Numerical Methods - Boundary Value Problems for PDEs

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2013

Outline

Classification of Second Order Linear PDEs

- Consider a Linear Second Order PDE:

$$a\frac{\partial^2 u}{\partial x^2} + b\frac{\partial^2 u}{\partial x\,\partial y} + c\frac{\partial^2 u}{\partial y^2} = f\left(x, y, u, \frac{\partial u}{\partial x}, \frac{\partial u}{\partial y}\right).$$

- The PDE is hyperbolic if $b^2 - 2ac > 0$:
  - Wave equation: $u_{tt} = c^2\nabla^2 u$
- The PDE is parabolic if $b^2 - 2ac = 0$:
  - Heat equation: $u_t = k\nabla^2 u$
  - Diffusion equation: $u_t = \nabla(D\nabla u) + \rho(x, y)$
- The PDE is elliptic if $b^2 - 2ac < 0$:
  - Laplace equation: $\nabla^2 u = 0$
  - Poisson equation: $\nabla^2 u = -4\pi\rho(x, y)$
  - Helmholtz equation: $\nabla^2 u = -k^2 u$

Boundary Conditions

- In order to solve the PDE uniquely, additional information are required and they are (1) initial conditions and (2) boundary conditions.
- For hyperbolic PDE, two initial conditions are required, as the PDE is second order in t.
- Similarly, one initial condition is required for parabolic PDE.
- All hyperbolic, parabolic and elliptic PDEs required the boundary of the regions where the PDEs defined to be specified:
  - Dirichlet condition: The value of u are specified at the boundary.
  - Neumann condition: The normal gradient $\nabla u \cdot \hat{\mathbf{n}}$ is specified at the boundary.

Outline

Elliptic Boundary Value Problem

We will consider the Poisson equation as an example for the elliptic problem:

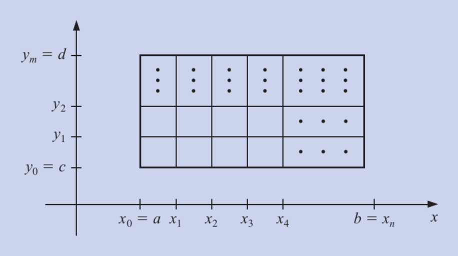
$$\begin{aligned} \text{PDE} &: \quad \nabla^2 u = u_{xx}(x,y) + u_{yy}(x,y) = f(x,y), \quad \text{for } (x,y) \in R \\ \text{B.C.} &: \quad u(x,y) = g(x,y), \quad \text{for } (x,y) \in S \end{aligned}$$

where $R = \{(x,y) | a < x < b, c < y < d\}$ and S is the boundary of R.

- This is an Dirichlet boundary value problem.
- If $f(x,y) = 0$ we have the Laplace equation.
- If f and g are continuous on R and S then there is a unique solution to this BVP.
- In this example R is rectangular, however there may be other possible BVP on domain Ω that is not rectangular.

Discretise BVP

- The main technique for most PDE is finite difference, and thus the domain R need to be discretise to a grid of $N \times M$ boxes.
  - partition $a < x < b$ into equally spaced N subintervals : $a = x_0 < x_1 < x_2 < \cdots < x_N = b$, or $x_i = a + ih$, where $h = (b - a)/N$.
  - partition $c < y < d$ into equally spaced M subintervals : $c = y_0 < y_1 < y_2 < \cdots < y_M = d$, or $y_j = a + jk$, where $k = (d - c)/M$.



  - The lines $x = x_i$ and $y = y_j$ are grid lines and the intersections points are the mesh points.
  - The values of u will be evaluated / approximated at these grid points.

Elliptic BVP - Finite Difference Method

- Central Difference:
  $u_{xx}(x_i, y_j) = \dfrac{u(x_i + h, y_j) - 2u(x_i, y_j) + u(x_i - h, y_j)}{h^2} + O(h^2)$ and
  $u_{yy}(x_i, y_j) = \dfrac{u(x_i, y_j + k) - 2u(x_i, y_j) + u(x_i, y_j - k)}{k^2} + O(k^2)$.
- Let $u_{i,j} \approx u(x_i, y_j)$, $f_{i,j} = f(x_i, y_j)$ and the discretised PDE is now:

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

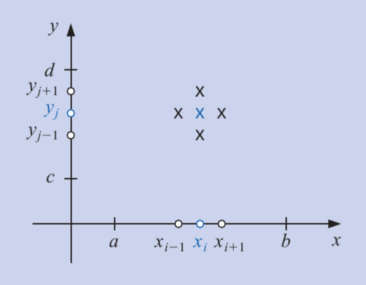
  with truncation error $O(h^2) + O(k^2)$.
- **(Interior Points)** $i = 1, 2, \ldots, N-1, j = 1, 2, \ldots, M-1$

$$2[(h/k)^2 + 1]u_{i,j} - (u_{i+1,j} + u_{i-1,j}) - (h/k)^2(u_{i,j+1} + u_{i,j-1}) = -h^2 f_{i,j}.$$

