Chapter 13 More about Boundary conditions

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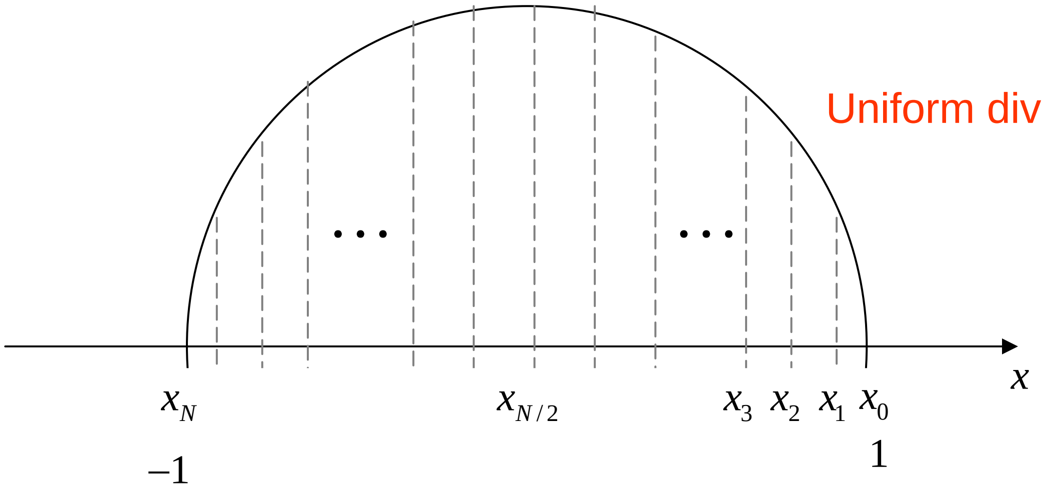
Book: Lloyd N. Trefethen, Spectral Methods in MATLAB

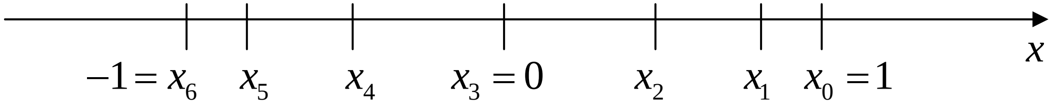
Preliminary: Chebyshev node and diff. matrix [1]

Consider $N+1$ Chebyshev node on $[-1,1]$, $x_j = \cos\left(\frac{j\pi}{N}\right)$ for $j = 0,1,2,\cdots,N$

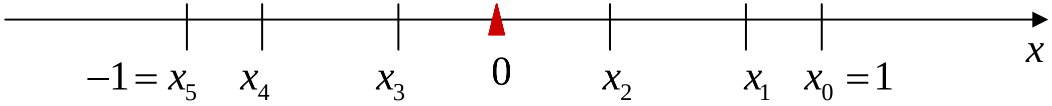


Uniform division in arc

Even case: $N = 6$



Odd case: $N = 5$



Preliminary: Chebyshev node and diff. matrix [2]

Given $N+1$ Chebyshev nodes , $x_j = \cos\left(\frac{j\pi}{N}\right)$ and corresponding function value v_j

We can construct a unique polynomial of degree N , called $p(x) = \sum_{j=0}^{N} v_j S_j(x)$

$S_j(x_k) = \begin{cases} 1 & k = j \\ 0 & k \neq j \end{cases}$ is a basis.

$p'(x_i) = \sum_{j=0}^{N} v_j S_j^{(1)}(x_i) = \sum_{j=0}^{N} D_{ij}^N v_j$ where differential matrix $D_N \triangleq \left(D_{ij}^N\right)$ is expressed as

$$D_{00}^N = \frac{2N^2+1}{6}, \quad D_{NN}^N = -\frac{2N^2+1}{6}, \quad D_{jj}^N = \frac{-x_j}{2\left(1-x_j^2\right)}, \text{ for } j = 1, 2, \cdots, N-1$$

$$D_{ij}^N = \frac{c_i}{c_j}\frac{(-1)^{i+j}}{x_i - x_j}, \text{ for } i \neq j, \; i, j = 0, 1, 2, \cdots, N \qquad \text{where } c_i = \begin{cases} 2 & i = 0, N \\ 1 & \text{otherwise} \end{cases}$$

with identity $D_{ii}^N = -\sum_{j=0, j\neq i}^{N} D_{ij}^N$

Second derivative matrix is $D_N^2 = D_N \cdot D_N$

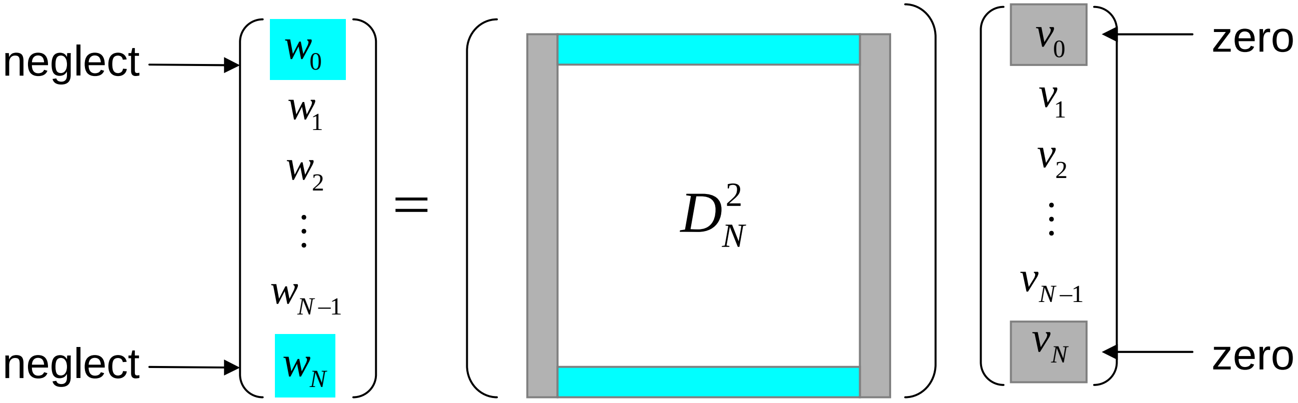
Preliminary: Chebyshev node and diff. matrix [3]

Let $p(x)$ be the unique polynomial of degree $\leq N$ with $p(\pm 1) = 0$ and $p(x_j) = v_j$

define $w_j = p''(x_j)$ and $z_j = p'(x_j)$ for $0 \leq j \leq N$

We abbreviate $w = D_N^2 \cdot v$, then impose B.C. $p(\pm 1) = 0$,that is, $v_0 = v_N = 0$

In order to keep solvability, we neglect $w_0 = w_N$,that is, $\tilde{D}_N^2 = D_N^2(1:N-1,1:N-1)$



Similarly, we also modify differential matrix as $\tilde{D}_N = D_N(1:N-1,1:N-1)$

Asymptotic behavior of spectrum of Chebyshev diff. matrix

In chapter 10, we have showed that spectrum of Chebyshev differential matrix $\tilde{D}_N^2$ (second order) approximates

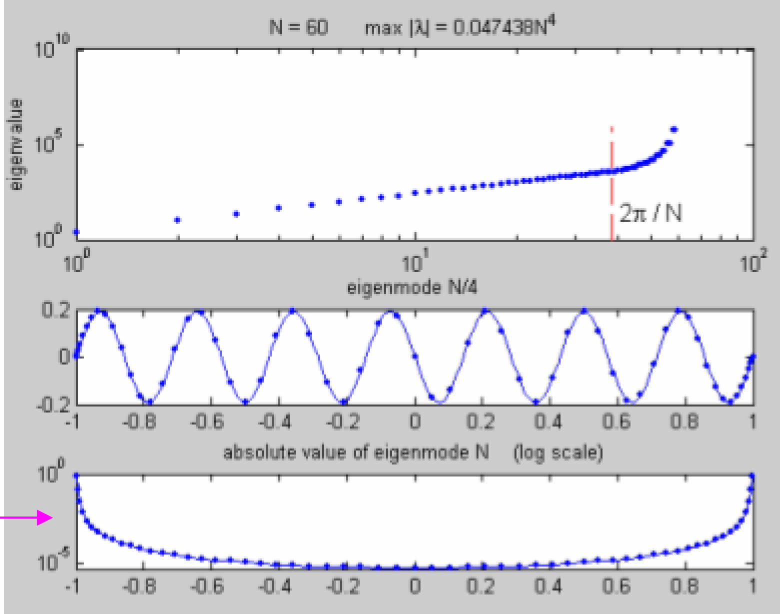
$$u_{xx} = \lambda u, \quad -1 < x < 1, \ \text{B.C. } u(\pm 1) = 0 \quad \text{with eigenmode } \lambda_k = -\frac{\pi^2}{4} k^2$$

1 Eigenvalue of $\tilde{D}_N^2$ is negative (real number) and $\boxed{\lambda_{\max} \approx -0.048 N^4}$

2 Large eigenmode of $\tilde{D}_N^2$ does not approximate to $\lambda_k = -\frac{\pi^2}{4} k^2$

Since ppw is too small such that

resolution is not enough



Mode *N* is spurious and localized near boundaries $x = \pm 1$

Preliminary: DFT [1]

Given a set of data point $\{v_1, v_2, \cdots, v_N\} \in R^N$ with $N = 2m$ is even, $h = \frac{2\pi}{N}$

Then *DFT* formula for $\{v_j\}$

$$\hat{v}_k = \frac{2\pi}{N} \sum_{j=1}^{N} v_j \exp\left(-ikx_j\right) \qquad \text{for} \quad k = -m, -m+1, \cdots, m-1, m$$

$$v_j = \frac{1}{2\pi} \sum_{k=-m+1}^{m} \hat{v}_k \exp\left(ikx_j\right) \qquad \text{for} \quad j = 1, 2, \cdots, N$$

Definition: band-limit interpolant of $\delta - \text{function}$, is periodic **sinc** function $S_N(x)$

$$S_N(x) \triangleq \frac{h}{2\pi} P \sum_{k=-m}^{m} e^{ikx} = \frac{\sin(\pi x / h)}{(2\pi / h)\tan(x/2)} = \frac{1}{2m} \frac{\sin(mx)}{\tan(x/2)}$$

If we write $v_j = \sum_{k=1}^{N} v_k \delta_{j-k} = \delta * v$, then $p(x) = \frac{1}{2\pi} P \sum_{k=-m}^{m} e^{ikx} \hat{v}_k = \sum_{k=1}^{N} v_k S_N(x - x_k)$

Also derivative is according to $w_j = p'(x_j) = \sum_{k=1}^{N} v_k S_N^{(1)}(x_j - x_k)$

Preliminary: DFT [2]

Direct computation of derivative of $S_N(x)=\dfrac{\sin(\pi x/h)}{(2\pi/h)\tan(x/2)}$, we have

$$S_N^{(1)}(x_j)=\begin{cases}0 & j=0(\bmod N)\\ \dfrac{1}{2}(-1)^j\cot\left(\dfrac{jh}{2}\right), & j\neq 0(\bmod N)\end{cases}$$

Example: $D_5=\left(S_5^{(1)}(x_j-x_k)\right)=\begin{pmatrix} 0 & S_5^{(1)}(-h) & S_5^{(1)}(-2h) & S_5^{(1)}(-3h) & S_5^{(1)}(-4h)\\ S_5^{(1)}(h) & 0 & S_5^{(1)}(-h) & S_5^{(1)}(-2h) & S_5^{(1)}(-3h)\\ S_5^{(1)}(2h) & S_5^{(1)}(h) & 0 & S_5^{(1)}(-h) & S_5^{(1)}(-2h)\\ S_5^{(1)}(3h) & S_5^{(1)}(2h) & S_5^{(1)}(h) & 0 & S_5^{(1)}(-h)\\ S_5^{(1)}(4h) & S_5^{(1)}(3h) & S_5^{(1)}(2h) & S_5^{(1)}(h) & 0\end{pmatrix}$

is a Toeplitz matrix.

Second derivative is $S_N^{(2)}(x_j)=\begin{cases}-\dfrac{1}{6}-\dfrac{\pi^2}{3h^2} & j=0(\bmod N)\\ -\dfrac{(-1)^j}{2\sin^2(jh/2)}, & j\neq 0(\bmod N)\end{cases}$

Preliminary: DFT [3]

$$S_N^{(2)}(x_j) = \begin{cases} -\frac{1}{6} - \frac{\pi^2}{3h^2} & j = 0(\mathrm{mod}\, N) \\ -\frac{(-1)^j}{2\sin^2(jh/2)}, & j \neq 0(\mathrm{mod}\, N) \end{cases}$$

For second derivative operation $w_j = p''(x_j) = \sum_{k=1}^{N} v_k S_N^{(2)}(x_j - x_k) \equiv \sum_{k=1}^{N} D_N^2(j,k) v_k$

second diff. matrix is explicitly defined by using Toeplitz matrix (command in MATLAB)

$$D_N^2 = \left(S_N^{(2)}(x_j - x_k)\right) = \begin{pmatrix} \ddots & \vdots & \\ \ddots & -\csc^2(2h/2)/2 & \\ \ddots & \csc^2(h/2)/2 & \\ \ddots & -\frac{1}{6} - \frac{\pi^2}{3h^2} & \ddots \\ & \csc^2(h/2)/2 & \ddots \\ & -\csc^2(2h/2)/2 & \ddots \end{pmatrix} = toeplitz\left(-\frac{1}{6} - \frac{\pi^2}{3h^2}, \frac{(-1)^{2:N}}{2\sin^2((1:N-1)h/2)}\right)$$

Symmetry property: $D_N^2 = \left(D_N^2\right)^T$

Preliminary: DFT [4]

Eigenvalue of Fourier differentiation matrix D_N is $\lambda_k = ik$ corresponding to eigenvector

$\varphi_k = \exp(ikx)$ for $k = -\frac{N}{2}+1, \cdots, \frac{N}{2}-1$ and $\lambda = 0$ has multiplicity 2

$$w_j = \sum_{k=1}^{N} v_k S_N^{(1)}\left(x_j - x_k\right), \quad S_N(x) = \frac{h}{2\pi} P \sum_{k=-m}^{m} e^{ikx} \quad \text{and} \quad \hat{v}_k = h \sum_{j=1}^{N} e^{-ikx_j} v_j$$

$$S_N^{(1)}\left(x - x_j\right) = \frac{h}{2\pi} \sum_{\substack{k=-m-1 \\ k \neq 0}}^{m-1} ike^{ik\left(x-x_j\right)} + \frac{h}{4\pi}\left[ime^{im\left(x-x_j\right)} - ime^{-im\left(x-x_j\right)}\right]$$

$$\hat{v}_m = \hat{v}_{-m}$$

$$\longrightarrow \quad \sum_{j=1}^{N} S_N^{(1)}\left(x - x_j\right) v_j = \frac{1}{2\pi} \sum_{\substack{k=-m-1 \\ k \neq 0}}^{m-1} ike^{ikx}\hat{v}_k + \frac{h}{4\pi}\left[\cancel{ime^{imx}\hat{v}_m - ime^{-imx}\hat{v}_{-m}}\right]$$

$$\longrightarrow \quad D_N v = \sum_{j=1}^{N} S_N^{(1)}\left(x_i - x_j\right) v_j = \frac{1}{2\pi} \sum_{\substack{k=-m-1 \\ k \neq 0}}^{m-1} ike^{ikx}\hat{v}_k$$

when $v \equiv 1\left(e^{i0x}\right)$ and $v = e^{imx}$, we have $D_N v = 0$

How to deal with boundary conditions

- Method I: Restrict attention to interpolants that satisfy the boundary conditions.

Example: chapter 7. Boundary value problems

Linear ODE: $u_{xx} = e^{4x}, \quad -1 < x < 1, \;\; u(\pm 1) = 0$

Nonlinear ODE: $u_{xx} = e^{u}, \quad -1 < x < 1, \;\; u(\pm 1) = 0$

Eigenvalue problem: $u_{xx} = \lambda u, \quad -1 < x < 1, \;\; u(\pm 1) = 0$

Poisson equation: $u_{xx} + u_{yy} = 10\sin\left(8x\left(y-1\right)\right), \quad -1 < x, y < 1, \;\; u = 0 \;\text{ on boundary}$

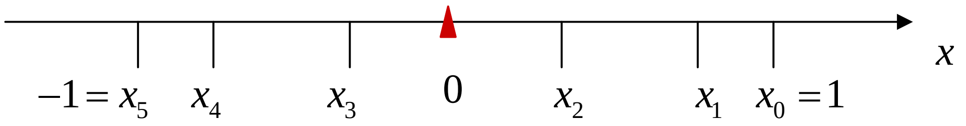
Helmholtz equation: $u_{xx} + u_{yy} + k^2 u = f\left(x, y\right), \quad -1 < x, y < 1, \;\; u = 0 \;\text{ on boundary}$

- Method II: Do not restrict the interpolants, but add additional equations to enforce the boundary condition.

