Numerical Approaches to the Heat Equation

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Introduction

The heat equation is a fundamental partial differential equation (PDE) that describes how heat diffuses through a medium over time.

It appears in a wide range of fields:

- Physics (e.g., heat conduction, diffusion processes)
- Engineering (e.g., thermal analysis)
- Finance (e.g., Black-Scholes equation)

What We'll Cover

- Introduction to the problem and methods
- An analytical solution to our problem
- Derivation of Numerical Method
- Physics Informed Neural Networks (PINNs)
- Implementation of each method
- Results Comparisons
- Conclusions and insight from data

The 1D Heat Equation

The classical 1D heat equation (On a rod of length L):

$$\frac{\partial u}{\partial t} = k\frac{\partial^2 u}{\partial x^2}, \quad x \in [0, L],\ t \geq 09$$

Where:

- $u(x, t)$ is the temperature at position x and time t
- k is the thermal diffusivity constant

Initial Condition (IC):

$$u(x, 0) = f(x) \quad \text{(initial temperature distribution)}$$

Boundary Conditions (BCs):

$$u(0, t) = T_1, \quad u(L, t) = T_2 \quad \text{(Dirichlet BCs – fixed temperature at ends)}$$

Obtaining the 1D Analytical Solution

We will now solve the 1D heat equation under the follwing conditions:

$$\frac{\partial u(x,t)}{\partial t} = k\frac{\partial^2 u(x,t)}{\partial x^2}$$

Initial Condition (IC):

- $u(x,0) = \sin(\pi x)$
- The sine function was chosen as the initial condition because it will give a clear initial temperature distribution across our domain, satisfying our boundary conditions

Boundary Conditions (BCs):

- $u(0,t) = 0$ and $u(1,t) = 0$
- These are homogeneous Dirichlet boundary conditions, meaning the temperature at the ends of our domain are fixed at 0

Obtaining the 1D analytical solution

To solve the heat equation, we will use the method of **separation of variables**.
We assume the solution has the form:

$$u(x,t) = \phi(x)G(t)$$

Where $\phi(x)$ is a function of x and $G(t)$ is a function of t.
We can subsitute this into our heat equation to get the following:

$$\phi(x)\frac{dG(t)}{dt} = kG(t)\frac{d^2\phi(x)}{dx^2}$$

Obtaining the 1D analytical solution

Dividing both sides by $\phi(x)G(t)$ to separate the variables:

$$\frac{1}{kG(t)}\frac{dG(t)}{dt} = \frac{1}{\phi(x)}\frac{d^2\phi(x)}{dx^2}$$

Both sides are equal to a constant, which we denote as $-\lambda$.
This results in two ordinary differential equations (ODEs):

$$\frac{d^2\phi(x)}{dx^2} + \lambda\phi(x) = 0$$

$$\frac{dG(t)}{dt} = -k\lambda G(t)$$

Obtaining the 1D analytical solution

We begin with the ODE for $\phi(x)$:

$$\frac{d^2\phi(x)}{dx^2} + \lambda\phi(x) = 0$$

This standard 2nd Order ODE has the general solution:

$$\phi(x) = A\sin(\sqrt{\lambda}x) + B\cos(\sqrt{\lambda}x)$$

Applying the boundary conditions: $\phi(0) = 0$ and $\phi(1) = 0$ gives $\sin(\sqrt{\lambda}) = 0$

Thus, $\sqrt{\lambda} = n\pi$ where n is a positive integer.

So, the eigenvalues are:

$$\lambda_n = (n\pi)^2$$

And the corresponding eigenfunctions are:

$$\phi_n(x) = A_n\sin(n\pi x)$$

Obtaining the 1D analytical solution

We now solve the ODE for $G(t)$:

$$\frac{dG(t)}{dt} = -k\lambda G(t)$$

This is a simple first-order linear differential equation. The solution is of the form:

$$G(t) = Ce^{-k\lambda t}$$

Now, we substitute the eigenvalue $\lambda_n = (n\pi)^2$ into this equation:

$$G_n(t) = C_n e^{-k(n\pi)^2 t}$$

So, the time-dependent part of the solution for each n is:

