

# Numerical Solution of PDE

## 2. Introduction to PDE

### 2.1 Classification of PDE

#### 1st order PDE

$$F(x, y, u_x, u_y) = 0$$

Eg:  $uu_x + u_t = 1$  shock waves in traffic flow and fluid mechanics

#### Solving 1st order PDE using the method of characteristics

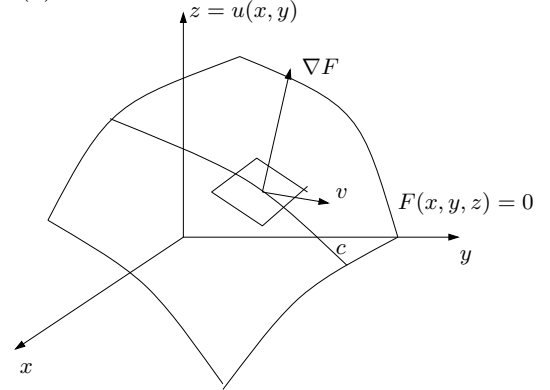
$$\boxed{a(x, y, u)u_x + b(x, y, u)u_y = c(x, y, u)} \quad (*)$$

The solution  $z = u(x, y)$  is a surface.

Now consider the surface

$$F(x, y, z) = u(x, y) - z = 0$$

Then  $\nabla F = (u_x, u_y, -1)$  is a normal to the surface  $F = 0$ .



Now the PDE (\*) can be rewritten in the form

$$\mathbf{v} \cdot \nabla F = (a, b, c) \cdot \left( \frac{\partial u}{\partial x}, \frac{\partial u}{\partial y}, -1 \right) = 0.$$

Thus  $\mathbf{v} = (a, b, c)$  represents a tangent vector to the solution surface  $F = 0$  at the point  $(x, y, z = u)$ .

We can construct a curve  $C : (x(t), y(t), z(t))$  lies in the solution surface for which  $\mathbf{v}$  is a tangent at each point. Since  $\mathbf{v}$  is tangent to  $c$  it follows that the tangent vector to  $c$  is

$$\left( \frac{dx}{dt}, \frac{dy}{dt}, \frac{dz}{dt} \right) \parallel (a, b, c) \Leftrightarrow \left( \frac{dx}{dt}, \frac{dy}{dt}, \frac{dz}{dt} \right) = \alpha(a, b, c) \quad \text{or equivalently}$$

$$\boxed{\frac{dx}{dt} = a(x, y, u) \quad \frac{dy}{dt} = b(x, y, u) \quad \frac{du}{dt} = c(x, y, u)} \quad (**)$$

by defining the arclength of  $C$  to be such that  $\alpha = 1$ . Thus the solution of the PDE (\*) has been reduced to solving the system of ODE's.

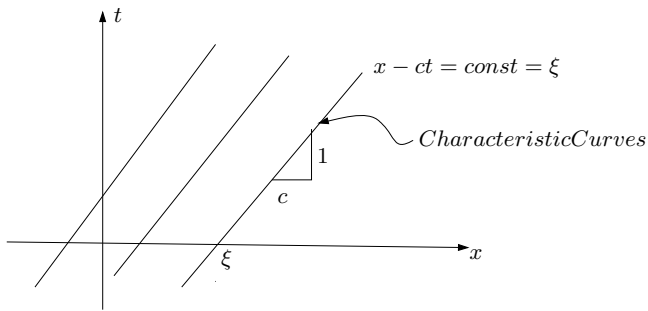
**Eg. 1:** 1D wave equation  $u_t + cu_x = 0$ ;  $u(x, 0) = f(x)$ .

$$\frac{dx}{dt} = \frac{c}{1}$$

$$\Rightarrow x - ct = \text{constant} = \xi \quad \frac{du}{d\xi} = 0 \Rightarrow u = \text{const} = B$$

$$u(x, 0) = f(x) = B \quad x - c \cdot 0 = \xi \Rightarrow x = \xi \Rightarrow B = f(\xi)$$

$$\therefore u(x, t) = f(x - ct).$$



### Cauchy problem

Given  $u(x, y)$  along  $C : y = y(x)$ , when can we determine  $u_x$  and  $u_y$ ?

$$\begin{aligned}
 u(x, y(x)) &= f(x) \\
 u_x + u_y y' &= f'(x) \\
 au_x + bu_y &= c \\
 \begin{bmatrix} 1 & y' \\ a & b \end{bmatrix} \begin{bmatrix} u_x \\ u_y \end{bmatrix} &= \begin{bmatrix} f' \\ c \end{bmatrix}
 \end{aligned}$$

Cannot calculate  $u_x$  and  $u_y$  when

$$\begin{aligned}
 \det \left( \begin{pmatrix} 1 & y' \\ a & b \end{pmatrix} \right) &= 0 \\
 \text{or} \quad b - ay' &= 0 \\
 b &= a \frac{dy}{dx}
 \end{aligned}$$

$$\boxed{\frac{dx}{a} = \frac{dy}{b}}$$

Cannot specify data along a characteristic curve.