- **(Boundary Points)**
  - $i = 0, u_{0,j} = g(x_0, y_j)$, for $j = 0, 1, \ldots, M$
  - $i = N, u_{N,j} = g(x_N, y_j)$, for $j = 0, 1, \ldots, M$
  - $j = 0, u_{i,0} = g(x_i, y_0)$, for $j = 1, 2, \ldots, N-1$
  - $j = M, u_{i,M} = g(x_i, y_M)$, for $j = 1, 2, \ldots, N-1$

- Note that for each of the interior points, $i = 1, 2, \ldots, N-1$, $j = 1, 2, \ldots, M-1$ there is one of the following equation:

$$2[(h/k)^2 + 1]u_{i,j} - (u_{i+1,j} + u_{i-1,j}) - (h/k)^2(u_{i,j+1} + u_{i,j-1}) = -h^2 f_{i,j}.$$



- The resulting $(N-1)(M-1)$ equations forms an $(N-1)(M-1) \times (N-1)(M-1)$ linear system and could be solved by various numerical methods.

Laplace Equation (example)

Example

Use a central finite difference scheme to solve the following BVP for Laplace equation with 3 equal subintervals for both x and y ranges:

$$\begin{aligned}
\text{PDE} &: \quad u_{xx} + u_{yy} = 0, \quad 0 < x < 0.3, 0 < y < 0.3 \\
\text{B.C.} &: \quad u(0, y) = 0, \quad 0 < y < 0.3 \\
\text{B.C.} &: \quad u(0.3, y) = 200y, \quad 0 < y < 0.3 \\
\text{B.C.} &: \quad u(x, 0) = 0, \quad 0 < x < 0.3 \\
\text{B.C.} &: \quad u(x, 0.3) = 200x, \quad 0 < x < 0.3
\end{aligned}$$

ANSWER:

- $h = k = 0.3/3 = 0.1$, and let $u_{i,j} \approx u(x_i, y_j) = u(ih, jk)$.
- Boundary points:
  - $i = 0$, $u_{0,j} = 0, j = 0, 1, 2, 3$, ie $u_{0,0} = u_{0,1} = u_{0,2} = u_{0,3} = 0$; similarly
  - $i = 3$, $u_{3,0} = 0, u_{3,1} = 20, u_{3,2} = 40, u_{3,3} = 60$;
  - $j = 0$, $u_{1,0} = u_{2,0} = 0$;
  - $j = 3$, $u_{1,3} = 20, u_{2,3} = 40$.

Laplace Equation (example)

Example

- since $h/k = 1$, we have $4u_{i,j} - (u_{i+1,j} + u_{i-1,j}) - (u_{i,j+1} + u_{i,j-1}) = 0$.
- Interior points:
  - $i = 1, j = 1$,
    $4u_{1,1} - u_{2,1} - u_{0,1} - u_{1,2} - u_{1,0} = 0 \implies 4u_{1,1} - u_{2,1} - u_{1,2} = 0$;
  - $i = 1, j = 2$,
    $4u_{1,2} - u_{2,2} - u_{0,2} - u_{1,3} - u_{1,1} = 0 \implies 4u_{1,2} - u_{2,2} - u_{1,1} = 20$;
  - $i = 2, j = 1$,
    $4u_{2,1} - u_{3,1} - u_{1,1} - u_{2,2} - u_{2,0} = 0 \implies 4u_{2,1} - u_{1,1} - u_{2,2} = 20$;
  - $i = 2, j = 2$,
    $4u_{2,2} - u_{3,2} - u_{1,2} - u_{2,3} - u_{2,1} = 0 \implies 4u_{2,2} - u_{1,2} - u_{2,1} = 80$.
- In matrix form

$$\begin{bmatrix} 4 & -1 & -1 & 0 \\ -1 & 4 & 0 & -1 \\ -1 & 0 & 4 & -1 \\ 0 & -1 & -1 & 4 \end{bmatrix} \begin{bmatrix} u_{1,1} \\ u_{1,2} \\ u_{2,1} \\ u_{2,2} \end{bmatrix} = \begin{bmatrix} 0 \\ 20 \\ 20 \\ 80 \end{bmatrix}$$

- Solve the matrix equation by direct method gives
  $[u_{1,1}, u_{1,2}, u_{2,1}, u_{2,2}]^T = [20/3, 40/3, 40/3, 80/3]^T$.

