Heat Equation

Partial Differential Equations

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Objectives

In this lesson we will:

- develop an explicit method for numerically approximating the solution to a heat/diffusion equation initial boundary value problem, and
- develop an implicit method (Crank-Nicolson) for numerically approximating the solution to a heat/diffusion equation initial boundary value problem.

Initial Boundary Value Problem

Numerically approximate the solution to the following Fourier problem:

$$
\begin{aligned}
u_t &= u_{xx} \text{ for } 0 < x < 1 \text{ and } t > 0 \\
u(0,t) &= u(1,t) = 0 \text{ for } t > 0 \\
u(x,0) &= 100 \text{ for } 0 < x < 1.
\end{aligned}
$$

The spatial interval $[0,1]$ must be subdivided into N intervals of length $h = 1/N$. A forward time step of size $k > 0$ must be chosen and a differencing scheme must be selected for the partial differential equation.

$$\frac{u(x,t+k) - u(x,t)}{k} \approx \frac{u(x+h,t) - 2u(x,t) + u(x-h,t)}{h^2}.$$

This finite difference approximation is classified as having truncation error $O(k) + O(h^2)$.

Explicit Scheme

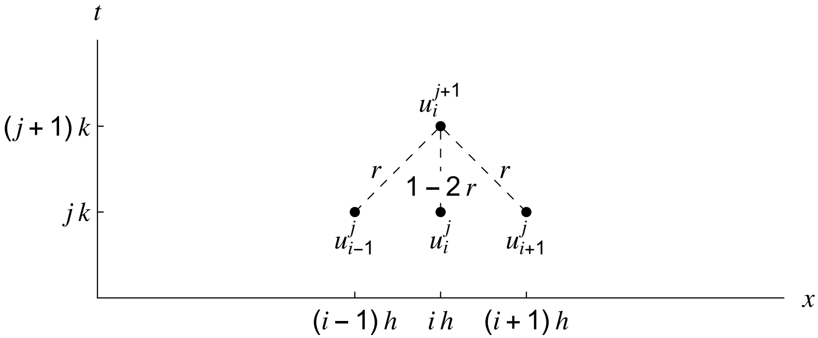
$$\frac{1}{k}(u_i^{j+1} - u_i^j) = \frac{1}{h^2}(u_{i+1}^j - 2u_i^j + u_{i-1}^j)$$
$$u_i^{j+1} = ru_{i-1}^j + (1-2r)u_i^j + ru_{i+1}^j$$

for $i = 1, 2, \ldots, N-1$, where $r = k/h^2$. This is an example of an **explicit** finite difference scheme.

For $i = 0$ and $i = N$ the homogeneous Dirichlet boundary conditions provide $u_0^j = u_N^j = 0$ for all $j \in \mathbb{N}$.

Note that the explicit scheme gives the value of u_i^{j+1} as a function of three values of u one time step earlier.

Stencil



The values of u_i^0 are the initial conditions and are thus known. This enables the solution to be approximated at $t = j\,k$ for $j \in \mathbb{N}$ iteratively.

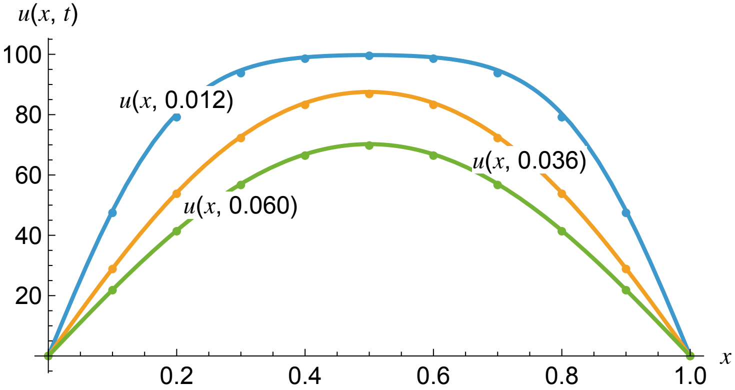
Matrix/Vector Form

If the vector $\mathbf{u}^{(j)} = (u_1^j, u_2^j, \ldots, u_{N-1}^j)^T$ then the system of equations may be written as $\mathbf{u}^{(j+1)} = A(r)\,\mathbf{u}^{(j)}$ or