$$G_n(t) = C_n e^{-kn^2\pi^2 t}$$

Obtaining the 1D analytical Solution

Now that we've solved both ODEs, the full solution is:

$$u(x,t) = \sum_{n=1}^{\infty} A_n \sin(n\pi x) e^{-k(n\pi)^2 t}$$

The constants A_n are determined using the initial condition:

$$u(x,0) = \sum_{n=1}^{\infty} A_n \sin(n\pi x) = \sin(\pi x)$$

This is a Fourier sine series, giving the following A values:

$$A_1 = 1, \quad A_n = 0 \text{ for } n \neq 1$$

Final Analytical Solution

Since only $A_1 = 1$ and all other $A_n = 0$, the infinite sum reduces to a single term.
The final solution is:

$$u(x, t) = \sin(\pi x)\, e^{-k\pi^2 t}$$

This function satisfies:

- The heat equation
- The boundary conditions: $u(0, t) = u(1, t) = 0$
- The initial condition: $u(x, 0) = \sin(\pi x)$

Numerical Approach: Crank-Nicolson Method

We now turn to a numerical method for solving the 1D heat equation:

$$\frac{\partial u}{\partial t} = k\frac{\partial^2 u}{\partial x^2}$$

We will use the **Crank-Nicolson method**, which is:

- Second-order accurate in both time and space.
- Unconditionally stable for linear problems.

It works by averaging the Forward Euler and Backward Euler methods, making it a balanced, more accurate approach

Crank-Nicolson Scheme Derivation

We start by discretizing the domain into a spacial grid and a time grid:

$$\textit{Space Grid}: \; x_i = i\Delta x, \; \textit{for } i = 0, 1, 2, 3...$$

$$\textit{Time Grid}: \; t^n = n\Delta t, \; \textit{for } n = 0, 1, 2, 3...$$

$$\textit{This gives}: \; u_i^n \approx u(x_i, t^n)$$

Crank-Nicolson Scheme Derivation

Next, we discretize the time derivative

$$\frac{\partial u}{\partial t}(x_i, t^{n+\frac{1}{2}}) \approx \frac{u_i^{n+1} - u_i^n}{\Delta t}$$

And then we average the central difference for space at time step n and $n+1$

$$\frac{\partial^2 u}{\partial x^2}(x_i, t^{n+\frac{1}{2}}) \approx \frac{1}{2} \left. \frac{u_{i+1}^n - 2u_i^n + u_{i-1}^n}{(\Delta x)^2} + \frac{u_{i+1}^{n+1} - 2u_i^{n+1} + u_{i-1}^{n+1}}{(\Delta x)^2} \right)$$

Crank-Nicolson Scheme Derivation

Now we can plug each of our approximations into the heat equation:

$$\frac{u_i^{n+1} - u_i^n}{\Delta t} = k \cdot \frac{1}{2} \left(\frac{u_{i+1}^n - 2u_i^n + u_{i-1}^n}{(\Delta x)^2} + \frac{u_{i+1}^{n+1} - 2u_i^{n+1} + u_{i-1}^{n+1}}{(\Delta x)^2} \right)$$

Next we multiply by Δt and factor $(\Delta x)^2$

$$u_i^{n+1} - u_i^n = \frac{k\,\Delta t}{2(\Delta x)^2} \left(u_{i+1}^n - 2u_i^n + u_{i-1}^n + u_{i+1}^{n+1} - 2u_i^{n+1} + u_{i-1}^{n+1} \right)$$

Crank-Nicolson Scheme Derivation

To simplify things we will let $s = \frac{k\Delta t}{(\Delta x)^2}$ to give us this:

$$u_i^{n+1} - u_i^n = \frac{s}{2}\left(u_{i+1}^n - 2u_i^n + u_{i-1}^n + u_{i+1}^{n+1} - 2u_i^{n+1} + u_{i-1}^{n+1}\right)$$

And lastly, we can rearrange and simplify our equation with all of our $n+1$ terms on the left.

$$(1+s)u_i^{n+1} - 2s\, u_{i+1}^{n+1} - 2s\, u_{i-1}^{n+1} = (1-s)u_i^n + 2s\, u_{i+1}^n + 2s\, u_{i-1}^n$$

Transition from Single Equation to System of Equations

In the Crank-Nicolson scheme, we have a single equation for each grid point in the spatial domain. We can apply this equation at every grid point in the domain, resulting in a set of equations, one for each spatial point. Thus, the system of equations becomes:

$$\begin{aligned}
u(x_1, t+\Delta t) &= \text{function of known values at time t} \\
u(x_2, t+\Delta t) &= \text{function of known values at time t} \\
&\vdots \\
u(x_N, t+\Delta t) &= \text{function of known values at time t}
\end{aligned}$$

This forms a linear system for all unknowns at $t + \Delta t$.