Recall linear ODE in chapter 7

$u_{xx} = e^{4x}, \quad -1 < x < 1, \quad u(\pm 1) = 0$ with exact solution $u = \frac{1}{16}\left(e^{4x} - x\sinh(4) - \cosh(4)\right)$

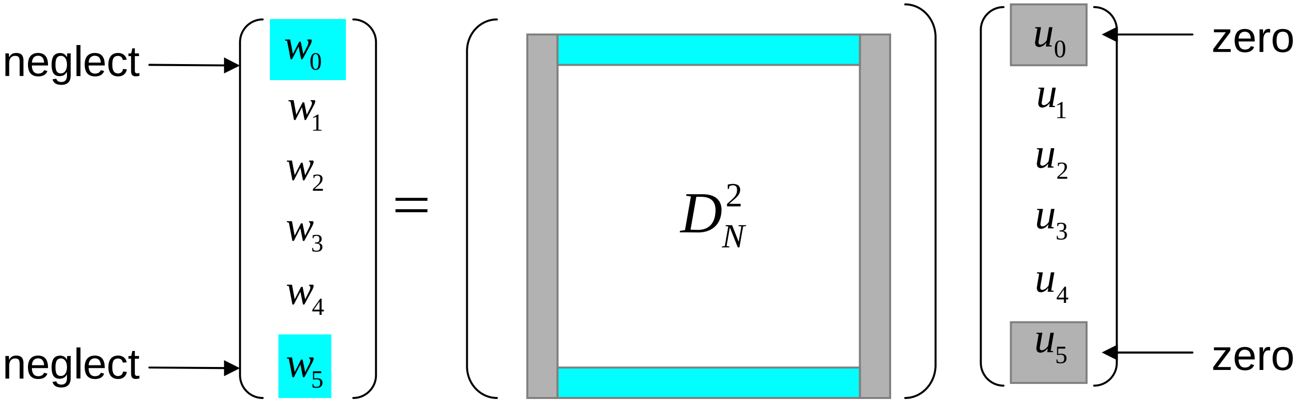
Chebyshev nodes:



① Let $p(x)$ be unique polynomial of degree $\le N$ with $\underline{p(\pm 1) = 0}$ and $p(x_j) = u_j$ for $1 \le j \le N-1$

Method I

② Set $w_j = p''(x_j)$ for $1 \le j \le N-1$



$$\tilde{D}_N^2 = D_N^2(1:N-1, 1:N-1)$$

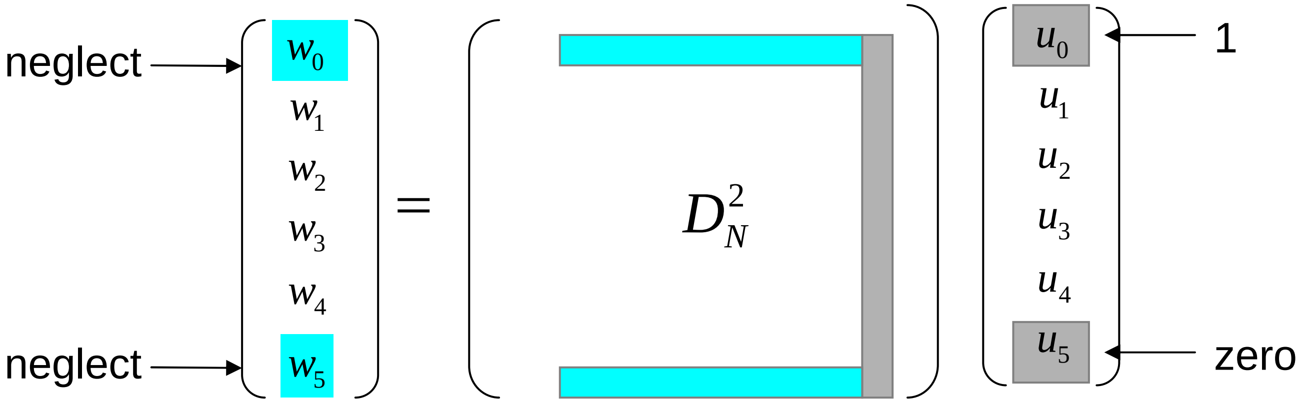
Inhomogeneous boundary data [1]

$$u_{xx} = e^{4x}, \quad -1 < x < 1, \; u(-1) = 0, \; u(1) = 1$$

Method I

① Let $p(x)$ be unique polynomial of degree $\leq N$ with $\underline{p(-1) = 0, \; p(1) = 1}$ and $p(x_j) = u_j$ for $1 \leq j \leq N-1$

② Set $w_j = p''(x_j)$ for $1 \leq j \leq N-1$



$$\begin{pmatrix} w_0 \\ w_1 \\ w_2 \\ w_3 \\ w_4 \\ w_5 \end{pmatrix} = \begin{pmatrix} & & \\ & D_N^2 & \\ & & \end{pmatrix} \begin{pmatrix} u_0 \\ u_1 \\ u_2 \\ u_3 \\ u_4 \\ u_5 \end{pmatrix}$$

or say

$$\begin{pmatrix} w_1 \\ w_2 \\ w_3 \\ w_4 \end{pmatrix} = D_N^2(1:4, 1:4) \begin{pmatrix} u_1 \\ u_2 \\ u_3 \\ u_4 \end{pmatrix} + D_N^2(1:4, 0)$$

Inhomogeneous boundary data [2]

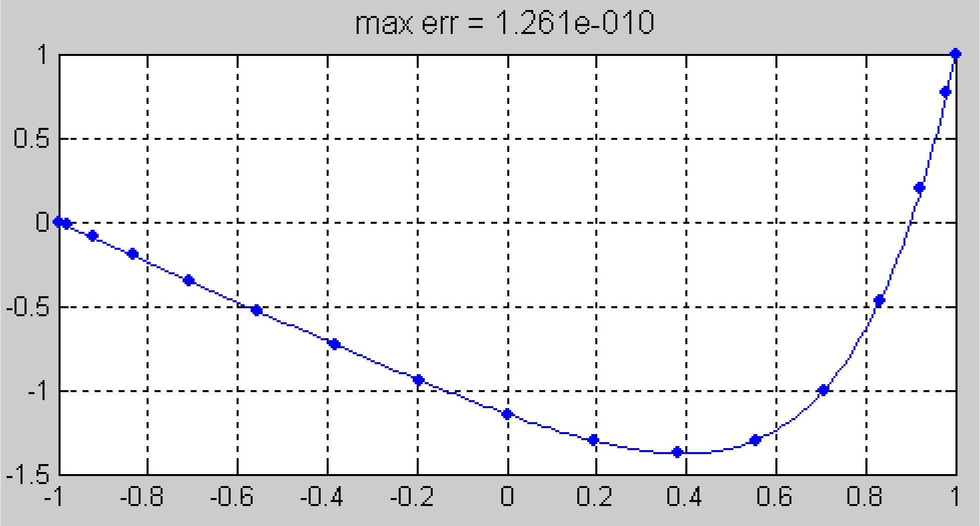
$$u_{xx} = e^{4x}, \quad -1 < x < 1, \ u(-1) = 0, \ u(1) = 1$$

Method of homogenization

$u_S = \dfrac{x+1}{2}$ satisfies $u_S(-1) = 0, \ u_S(1) = 1$, decompose $u = u_H + u_S$, then

$\dfrac{d^2}{dx^2} u_H = e^{4x}, \quad -1 < x < 1, \ u_H(\pm 1) = 0$ which can be solved by method I

Solution under **N = 16**



u_1 : ***method I*** directly

u_2 : method of homogenization

$$\left\| u_2 - u_1 \right\| = 7.5336E - 15$$

method I is good even for inhomogeneous boundary data

exact solution $u = \dfrac{1}{16}\left(e^{4x} - x\sinh(4) - \cosh(4)\right) + \dfrac{x+1}{2}$

Mixed type B.C. [1]

$$u_{xx} = e^{4x}, \quad -1 < x < 1, \ u_x(-1) = 0, \ u(1) = 0$$

Method I

① Let $p(x)$ be unique polynomial of degree $\leq N$ with $\boxed{p_x(-1) = 0,}$ $p(1) = 0$ and

$p(x_j) = u_j$ for $1 \leq j \leq N-1$

How to do?

② Set $w_j = p''(x_j)$ for $1 \leq j \leq N-1$

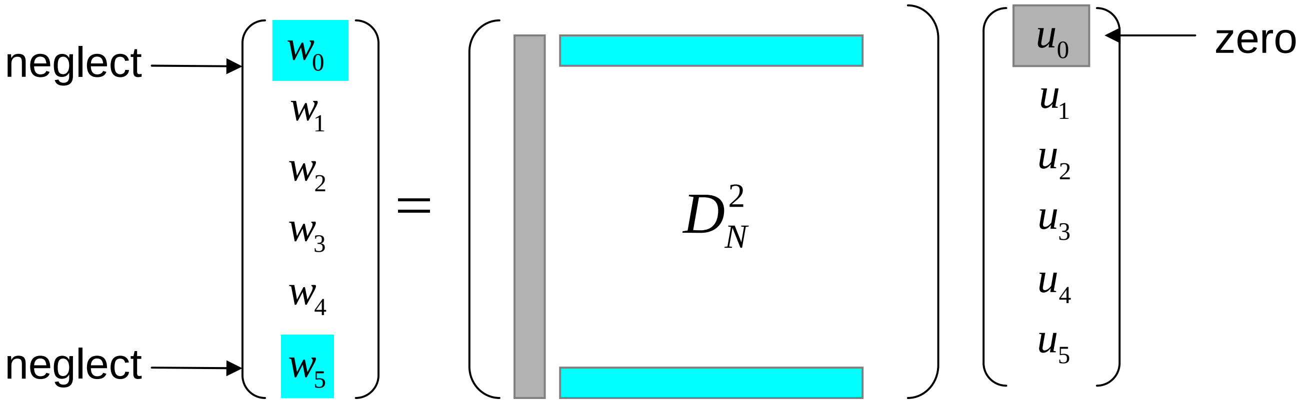
Method II

1 Let $p(x)$ be unique polynomial of degree $\leq N$ with $\boxed{p(1) = 0}$ and

$p(x_j) = u_j$ for $1 \leq j \leq N$

easy to do

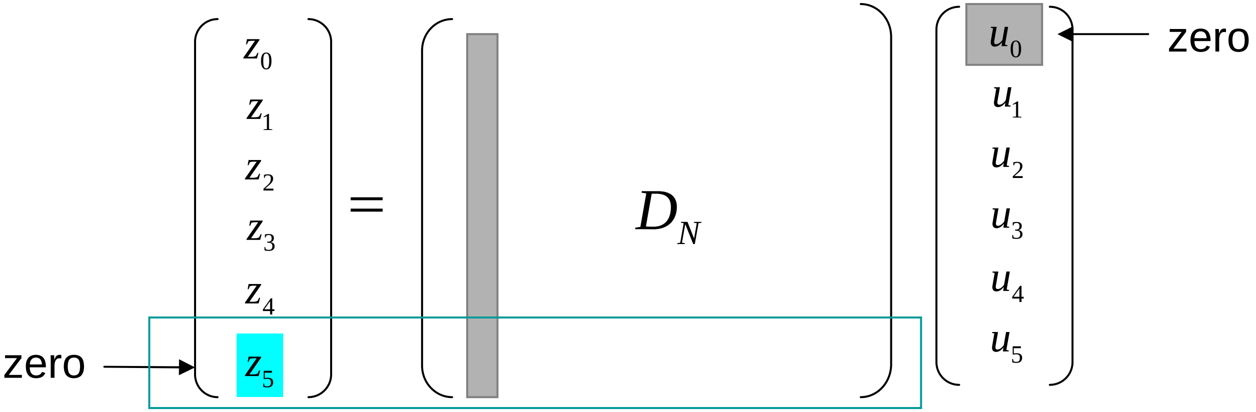
2 Set $w_j = p''(x_j)$ for $1 \leq j \leq N-1$



$$\begin{pmatrix} w_0 \\ w_1 \\ w_2 \\ w_3 \\ w_4 \\ w_5 \end{pmatrix} = \Big(\ D_N^2 \ \Big) \begin{pmatrix} u_0 \\ u_1 \\ u_2 \\ u_3 \\ u_4 \\ u_5 \end{pmatrix}$$

Mixed type B.C. [2]

3 Set $z_j = p'\left(x_j\right)$, we add one more constraint (equation) $z_N = p'\left(-1\right) = 0$



Active variable $\left(u_1 \,|\, u_2 \,|\, u_3 \,|\, u_4 \,|\, u_5\right)^T$ with governing equation

$$\begin{pmatrix} D_N^2\left(1:4,1:5\right) \\ D_N\left(5,1:5\right) \end{pmatrix} \begin{pmatrix} u_1 \\ u_2 \\ u_3 \\ u_4 \\ u_5 \end{pmatrix} = \begin{pmatrix} f_1 \\ f_2 \\ f_3 \\ f_4 \\ 0 \end{pmatrix} \left.\begin{matrix} \\ \\ \\ \\ \end{matrix}\right\}$$

from interior point

from Neumann condition

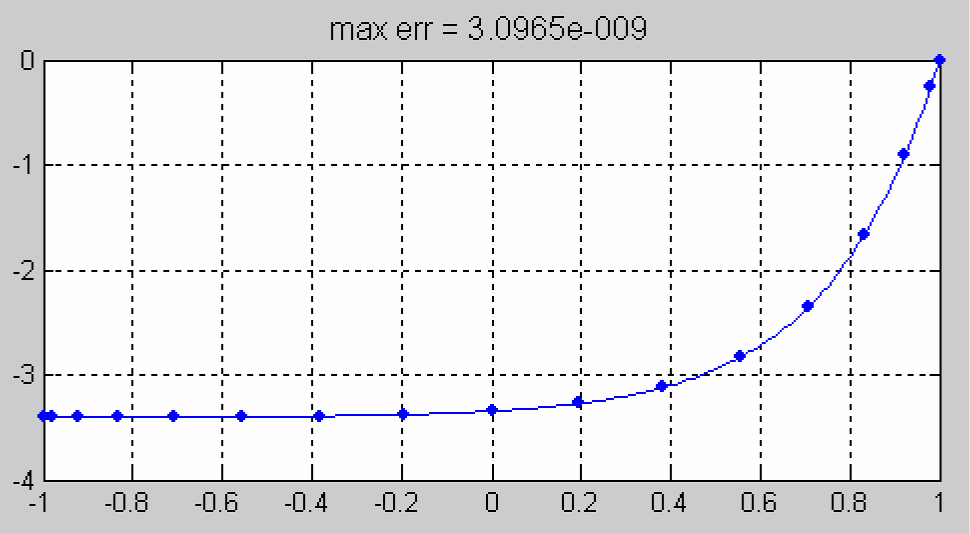
In general, replace 5 by N since the method works for $N = 5$

Mixed type B.C.   [3]

$$u_{xx} = e^{4x}, \quad -1 < x < 1, \; u_x(-1) = 0, \; u(1) = 1$$

exact solution $u = \frac{1}{16}\left(e^{4x} - 4e^{-4}(x-1) - e^4\right)$

Solution under **N = 16**



Allen-Cahn (bistable equation) [1]

Nonlinear reaction-diffusion equation: $u_t = \varepsilon \cdot u_{xx} + u - u^3, \quad -1 < x < 1$

where ε is a parameter

① This equation has three constant steady state, $u = 0,\ u = -1,\ u = 1$

(consider *ODE* $u_t = u - u^3$, equilibrium occurs at zero forcing $u - u^3 = 0$)

② $u = 0$ is unstable and $u = \pm 1$ is attractor.

$$u_t = u - u^3 \longrightarrow uu_t = u^2\left(1-u^2\right) \longrightarrow \frac{d}{dt}u^2 = 2u^2\left(1-u^2\right)$$

$$\xrightarrow{x := u^2} \begin{cases} \dfrac{dx}{dt} = 2x(1-x) \\ x(0) \ge 0 \end{cases}$$ is Logistic equation.

$$x(t) = \frac{ce^{2t}}{1+ce^{2t}}, \quad c = \frac{x(0)}{1-x(0)} \longrightarrow \lim_{t\to\infty} x(t) = 1 \ \text{ for } \ x(0) > 0$$

$$\left.\begin{array}{l} 1 > x(0) > 0 \ \Rightarrow \ \dfrac{dx}{dt} > 0 \ \Rightarrow \ x(t) \nearrow 1 \\ 1 < x(0) \ \Rightarrow \ \dfrac{dx}{dt} < 0 \ \Rightarrow \ x(t) \searrow 1 \end{array}\right\} x \equiv 0 : \text{unstable}$$