Laplace Equation (example)

Example

- More often the number of mesh points is large and we cannot effort to compute the inverse of the coefficient matrix, instead we use iterative method.
- For example, we use Gauss-Seidel iterations:
  - $u_{1,1}^{(n+1)} = 1/4(u_{2,1}^{(n)} + u_{1,2}^{(n)})$;
  - $u_{1,2}^{(n+1)} = 1/4(20 + u_{2,2}^{(n)} + u_{1,1}^{(n+1)})$;
  - $u_{2,1}^{(n+1)} = 1/4(20 + u_{1,1}^{(n+1)} + u_{2,2}^{(n)})$;
  - $u_{2,2}^{(n+1)} = 1/4(80 + u_{1,2}^{(n+1)} + u_{2,1}^{(n+1)})$.
-

n	$u_{1,1}$	$u_{1,2}$	$u_{2,1}$	$u_{2,2}$
0	0	0	0	0
1	0	5	5	22.5
2	2.5	11.25	11.25	25.625
3	5.625	12.812	12.812	26.406
4	6.4062	13.203	13.203	26.602
5	6.6016	13.301	13.301	26.650
⋮				⋮

Outline

Parabolic Boundary Value Problem

We will consider the Heat equation as an example for the parabolic problem:

$$\begin{aligned}
\text{PDE} &: \quad u_t(x,t) - \alpha^2 u_{xx}(x,t) = 0, \quad \text{for } 0 < x < l, t > 0, \\
\text{B.C.} &: \quad u(0,t) = u(l,t) = 0, \quad \text{for } t > 0, \\
\text{I.C.} &: \quad u(x,0) = f(x), 0 < x < l.
\end{aligned}$$

- This is an Dirichlet boundary value problem.
- Strategy:
  - Discretise the space and time variables into grid of x_i and t_j.
  - Discretise the PDE $u_{i,j} \approx u(x_i, t_j)$
  - Evaluate the values of u at the boundaries (apply B.C.)
  - Evaluate the values of u at $t_0 = 0$ (apply I.C.)
  - Evaluate the values of u in the next time steps $t_1, t_2, \ldots$ by using the values of u of the previous time steps, as in the IVP.

Parabolic BVP - Finite Difference Method (FTCS)

- Discretise the space and time variables
  - Let h be the step size and N be the number of partitions in x. Then $x_i = ih, i = 0, 1, \ldots, N$.
  - Let k be the time-step size, then $t_j = jk, j = 0, 1, 2, \ldots$.
- Discritise PDE: Denote $u_{i,j} \approx u(x_i, t_j)$
  - Forward-Time : $u_t(x_i, t_j) \approx \dfrac{u_{i,j+1} - u_{i,j}}{k} + O(k)$
  - Center-Space : $u_{xx}(x_i, y_j) \approx \dfrac{u_{i+1,j} - 2u_{i,j} + u_{i-1,j}}{h^2} + O(h^2)$
  - Ignore error terms $O(h^2) + O(k)$: $\dfrac{u_{i,j+1} - u_{i,j}}{k} - \alpha^2 \dfrac{u_{i+1,j} - 2u_{i,j} + u_{i-1,j}}{h^2} = 0.$
  - Re-arrange **(Interior Points)** :

$$u_{i,j+1} = (1 - \frac{2\alpha^2 k}{h^2})u_{i,j} + \frac{\alpha^2 k}{h^2}(u_{i+1,j} + u_{i-1,j}),$$

for $i = 1, 2, \ldots, N-1, j = 1, 2, \ldots$.

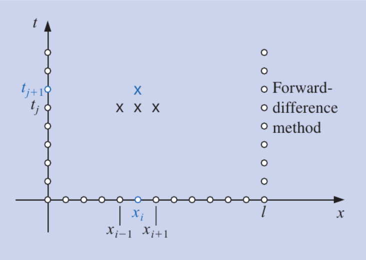
Parabolic BVP - Finite Difference Method (FTCS)

- Evaluate u at boundary **(Boundary Points)**
  - $u(0,t) = 0 \implies i = 0, u_{0,j} = 0$, for $j = 0, 1, \dots$
  - $u(l,t) = 0 \implies i = N, u_{N,j} = 0$, for $j = 0, 1, \dots$
- Evaluate u at $t = 0$ **(Initial Points)**
  - $u(x,0) = f(x) \implies j = 0, u_{i,0} = f(x_i)$, for $i = 1, 2, \dots, N-1$.
- Evaluate u for $j = 1, 2, \dots$ **(time marching)**
  - Let $\mathbf{u}_j = [u_{1,j}, u_{2,j}, \dots, u_{N-1,j}]^T$ be the interior points at time-step $t_j = jk$, then the value of the interior points at t_{j+1} is $\mathbf{u}_{j+1} = \mathbf{A}\mathbf{u}_j$, where

$$\mathbf{A} = \begin{bmatrix} (1-2\lambda) & \lambda & 0 & \dots & 0 \\ \lambda & (1-2\lambda) & \lambda & \dots & 0 \\ 0 & \lambda & (1-2\lambda) & \dots & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & 0 & \dots & (1-2\lambda) \end{bmatrix}$$

  and $\lambda = \alpha k / h^2$.
  - This is known as **FTCS** method and it is of order $O(k + h^2)$.