$$\begin{bmatrix} u_1^{j+1} \\ u_2^{j+1} \\ u_3^{j+1} \\ \vdots \\ u_{N-3}^{j+1} \\ u_{N-2}^{j+1} \\ u_{N-1}^{j+1} \end{bmatrix} = \begin{bmatrix} 1-2r & r & 0 & \cdots & 0 & 0 & 0 \\ r & 1-2r & r & \cdots & 0 & 0 & 0 \\ 0 & r & 1-2r & \cdots & 0 & 0 & 0 \\ \vdots & \vdots & \vdots & & \vdots & \vdots & \vdots \\ 0 & 0 & 0 & \cdots & 1-2r & r & 0 \\ 0 & 0 & 0 & \cdots & r & 1-2r & r \\ 0 & 0 & 0 & \cdots & 0 & r & 1-2r \end{bmatrix} \begin{bmatrix} u_1^j \\ u_2^j \\ u_3^j \\ \vdots \\ u_{N-3}^j \\ u_{N-2}^j \\ u_{N-1}^j \end{bmatrix}.$$

Results

If $h = 1/10$ and $k = 1/1000$ then $r = 1/10$ and the values of $u(x, t)$ are shown for $t = 0.012$, $t = 0.036$, and $t = 0.060$.



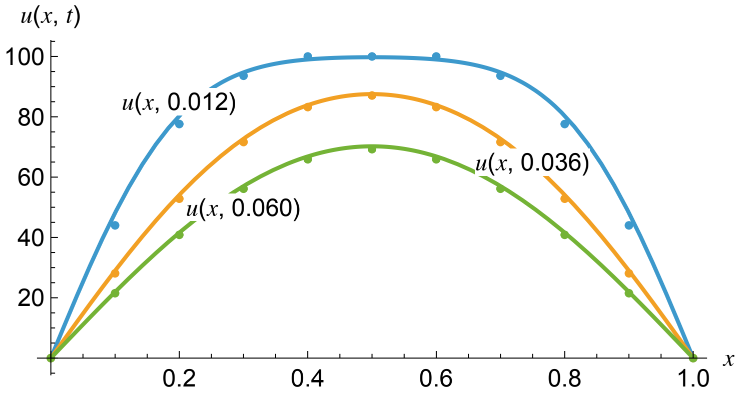
The solid curves provide a comparison with the Fourier series solution.

Remarks

- Since the forward time step size is $k = 0.001$, one thousand iterations of the explicit formula are required to approximate the solution for $0 < t \leq 1$.
- To reduce the number of iterations required to reach the $t = 1$ milestone, k could be increased.
- If $k = 0.004$ only two hundred fifty iterations are required.

Results

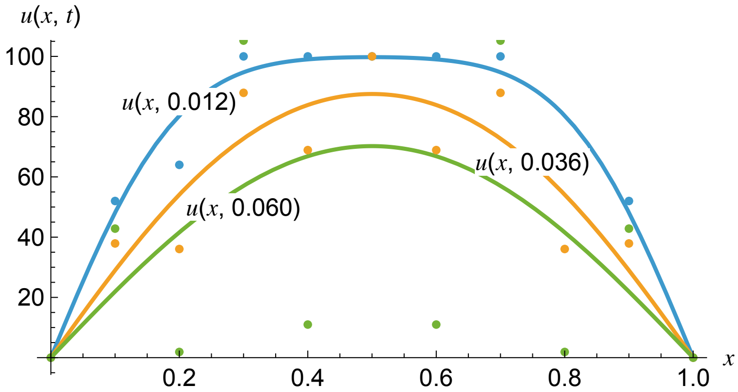
If $h = 1/10$ and $k = 0.004$ then $r = 0.4$ and the values of $u(x, t)$ are shown for $t = 0.012$, $t = 0.036$, and $t = 0.060$.