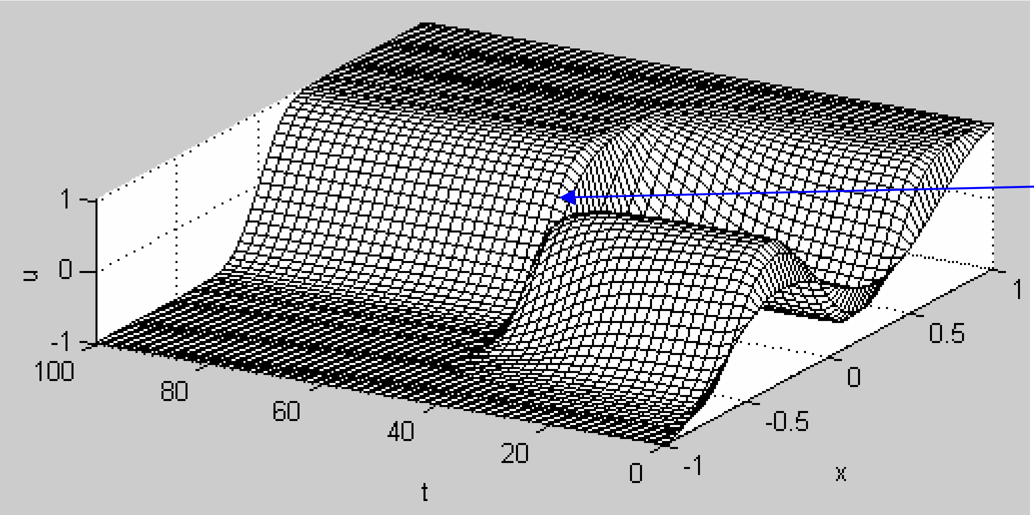
Allen-Cahn (bistable equation) [2]

for $u_t = u\left(1-u^2\right)$

$$\left\{\begin{array}{llllll} 1 > u(0) > 0 & \Rightarrow & \dfrac{du}{dt} > 0 & \Rightarrow & u(t) \nearrow 1 \\ 1 < u(0) & \Rightarrow & \dfrac{du}{dt} < 0 & \Rightarrow & u(t) \searrow 1 \\ 0 > u(0) > -1 & \Rightarrow & \dfrac{du}{dt} < 0 & \Rightarrow & u(t) \searrow -1 \\ -1 > u(0) & \Rightarrow & \dfrac{du}{dt} > 0 & \Rightarrow & u(t) \nearrow -1 \end{array}\right\} u \equiv 0 : \text{unstable}$$

③ Solution tends to exhibit flat areas close to $u = \pm 1$, separated by interfaces

That may coalesce or vanish on a long time scale, called metastability.



interface

boundary value: $u(t, x = \pm 1) = \pm 1$

Allen-Cahn : example 1 [1]

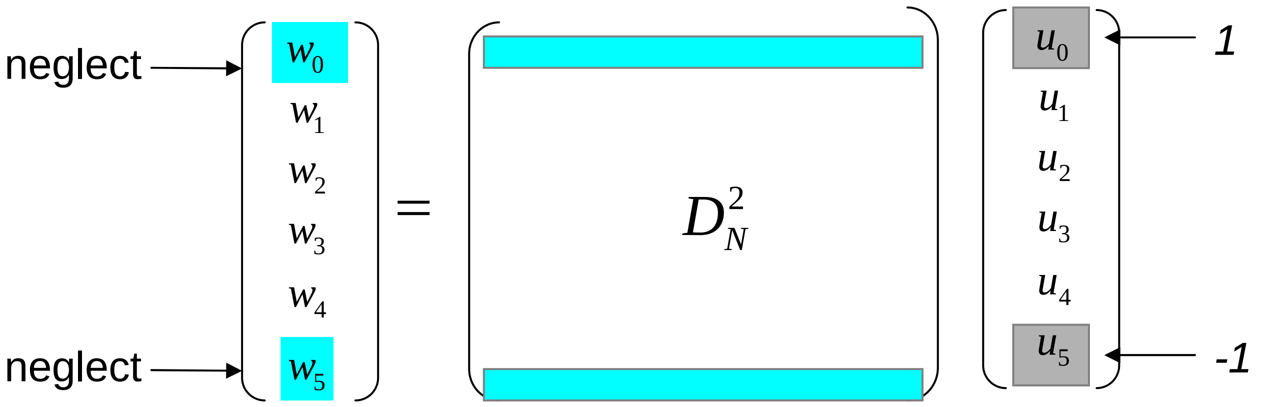
$$u_t = \varepsilon \cdot u_{xx} + u - u^3, \quad -1 < x < 1, \;\; u(-1) = -1, \;\; u(1) = 1$$

with parameter $\varepsilon = 0.01$ and initial condition $u(t=0) = 0.53x + 0.47\sin\left(-\frac{3\pi}{2}x\right)$

Method I

① Let $p(x)$ be unique polynomial of degree $\leq N$ with $p(-1) = -1, \;\; p(1) = 1$ and $p(x_j) = u_j$ for $1 \leq j \leq N-1$

② Set $w_j = p''(x_j)$ for $1 \leq j \leq N-1$



or say
$$\begin{pmatrix} w_1 \\ w_2 \\ w_3 \\ w_4 \end{pmatrix} = D_N^2(1:4,1:4)\begin{pmatrix} u_1 \\ u_2 \\ u_3 \\ u_4 \end{pmatrix} + D_N^2(1:4,0) - D_N^2(1:4,5)$$

Allen-Cahn : example 1   [2]

Temporal discretization: forward Euler with ***CFL*** condition $dt = \min\left(0.01,\ 50N^{-4}/\varepsilon\right)$

(eigenvalue of $\tilde{D}_N^2$ is negative (real number) and $\lambda_{\max} \approx -0.048N^4$)

$$\frac{\begin{pmatrix}u_1\\u_2\\u_3\\u_4\end{pmatrix}^{(k+1)} - \begin{pmatrix}u_1\\u_2\\u_3\\u_4\end{pmatrix}^{(k)}}{dt} = \varepsilon\cdot D_N^2\left(1:4,0:5\right)\begin{pmatrix}u_0=1\\u_1\\u_2\\u_3\\u_4\\u_5=-1\end{pmatrix}^{(k)} + \begin{pmatrix}u_1\\u_2\\u_3\\u_4\end{pmatrix}^{(k)} - \left(\begin{pmatrix}u_1\\u_2\\u_3\\u_4\end{pmatrix}^{(k)}\right)^3$$

One can simplify above equation by using equilibrium of $u=\pm1$ at boundary point.

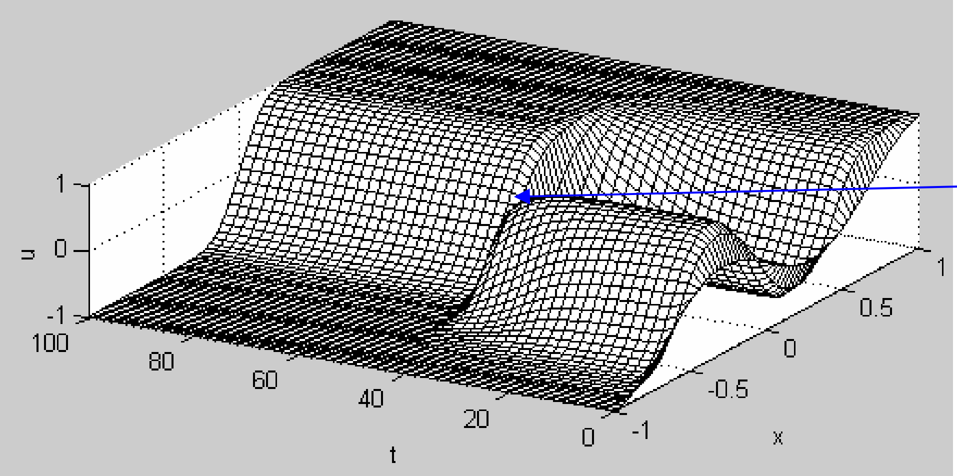
$$\frac{1}{dt}\left(\begin{pmatrix}u_0\\u_1\\u_2\\u_3\\u_4\\u_5\end{pmatrix}^{(k+1)} - \begin{pmatrix}u_0\\u_1\\u_2\\u_3\\u_4\\u_5\end{pmatrix}^{(k)}\right) = \varepsilon\cdot\begin{pmatrix}0\\D_N^2\left(1:4,0:5\right)\\0\end{pmatrix}\begin{pmatrix}u_0\\u_1\\u_2\\u_3\\u_4\\u_5\end{pmatrix}^{(k)} + \begin{pmatrix}u_0\\u_1\\u_2\\u_3\\u_4\\u_5\end{pmatrix}^{(k)} - \left(\begin{pmatrix}u_0\\u_1\\u_2\\u_3\\u_4\\u_5\end{pmatrix}^{(k)}\right)^3$$

Allen-Cahn : example 1 [3]

$$u_t = \varepsilon \cdot u_{xx} + u - u^3, \quad -1 < x < 1, \ u(-1) = -1, \ u(1) = 1$$

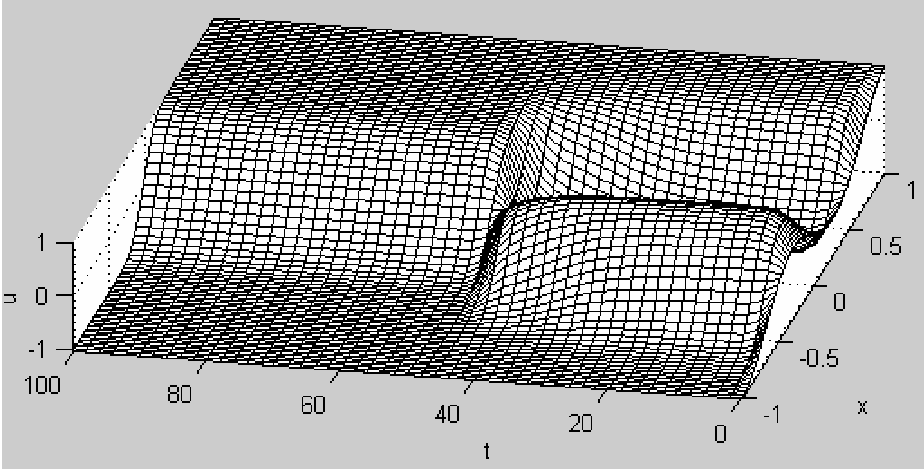
with parameter $\varepsilon = 0.01$ and initial condition $u(t=0) = 0.53x + 0.47\sin\left(-\frac{3\pi}{2}x\right)$

Solution under **N = 20**



boundary value: $u(t, x = \pm 1) = \pm 1$

interface



Metastability up to $t \approx 45$ followed by rapid transition to a solution with just one interface.

Allen-Cahn : example 2 [1]

$$u_t = \varepsilon \cdot u_{xx} + u - u^3, \quad -1 < x < 1, \ u(-1,t) = -1, \ u(1,t) = 1 + \sin^2(t/5)$$

with parameter $\varepsilon = 0.01$ and initial condition $u(t=0) = 0.53x + 0.47\sin\left(-\frac{3\pi}{2}x\right)$

Method I

1 Let $p(x)$ be unique polynomial of degree $\le N$ with $p(-1) = -1$, $\underline{p(1) = 1 + \sin^2(t/5)}$

and $p(x_j) = u_j$ for $1 \le j \le N-1$

2 Set $w_j = p''(x_j)$ for $1 \le j \le N-1$

$$\frac{\begin{pmatrix} u_1 \\ u_2 \\ u_3 \\ u_4 \end{pmatrix}^{(k+1)} - \begin{pmatrix} u_1 \\ u_2 \\ u_3 \\ u_4 \end{pmatrix}^{(k)}}{dt} = \varepsilon \cdot D_N^2(1:4, 0:5) \begin{pmatrix} \underline{u_0 = 1 + \sin^2(t_k/5)} \\ u_1 \\ u_2 \\ u_3 \\ u_4 \\ u_5 = -1 \end{pmatrix}^{(k)} + \begin{pmatrix} u_1 \\ u_2 \\ u_3 \\ u_4 \end{pmatrix}^{(k)} - \left[\begin{pmatrix} u_1 \\ u_2 \\ u_3 \\ u_4 \end{pmatrix}^{(k)}\right]^3$$

Second, set $u_0^{(k+1)} = 1 + \sin^2(t_{k+1}/5)$

Allen-Cahn : example 2 [2]

However we cannot simplify as following form

$$\xcancel{\frac{1}{dt}\left[\begin{pmatrix}u_0\\u_1\\u_2\\u_3\\u_4\\u_5\end{pmatrix}^{(k+1)}-\begin{pmatrix}u_0\\u_1\\u_2\\u_3\\u_4\\u_5\end{pmatrix}^{(k)}\right]=\varepsilon\cdot\begin{pmatrix}0\\D_N^2\,(1:4,0:5)\\0\end{pmatrix}\begin{pmatrix}u_0\\u_1\\u_2\\u_3\\u_4\\u_5\end{pmatrix}^{(k)}+\begin{pmatrix}u_0\\u_1\\u_2\\u_3\\u_4\\u_5\end{pmatrix}^{(k)}-\left[\begin{pmatrix}u_0\\u_1\\u_2\\u_3\\u_4\\u_5\end{pmatrix}^{(k)}\right]^3}$$

since $u(1,t)=1+\sin^2(t/5)$ is NOT an equilibrium.

Method II

1 Let $p(x)$ be unique polynomial of degree $\le N$ with $p(x_j)=u_j$ for $0\le j\le N$

2 Set $w_j = p''(x_j)$ for $0\le j\le N$

3 Neglect $u_0,\ u_N$ computed from 2 , and reset $u_0 = 1+\sin^2(t/5),\ u_N = -1$

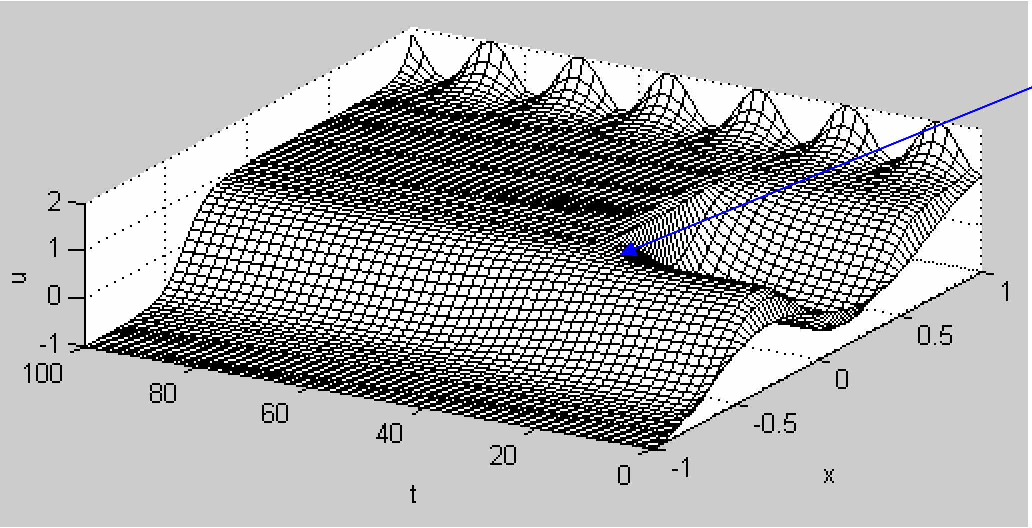
Allen-Cahn : example 2 [3]

Step 1:

$$\frac{1}{dt}\left(\begin{pmatrix}u_0\\u_1\\u_2\\u_3\\u_4\\u_5\end{pmatrix}^{(k+1)}-\begin{pmatrix}u_0\\u_1\\u_2\\u_3\\u_4\\u_5\end{pmatrix}^{(k)}\right)=\varepsilon\cdot D_N^2\begin{pmatrix}u_0\\u_1\\u_2\\u_3\\u_4\\u_5\end{pmatrix}^{(k)}+\begin{pmatrix}u_0\\u_1\\u_2\\u_3\\u_4\\u_5\end{pmatrix}^{(k)}-\left(\begin{pmatrix}u_0\\u_1\\u_2\\u_3\\u_4\\u_5\end{pmatrix}^{(k)}\right)^3$$

Step 2: $u_0^{(k+1)}=1+\sin^2\left(t_{k+1}/5\right),\ u_N^{(k+1)}=-1$

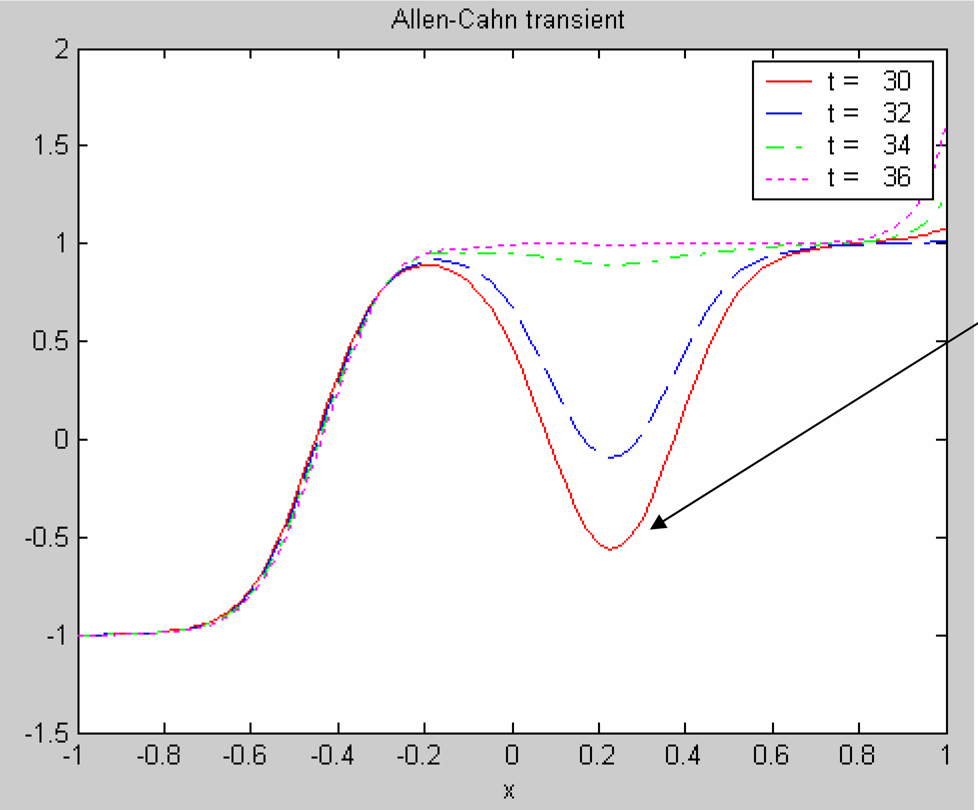
Solution under **N = 20,** *method II*



Final interface is moved from $x=0$ to $x\approx-0.4$ and transients vanish earlier at $t\approx 30$ instead of $t\approx 45$

$dt=0.01$ and $tplot=2$

Allen-Cahn : example 2 [4]



graph concave up $\Rightarrow \quad u_{xx} > 0$

$0 > u > -1 \quad \Rightarrow \quad -|u| < u\left(1-u^2\right) < 0$

$u_t = \varepsilon \cdot u_{xx} + u\left(1-u^2\right) > 0$?