Solving each system of equations

Each time step involves solving a linear system to find the values of $u(x, t)$ at every spatial point x for that specific time.

- The size of each system corresponds to the number of spatial points N_x in the discretized domain.
- At each time step t_n, the linear system has N_x unknowns, representing the values of $u(x, t_n)$ for each x.
- The system is solved for each t_n, yielding a vector $\mathbf{u}^n$ of length N_x.

Once the system is solved at each time step, the solutions are pieced together:

$$\mathbf{u}(x, t_0), \mathbf{u}(x, t_1), \ldots, \mathbf{u}(x, t_{N_t})$$

In this way, the numerical solution is built layer by layer, starting from the initial condition and iterating forward in time.

Introduction to PINNs

Physics-Informed Neural Networks (PINNs) are a type of machine learning approach to solving equations.

- PINNs utilize neural networks and governing (PDEs) by embedding the physics directly into the network's training process.
- PINNs learn continuous solutions that satisfy the PDE, boundary, and initial conditions.

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Key Components of PINNs:

- **Neural Network**: A feed-forward neural network that takes space and time coordinates as inputs, then outputs the solution
- **Loss Function**: A combination of:
  - **Physics-based loss**: Penalizes the network for not satisfying the PDE.
  - **Boundary/Initial Condition loss**: Ensures the network adheres to the boundary or initial conditions.

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Why PINNs?

- They can solve complex PDEs without discretizing the domain.
- They handle higher dimensions better
- They can work inversely

Neural Network Architecture in PINNs

The PINN uses a neural network with 3 parts to learn the solution

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- **Hidden Layers**: The network has one or more hidden layers made of nodes (neurons) that process the information. This is where the learning and adjustments of the NN are done.
- **Output Layer**: The final layer of the network outputs the solution to the PDE at the given coordinates x and t.

The goal of the network is to approximate the solution of the PDE without explicitly solving it through traditional methods.

Loss Function in PINNs

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- **Boundary Condition Loss**: This ensures that the network respects the boundary conditions (values at the edges of the domain).
- **Initial Condition Loss**: The network is also penalized if it doesn't match the initial condition (the solution at the start of the process).

Training the PINN (Data Generation & Loss Function)

The PINN is trained by optimizing the loss function.

- **Step 1: Data Generation**
  - The input data consists of random samples for spatial x and temporal t values.
  - These points are fed into the network to generate predictions for the solution $u(x, t)$.
- **Step 2: Loss Function Calculation**
  - The loss function combines multiple components, each weighted differently:
    - **Physics-based loss**: Ensures the network satisfies the PDE by penalizing deviations from the PDE.
    - **Boundary Condition loss**: Enforces the correct values at the boundaries of the spatial domain.
    - **Initial Condition loss**: Ensures the solution is correct at $t = 0$.

Training the PINN (Backpropagation & Repetition)

- **Step 3: Backpropagation and Optimization**
  - Using the computed loss, backpropagation is performed to penalize the neural network
  - The optimizer adjusts the weights and biases of the network to minimize the total loss.
- **Step 4: Repeat**
  - This process is repeated over multiple training iterations, or "epochs" to improve the model's accuracy.