**2nd order PDE**  $F(x, y, u, u_x, u_y, u_{xx}, u_{xy}, u_{yy}) = 0$  (\*)

- Higher order PDE often occur, but we already have an extremely rich class of PDE in (\*).
- Linear if  $F$  is linear in each term involving  $u$ .
- Quasilinear if linear in the highest derivatives.

**Eg:**

Heat Eq:	$u_t = u_{xx}$	
Wave Eq:	$u_{tt} = c^2 u_{xx}$	
Laplace's Eq:	$u_{xx} + u_{yy} = 0$	
Burger's Eq:	$u_t + uu_x = u_{xx}$	quasilinear, shocks smoothed by viscosity
Porous Media Eq:	$u_t = (\beta(u)u_x)_x$	nonlinear

## Classification of general 2nd order linear PDE

$$Lu = \underbrace{au_{xx} + bu_{xy} + cu_{yy}}_{\text{Principal part}} + \underbrace{du_x + eu_y + fu}_{\text{Lower order terms}} = \underbrace{g}_{\text{Inhomogeneous term}} \quad a = a(x, y) \text{ variable?}$$

by analogy with quadratic forms  $aX^2 + bXY + cY^2 + \dots$  we define the equations to be

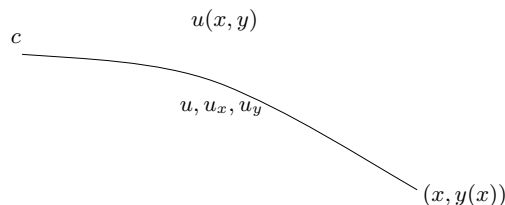
- (a) Hyperbolic if  $b^2 - 4ac > 0$
- (b) Parabolic if  $b^2 - 4ac = 0$
- (c) Elliptic if  $b^2 - 4ac < 0$ .

## Cauchy Problem

If we are given  $u, u_x, u_y$  along some curve  $c : y = y(x)$ , i.e.,  $u(x, y(x)) = F(x)$ ,  $u_x(x, y(x)) = G(x)$ ,  $u_y(x, y(x)) = H(x)$ . Can we determine  $u(x, y)$  at some neighboring point?

$$\begin{aligned} u_{xx} + u_{xy}y' &= G'(x) \\ u_{xy} + u_{yy}y' &= H'(x) \\ a u_{xx} + b u_{xy} + c u_{yy} &= g - \text{LOT} = K(x) \end{aligned}$$

$$\begin{bmatrix} 1 & y' & 0 \\ 0 & 1 & y' \\ a & b & c \end{bmatrix} \begin{bmatrix} u_{xx} \\ u_{xy} \\ u_{yy} \end{bmatrix} = \begin{bmatrix} G' \\ H' \\ K \end{bmatrix}$$

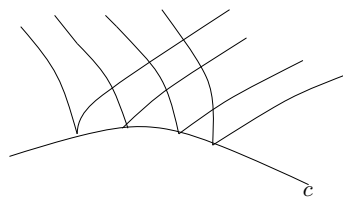


We can calculate  $u_{xx}, u_{xy}$  and  $u_{yy}$  provided  $\det(\cdot) = a(y')^2 - by' + c \neq 0$

- (i) If  $b^2 - 4ac > 0$  we get 2 curves along which data cannot be specified and used to get a neighboring solution. These curves are called characteristics and are defined by  $y' = \frac{b \pm \sqrt{b^2 - 4ac}}{2a}$ .

Eg: Wave equation

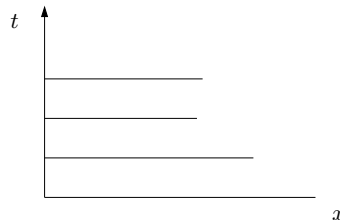
$$\begin{aligned} \left( \frac{\partial z}{\partial t^2} - c^2 \frac{\partial^2}{\partial x^2} \right) u &= \left( \frac{\partial}{\partial t} - c \frac{\partial}{\partial x} \right) \left( \frac{\partial}{\partial t} + c \frac{\partial}{\partial x} \right) u = 0 \\ b^2 - 4ac &= 0^2 - 4(1)(-c^2) = 4c^2 > 0 \\ x \pm ct &= \text{const are characteristics} \end{aligned}$$