Threshold is $\varepsilon \cdot u_{xx} - |u| \geq 0$

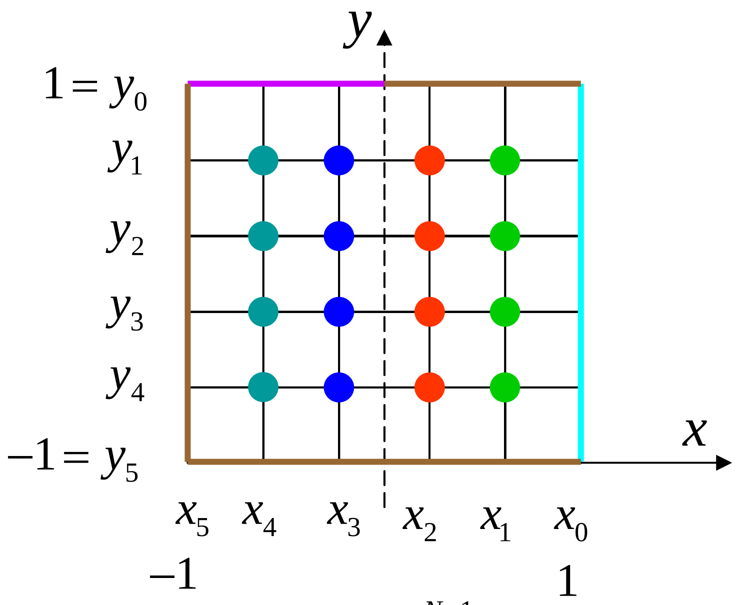
In fact we can estimate trend of transient at point $x = 0.2$

$u_x\left(x = 0.2^+\right) \approx \dfrac{0.5-(-0.5)}{0.2} = 5$ and $u_x\left(x = 0.2^-\right) \approx -u_x\left(x = 0.2^+\right) = -5$

$u_{xx}(0.2) \approx \dfrac{u_x\left(0.2^+\right) - u_x\left(0.2^-\right)}{0.2} = 50$, then $\varepsilon \cdot u_{xx}(0.2) \approx 0.5$ but $u\left(1-u^2\right)|_{x=0.2} \approx -0.375$

Laplace equation [1]

$u_{xx}+u_{yy}=0, \quad -1<x,y<1$ subject to *B.C.* $u(x,y)=\begin{cases}\sin^4(\pi x) & y=1 \ \ and \ \ -1<x<0 \\ \frac{1}{5}\sin(3\pi y) & x=1 \\ 0, & \text{otherwise}\end{cases}$



$\sin^4(\pi x)$

$\frac{1}{5}\sin(3\pi y)$

0

boundary data is continuous

Method I

① Let $P(x,y)=\sum_{i,j=1}^{N-1} u_{i,j}\,p_i(x)\,p_j(y)$ be unique polynomial, $P(x_i,y_j)=u_{i,j}$ for $1\le i,j\le N-1$ (interior point) and $P(x_i,y_j)=B.C.$ for $i=0,N \ or \ j=0,N$

② Set $w_{i,j}=\Delta P(x_i,y_j)$ for $1\le i,j\le N-1$

Briefly speaking, *method I* take active variables as ● ● ● ●

However method 1 is not intuitive to write down linear system if we choose Kronecker-product

Laplace equation [2]

Method II

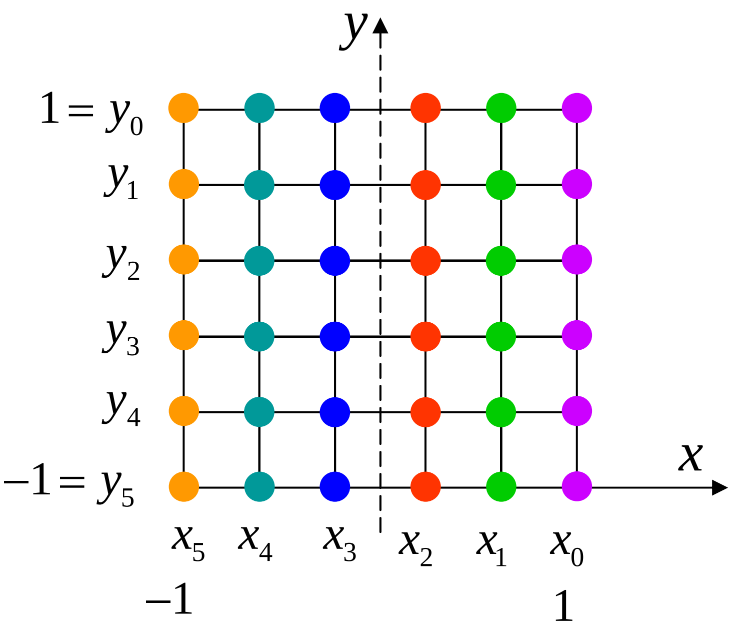
1 Let $P(x,y)=\sum_{i,j=1}^{N-1} u_{i,j}\, p_i(x)\, p_j(y)$ be unique polynomial, $P(x_i,y_j)=u_{i,j}$ for

$0 \le i, j \le N$ (all points)

2 Set $w_{i,j} = \Delta P(x_i, y_j)$ for $1 \le i, j \le N-1$ (interior points)

3 Additional constraints (equations) for boundary condition.

$u_{i,j} = B.C.$ for $i = 0, N \;or\; j = 0, N$



method II take active variables as ● ● ● ● ● ●

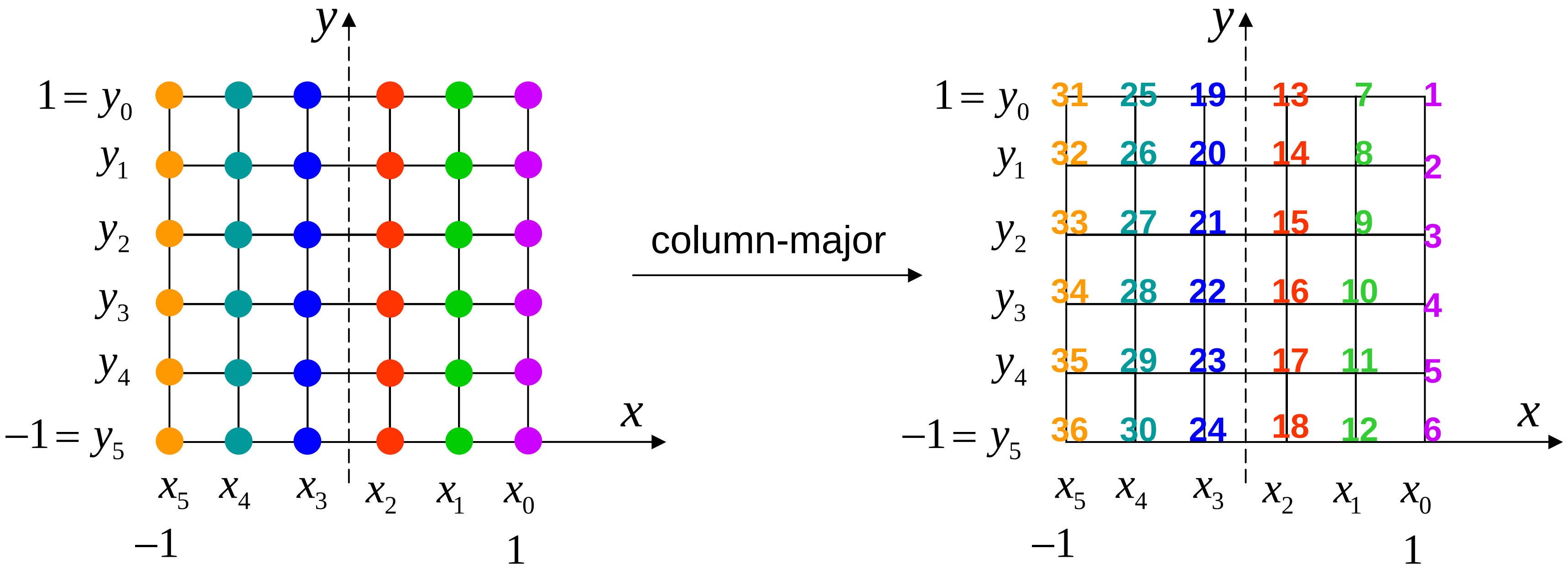
Technical problem:

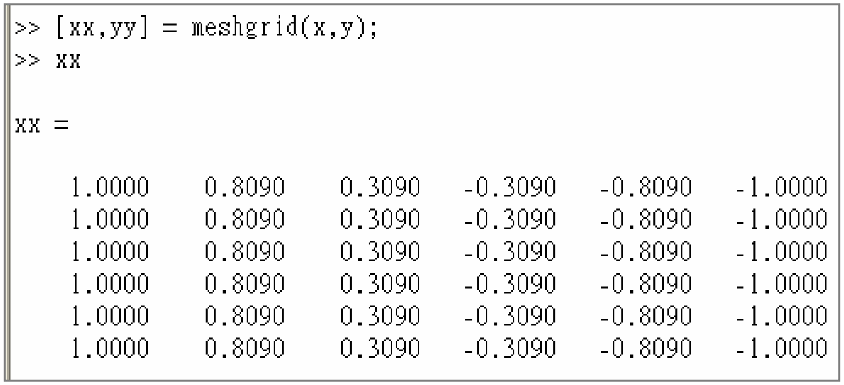
1. How to order the active variables
2. How to build up linear system (matrix)
   (including second derivative and additional equation)
3. How to write down right hand side vector

Laplace equation : order active variable [3]

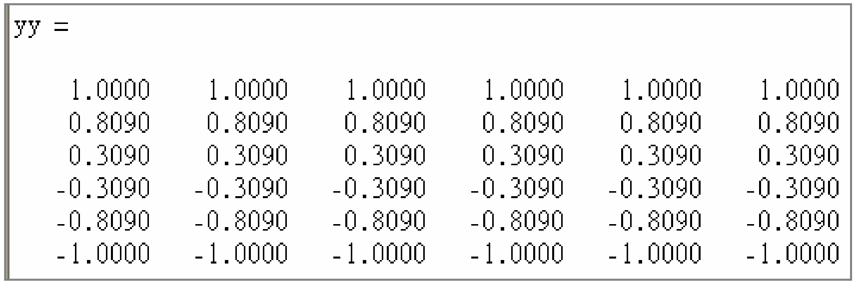
MATLAB use column-major, so we index active variable by column-major

$$x = \left(x_0 \,|\, x_1 \,|\, x_2 \,|\, x_3 \,|\, x_4 \,|\, x_5\right)^T = \left(1 \,|\, 0.809 \,|\, 0.309 \,|\, -0.309 \,|\, -0.809 \,|\, -1\right)^T \quad \text{and} \quad y = x$$



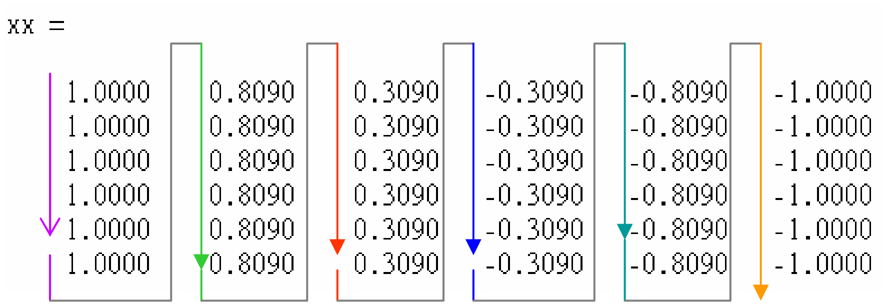


```
>> [xx,yy] = meshgrid(x,y);
>> xx

xx =

    1.0000    0.8090    0.3090   -0.3090   -0.8090   -1.0000
    1.0000    0.8090    0.3090   -0.3090   -0.8090   -1.0000
    1.0000    0.8090    0.3090   -0.3090   -0.8090   -1.0000
    1.0000    0.8090    0.3090   -0.3090   -0.8090   -1.0000
    1.0000    0.8090    0.3090   -0.3090   -0.8090   -1.0000
    1.0000    0.8090    0.3090   -0.3090   -0.8090   -1.0000
```

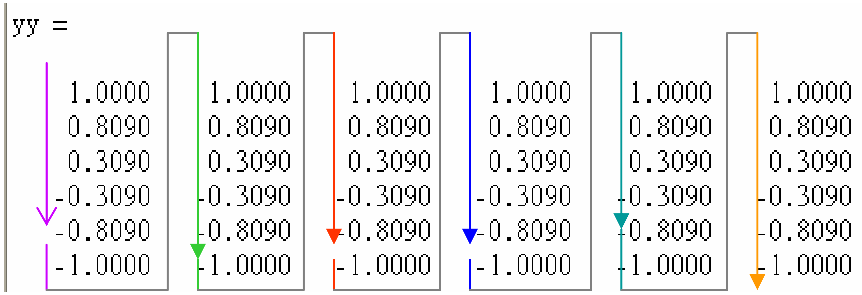


```
yy =

    1.0000    1.0000    1.0000    1.0000    1.0000    1.0000
    0.8090    0.8090    0.8090    0.8090    0.8090    0.8090
    0.3090    0.3090    0.3090    0.3090    0.3090    0.3090
   -0.3090   -0.3090   -0.3090   -0.3090   -0.3090   -0.3090
   -0.8090   -0.8090   -0.8090   -0.8090   -0.8090   -0.8090
   -1.0000   -1.0000   -1.0000   -1.0000   -1.0000   -1.0000
```

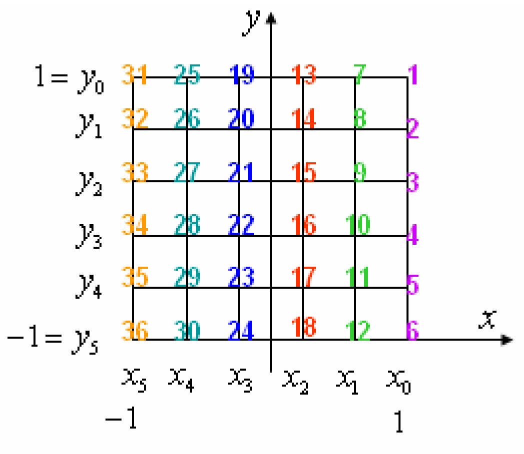
Laplace equation : order active variable [4]