Stability of FTCS



- Let the initial point $\mathbf{u}_0$ used in FTCS scheme in not exact but comes with an error $\mathbf{e}_0 = [e_1, e_2, \ldots, e_{N-1}]^T$.
- In every time steps, the initial error propagates through $\mathbf{u}_n = \mathbf{A}^n(\mathbf{u}_0 - \mathbf{e}_0)$.
- Thus, the method is only stable if $\|\mathbf{A}^n \mathbf{e}_0\| < \|\mathbf{e}_0\|$ for all n, ie $\|A^n\| \leq 1$, or the spectral radius $\rho(\mathbf{A}^n) = \rho(\mathbf{A})^n \leq 1$.
- The eigenvalues of $\mathbf{A}$ is $1 - 4\lambda \sin^2(i\pi/2N), i = 1, 2, \ldots, N-1$.
- From $\rho(\mathbf{A}) \leq 1$ and stability condition requires to hold as $h \to 0$, simplify to

$$0 \leq \lambda \leq \frac{1}{2}, \text{ or } \alpha^2 \frac{k}{h^2} \leq \frac{1}{2}.$$

Heat Equation (Example)

Example

Use a FTCS explicit scheme to solve the following BVP for the Heat equation with 4 equal subintervals for $[0, 1]$ and let $k = 0.01$:

$$\begin{aligned} \text{PDE} &: \quad u_t(x,t) - u_{xx}(x,t) = 0, \quad \text{for } 0 < x < 1, t > 0, \\ \text{B.C.} &: \quad u(0,t) = u(1,t) = 0, \quad \text{for } t > 0, \\ \text{I.C.} &: \quad u(x,0) = \sin(\pi x), 0 < x < 1. \end{aligned}$$

ANSWER:

- Discretise x and given $k = 0.01$:
  - $h = 1/4 = 0.25$, thus $x_i = ih, i = 0, 1, 2, 3, 4$
  - Given $k = 0.01$, thus $\lambda = \alpha^2(k/h^2) = 0.16$ ($< 1/2$, FTCS should be stable.)
- Discretise PDE:
  - Let $u_{i,j} \approx u(x_i, t_j) = u(ih, jk)$.
  - $u_{i,j+1} = (1 - 2\lambda)u_{i,j} + \lambda(u_{i+1,j} + u_{i-1,j})$, for $i = 0, 1, 2, 3, 4,$ and $j \geq 0$.
- Boundary points:
  - $i = 0$, $u_{0,j} = u(0,t) = 0, j \geq 0$.
  - $i = 4$, $u_{4,j} = u(1,t) = 0, j \geq 0$.

Heat Equation (example)

Example

- Initial points, $k = 0$:
  - $u_{i,0} = u(x_i, 0) = \sin(\pi x), 0 \le u \le 4$.
  - $u_{0,0} = 0, u_{1,0} = 0.70710678, u_{2,0} = 1, u_{3,0} = 0.70710678, u_{4,0} = 0$.
- Time marching, $k \ge 1$:
  - Let $\mathbf{u}_j = [u_{1,j}, u_{2,j}, u_{3,j}]^T$, and $\mathbf{u}_{j+1} = \mathbf{A}\mathbf{u}_j$, where
    $$\mathbf{A} = \begin{bmatrix} (1-2\lambda) & \lambda & 0 \\ \lambda & (1-2\lambda) & \lambda \\ 0 & \lambda & (1-2\lambda) \end{bmatrix} = \begin{bmatrix} 0.68 & 0.16 & 0 \\ 0.16 & 0.68 & 0.16 \\ 0 & 0.16 & 0.68 \end{bmatrix}$$ and
    $\mathbf{u}_0 = [0.70710678, 1, 0.70710678]^T$
  -

x_i	$u_{0,j}$	$u_{1,j}$	$u_{2,j}$	$u_{3,j}$	$u_{4,j}$
$j = 0, t_0 = 0.00$	0	0.70710678	1	0.70710678	0
$j = 1, t_1 = 0.01$	0	0.64083261	0.90627420	0.64083261	0
$j = 2, t_2 = 0.02$	0	0.58077004	0.82133287	0.58077004	0
$j = 3, t_3 = 0.03$	0	0.52633689	0.74435277	0.52633689	0
$j = 4, t_4 = 0.04$	**0**	**0.47700553**	**0.67458769**	**0.47700553**	**0**
$\vdots$				$\vdots$	

Parabolic BVP - Finite Difference Method (BTCS)