The solid curves provide a comparison with the Fourier series solution. The numerical solution does not appear to agree as well with the infinite series solution when $r = 0.4$.

Results

If $h = 1/10$ and $k = 0.006$ then $r = 0.6$ and the values of $u(x, t)$ are shown for $t = 0.012$, $t = 0.036$, and $t = 0.060$.



The solid curves provide a comparison with the Fourier series solution. The numerical solution does not agree well with the infinite series solution when $r = 0.6$.

Crank-Nicolson Method

Suppose f is a twice continuously differentiable function on a neighborhood of $t+k/2$, and expand f as a Taylor polynomial about $t+k/2$.

$$f(s) = f\left(t+\frac{k}{2}\right) + f'\left(t+\frac{k}{2}\right)\left(s-t-\frac{k}{2}\right) + O\left(\left(s-t-\frac{k}{2}\right)^2\right),$$

for s close to $t+k/2$. Replace s by t and again by $t+k$:

$$f(t) = f\left(t+\frac{k}{2}\right) - f'\left(t+\frac{k}{2}\right)\left(\frac{k}{2}\right) + O(k^2)$$
$$f(t+k) = f\left(t+\frac{k}{2}\right) + f'\left(t+\frac{k}{2}\right)\left(\frac{k}{2}\right) + O(k^2).$$

Add these two equations and solve for $f(t+k/2)$.

$$f\left(t+\frac{k}{2}\right) = \frac{f(t)+f(t+k)}{2} + O(k^2),$$

which has an $O(k^2)$ truncation error.

Developing an Implicit Scheme

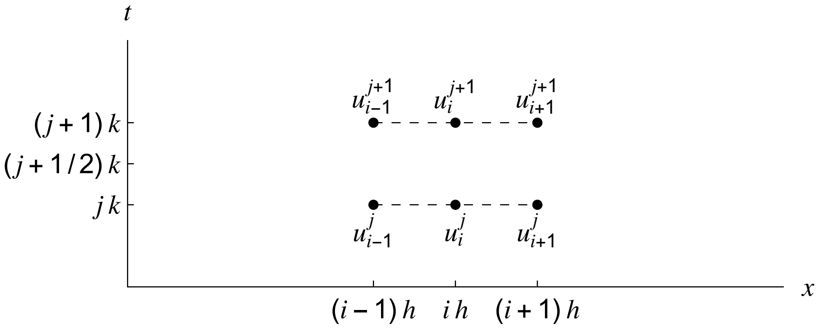
Choose f to be $u_{xx}(x,t)$, then

$$\begin{aligned}
u_{xx}(x,t+k/2) &= \frac{u_{xx}(x,t)+u_{xx}(x,t+k)}{2} + O(k^2) \\
&= \frac{u(x+h,t)-2u(x,t)+u(x-h,t)}{2h^2} \\
&\quad + \frac{u(x+h,t+k)-2u(x,t+k)+u(x-h,t+k)}{2h^2} \\
&\quad + O(k^2)+O(h^2).
\end{aligned}$$

A formula for $u_{xx}(x,t+k/2)$ has been found by averaging the three-point formulas for the second derivative at times $t = kj$ and $t = k(j+1)$.

This formula has $O(k^2)+O(h^2)$ accuracy as $h,\ k \to 0$.

Stencil



Developing an Implicit Scheme

The heat equation can be discretized as

$$\frac{u_i^{j+1} - u_i^j}{k} = \frac{u_{i-1}^j - 2u_i^j + u_{i+1}^j}{2h^2} + \frac{u_{i-1}^{j+1} - 2u_i^{j+1} + u_{i+1}^{j+1}}{2h^2}$$

or equivalently as,

$$-ru_{i-1}^{j+1} + 2(1+r)u_i^{j+1} - ru_{i+1}^{j+1} = ru_{i-1}^j + 2(1-r)u_i^j + ru_{i+1}^j$$

for $i = 1, 2, \ldots, N-1$ and where $r = k/h^2$.