- (ii) If  $b^2 - 4ac = 0$  we get 1 characteristic curve

Eg.

$$\begin{aligned} u_t - u_{xx} &= 0 \\ b^2 - 4ac &= 0 - 4(-1)(0) = 0 \\ \frac{dt}{dx} &= 0 \text{ is a characteristic} \\ t &= \text{const are characteristics} \\ \text{(Signals propagate with infinite speed.)} \end{aligned}$$



(iii) If  $b^2 - 4ac < 0$  there are no characteristic curves

Eg: Laplace's equation  $u_{xx} + u_{yy} = 0$

$$b^2 - 4ac = 0 - 4 = -4 < 0$$

Thus, Cauchy data can be specified for any curve to obtain a neighboring solution. This presents a problem if Cauchy data are specified for a boundary value problem – over specified.

$$\boxed{u_{xx} + u_{yy} = 0}$$

### Prototype parabolic problem

$$u_t = \underbrace{Du_{xx}}_{\text{Diffusion}} - \underbrace{cu_x}_{\text{Convection}} - \underbrace{bu}_{\text{Cooling}} + \underbrace{f(x,t)}_{\text{External input/output of heat}} \quad x \in \Omega$$

$D > 0$  – Diffusion coefficient

$c$  – Wave speed ( $c > 0 \Rightarrow$  wave moves in positive  $x$  direction)

$b$  – heat transfer coefficient ( $b > 0$  heat loss,  $b < 0$  heat gain)

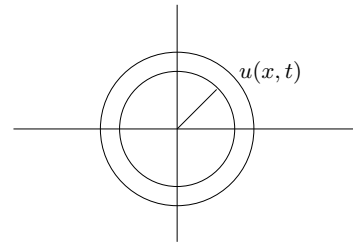
Later we will consider the cases  $b(x)$  – variable coefficients

$b(x, u)$  – quasilinear

### Different types of boundary conditions:

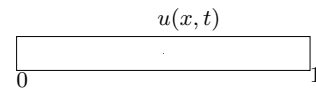
1) Periodic BC – temperature in a conducting ring

- $\Omega = (0, 2\pi)$
- ‘Boundary Condition’:  $u(x, t) = u(x + 2\pi, t)$  –  $u$  is periodic
- Initial Condition  $u(x, 0) = u_0(x)$
- For the solution to make physical sense  $b > 0$  otherwise  $u \Rightarrow \infty$ .



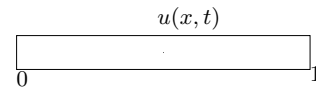
2) Dirichlet BC – temperature in a bar with fixed end temperature

- $\Omega = (0, 1)$
- Dirichlet BC –  $u(0, t) = \alpha(t)$      $u(1, t) = \beta(t)$
- Initial Condition:  $u(x, 0) = u_0(x)$ .



3) Mixed BC – Temperature in a bar with one end at a specified temperature and the other at a specified flux.

- $\Omega = (0, 1)$
- Mixed BC     $u(0, t) = \alpha(t), \quad \frac{\partial u}{\partial x}(1, t) = \beta(t)$



## Time Independent Problem

- Will return to the parabolic problem later.
- Assume  $f$ ,  $\alpha$  and  $\beta$  do not depend on time. Then we can show that  $u(x, t) \xrightarrow{t \rightarrow \infty} u(x)$  a steady state.

$u(x)$  satisfies the steady state equation:

$D u_{xx} - cu_x - bu = f(x)$ <ul style="list-style-type: none"> <li>• <math>u</math> satisfies periodic, Dirichlet or mixed BC.</li> </ul>
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## This is our prototype elliptic problem

- Elliptic problems arise in
  - Steady state for problems with diffusion or viscosity.
  - Potential problems.
- Mathematical characterization of elliptic problems.
  - Unique solutions that are smoother (i.e., have more derivatives) than the data function  $f$ .
- Why is this a prototype problem?
  - Only 1 space dimension – problem character does not change in 2D or 3D but there are extra numerical issues that arise (e.g. iterative solution methods, boundary conditions).
  - For periodic problem there are no boundary conditions, which makes the analysis easier.