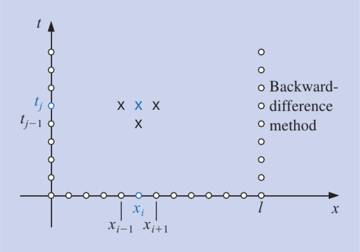
- The FTCS scheme is not stable when $\lambda > 1/2$.
- A more stable method is obtained by using a backward difference in time and central difference in space, thus **BTCS** scheme.
- Discritise PDE: Denote $u_{i,j} \approx u(x_i, t_j)$
  - Backward-Time : $u_t(x_i, t_j) \approx \dfrac{u_{i,j} - u_{i,j-1}}{k} + O(k)$
  - Center-Space : $u_{xx}(x_i, y_j) \approx \dfrac{u_{i+1,j} - 2u_{i,j} + u_{i-1,j}}{h^2} + O(h^2)$
  - PDE : $\dfrac{u_{i,j} - u_{i,j-1}}{k} - \alpha^2 \dfrac{u_{i+1,j} - 2u_{i,j} + u_{i-1,j}}{h^2} = 0.$
  - Re-arrange **(Interior Points)** :

$$(1+2\lambda)u_{i,j} - \lambda u_{i+1,j} - \lambda u_{i-1,j} = u_{i,j-1},$$

  for $i = 1, 2, \ldots, N-1, j = 1, 2, \ldots$ and $\lambda = \alpha^2 k/h^2$.
  - In matrix form $\mathbf{B}\mathbf{u}_j = \mathbf{u}_{j-1}$, where

$$\begin{bmatrix} (1+2\lambda) & -\lambda & 0 & \ldots & 0 \\ -\lambda & (1+2\lambda) & -\lambda & \ldots & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & 0 & \ldots & (1+2\lambda) \end{bmatrix} \begin{bmatrix} u_{1,j} \\ u_{2,j} \\ \vdots \\ u_{N-1,j} \end{bmatrix} = \begin{bmatrix} u_{1,j-1} \\ u_{2,j-1} \\ \vdots \\ u_{N-1,j-1} \end{bmatrix}$$

Stability of BTCS



- Truncation error for BTCS is of order $O(k + h^2)$.
- The eigenvalues of $\mathbf{B}$ is $1 + 4\lambda \sin^2(i\pi/2N) > 1$, for all $i = 1, 2, \ldots, N-1$.
- This implies $\mathbf{B}^{-1}$ exists.
- Thus, an error $\mathbf{e}_0$ in the initial data produces an error $(\mathbf{B}^{-1})^n \mathbf{e}_0$ after n time steps.
- Since $\mathbf{B}^{-1}$ is bounded above by 1, thus the method is unconditionally stable, ie independent of the choice of λ.

Example

Repeat the same BVP as for FTCS case, but using at BTCS scheme with $k = 0.04$.

ANSWER :

- Given $k = 0.04$, then $\lambda = \alpha^2 k/h^2 = 0.64$.
- Let $\mathbf{u}_j = [u_{1,j}, u_{2,j}, u_{3,j}]^T$, and solve for $\mathbf{B}\mathbf{u}_j = \mathbf{u}_{j-1}$:
  - Initial points, $j = 0$: $\mathbf{u}_0 = [u_{1,0}, u_{2,0}, u_{3,0}]^T = [0.70710678, 1, 0.70710678]^T$.
  - $\mathbf{B} = \begin{bmatrix} (1+2\lambda) & -\lambda & 0 \\ -\lambda & (1+2\lambda) & -\lambda \\ 0 & -\lambda & (1+2\lambda) \end{bmatrix} = \begin{bmatrix} 2.28 & -0.64 & 0 \\ -0.64 & 2.28 & -0.64 \\ 0 & -0.64 & 2.28 \end{bmatrix}$
  -

x_i	$u_{0,j}$	$u_{1,j}$	$u_{2,j}$	$u_{3,j}$	$u_{4,j}$
$j = 0, t_0 = 0$	0	0.70710678	1	0.70710678	0
$j = 1, t_1 = 0.04$	**0**	**0.51429564**	**0.72732387**	**0.51429564**	**0**
$j = 2, t_1 = 0.08$	0	0.37405949	0.52900001	0.37405949	0
$j = 3, t_1 = 0.12$	0	0.27206240	0.38475433	0.27206240	0
$\vdots$				$\vdots$	

Parabolic BVP - Crank-Nicolson Method

- Both FTCS and BTCS are $O(k+h^2)$ schemes
- We can improve the accuracy of the scheme by averaging j-th step in FTCS and $(j+1)$-th step in BTCS:
  - FTCS (j-th step) :
    $\frac{u_{i,j+1}-u_{i,j}}{k} - \alpha^2 \frac{u_{i+1,j}-2u_{i,j}+u_{i-1,j}}{h^2} + \frac{k}{2} u_{tt}(x_i, \xi_j) + O(h^2) = 0.$
  - BTCS ($(j+1)$-th step) :
    $\frac{u_{i,j+1}-u_{i,j}}{k} - \alpha^2 \frac{u_{i+1,j+1}-2u_{i,j+1}+u_{i-1,j+1}}{h^2} - \frac{k}{2} u_{tt}(x_i, \xi_{j+1}) + O(h^2) = 0.$
  - Assuming $\frac{k}{2} u_{tt}(x_i, \xi_j) \approx \frac{k}{2} u_{tt}(x_i, \xi_{j+1})$, then averaging the two schemes eliminates the error of $O(k)$.
  - **Crank-Nicolson** :

$$\frac{u_{i,j+1}-u_{i,j}}{k} - \frac{\alpha^2}{2} \left[\frac{u_{i+1,j}-2u_{i,j}+u_{i-1,j}}{h^2} + \frac{u_{i+1,j+1}-2u_{i,j+1}+u_{i-1,j+1}}{h^2} \right] = 0,$$

which has error of order $O(k^2+h^2)$.