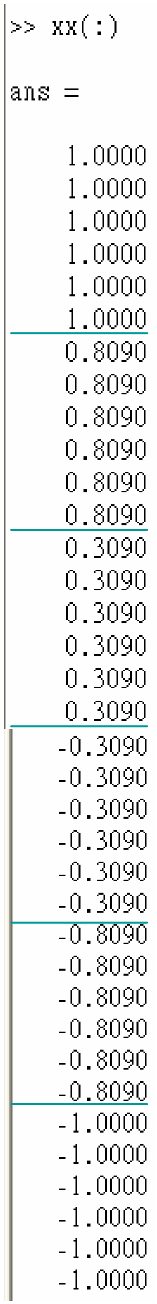


```
xx =

    1.0000    0.8090    0.3090   -0.3090   -0.8090   -1.0000
    1.0000    0.8090    0.3090   -0.3090   -0.8090   -1.0000
    1.0000    0.8090    0.3090   -0.3090   -0.8090   -1.0000
    1.0000    0.8090    0.3090   -0.3090   -0.8090   -1.0000
    1.0000    0.8090    0.3090   -0.3090   -0.8090   -1.0000
    1.0000    0.8090    0.3090   -0.3090   -0.8090   -1.0000
```

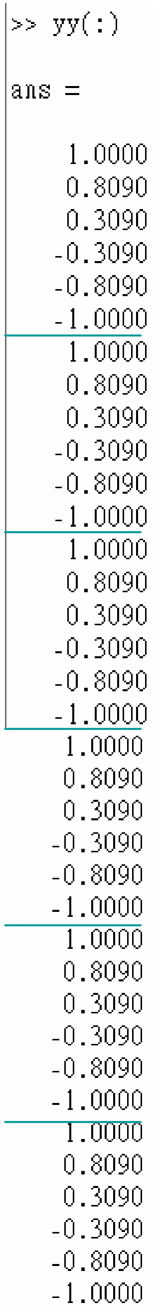


```
yy =

    1.0000    1.0000    1.0000    1.0000    1.0000    1.0000
    0.8090    0.8090    0.8090    0.8090    0.8090    0.8090
    0.3090    0.3090    0.3090    0.3090    0.3090    0.3090
   -0.3090   -0.3090   -0.3090   -0.3090   -0.3090   -0.3090
   -0.8090   -0.8090   -0.8090   -0.8090   -0.8090   -0.8090
   -1.0000   -1.0000   -1.0000   -1.0000   -1.0000   -1.0000
```



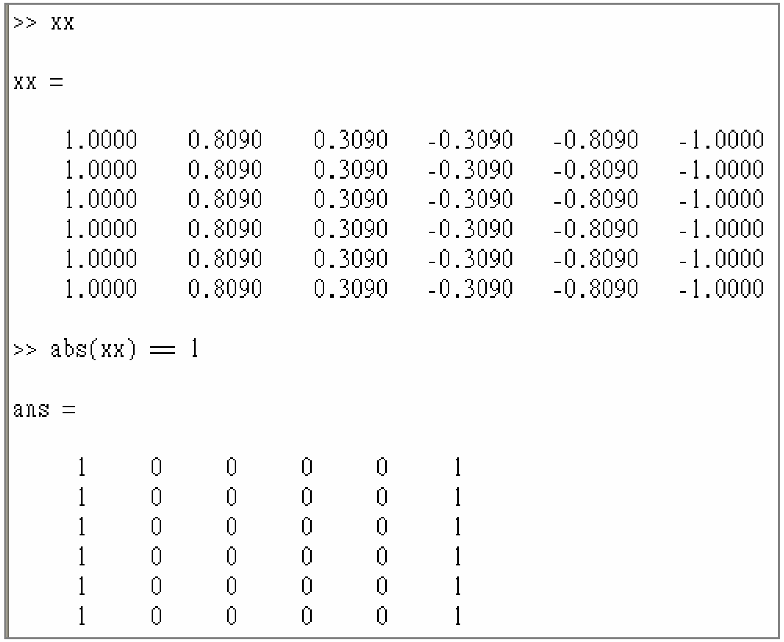


```
>> xx(:)

ans =

    1.0000
    1.0000
    1.0000
    1.0000
    1.0000
    1.0000
    0.8090
    0.8090
    0.8090
    0.8090
    0.8090
    0.8090
    0.3090
    0.3090
    0.3090
    0.3090
    0.3090
    0.3090
   -0.3090
   -0.3090
   -0.3090
   -0.3090
   -0.3090
   -0.3090
   -0.8090
   -0.8090
   -0.8090
   -0.8090
   -0.8090
   -0.8090
   -1.0000
   -1.0000
   -1.0000
   -1.0000
   -1.0000
   -1.0000
```

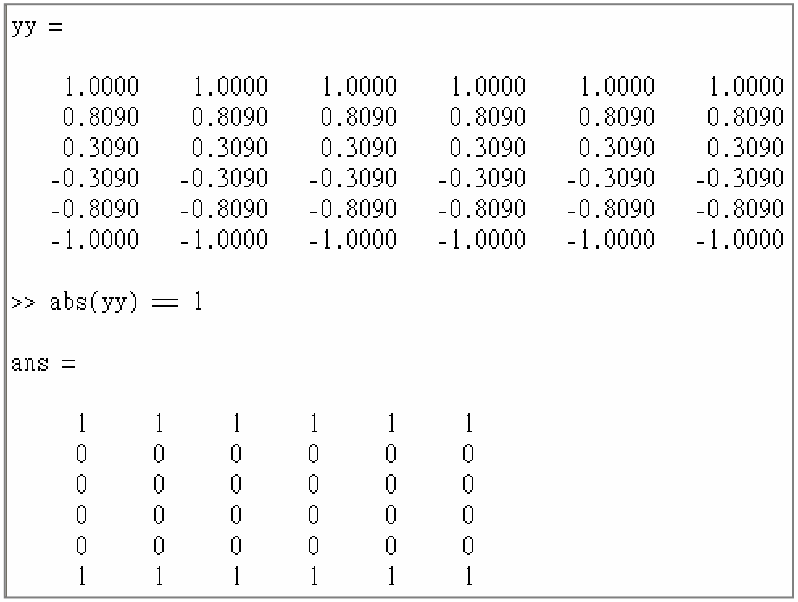


```
>> yy(:)

ans =

    1.0000
    0.8090
    0.3090
   -0.3090
   -0.8090
   -1.0000
    1.0000
    0.8090
    0.3090
   -0.3090
   -0.8090
   -1.0000
    1.0000
    0.8090
    0.3090
   -0.3090
   -0.8090
   -1.0000
    1.0000
    0.8090
    0.3090
   -0.3090
   -0.8090
   -1.0000
    1.0000
    0.8090
    0.3090
   -0.3090
   -0.8090
   -1.0000
    1.0000
    0.8090
    0.3090
   -0.3090
   -0.8090
   -1.0000
```

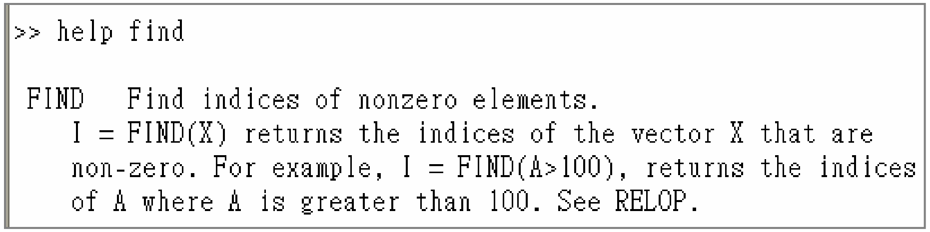
Laplace equation : find boundary point [5]



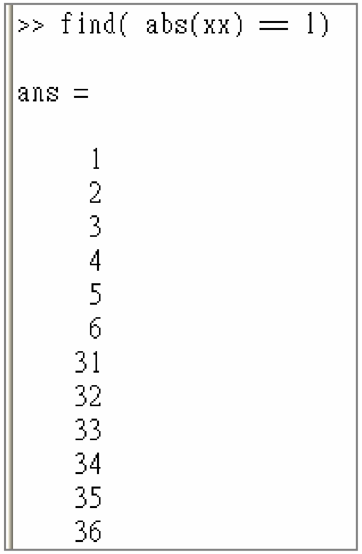
```
>> xx

xx =

    1.0000    0.8090    0.3090   -0.3090   -0.8090   -1.0000
    1.0000    0.8090    0.3090   -0.3090   -0.8090   -1.0000
    1.0000    0.8090    0.3090   -0.3090   -0.8090   -1.0000
    1.0000    0.8090    0.3090   -0.3090   -0.8090   -1.0000
    1.0000    0.8090    0.3090   -0.3090   -0.8090   -1.0000
    1.0000    0.8090    0.3090   -0.3090   -0.8090   -1.0000

>> abs(xx) == 1

ans =

     1     0     0     0     0     1
     1     0     0     0     0     1
     1     0     0     0     0     1
     1     0     0     0     0     1
     1     0     0     0     0     1
     1     0     0     0     0     1
```



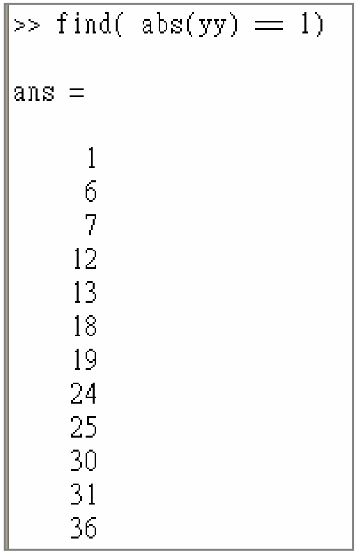
```
yy =

    1.0000    1.0000    1.0000    1.0000    1.0000    1.0000
    0.8090    0.8090    0.8090    0.8090    0.8090    0.8090
    0.3090    0.3090    0.3090    0.3090    0.3090    0.3090
   -0.3090   -0.3090   -0.3090   -0.3090   -0.3090   -0.3090
   -0.8090   -0.8090   -0.8090   -0.8090   -0.8090   -0.8090
   -1.0000   -1.0000   -1.0000   -1.0000   -1.0000   -1.0000

>> abs(yy) == 1

ans =

     1     1     1     1     1     1
     0     0     0     0     0     0
     0     0     0     0     0     0
     0     0     0     0     0     0
     0     0     0     0     0     0
     1     1     1     1     1     1
```



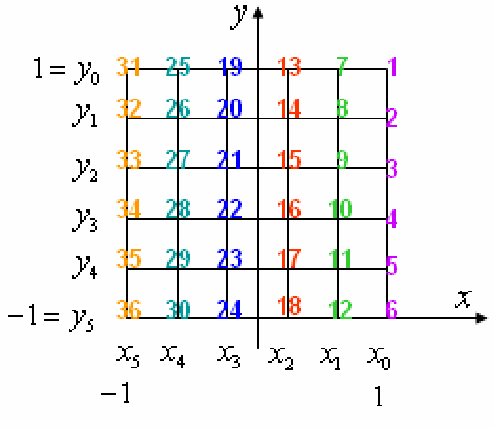
```
>> help find

 FIND   Find indices of nonzero elements.
    I = FIND(X) returns the indices of the vector X that are
    non-zero. For example, I = FIND(A>100), returns the indices
    of A where A is greater than 100. See RELOP.
```



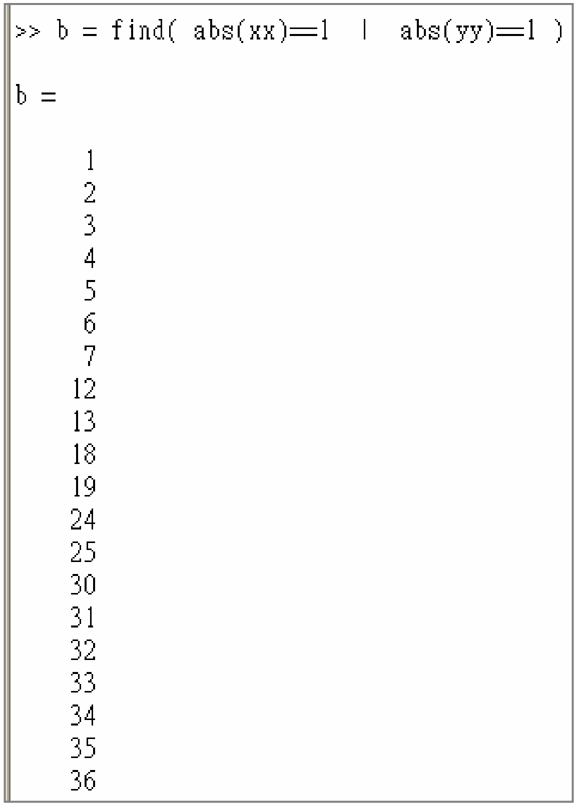
```
>> find( abs(xx) == 1)

ans =

     1
     2
     3
     4
     5
     6
    31
    32
    33
    34
    35
    36
```



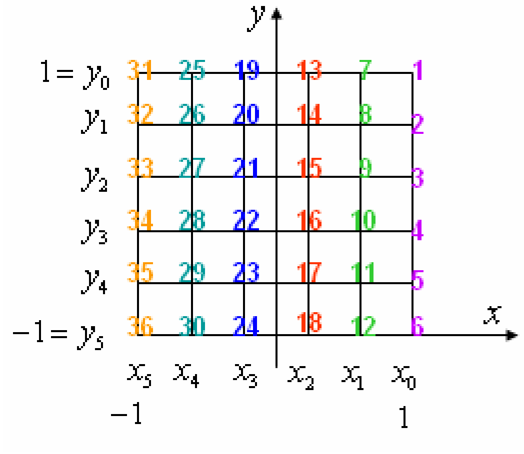
```
>> find( abs(yy) == 1)

ans =

     1
     6
     7
    12
    13
    18
    19
    24
    25
    30
    31
    36
```



Laplace equation : find boundary point [6]



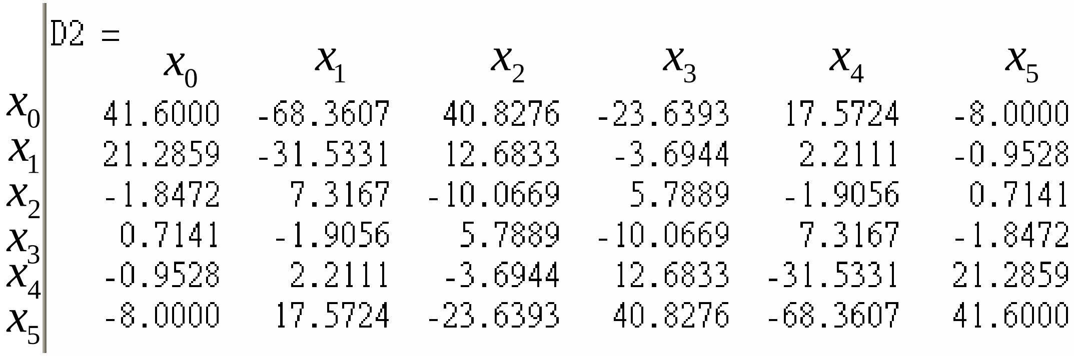
```
>> b = find( abs(xx)==1  |  abs(yy)==1 )

b =

     1
     2
     3
     4
     5
     6
     7
    12
    13
    18
    19
    24
    25
    30
    31
    32
    33
    34
    35
    36
```



b is index set of boundary points, if we write down equations according to index of active variables, then we can use index set ***b*** to modify the linear system.