## Discretization Process:

- Periodic case:  $\Omega = [0, 2\pi]$   
Divide domain into  $N$  sample points

$$\begin{array}{c}
 \begin{array}{ccc}
 0 & \text{---} & N-1 \\
 | & & | \\
 0 & & 2\pi
 \end{array} \\
 \\
 x_k = (2\pi/N)k \quad k = 0, 1, \dots, N-1 \\
 h = (2\pi)/N
 \end{array}$$

- Dirichlet and mixed cases:  $\Omega = (0, 1)$   
Divide domain into  $N + 1$  sample points

$$\begin{array}{c}
 \begin{array}{ccc}
 0 & \text{---} & N \\
 | & & | \\
 0 & & 1
 \end{array} \\
 \\
 x_k = (1/N)k \quad k = 0, \dots, N \quad h = 1/N
 \end{array}$$

Sample  $u$  at each of the grid points with a uniform spacing  $h$ . We use capital letters to denote approximate values at grid points:

$$\left. \begin{array}{l}
 U_k \simeq u(x_k) \\
 F_k = f(x_k) \\
 C_k = c(x_k) \\
 B_k = b(x_k)
 \end{array} \right\} \text{Exact}$$

We will consider the following types of discretizations for the prototype problem.

- (I) Finite Difference
- (II) Spectral – For the periodic case
- (III) The method of weighted residuals

- Collocation
- Galerkin

(IV) The finite element method

### The finite difference method

**Idea:** Approximate derivatives by difference quotients.

**Periodic Problem:**  $-D u_{xx} + bu = f, \quad u(x + 2\pi) - u(x), \quad D = 1$

$$u_{xx} \simeq \frac{\delta^2 U_n}{h^2} = \frac{U_{n+1} - 2U_n + U_{n-1}}{h^2}$$

$$\therefore \boxed{\frac{-1}{h^2} U_{n+1} + \left(\frac{2}{h^2} + B_n\right) U_n - \frac{U_{n-1}}{h^2} = F_n} \quad n = 0, \dots, N-1$$

Periodicity  $\Rightarrow U_N = U_0 \quad U_{N-1} = U_{-1}$

so we have the matrix problem

$$A^h U = F^h$$

where  $A^h = \begin{bmatrix} (2/h^2 + B_0) & -1/h^2 & 0 \dots 0 & -1/h^2 \\ -1/h^2 & (2/h^2 + B_1) & -1/h^2 & 0 \dots 0 \\ & 0 & \ddots & \\ \vdots & & & \\ 0 & & & \\ -1/h^2 & 0 \dots 0 & -1/h^2 & (2/h^2 + B_{N-1}) \end{bmatrix}$

### Properties of A:

- A is symmetric
- A is positive definite
- A is diagonally dominant i.e.,  $|A_{ii}| \geq \sum_{\substack{j=1 \\ j \neq i}}^N |A_{ij}|$
- A is almost tridiagonal – can be solved in  $O(N)$  operations

### Questions:

- (1) Is  $AU = F$  solvable? Yes, all eigenvalues are positive.
- (2) How close is  $U$  to  $u$ ?  
We expect  $\|U - u\| \leq kh^2$  but we need to do some work to prove this.

**Truncation Error:** The truncation error (T.E.) is the remainder you get when you substitute the exact solution to  $-Du_{xx} + bu = f(*)$  into the difference equation.

$$\text{i.e.:} \quad T_h = -\frac{\delta^2}{h^2}u_i + B_i u_i - F_i = O(h^2).$$

A difference scheme is *consistent* with the differential equation (\*) if  $T_h \Rightarrow 0$  as  $h \Rightarrow 0$ .

### Vector and Matrix Norms

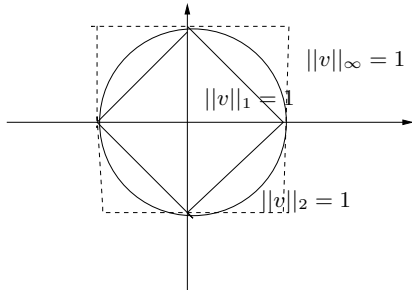
**Vector Norms:** Let  $\mathbf{x} \in \mathbb{R}^N$ , then  $\|\cdot\| : \mathbb{R}^N \rightarrow \mathbb{R}^+$  is a real valued function satisfying:

- (i)  $\|x\| \geq 0 \quad \forall \mathbf{x} \in \mathbb{R}^N \quad \|x\| = 0 \Leftrightarrow \mathbf{x} = 0$
- (ii)  $\|c\mathbf{x}\| = |c| \|\mathbf{x}\| \quad \forall \mathbf{x} \in \mathbb{R}^N, c \in \mathbb{R}$
- (iii)  $\|\mathbf{x} + \mathbf{y}\| \leq \|\mathbf{x}\| + \|\mathbf{y}\| \quad \forall \mathbf{x}, \mathbf{y} \in \mathbb{R}^N \quad \Delta \text{ inequality.}$

If  $\|\cdot\|$  satisfies (i)–(iii) then it is called a vector norm.