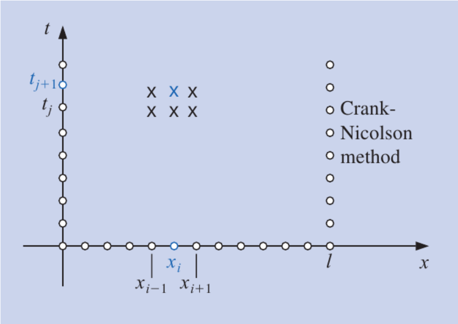
- The Crank-Nicolson method in matrix form: $\mathbf{P}\mathbf{u}_{j+1} = \mathbf{Q}\mathbf{u}_j$, where

$$\mathbf{P} = \begin{bmatrix} (1+\lambda) & -\lambda/2 & 0 & \dots & 0 & 0 \\ -\lambda/2 & (1+\lambda) & -\lambda/2 & \dots & 0 & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & 0 & \dots & -\lambda/2 & (1+\lambda) \end{bmatrix}$$

$$\mathbf{Q} = \begin{bmatrix} (1-\lambda) & \lambda/2 & 0 & \dots & 0 & 0 \\ \lambda/2 & (1-\lambda) & \lambda/2 & \dots & 0 & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & 0 & \dots & \lambda/2 & (1-\lambda) \end{bmatrix}$$

- Since $\mathbf{P}$ is positive, strictly diagonal dominant and tri diagonal, $\mathbf{P}$ is nonsingular.
- The system could be solved by Gauss-Seidel or SOR method to obtain $\mathbf{u}_{j+1}$ from $\mathbf{u}_j$ for $j = 0, 1, 2, 3, \dots$.

Parabolic BVP - Crank-Nicolson Method



Example

Repeat the same BVP by using at Crank-Nicolson scheme with $k = 0.04$.

ANSWER :

- Given $k = 0.04$, then $\lambda = \alpha^2 k/h^2 = 0.64$.
- Let $\mathbf{u}_j = [u_{1,j}, u_{2,j}, u_{3,j}]^T$, and solve for $\mathbf{P}\mathbf{u}_{j+1} = \mathbf{Q}\mathbf{u}_j$:
  - Initial points, $j = 0$: $\mathbf{u}_0 = [u_{1,0}, u_{2,0}, u_{3,0}]^T = [0.70710678, 1, 0.70710678]^T$.
  - $\mathbf{P} = \begin{bmatrix} 1.64 & -0.32 & 0 \\ -0.32 & 1.64 & -0.32 \\ 0 & -0.32 & 1.64 \end{bmatrix}, \quad \mathbf{Q} = \begin{bmatrix} 0.36 & 0.32 & 0 \\ 0.32 & 0.36 & 0.32 \\ 0 & 0.32 & 1.36 \end{bmatrix}$
  - $\mathbf{P}^{-1}\mathbf{Q} = \begin{bmatrix} 0.269769 & 0.257566 & 0.050257 \\ 0.257566 & 0.320026 & 0.257566 \\ 0.050257 & 0.257566 & 0.269769 \end{bmatrix}$
  -

x_i	$u_{0,j}$	$u_{1,j}$	$u_{2,j}$	$u_{3,j}$	$u_{4,j}$
$j = 0, t_0 = 0$	0	0.70710678	1	0.70710678	0
$j = 1, t_1 = 0.04$	**0**	**0.48385838**	**0.68427909**	**0.48385838**	**0**
$j = 2, t_1 = 0.08$	0	0.33109417	0.46823787	0.33109417	0
$j = 3, t_1 = 0.12$	0	0.22656082	0.32040538	0.22656082	0
⋮				⋮	

Outline

Hyperbolic Boundary Value Problem

We will consider the wave equation as an example for the hyperbolic problem:

$$\begin{aligned}
\text{PDE} &: \quad u_{tt}(x,t) - \alpha^2 u_{xx}(x,t) = 0, \quad \text{for } 0 < x < l, t > 0, \\
\text{B.C.} &: \quad u(0,t) = u(l,t) = 0, \quad \text{for } t > 0, \\
\text{I.C.} &: \quad u(x,0) = f(x), 0 < x < l, \\
\text{I.C.} &: \quad u_t(x,0) = g(x), 0 < x < l.
\end{aligned}$$

- This is an Dirichlet boundary value problem.
- Strategy:
  - Discretise the space and time variables into grid of x_i and t_j.
  - Discretise the PDE $u_{i,j} \approx u(x_i, t_j)$
  - Evaluate the values of u at the boundaries (apply B.C.)
  - Evaluate the values of u at $t_0 = 0$. (apply I.C.)
  - Evaluate the values of u at $t_1 = k$. (apply I.C.)
  - Evaluate the values of u in the next time steps $t_2, t_3, \ldots$ by using the values of u of the previous time steps, as in the IVP.