Chebyshev differentiation matrix:

(second order)

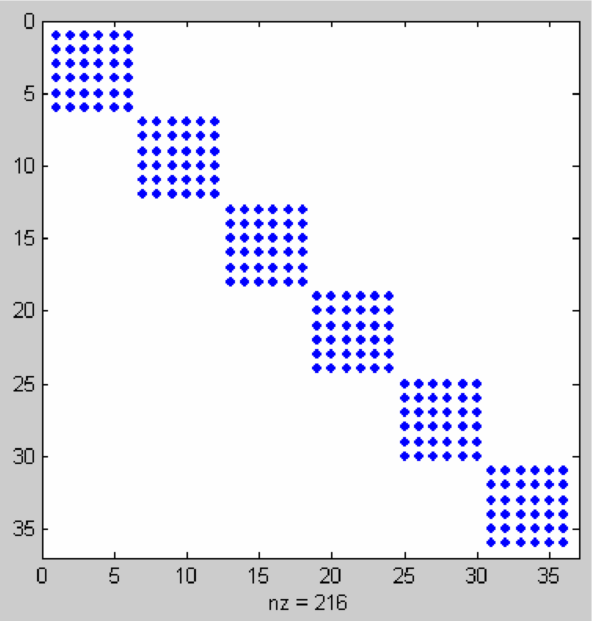


D2 =

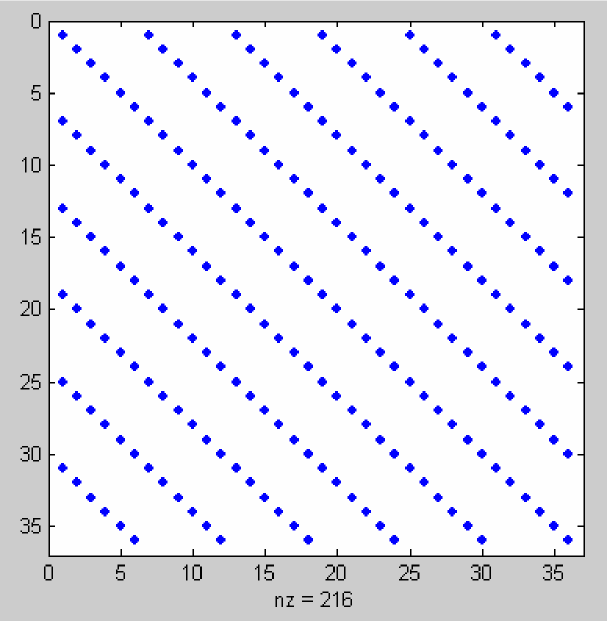
$$
\begin{array}{c|rrrrrr}
 & x_0 & x_1 & x_2 & x_3 & x_4 & x_5 \\
x_0 & 41.6000 & -68.3607 & 40.8276 & -23.6393 & 17.5724 & -8.0000 \\
x_1 & 21.2859 & -31.5331 & 12.6833 & -3.6944 & 2.2111 & -0.9528 \\
x_2 & -1.8472 & 7.3167 & -10.0669 & 5.7889 & -1.9056 & 0.7141 \\
x_3 & 0.7141 & -1.9056 & 5.7889 & -10.0669 & 7.3167 & -1.8472 \\
x_4 & -0.9528 & 2.2111 & -3.6944 & 12.6833 & -31.5331 & 21.2859 \\
x_5 & -8.0000 & 17.5724 & -23.6393 & 40.8276 & -68.3607 & 41.6000
\end{array}
$$

Laplace equation : construct matrix [7]

$kron\left(I_6, D2\right)$



$kron\left(D2, I_6\right)$



2 Set $w_{i,j} = \Delta P\left(x_i, y_j\right)$ for $1 \le i, j \le N-1$ (interior points)

$$w_{i,j} = \Delta P\left(x_i, y_j\right) \quad \Rightarrow \quad w = \left[kron\left(I_6, D2\right) + kron\left(D2, I_6\right)\right]u \equiv Lu$$

Definition: Kronecker product is defined by $A \oplus B = \begin{pmatrix} a_{11}B & a_{12}B & \cdots & a_{1n}B \\ a_{12}B & a_{22}B & \cdots & a_{2n}B \\ \vdots & \cdots & \ddots & \vdots \\ a_{m1}B & a_{m2}B & \cdots & a_{mn}B \end{pmatrix}$

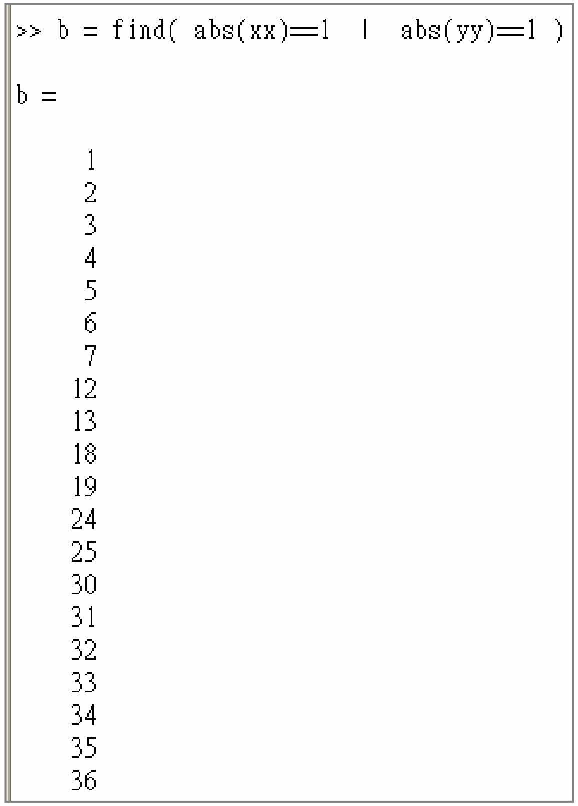
Laplace equation : construct matrix [8]

3 Additional constraints (equations) for boundary condition.

$u_{i,j} = B.C.$ for $i=0,N \ or \ j=0,N$

We need to replace equation of $w = Lu$ on boundary points by $u_{i,j} = B.C.$

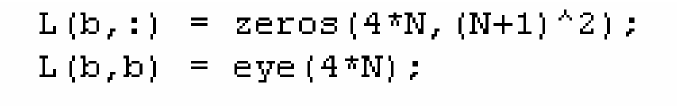
Index of boundary points



```
>> b = find( abs(xx)==1  |  abs(yy)==1 )

b =

     1
     2
     3
     4
     5
     6
     7
    12
    13
    18
    19
    24
    25
    30
    31
    32
    33
    34
    35
    36
```

$L(k,:) \rightarrow e_k^T$ for $k \in b$

such that $(Lu)(k) = L(k,:)u = e_k^T u = u_k$ (boundary point)



```
L(b,:)  = zeros(4*N,(N+1)^2);
L(b,b)  = eye(4*N);
```

where $size(b) = \underline{4(N-1)} + 4 = 4N$

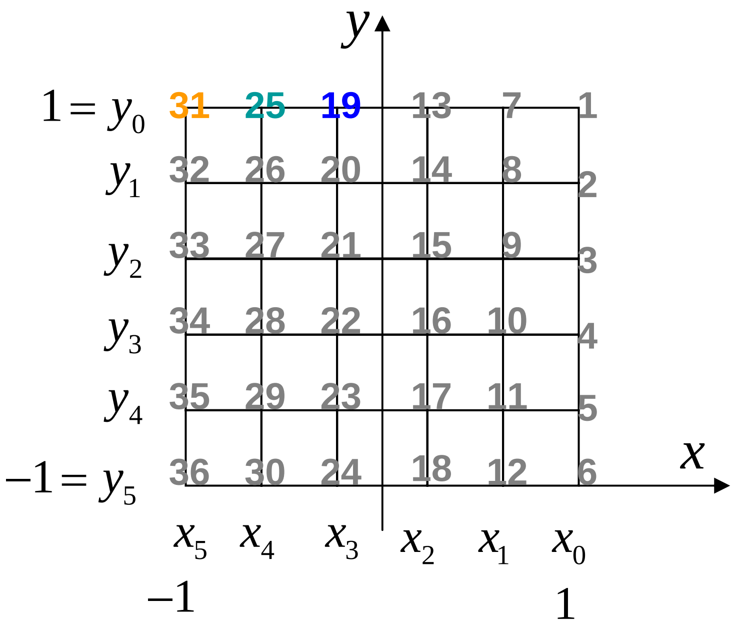
four corner points

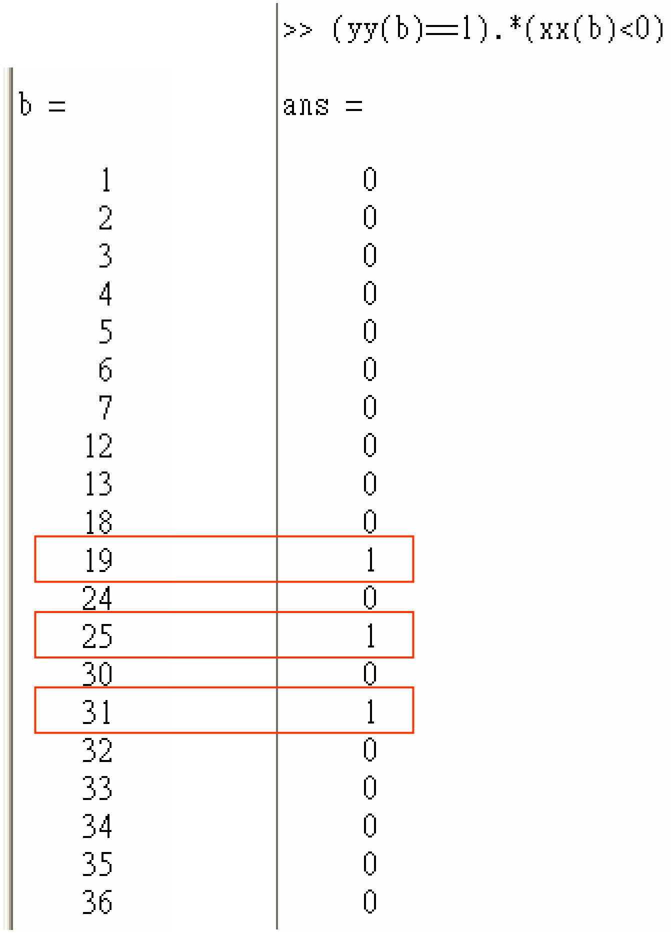
each edge has ***N-1*** points

Laplace equation : right hand side vector [9]

Boundary data: $$u(x,y)=\begin{cases}\sin^4(\pi x) & y=1 \ \ and \ \ -1<x<0\\ \frac{1}{5}\sin(3\pi y) & x=1\\ 0, & \text{otherwise}\end{cases}$$

identify $y=1 \ \ and \ \ -1<x<0$





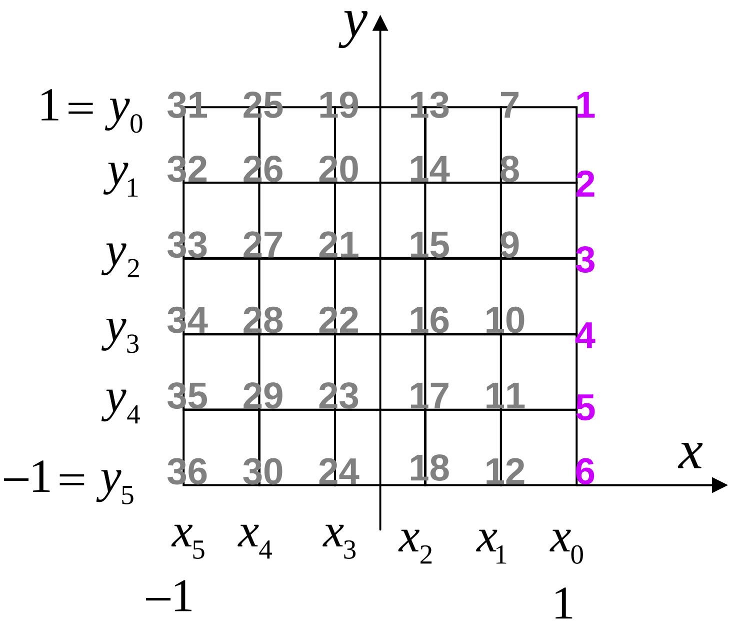
```
                    >> (yy(b)==1).*(xx(b)<0)

b =                 ans =

     1                   0
     2                   0
     3                   0
     4                   0
     5                   0
     6                   0
     7                   0
    12                   0
    13                   0
    18                   0
    19                   1
    24                   0
    25                   1
    30                   0
    31                   1
    32                   0
    33                   0
    34                   0
    35                   0
    36                   0
```

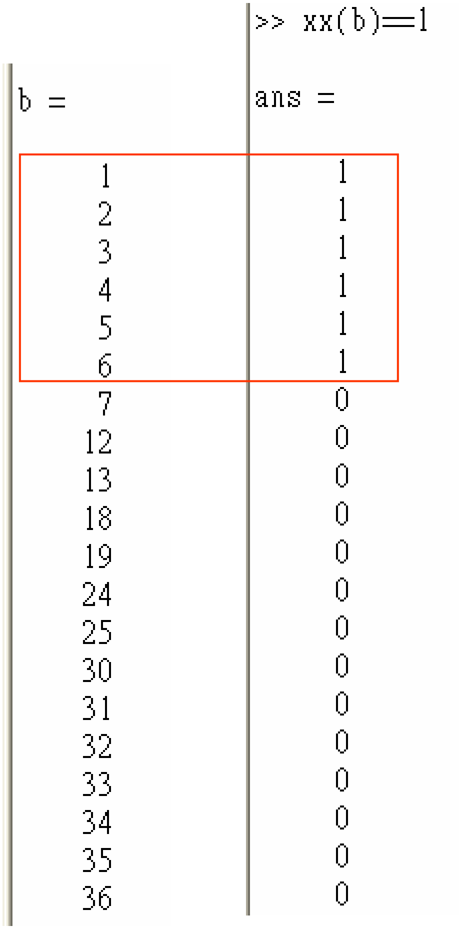
Laplace equation : right hand side vector

Boundary data:

$$u(x,y)=\begin{cases}\sin^4(\pi x) & y=1 \;\; and \quad -1<x<0\\ \dfrac{1}{5}\sin(3\pi y) & x=1\\ 0, & \text{otherwise}\end{cases}$$

identify $x=1$





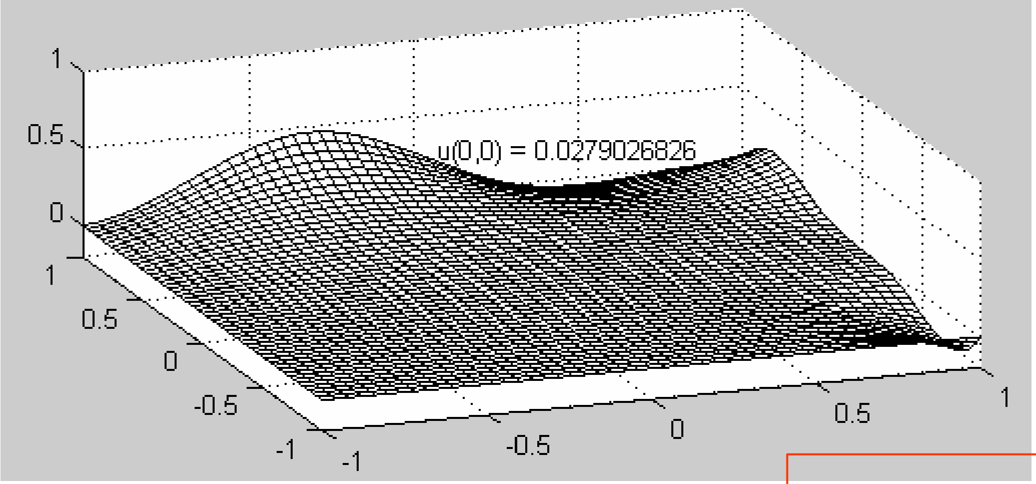
```
b =

     1
     2
     3
     4
     5
     6
     7
    12
    13
    18
    19
    24
    25
    30
    31
    32
    33
    34
    35
    36
```

```
>> xx(b)==1

ans =

     1
     1
     1
     1
     1
     1
     0
     0
     0
     0
     0
     0
     0
     0
     0
     0
     0
     0
     0
     0
```

```
rhs = zeros((N+1)^2,1);
rhs(b)  = (yy(b)==1).*(xx(b)<0).*sin(pi*xx(b)).^4 + ...
          .2*(xx(b)==1).*sin(3*pi*yy(b));
```

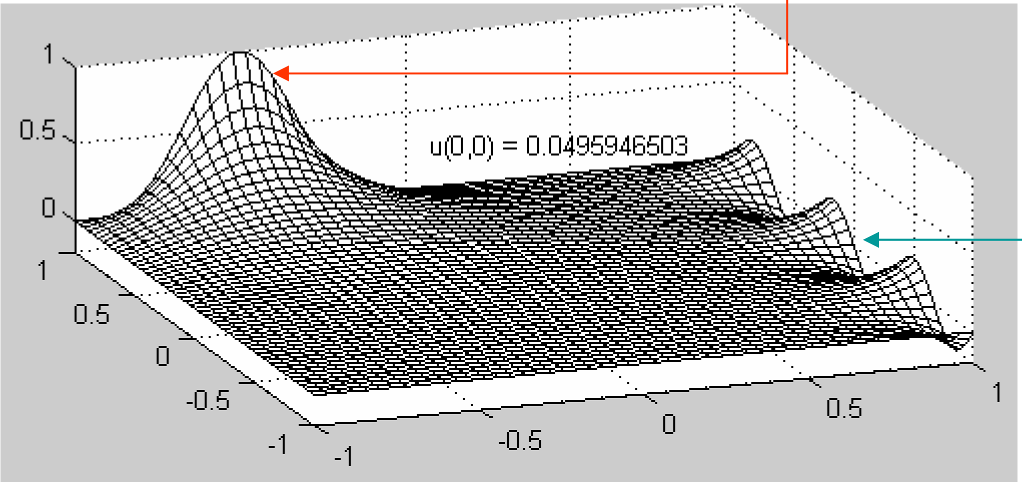
Laplace equation : results [11]

Solution under **N = 5,** *method II*



$$u(x,y)=\begin{cases}\sin^4(\pi x) & y=1 \ \ \mathit{and} \ \ -1<x<0\\ \frac{1}{5}\sin(3\pi y) & x=1\\ 0, & \text{otherwise}\end{cases}$$

Solution under **N = 24,** *method II*



Wave equation [1]

$u_{tt} = u_{xx} + u_{yy}, \quad -3 < x < 3, \quad -1 < y < 1$ subject to *B.C.* $\begin{cases} u_y(x, \pm 1, t) = 0 & \text{Neumann in } y \\ u(-3, y, t) = u(3, y, t) & \text{Periodic in } x \end{cases}$

Separation of variables leads to

① Periodic B.C. in ***x***-coordinate ⇒ Fourier discretization in ***x***

② Chebyshev discretization in ***y***, we must deal with Neumann B.C.