### Examples:

$$\begin{aligned} \|\mathbf{x}\|_1 &= \sum_{i=1}^N |x_i| && \text{absolute sum norm} \\ \|\mathbf{x}\|_2 &= \left( \sum_{i=1}^N |x_i|^2 \right)^{1/2} && \text{Euclidean norm} \\ \|\mathbf{x}\|_\infty &= \max_i |x_i| && \text{maximum norm} \end{aligned}$$



The sets of points in  $\mathbb{R}^2$  for which the various norms are 1 i.e. unit circles.

### Matrix Norms:

A matrix norm is a function  $\|\cdot\| : \mathbb{R}^N \times \mathbb{R}^N \Rightarrow \mathbb{R}^+$  which satisfies the properties

- (i)  $\|A\| > 0 \quad \|A\| = 0 \Leftrightarrow A \equiv 0$
- (ii)  $\|cA\| = |c| \|A\|$
- (iii)  $\|A + B\| \leq \|A\| + \|B\|$

A matrix norm with the property  $\|AB\| \leq \|A\| \|B\|$  is called *multiplicative*.

A matrix norm and a vector norm are *consistent* if

$$\|Ax\| \leq \|A\| \|x\| \quad \|x\| \neq 0 \Rightarrow \frac{\|Ax\|}{\|x\|} \leq \|A\|.$$

**Induced matrix norms:**

Define  $\|A\| = \max_{\|x\| \neq 0} \frac{\|Ax\|}{\|x\|} = \max_{\|x\|=1} \|Ax\|$  – Lengths of images of the unit sphere.

Example 1.  $\|A\|_\infty = \max$  row sum of the elements of  $A = \max_i \sum_j |a_{ij}|$

**Proof:**

$$\begin{aligned} \|x\|_\infty &= \max_i |x_i| \\ \|Ax\|_\infty &= \max_i \left| \sum_j a_{ij} x_j \right| \stackrel{\Delta \text{ineq}}{\leq} \max_i \sum_j |a_{ij} x_j| \leq \left( \max_i \sum_j |a_{ij}| \right) \|x\|_\infty \\ \therefore \frac{\|Ax\|_\infty}{\|x\|_\infty} &\leq \left( \max_i \sum_j |a_{ij}| \right) \therefore \|A\|_\infty \leq \max_i \sum_j |a_{ij}| \quad (*) \end{aligned}$$

If  $\max_i \sum_j |a_{ij}| = \sum_j |a_{kj}|$  for some row index  $k$ , then let

$$\hat{x} = (\bar{a}_{k1}/|a_{k1}|, \dots, \bar{a}_{kN}/|a_{kN}|) \Rightarrow \sum_j a_{kj} \hat{x}_j = \sum_j |a_{kj}|^2 / |a_{kj}| = \sum_j |a_{kj}|.$$

If for some index  $j$ ,  $a_{kj} = 0$  then let  $\hat{x}_j = 1$ . Then  $\|\hat{x}\|_\infty = 1$ , and

$$\begin{aligned} \|A\hat{x}\|_\infty &= \max_i \left| \sum_j a_{ij} \hat{x}_j \right| \geq \sum_j |a_{kj}| = \sum_j |a_{kj}| \|\hat{x}\|_\infty = \max_i \sum_j |a_{ij}| \|\hat{x}\|_\infty \\ \|A\|_\infty &\geq \frac{\|A\hat{x}\|_\infty}{\|\hat{x}\|_\infty} \geq \max_i \sum_j |a_{ij}| \quad (**) \end{aligned}$$

Combining (\*) and (\*\*) we have  $\|A\|_\infty = \max_i \sum_j |a_{ij}|$

**Exercise 2:**  $\|A\|_1 = \max$  column sum of the moduli of elements of  $A = \max_j \sum_i |a_{ij}|$

**Example 3:**  $\|A\|_2 = (\text{maximum eigenvalue of } A^*A)^{1/2} = \rho(A^*A)$  where  $\rho(B) = \max_j |\lambda_j|$  where  $\lambda_j$  are the eigenvalues of  $B$ , is known as the spectral radius of  $B$ .