- Discretise the space and time variables
  - Let h be the step size and N be the number of partitions in x. Then $x_i = ih, i = 0, 1, \ldots, N$.
  - Let k be the time-step size, then $t_j = jk, j = 0, 1, 2, \ldots$.
- Discritise PDE: Denote $u_{i,j} \approx u(x_i, t_j)$
  - Center-Time : $u_{tt}(x_i, t_j) \approx \dfrac{u_{i,j+1} - 2u_{i,j} + u_{i,j-1}}{k^2} + O(k^2)$
  - Center-Space : $u_{xx}(x_i, y_j) \approx \dfrac{u_{i+1,j} - 2u_{i,j} + u_{i-1,j}}{h^2} + O(h^2)$
  - Ignore error terms $O(h^2) + O(k^2)$: $\dfrac{u_{i,j+1} - 2u_{i,j} + u_{i,j-1}}{k^2} - \alpha^2 \dfrac{u_{i+1,j} - 2u_{i,j} + u_{i-1,j}}{h^2} = 0.$
  - Re-arrange **(Interior Points)** :

$$u_{i,j+1} = 2(1 - \lambda^2)u_{i,j} + \lambda^2(u_{i+1,j} + u_{i-1,j}) - u_{i,j-1},$$

for $i = 1, 2, \ldots, N - 1, j = 2, 3, \ldots,$ where $\lambda = \alpha k/h$.

Hyperbolic BVP - Finite Difference Method (CTCS)

- Evaluate u at boundary **(Boundary Points)**
  - $u(0,t) = 0 \implies i = 0, u_{0,j} = 0$, for $j = 0, 1, \ldots$
  - $u(l,t) = 0 \implies i = N, u_{N,j} = 0$, for $j = 0, 1, \ldots$
- Evaluate u at $t_0 = 0$ **(Initial Points)**
  - $u(x,0) = f(x) \implies j = 0, u_{i,0} = f(x_i)$, for $i = 1, 2, \ldots, N-1$.
- Evaluate u at $t_1 = k$ **(Initial Points)**
  - The value of $u_{i,1}$ could be obtained from $u_t(x,0) = g(x), 0 \le x \le l$.
  - At $t_1 = k$, $u(x_i, t_1) = u(x_i, 0) + k u_t(x_i, 0) + \frac{k^2}{2} u_{tt}(x_i, \xi_1)$.
  - Thus, $u_{i,1} = u_{i,0} + k g(x_i)$ with error $O(k^2)$.
- (Improved value of u at $t_1 = k$ **(Initial Points)**):
  - The value of $u_{i,1}$ could be improved if f'' exists.
  - At $t_1 = k$, $u(x_i, t_1) = u(x_i, 0) + k u_t(x_i, 0) + \frac{k^2}{2} u_{tt}(x_i, 0) + \frac{k^3}{6} u_{ttt}(x_i, \xi_2)$.
  - Since $u_{tt}(x_i, 0) = \alpha^2 u_{xx}(x_i, 0) = \alpha^2 f''(x_i)$, we have,
    $u_{i,1} = u_{i,0} + k g(x_i) + \frac{\alpha^2 k^2}{2} f''(x_i)$ with error $O(k^3)$.
  - If f'' is not available, we replace it by central difference:
    $f''(x) = \frac{f(x_{i+1}) - 2f(x_i) + f(x_{i-1})}{h^2} + O(h^2)$.
  - That gives, $u_{i,1} = u_{i,0} + k g(x_i) + \frac{\lambda^2}{2}[f(x_{i+1}) - 2f(x_i) + f(x_{i-1})]$ with error $O(k^3 + h^2 k^2)$.