③ Leap-frog formula in time

$$u_{tt} = \lambda u \xrightarrow{\text{Leap-frog}} \frac{u^{(n+1)} - 2u^{(n)} + u^{(n-1)}}{(\Delta t)^2} = \lambda u^{(n)} \longrightarrow \lambda (\Delta t)^2 \in (-4, 0)$$

eigenvalue of $\tilde{D}_N^2$ (chebyshev diff. matrix) is negative and $\lambda_{\max} \approx -0.048 N^4$

eigenvalue of $D_{N,f}$ (Fourier diff. matrix) is $\lambda_k = ik, \quad k = -N/2+1, \cdots, N/2-1$

eigenvalue of $D_{N,f}^2$ (Fourier diff. matrix) is negative and $\lambda_{\max} = -(N/2-1)^2$

Hence stability requirement of $u_{tt} = u_{xx} + u_{yy}$ is $\left[0.048 N_y^4 + (N_x/2-1)^2\right](\Delta t)^2 \leq 4$

$$\Delta t \approx \frac{9}{N_y^2 \sqrt{1 + 5N_x^2 / N_y^4}}$$

(author chooses $\Delta t = \dfrac{5}{N_y^2 + N_x}$)

Wave equation [2]

① Periodic B.C. in ***x***-coordinate ⇒ Fourier discretization in ***x***

$$x = \left(x_1 \mid x_2 \mid x_3 \mid x_4 \mid x_5 \mid x_6 \right) = \left(-2, -1, 0, 1, 2, 3 \right)$$

② Chebyshev discretization in ***y***

$$y = \left(y_0 \mid y_1 \mid y_2 \mid y_3 \mid y_4 \mid y_5 \right)^T = \left(1 \mid 0.809 \mid 0.309 \mid -0.309 \mid -0.809 \mid -1 \right)^T$$

Method II

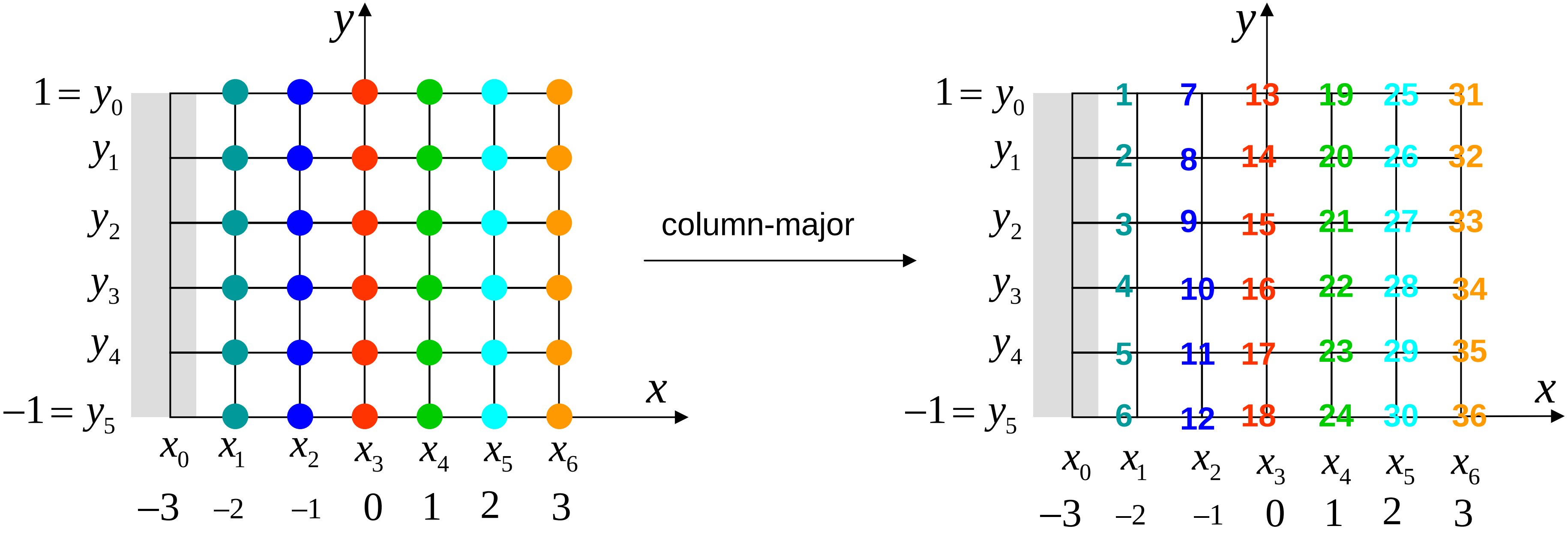
1. Let $p(y)$ be unique polynomial of degree $\le N$ with $p\left(y_j\right) = u_j$ for $0 \le j \le N_y$
2. Set $w_j = p''\left(y_j\right)$ for $0 \le j \le N_y$
3. replace $u\left(x, y_0\right),\ u\left(x, y_{N_y}\right)$ computed from 2 by Neumann B.C.

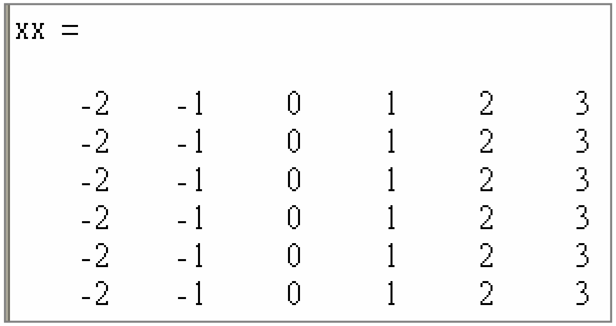
$$\left[D_{N_y} u\left(x,:\right) \right]_0 = \left[D_{N_y} u\left(x,:\right) \right]_{N_y} = 0$$

Chebyshev diff. matrix

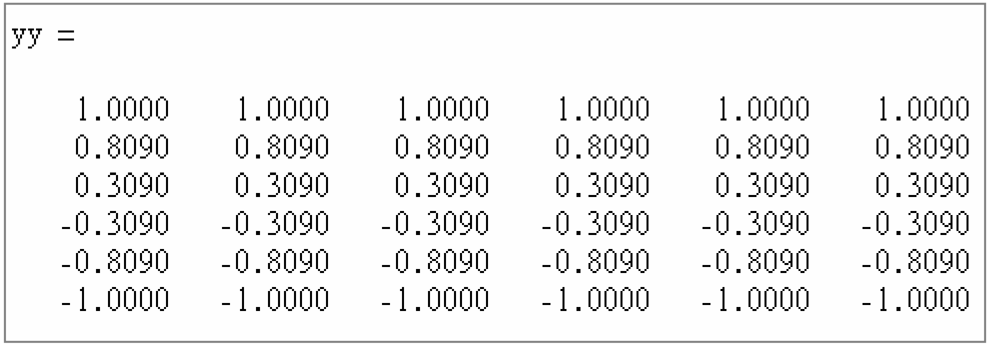
$$D_{N_y} = \begin{pmatrix} 8.5000 & -10.4721 & 2.8944 & -1.5279 & 1.1056 & -0.5000 \\ 2.6180 & -1.1708 & -2.0000 & 0.8944 & -0.6180 & 0.2764 \\ -0.7236 & 2.0000 & -0.1708 & -1.6180 & 0.8944 & -0.3820 \\ 0.3820 & -0.8944 & 1.6180 & 0.1708 & -2.0000 & 0.7236 \\ -0.2764 & 0.6180 & -0.8944 & 2.0000 & 1.1708 & -2.6180 \\ 0.5000 & -1.1056 & 1.5279 & -2.8944 & 10.4721 & -8.5000 \end{pmatrix}$$

Wave equation: order active variable [3]





```
xx =

    -2    -1     0     1     2     3
    -2    -1     0     1     2     3
    -2    -1     0     1     2     3
    -2    -1     0     1     2     3
    -2    -1     0     1     2     3
    -2    -1     0     1     2     3
```



```
yy =

    1.0000    1.0000    1.0000    1.0000    1.0000    1.0000
    0.8090    0.8090    0.8090    0.8090    0.8090    0.8090
    0.3090    0.3090    0.3090    0.3090    0.3090    0.3090
   -0.3090   -0.3090   -0.3090   -0.3090   -0.3090   -0.3090
   -0.8090   -0.8090   -0.8090   -0.8090   -0.8090   -0.8090
   -1.0000   -1.0000   -1.0000   -1.0000   -1.0000   -1.0000
```

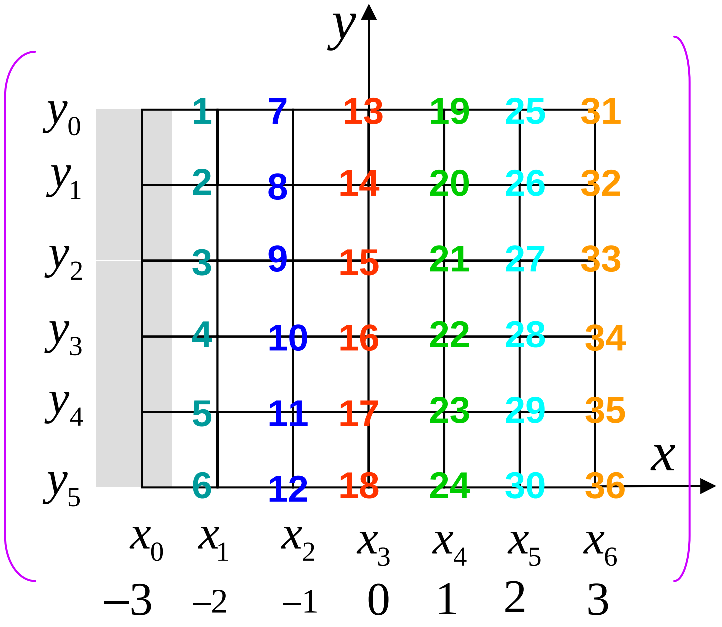
In this example, we don't arrange $u\left(x_i, y_j\right)$ as vector $vec\left(u\right)$ but keep in 2-dimensional form say $u_{i,j} = u\left(x_i, y_j\right)$, the same arrangement of ***xx*** and ***yy*** generated by ***meshgrid(x,y)***

Wave equation: action of Chebyshev operator [4]

Chebyshev 2nd diff. matrix $D^2_{N_y} =$

$$
\begin{array}{c|cccccc|c}
 & y_0 & y_1 & y_2 & y_3 & y_4 & y_5 & \\
\hline
 & 41.6000 & -68.3607 & 40.8276 & -23.6393 & 17.5724 & -8.0000 & y_0 \\
 & 21.2859 & -31.5331 & 12.6833 & -3.6944 & 2.2111 & -0.9528 & y_1 \\
 & -1.8472 & 7.3167 & -10.0669 & 5.7889 & -1.9056 & 0.7141 & y_2 \\
 & 0.7141 & -1.9056 & 5.7889 & -10.0669 & 7.3167 & -1.8472 & y_3 \\
 & -0.9528 & 2.2111 & -3.6944 & 12.6833 & -31.5331 & 21.2859 & y_4 \\
 & -8.0000 & 17.5724 & -23.6393 & 40.8276 & -68.3607 & 41.6000 & y_5
\end{array}
$$

$D^2_{N_y} \cdot$



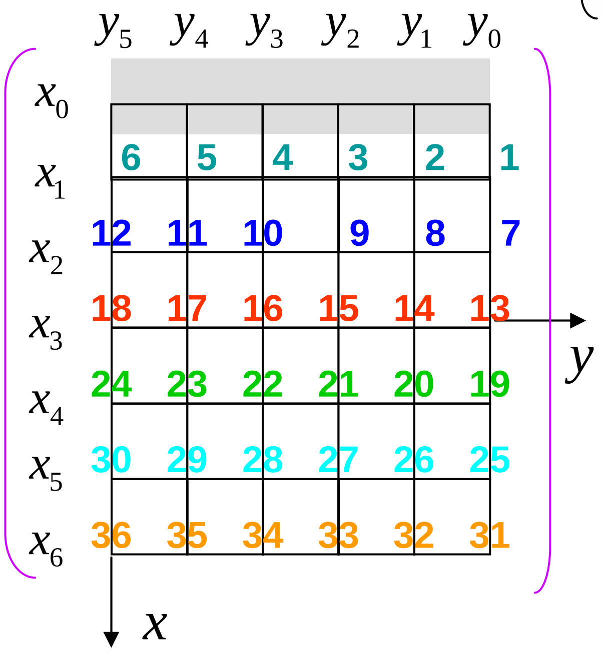
$$
= D^2_{N_y} \cdot \begin{pmatrix}
u_{1,0} & u_{2,0} & u_{3,0} & u_{4,0} & u_{5,0} & u_{6,0} \\
u_{1,1} & u_{2,1} & u_{3,1} & u_{4,1} & u_{5,1} & u_{6,1} \\
u_{1,2} & u_{2,2} & u_{3,2} & u_{4,2} & u_{5,2} & u_{6,2} \\
u_{1,3} & u_{2,3} & u_{3,3} & u_{4,3} & u_{5,3} & u_{6,3} \\
u_{1,4} & u_{2,4} & u_{3,4} & u_{4,4} & u_{5,4} & u_{6,4} \\
u_{1,5} & u_{2,5} & u_{3,5} & u_{4,5} & u_{5,5} & u_{6,5}
\end{pmatrix}
$$

$u_{i,j} = u\left(x_i, y_j\right)$ index *(i,j)* is logical index according to index of ordinates ***x***, ***y***

Wave equation: action of Fourier operator [5]

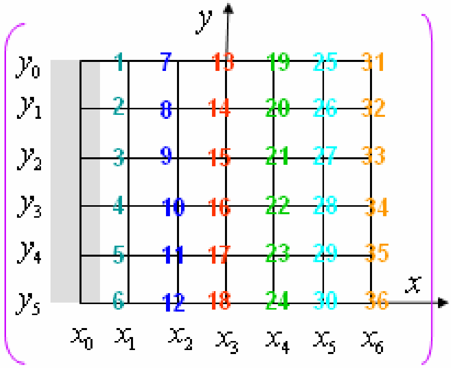
Fourier 2nd diff. matrix $D^2_{N_x} = \begin{array}{c|cccccc|c} & x_1 & x_2 & x_3 & x_4 & x_5 & x_6 & \\ \hline & -3.4726 & 2.1932 & -0.7311 & 0.5483 & -0.7311 & 2.1932 & x_1 \\ & 2.1932 & -3.4726 & 2.1932 & -0.7311 & 0.5483 & -0.7311 & x_2 \\ & -0.7311 & 2.1932 & -3.4726 & 2.1932 & -0.7311 & 0.5483 & x_3 \\ & 0.5483 & -0.7311 & 2.1932 & -3.4726 & 2.1932 & -0.7311 & x_4 \\ & -0.7311 & 0.5483 & -0.7311 & 2.1932 & -3.4726 & 2.1932 & x_5 \\ & 2.1932 & -0.7311 & 0.5483 & -0.7311 & 2.1932 & -3.4726 & x_6 \end{array}$

$D^2_{N_x} \cdot$



$$= D^2_{N_x} \cdot \begin{pmatrix} u_{1,0} & u_{2,0} & u_{3,0} & u_{4,0} & u_{5,0} & u_{6,0} \\ u_{1,1} & u_{2,1} & u_{3,1} & u_{4,1} & u_{5,1} & u_{6,1} \\ u_{1,2} & u_{2,2} & u_{3,2} & u_{4,2} & u_{5,2} & u_{6,2} \\ u_{1,3} & u_{2,3} & u_{3,3} & u_{4,3} & u_{5,3} & u_{6,3} \\ u_{1,4} & u_{2,4} & u_{3,4} & u_{4,4} & u_{5,4} & u_{6,4} \\ u_{1,5} & u_{2,5} & u_{3,5} & u_{4,5} & u_{5,5} & u_{6,5} \end{pmatrix}^T$$

Take transpose →



$\cdot \left(D^2_{N_x}\right)^T$

Wave equation: action of operator [6]