**Proof:** Since  $A^*A$  is Hermitian there exists a unitary matrix  $u$  (for which  $u^*u = I$ ) such that

$$u^*(A^*A)u = \begin{bmatrix} \mu_1 & 0 \\ 0 & \mu_N \end{bmatrix}$$

where  $\mu_i \geq 0$  are the eigenvalues of  $A^*A$ . Let  $y = u^*x$  so that  $x = uy$ . Then

$$\begin{aligned} \|A\|_2 &= \max_{\|x\| \neq 0} \frac{\|Ax\|_2}{\|x\|_2} = \max_{\|x\| \neq 0} \sqrt{\frac{\langle A^*Ax, x \rangle}{\langle x, x \rangle}} & \|Ax\| &= (Ax)^*(Ax) \\ & & &= (A^*Ax)(x) \\ &= \max_{\|y\| \neq 0} \sqrt{\frac{\langle u^*A^*Auy, y \rangle}{\langle u^*uy, y \rangle}} \end{aligned}$$



$$\begin{aligned}
&= \max_{\|y\| \neq 0} \sqrt{\frac{\sum_i \mu_i |y_i|^2}{\sum |y_i|^2}} \\
&= \sqrt{\max |\mu_i|} \\
\therefore \|A\|_2 &= \rho(A^*A)
\end{aligned}$$

■

**Note:** If  $A$  is symmetric  $\|A\|_2 = \max_i |\lambda_i|$ . Also  $\|A^{-1}\|_2 = \frac{1}{\min |\lambda_i|}$ .

**Error estimate for the finite difference method:**

Let us look at the size of the error  $e = u - U$ .

$$AU = F \tag{1}$$

$$Au = F + T_h \tag{2}$$

where  $T_h$  is the truncation error and  $\|T_h\|_\infty = O(h^2)$  and  $\|T_h\|_2 = O(h^2)$ . Subtract (1) from (2):

$$\begin{aligned}
Ae &= T_h \\
e &= A^{-1}T_h.
\end{aligned}$$

We want  $\|e\|_?$  to be  $O(h^2)$  the same as  $T_h$ , so we must have that  $\|A^{-1}\|_?$  is bounded independent of  $h$ .

**Definition:** (Norm stability)

A discretization  $A^h u^h = F^h$  for any elliptic problem

$\ell_\infty$  : is said to be *max-norm stable* if

$$\|(A^h)^{-1}\|_\infty \leq K \quad \text{for all } h.$$

$\ell_2$  : is said to be  $\ell_2$  norm stable if

$$\|(A^h)^{-1}\|_2 \leq K \quad \text{for all } h.$$

**Convergence Theorem:**

A consistent, stable discretization for a linear elliptic problem converges with the order of the truncation error:

**PF:**  $\|e\|_\infty \leq k\|T_h\|_\infty \quad \|e\|_2 \leq k\|T_h\|_2.$

**Claim 1:** The finite difference matrix for the periodic problem with constant heat transfer coefficient  $B_n = B$ :

$$A^h = -\frac{E}{h^2} + \left(\frac{2}{h^2} + B\right)I - \frac{E^{-1}}{h^2}$$

is  $\ell_2$  -norm stable.

Observe that the DFT basis vectors  $\phi_j^k = e^{i\frac{2\pi}{N}jk}$   $k = 0, 1, \dots, N-1$  are eigenvectors of  $A^h$

$$\begin{aligned} A^h \phi_j^k &= -\frac{e^{i(\frac{2\pi}{N})k(j+1)h}}{h^2} + \left(\frac{2}{h^2} + B\right) e^{i(\frac{2\pi}{N})kjh} - \frac{e^{i(\frac{2\pi}{N})k(j-1)h}}{h^2} \\ &= \left\{ \frac{2 - 2\cos(kh\pi/N)}{h^2} + B \right\} \phi_j^k \\ &= \left\{ \frac{4\sin^2(kh\pi/2N)}{h^2} + B \right\} \phi_j^k \\ &= \lambda^k \phi_j^k \end{aligned}$$

**Note:**

- Eigenvalues  $\lambda^k$  are all positive.
- $\|A^{-1}\|_2 = \frac{1}{\min|\lambda^k|} = \frac{1}{B}$  which is bounded independent of  $h$ .
- The fact that the DFT basis vectors  $\phi_j^k$  diagonalize  $A^h$  can be used as a computational device to invert the matrix  $A^h$ . Let  $\hat{u}^k = FFT(U)$  and  $\hat{F}^k = FFT(F)$ . Then since  $A^h \phi^k = \lambda^k \phi^k$  and  $U = \sum \hat{u}^k \phi^k$ ,  $F = \sum \hat{F}^k \phi^k$ . It follows that  $\lambda^k \hat{U}^k = \hat{F}^k$ .

$$\therefore \hat{U}^k = \hat{F}^k / \lambda^k$$

so that  $u = FFT^{-1}(\hat{U}^k)$ .

- The above analysis and inversion technique only works for constant coefficients  $b$ . It is possible to analyze the stability of a variable coefficient problem by freezing coefficients and performing a DFT stability analysis.