- Evaluate u for $j = 2, 3, \ldots$ **(time marching)**
  - The discretised PDE at the interior points

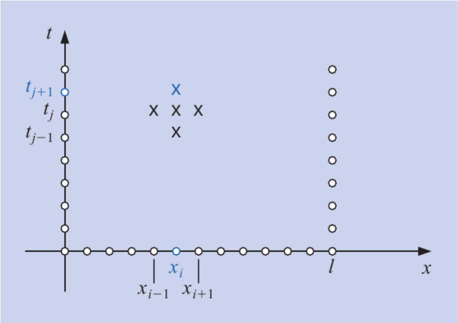
$$u_{i,j+1} = 2(1-\lambda^2)u_{i,j} + \lambda^2(u_{i+1,j} + u_{i-1,j}) - u_{i,j-1},$$

    could be re-written in matrix form.
  - Let $\mathbf{u}_j = [u_{1,j}, u_{2,j}, \ldots, u_{N-1,j}]^T$ be the interior points at time-step $t_j = jk$, then the value of the interior points at t_{j+1} is $\mathbf{u}_{j+1} = \mathbf{A}\mathbf{u}_j - \mathbf{u}_{j-1}$, where

$$\mathbf{A} = \begin{bmatrix} 2(1-\lambda^2) & \lambda^2 & 0 & \ldots & 0 \\ \lambda^2 & 2(1-\lambda^2) & \lambda^2 & \ldots & 0 \\ 0 & \lambda^2 & (1-\lambda^2) & \ldots & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & 0 & \ldots & (1-\lambda^2) \end{bmatrix}$$

    and $\lambda = \alpha k/h$.
  - This is known as **CTCS** method and it is of order $O(k^2)$.

Hyperbolic BVP - Finite Difference Method (CTCS)



Wave Equation (Example)

Example

Use a CTCS explicit scheme to solve the following BVP for the Wave equation with 4 equal subintervals for $[0,1]$ and let $k = 0.01$:

$$\begin{aligned}
\text{PDE} &: \quad u_t(x,t) - 4u_{xx}(x,t) = 0, \quad \text{for } 0 < x < 1, t > 0, \\
\text{B.C.} &: \quad u(0,t) = u(1,t) = 0, \quad \text{for } t > 0, \\
\text{I.C.} &: \quad u(x,0) = 2\sin(3\pi x), 0 < x < 1, \\
\text{I.C.} &: \quad u_t(x,0) = -12\sin(2\pi x), 0 < x < 1.
\end{aligned}$$

ANSWER:

- Discretise x and given $k = 0.01$:
  - $h = 1/4 = 0.25$, thus $x_i = ih, i = 0, 1, 2, 3, 4$
  - Given $k = 0.01$, thus $\lambda = \alpha k/h = 0.16$
- Discretise PDE:
  - Let $u_{i,j} \approx u(x_i, t_j) = u(ih, jk)$.
  - $u_{i,j+1} = 2(1 - \lambda^2)u_{i,j} + \lambda^2(u_{i+1,j} + u_{i-1,j}) - u_{i,j-1}$, for $i = 0, 1, 2, 3, 4,$ and $j \geq 1$.

Wave Equation (example)

Example

- Boundary points:
  - $i = 0,\ u_{0,j} = u(0,t) = 0, j \geq 0.$
  - $i = 4,\ u_{4,j} = u(1,t) = 0, j \geq 0.$
- Initial points, $j = 0$:
  - $u_{i,0} = u(x_i, 0) = 2\sin(3\pi x), 0 \leq u \leq 4.$
  - $\mathbf{u}_0 = [u_{1,0}, u_{2,0}, u_{3,0}] = [1.41421356, -2.0, 1.41421356]$
- Initial points, $j = 1$:
  - $u_t(x, 0) = g(x) = -12\sin(2\pi x)$
  - $u_{i,1} = u_{i,0} + kg(x_i), 0 \leq u \leq 4.$
  - $\mathbf{u}_1 = [u_{1,0}, u_{2,0}, u_{3,0}] = [1.2942136, -2, 1.5342136];$

Wave Equation (example)

Example

- Time marching, $k \geq 1$:
  - Let $\mathbf{u}_j = [u_{1,j}, u_{2,j}, u_{3,j}]^T$, and $\mathbf{u}_{j+1} = \mathbf{A}\mathbf{u}_j - \mathbf{u}_{j-1}$, where

$$\mathbf{A} = \begin{bmatrix} 2(1-\lambda^2) & \lambda^2 & 0 \\ \lambda^2 & 2(1-\lambda^2) & \lambda^2 \\ 0 & \lambda^2 & 2(1-\lambda^2) \end{bmatrix} = \begin{bmatrix} 1.94880 & 0.02560 & 0.00000 \\ 0.02560 & 1.94880 & 0.02560 \\ 0.00000 & 0.02560 & 1.94880 \end{bmatrix}$$

  -

x_i	$u_{0,j}$	$u_{1,j}$	$u_{2,j}$	$u_{3,j}$	$u_{4,j}$
$j = 0, t_0 = 0.00$	0	1.414213562	-2.00	1.414213562	0
$j = 1, t_1 = 0.01$	0	1.294213562	-2.00	1.534213562	0
$j = 2, t_2 = 0.02$	0	1.056749828	-1.82519227	1.524461828	0
$j = 3, t_3 = 0.03$	0	0.718455580	-1.49085567	1.389932726	0
$j = 4, t_4 = 0.04$	0	0.305210502	-1.02621252	1.146073163	0
$\vdots$				$\vdots$	

THE END