Let active variable be $U \triangleq \begin{pmatrix} u_{1,0} & u_{2,0} & u_{3,0} & u_{4,0} & u_{5,0} & u_{6,0} \\ u_{1,1} & u_{2,1} & u_{3,1} & u_{4,1} & u_{5,1} & u_{6,1} \\ u_{1,2} & u_{2,2} & u_{3,2} & u_{4,2} & u_{5,2} & u_{6,2} \\ u_{1,3} & u_{2,3} & u_{3,3} & u_{4,3} & u_{5,3} & u_{6,3} \\ u_{1,4} & u_{2,4} & u_{3,4} & u_{4,4} & u_{5,4} & u_{6,4} \\ u_{1,5} & u_{2,5} & u_{3,5} & u_{4,5} & u_{5,5} & u_{6,5} \end{pmatrix}$, then operator for Laplacian is

$$u_{xx} + u_{yy} \longrightarrow LU \equiv U \cdot D_{N_x}^2 + D_{N_y}^2 \cdot U \qquad \boxed{\left(D_{N_x}^2\right)^T = D_{N_x}^2}$$

Combine with Leap-frog formula in time

$$u_{tt} = u_{xx} + u_{yy} \longrightarrow \frac{U^{(k+1)} - 2U^{(k)} + U^{(k-1)}}{(\Delta t)^2} = LU^{(k)}$$

where initial condition is Gaussian pilse traveling rightward at speed 1

$$U^{(0)} = u(x, y, 0) = \exp\left[-8\left((x+1.5)^2 + y^2\right)\right]$$

$$U^{(-1)} = u(x, y, -\Delta t) = \exp\left[-8\left((x+\Delta t 1.5)^2 + y^2\right)\right]$$

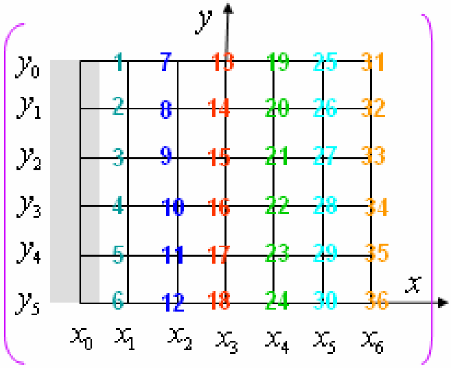
Question: how to match Neumann boundary condition $u_y(x, \pm 1, t) = 0$

Wave equation: Neumann B.C. in *y*-coordinate [7]

3 replace $u(x, y_0),\ u\left(x, y_{N_y}\right)$ computed from **2** by Neumann B.C.

$$\left[D_{N_y} u(x,:)\right]_0 = \left[D_{N_y} u(x,:)\right]_{N_y} = 0$$

$$\begin{pmatrix}
8.5000 & -10.4721 & 2.8944 & -1.5279 & 1.1056 & -0.5000 \\
2.6180 & -1.1708 & -2.0000 & 0.8944 & -0.6180 & 0.2764 \\
-0.7236 & 2.0000 & -0.1708 & -1.6180 & 0.8944 & -0.3820 \\
0.3820 & -0.8944 & 1.6180 & 0.1708 & -2.0000 & 0.7236 \\
-0.2764 & 0.6180 & -0.8944 & 2.0000 & 1.1708 & -2.6180 \\
0.5000 & -1.1056 & 1.5279 & -2.8944 & 10.4721 & -8.5000
\end{pmatrix}$$



$$= D_{N_y} U(:,x)$$

We require $\left[D_{N_y} U(:,x)\right]_0 = \left[D_{N_y} U(:,x)\right]_{N_y} = 0$

or say

$$\begin{pmatrix}
8.5 & -10.4721 & 2.8944 & -1.5279 & 1.1056 & -0.5 \\
0.5 & -1.1056 & 1.5279 & -2.8944 & 10.4721 & -8.5
\end{pmatrix}
\begin{pmatrix} U_{i,0} \\ U_{i,1} \\ U_{i,2} \\ U_{i,3} \\ U_{i,4} \\ U_{i,5} \end{pmatrix}
= \begin{pmatrix} 0 \\ 0 \end{pmatrix}$$

for $1 \le i \le 6$

Wave equation: Neumann B.C. in *y*-coordinate [8]

or say $$\begin{pmatrix} 8.5 & -0.5 \\ 0.5 & -8.5 \end{pmatrix}\begin{pmatrix} U_{i,0} \\ U_{i,5} \end{pmatrix} = -\begin{pmatrix} -10.4721 & 2.8944 & -1.5279 & 1.1056 \\ -1.1056 & 1.5279 & -2.8944 & 10.4721 \end{pmatrix}\begin{pmatrix} U_{i,1} \\ U_{i,2} \\ U_{i,3} \\ U_{i,4} \end{pmatrix}$$

written as $$\begin{pmatrix} U_{i,0} \\ U_{i,5} \end{pmatrix} = M_{BC}\begin{pmatrix} U_{i,1} \\ U_{i,2} \\ U_{i,3} \\ U_{i,4} \end{pmatrix}$$ where $$M_{BC} = -\begin{pmatrix} 8.5 & -0.5 \\ 0.5 & -8.5 \end{pmatrix}^{-1}\begin{pmatrix} -10.4721 & 2.8944 & -1.5279 & 1.1056 \\ -1.1056 & 1.5279 & -2.8944 & 10.4721 \end{pmatrix}$$

Procedure of wave equation simulation

Given $U^{(0)}, U^{(-1)}$

Step 1: time evolution by Leap-frog $$\frac{U^{(k+1)} - 2U^{(k)} + U^{(k-1)}}{(\Delta t)^2} = LU^{(k)}$$

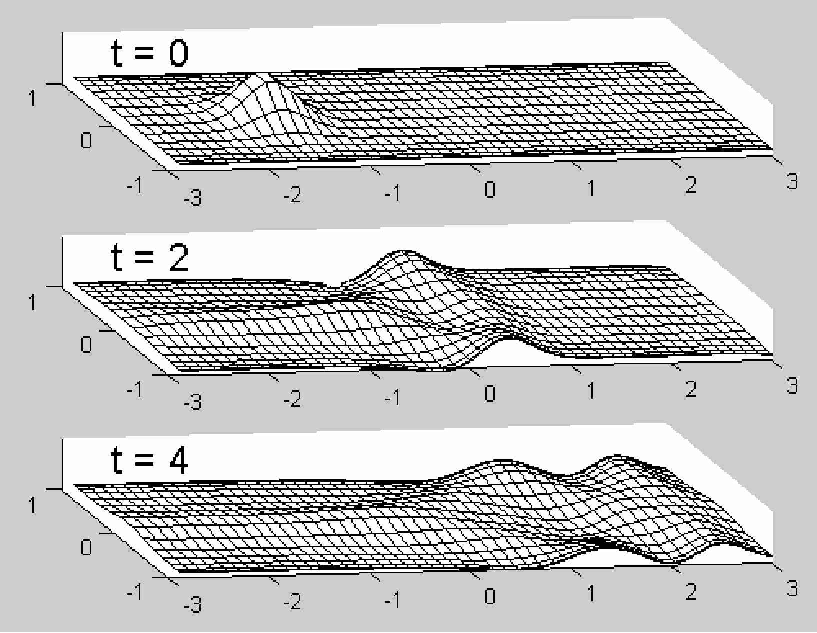
Step 2: correct boundary data $$U^{(k+1)}\left([1, N_y+1],\ :\ \right) = M_{BC}U^{(k+1)}\left(2:N_y,\ :\ \right)$$

where $$M_{BC} = -D_{N_y}\left([1, N_y+1],[1, N_y+1]\right)^{-1} D_{N_y}\left([1, N_y+1], 2:N_y\right)$$

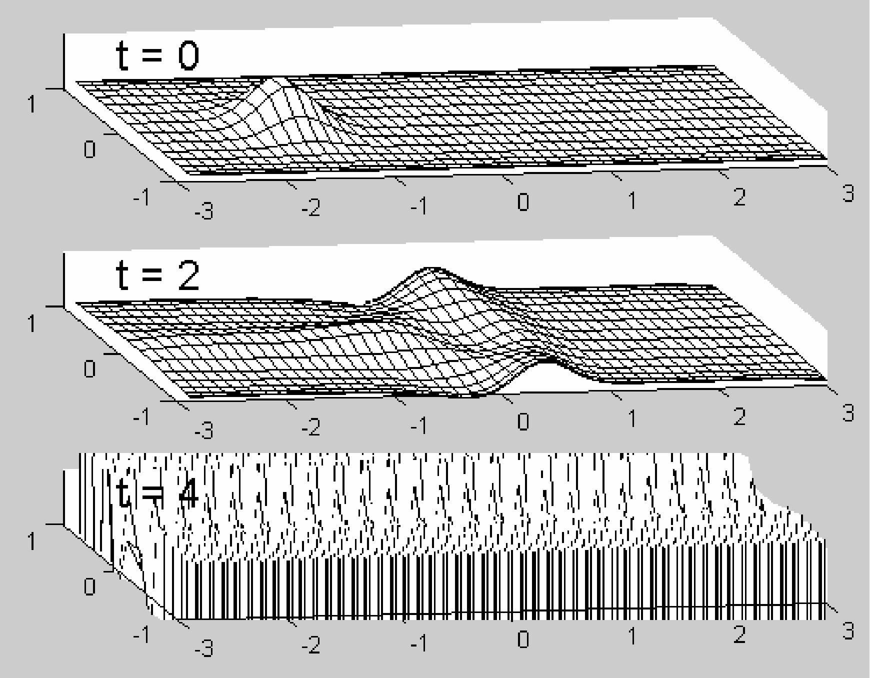
Wave equation: result [9]

Solution under $N_x = 50,\ N_y = 15$, ***method II***

$$\Delta t = \frac{5}{N_x + N_y^2} = 0.0182$$



$$\Delta t = \frac{3}{\sqrt{0.048 N_y^4 + \left(N_x/2-1\right)^2}} = 0.0547$$



Theoretical optimal value is $\Delta t = \frac{2}{\sqrt{0.048 N_y^4 + \left(N_x/2-1\right)^2}} = 0.0365$ (see exercise 13.4)

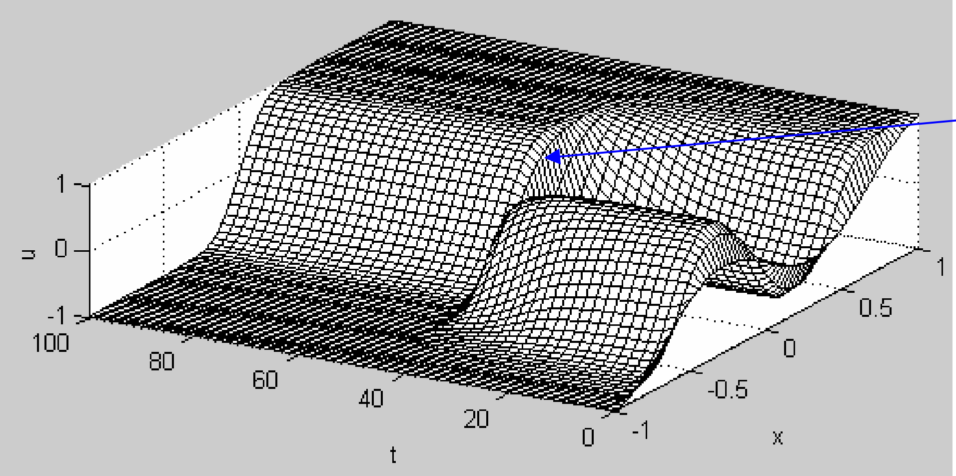
Exercise 13.2 [1]

The lifetime $T(\varepsilon)$ of metastable state depends strongly on the diffusion constant ε

$T(\varepsilon) =$ The value of ***t*** at which $u(x,t)$ first becomes monotonic in ***x***.

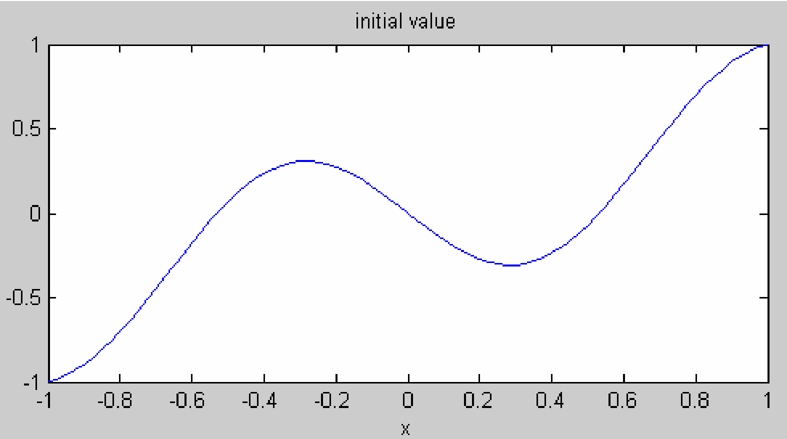
$$u_t = \varepsilon \cdot u_{xx} + u - u^3, \quad -1 < x < 1, \ u(-1) = -1, \ u(1) = 1$$

with parameter $\varepsilon = 0.01$ and initial condition $u(t=0) = 0.53x + 0.47\sin\left(-\frac{3\pi}{2}x\right)$



$T(0.01) = 47.36$

$$u(t=0) = 0.53x + 0.47\sin\left(-\frac{3\pi}{2}x\right)$$

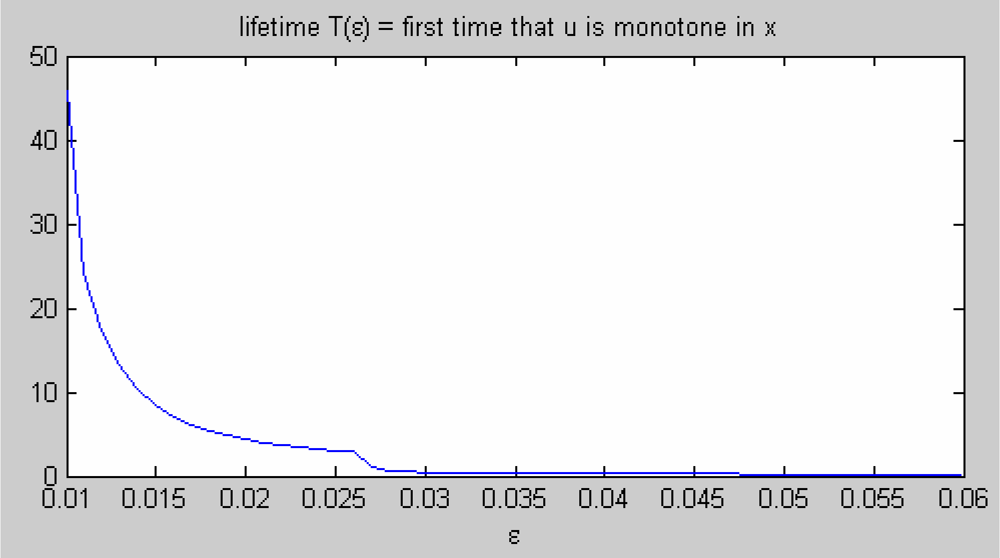


① what is graph of $T(\varepsilon)$

② Asymptotic behavior of $T(\varepsilon)$

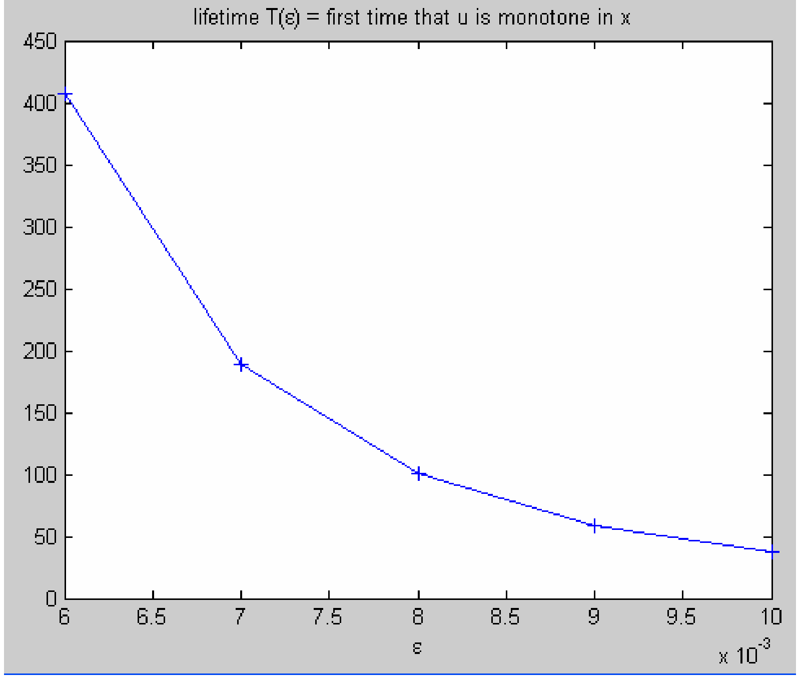
as $\varepsilon \to 0$

Exercise 13.2 [2]



$$\max T(\varepsilon) = 47.36$$

$$\min T(\varepsilon) = 0.1927$$



(1) Resolution is adaptive and

(2) Monotone under tolerance $1.E-7$