**The Dirichlet Problem:**

$$\begin{aligned} y'' &= f(x, y, y') \\ y(0) &= \alpha \quad y(1) = \beta. \end{aligned}$$

$$y_{n+1} - 2y_n + y_{n-1} = h^2 f\left(x_n, y_n, \frac{y_{n+1} - y_{n-1}}{2h}\right) = h^2 f_n \quad (3)$$

$$y_0 = \alpha \quad y_N = \beta$$

↓ from B.-C.

$$\begin{bmatrix} -2 & 1 & 0 & \cdots & 0 \\ 1 & -2 & 1 & \cdots & 0 \\ & & \ddots & & \vdots \\ & & \ddots & & 0 \\ & & & \ddots & 1 \\ 0 & & & & 1-2 \end{bmatrix} \begin{bmatrix} y_1 \\ \vdots \\ \vdots \\ y_{N-1} \end{bmatrix} = h^2 \begin{bmatrix} f_1 \\ \vdots \\ \vdots \\ f_{N-1} \end{bmatrix} - \begin{bmatrix} \alpha \\ 0 \\ \vdots \\ 0 \\ \beta \end{bmatrix}$$

Tridiagonal  $A\mathbf{y} = h^2\mathbf{f}(\mathbf{y}) - \mathbf{r}$

$$0 = \mathbf{g}(\mathbf{y}^{k+1}) = \mathbf{g}(\mathbf{y}^k) + \frac{\partial \mathbf{g}}{\partial \mathbf{y}}(\mathbf{y}^k)(\mathbf{y}^{k+1} - \mathbf{y}^k)$$

$$\therefore \mathbf{y}^{k+1} = \mathbf{y}^k - \left[ \frac{\partial \mathbf{g}}{\partial \mathbf{y}}(\mathbf{y}^k) \right]^{-1} \mathbf{g}(\mathbf{y}^k)$$

Solve using Newton Iteration

$$\mathbf{g}(\mathbf{y}) = A\mathbf{y} - h^2\mathbf{f}(\mathbf{y}) + \mathbf{r} = 0$$

$$\mathbf{y}^{(k+1)} = \mathbf{y}^{(k)} - \left[ \frac{\partial \mathbf{g}}{\partial \mathbf{y}}(\mathbf{y}^{(k)}) \right]^{-1} \mathbf{g}(\mathbf{y}^{(k)})$$

**Eg. 1**  $y'' = 0 \quad y(0) = 0 \quad y(1) = 1 \Rightarrow y(x) = x$

$$y_{n+1} - 2y_n + y_{n-1} = 0 \quad 1 \leq n \leq N-1$$

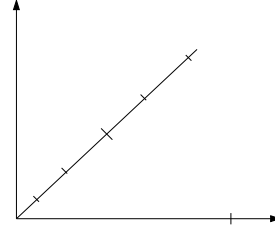
$$y_n = \theta^n \Rightarrow \theta^2 - 2\theta + 1 = 0$$

$$\theta = 1, 1$$

$$y_n = A + Bn$$

$$y_0 = A = 0$$

$$y_N = BN = 1 \Rightarrow y_n = \left(\frac{n}{N}\right) = nh = x_n$$

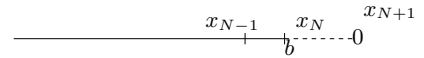


- Shape of solution was captured exactly by the quadratic variation assumed by the difference approximation.

**Special Tricks:**

(1) **For derivative boundary conditions:**

$$y'(b) = \beta \text{ say}$$



we introduce the pseudo meshpoint  $x_{N+1}$  and we have the condition

$$\frac{y_{N+1} - y_{N-1}}{2h} = \beta \implies y_{N+1} = (y_{N-1} + 2h\beta)$$

Let's look at the effect on the simple problem  $y'' = 0 \quad y(a) = \alpha \quad y'(b) = \beta$

$$y_1 \quad y_2$$

$$\begin{bmatrix} -2 & 1 & 0 & \dots & 0 \\ 1 & & & & \\ & \ddots & & \ddots & \\ & & 1 & & \\ & & 2 & & -2 \end{bmatrix} \begin{bmatrix} y_1 \\ \vdots \\ y_N \end{bmatrix} = - \begin{bmatrix} \alpha \\ 0 \\ \vdots \\ 0 \\ 2h\beta \end{bmatrix}$$

(2) For self-adjoint problems we often have:  $(p(x)y')' + q(x)y = T(x)$ . In this case we use

$$\frac{1}{h} \left[ p_{n+1/2} \left( \frac{y_{n+1} - y_n}{h} \right) - p_{n-1/2} \left( \frac{y_n - y_{n-1}}{h} \right) \right]$$