Crank-Nicolson Implementation Details

Simulation Parameters

- Domain: $x \in [0, 1]$, $t \in [0, 1]$
- Diffusivity coefficient: $k = 0.1$
- Initial condition: $u(x, 0) = \sin(\pi x)$
- Boundary conditions: $u(0, t) = u(1, t) = 0$

Discretization Details

- Spatial steps: $N_x = 400 \quad (\Delta x = 0.0025)$
- Time steps: $N_t = 20000 \quad (\Delta t = 0.00005)$
- Total Points: 8,000,000
- Central difference in space, trapezoidal rule in time

Computational Methods

- Solved for every interior point iteratively, then graphed
- Utilized the structure of matrices produced from CN scheme to speed up computation

PINN Methodology and Setup

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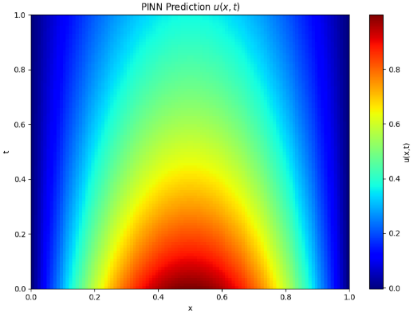
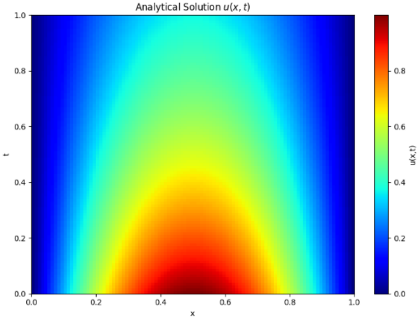
Training Parameters

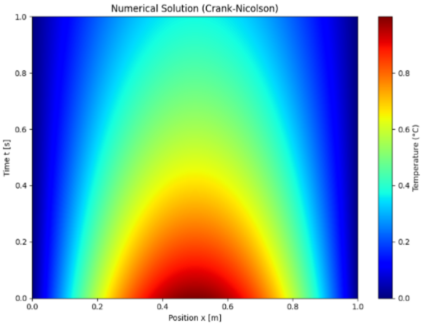
- **Number of Training Points**: 2000 randomly sampled points within the spatial and temporal domains
- **Epochs**: 15000 epochs for training
- **Weights**: PDE = 10, IC = 1, BC = 1
- **Learning Rate**: .001

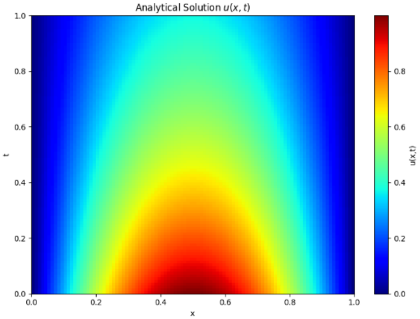
PINN vs Analytical Solution



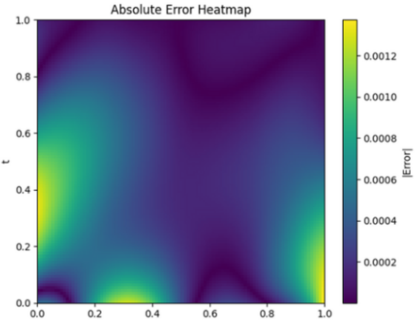


Crank-Nicolson vs Analytical Solution

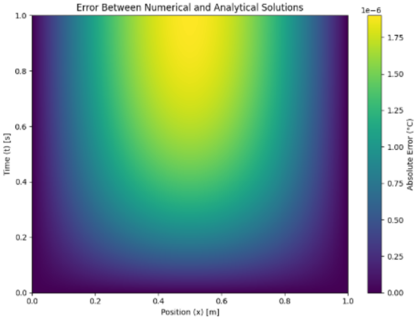




PINN Error vs Crank Nicolson Error




```
_____PINN Metrics_____
Maximum Absolute Error (Max Error): 0.001374
Mean Squared Error (MSE): 0.000000
Mean Absolute Error (MAE): 0.000333
```




```
_____Crank Nicolson Metrics_____
Max Error: 0.000002 °C
Mean Squared Error (MSE): 0.000000 °C²
Mean Absolute Error (MAE): 0.000001 °C
```

Conclusions

- Both the PINN and Numerical Method did an exceptional job at approximating the solution
- Overall, the numerical methods error metrics were better than the PINNs
- The numerical method was implemented more efficiently, and both were ran on the CPU
- The error maps show clear patterns for the numerical method, and unpredictable patterns for the PINN
- The PINN graphed better than the numerical method because of discretization