- Relative to the point at $(x, t) = (i\,h, (j + 1/2)k)$, the first derivative in t and the second derivative in x have been replaced with central difference approximations which, in general, are more accurate than forward (or backward) difference approximations.
- The three values u_{i-1}^{j+1}, u_i^{j+1}, and u_{i+1}^{j+1} are unknown and must be solved for simultaneously and depend on values found on the $t = j\,k$ row (which were either given as initial conditions or were calculated previously).

Matrix/Vector Form

If the boundary conditions are of homogeneous Dirichlet type, the system of equations can be written in matrix/vector form as

$$A(r)\mathbf{u}^{(j+1)} = A(-r)\mathbf{u}^{(j)}$$

where

$$A(r) = \begin{bmatrix} 2(1+r) & -r & 0 & \cdots & 0 & 0 & 0 \\ -r & 2(1+r) & -r & \cdots & 0 & 0 & 0 \\ \vdots & \vdots & \vdots & & \vdots & \vdots & \vdots \\ 0 & 0 & 0 & \cdots & -r & 2(1+r) & -r \\ 0 & 0 & 0 & \cdots & 0 & -r & 2(1+r) \end{bmatrix}.$$

Remarks

- A unique solution exists if and only if $A(r)$ is invertible.
- The inverse of $A(r)$ always exists for any $r > 0$ since the matrix is **strictly diagonally dominant**.
- The placement of the nonzero entries in this matrix gives it a special structure known as a **tridiagonal matrix** which is easily inverted.
- A system of equations of the form $A\mathbf{x} = \mathbf{b}$ where A is an $n \times n$ tridiagonal matrix can be solved by a Gaussian elimination algorithm requiring $O(n)$ operations (multiplications and additions).
- The matrix is **symmetric** and the off-diagonal elements of the matrix are all identical.

Example

Consider the following initial boundary value problem for the heat equation:

$$u_t = u_{xx} \text{ for } 0 < x < 1 \text{ and } t > 0$$
$$u(0,t) = u(1,t) = 0 \text{ for } t > 0$$
$$u(x,0) = x(1-x)^2 \text{ for } 0 < x < 1.$$

Approximate the solution for $0 \leq t \leq 1/10$ using the Crank-Nicolson method with $h = 1/10$ and $k = 1/100$.

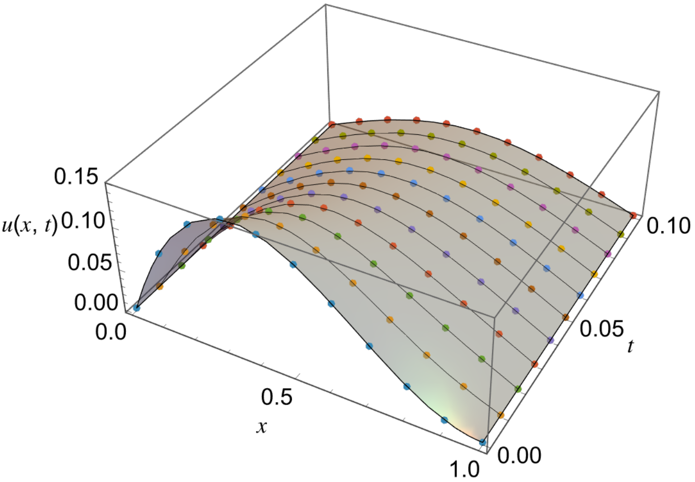
Solution (1 of 2)

For these choices of h and k the parameter $r = 1$.

