Lemma 1 The convolution of a function with the delta function is the function itself.

Proof.

$$
\begin{aligned}
f(t) * \delta(t) &= \int_{-\infty}^{\infty} f(\tau)\delta(t-\tau)\,d\tau \\
&= \int_{-\infty}^{\infty} f(\tau)\delta(\tau-t)\,d\tau \text{ (Since the delta function is symmetric in y axis)} \\
&= f(t).
\end{aligned}
$$

The last equality is true due to properties of the delta function: $\delta(\tau - t) \neq 0$ if and only if $\tau - t = 0$ if and only if $\tau = t$. Since the integral on the previous line is a function in t, we see that the integrad is non-zero only when $\tau = t$. I'm very inclined on obmitting this proof for many reasons.... in which case I'll just take this lemma for granted. Is that okay?

□

Lemma 2 Suppose u a continuous function whose n^{th} derivative exists and is also continuous, ϕ a compactly supported and infinitely differentiable function, then for any mixed partial ∂^α, $\partial^\alpha(u * \phi) = (\partial^\alpha u) * (\phi)$.

Proof.

$$
\begin{aligned}
\partial^\alpha(u*\phi) &= \partial^\alpha\Big(\int_{-\infty}^{\infty} u(x-z)\phi(x)\,dx\Big) \\
&= \int_{-\infty}^{\infty} \partial^\alpha(u(x-z)\phi(x))\,dx \qquad \text{by continuity} \\
&= \int_{-\infty}^{\infty} (\partial^\alpha u(x-z))\phi(x)\,dx \qquad \text{partial acts on u because the integral}
\end{aligned}
$$

is a function in z.

$$= (\partial^\alpha u) * \phi \qquad \text{as desired.}$$

Remark: We needed compact support to guarantee the existance of their convolution. The identity is true as long as the convolution makes sense. i.e., the integral $< \infty$. □

Theorem If $(\partial_t - \partial_{xx})u = f$, then $u = K * f$.

Proof.

$$(\partial_t - \partial_{xx})(K * f) = ((\partial_t - \partial_{xx})K) * f = \delta * f = f$$

The first equality is true by lemma 2. The second equality is true by the definition of the heat fundamental solution. The thrid equality is true by lemma 1. □

5.4.3 Formulat for Fundamental Solution and example problem

Now hopefully you believe that, if we know the fundamental solution $K(x,t)$, we can find the solution u to the inhomogeneous equation $(\partial_t - \partial_{xx})u = f$. Though we never formally introduced it, intuitively, K should have both a time and space variable, represented by t and x, to model the dispersal of heat in a system over time. In the real world, physical intuition tells us that introducing heat should have no effect on its heat concentration in the past. This is taken into account in our fundamental solution by a Heaviside step function $H(t) = 1$ when $t \geq 0$ and 0 otherwise.

Theorem The heat fundamental solution is given by $K(x,t) = \frac{1}{(4\pi t)^{n/2}} e^{\frac{-|x|^2}{4t}} H(t)$, where n is the number of dimension you are considering, generally 2 or 3.

Proof.
Obmit. It uses green's function and some weird trick. Not very relevant... I think? Also it's going to be about a page long. □

Example Let $(\partial_t - \partial_{xx})u = x^2 \sin(x)$, find u.

Proof.

$$\begin{aligned} u = K * f &= \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} K(x-y, t-s) f(y,s)\, dy\, ds \\ &= \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} H(t-s) \frac{1}{(4\pi(t-s))^{n/2}} e^{\frac{-|x-y|^2}{4(s-t)}} y^2 \sin(y)\, dy\, ds \\ &= \int_{t>s} \int_{-\infty}^{\infty} \frac{1}{(4\pi(t-s))^{n/2}} e^{\frac{-|x-y|^2}{4(s-t)}} y^2 \sin(y)\, dy\, ds \end{aligned}$$

Remark: Note that since $f(x)$ is time independent, the physical interpretation is that heat is constantly added.
Need some guidance: We need to check that this integral is not infinite, but we're not sure how? □

5.4.4 Philosophical Implications: Speed of Propagation

As we try to model the dispersion of heat through some material, a logical question to ask is *how fast* does heat travel through it? More precisely, what is the heat at x after t amount of time has passed since f occurred? As we have seen, this type of phenomenon is completely modelled by $K(x,t)$.

Here we make a crutial observation: the definition of K given by $\frac{1}{(4\pi t)^{n/2}} e^{\frac{-|x|^2}{4t}} H(t)$ is *strictly* positive for any $t > 0$. To fully appreciate this fact, let us consider a metal rod with the same length as the observable universe at equilibrium, and added heat to one end. Then at $t = 0.000001$ seconds, the heat at the other end is at a super tiny amount, *positive*. So in a perfectly mathematical universe, **heat travels with infinite speed!**

This is a manifestation of infinite speed of propagation for the heat equation. Other PDEs may or may not share this property. For instance, the wave equation have a different form of fundamental solution (the time variable is not exponentiated) and exhibits finite speed of propagation. In the real world, of course, heat can't travel faster than light speed by general relativity.

6 Conclusion