$$\begin{bmatrix} 4 & -1 & 0 & \cdots & 0 & 0 \\ -1 & 4 & -1 & \cdots & 0 & 0 \\ 0 & -1 & 4 & \cdots & 0 & 0 \\ \vdots & \vdots & \vdots & & \vdots & \vdots \\ 0 & 0 & 0 & \cdots & 4 & -1 \\ 0 & 0 & 0 & \cdots & -1 & 4 \end{bmatrix} \begin{bmatrix} u_1^{j+1} \\ u_2^{j+1} \\ u_3^{j+1} \\ \vdots \\ u_{N-2}^{j+1} \\ u_{N-1}^{j+1} \end{bmatrix} = \begin{bmatrix} 0 & 1 & 0 & \cdots & 0 & 0 \\ 1 & 0 & 1 & \cdots & 0 & 0 \\ 0 & 1 & 0 & \cdots & 0 & 0 \\ \vdots & \vdots & \vdots & & \vdots & \vdots \\ 0 & 0 & 0 & \cdots & 0 & 1 \\ 0 & 0 & 0 & \cdots & 1 & 0 \end{bmatrix} \begin{bmatrix} u_1^{j} \\ u_2^{j} \\ u_3^{j} \\ \vdots \\ u_{N-2}^{j} \\ u_{N-1}^{j} \end{bmatrix}$$

Let $u_i^0 = (ih)(1 - ih)^2$ with $h = 1/10$ for $i = 1, 2, \ldots, 9$.

Solution (2 of 2)



Robin Boundary Conditions

Consider the initial boundary value problem,

$$\begin{aligned} u_t &= u_{xx} \text{ for } 0 < x < 1 \text{ and } t > 0 \\ u_x(0,t) &= u(0,t) - e^{-t} \text{ for } t > 0 \\ -u_x(1,t) &= 2u(1,t) - t \text{ for } t > 0 \\ u(x,0) &= \frac{1}{3}e^{-2x} \text{ for } 0 < x < 1. \end{aligned}$$

Introduce fictitious points u_{-1}^j and the discretized form of the boundary condition at $x = 0$ can be written as

$$\frac{u_1^j - u_{-1}^j}{2h} = u_0^j - e^{-jk},$$

which implies the values at the fictitious points are

$$u_{-1}^j = -2hu_0^j + u_1^j + 2he^{-jk}.$$

Crank-Nicolson Formulation

The boundary condition at $x = 0$ can be discretized as

$$(1 + r + hr)u_0^{j+1} - ru_1^{j+1} = (1 - r - hr)u_0^j + ru_1^j + hr(e^{-(j+1)k} + e^{-jk}).$$

Similarly the boundary condition at $x = 1$ can be approximated using the central difference formula as

$$-\frac{u_{N+1}^j - u_{N-1}^j}{2h} = 2u_N^j - jk.$$

Solving for the fictitious point where $i = N + 1$ yields

$$u_{N+1}^j = u_{N-1}^j - 4hu_N^j + 2hjk.$$

Hence the boundary condition at $x = 1$ can be discretized as

$$-ru_{N-1}^{j+1} + (1 + r + 2hr)u_N^{j+1} = ru_{N-1}^j + (1 - r - 2hr)u_N^j + hr(2j + 1)k.$$

Matrix/Vector Form

The linear system can be expressed as

$$A(r)\,\mathbf{u}^{j+1} = A(-r)\,\mathbf{u}^{j} + \begin{bmatrix} hr(e^{-(j+1)k} + e^{-jk}) \\ 0 \\ \vdots \\ 0 \\ hr(2j+1)k \end{bmatrix}$$

where

$$A(r) = \begin{bmatrix} 1+r+hr & -r & 0 & \cdots & 0 & 0 & 0 \\ -r & 2(1+r) & -r & \cdots & 0 & 0 & 0 \\ \vdots & \vdots & \vdots & & \vdots & \vdots & \vdots \\ 0 & 0 & 0 & \cdots & -r & 2(1+r) & -r \\ 0 & 0 & 0 & \cdots & 0 & -r & 1+r+2hr \end{bmatrix}.$$