**Eg. 1 with derivative BC:**

$$\begin{aligned}
 y'' &= x & y(0) &= 0 & y'(1) &= 0 \\
 y &= \frac{x^3}{6} + Ax + B & y(0) &= B = 0 \\
 y'(x) &= \frac{x^2}{2} + A \Rightarrow y'(1) = \frac{1}{2} + A = 0 \Rightarrow A = -\frac{1}{2} \\
 \therefore y(x) &= \boxed{\frac{x^3}{6} - \frac{x}{2}}.
 \end{aligned}$$

Homog. eq.

$$\begin{aligned}
 y_{n+1} - 2y_n + y_{n-1} &= 0 & O(h^2) \\
 y_n = \theta^n \Rightarrow (\theta - 1)^2 &= 0 \Rightarrow \theta = 1, 1 \\
 y_n &= an + b
 \end{aligned}$$

Particular solution

$$\begin{aligned}
 y_{n+1} - 2y_n + y_{n-1} &= h^2 \overset{x_n}{\parallel} (nh) = h^3 n \\
 y_n = cn^3 \Rightarrow c \left[ (n+1)^3 - 2n^3 + (n-1)^3 \right] \\
 &= c \left[ n^3 + 3n^2 + 3n + 1 - 2n^3 + n^2 - 3n^2 + 3n - 1 \right] \\
 &= 6nc = h^3 n \\
 \therefore c &= \frac{h^3}{6} \\
 \therefore y_n = \frac{n^3 h^3}{6} + an + b &= \frac{(nh)^3}{6} + an + b.
 \end{aligned}$$

$$y_0 = 0 \rightarrow b = 0.$$

**BC 1:**

$$\frac{y_N - y_{N-1}}{h} = 0 \quad O(h)$$

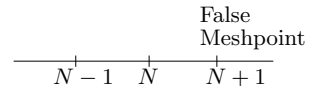
$$\begin{aligned}
 0 &= \frac{N^3 h^3}{6} + aN - \left[ \frac{(N-1)^3 h^3}{6} + a(N-1) \right] \Rightarrow a[N - (N-1)] = \frac{-h^3}{6} [N^3 - (N-1)^3] \\
 \therefore a &= -\frac{h^3}{6} [N^3 - N^3 + 3N^2 - 3N + 1] = -\frac{h^3}{6} [3N^2 - 3N + 1]
 \end{aligned}$$

$$hN = 1$$

$$\begin{aligned}
 y_n &= \frac{x_n^3}{6} - \frac{nh^3}{6} [3N^2 - 3N + 1] = \frac{x_n^3}{6} - \frac{x_n}{2} \left[ h^2 N^2 - h(hN) + \frac{1}{3} h^2 \right] \\
 &= \frac{x_n^3}{6} - \frac{x_n}{2} + \frac{x_n}{2} \left( h - \frac{h^2}{3} \right) \Leftarrow O(h) \rightarrow (\text{comes from BC})
 \end{aligned}$$

**BC 2:**

$$\begin{aligned}
 \frac{y_{N+1} - y_{N-1}}{2h} = 0 \Rightarrow y_{N+1} &= y_{N-1} \\
 \frac{(N+1)^3 h^3}{6} + a(N+1) &= \frac{(N-1)^3 h^3}{6} + a(N-1)
 \end{aligned}$$



$$\begin{aligned}
\therefore 2a &= \frac{h^3}{6} [(N-1)^3 - (N+1)^3] \\
&= -\frac{h^3}{6} [N^3 + 3N^2 + 3N + 1 - N^3 + 3N^2 - 3N + 1] \\
a &= -\frac{h^3}{6} [3N^2 + 1] \\
\therefore y_n &= \frac{x_n^3}{6} - \frac{(nh)h^2}{6} (3N^2 + 1) \\
&= \underbrace{\frac{x_n^3}{6}}_{\text{exact}} - \underbrace{\frac{x_n h^2}{6}}_{\text{error}} \longrightarrow O(h^2)
\end{aligned}$$

**Eg:**

$$\begin{aligned}
y'' + 4y &= 0 \\
y(0) &= 0 \quad y(1) = 1 \\
y &= A \sin 2x + B \cos 2x \\
y(0) &= 0 \Rightarrow B = 0 \\
y(1) &= 1 \Rightarrow A \sin 2 = 1 \Rightarrow A = \frac{1}{\sin 2} \\
\therefore y(x) &= \frac{\sin 2x}{\sin 2}
\end{aligned}$$

$$y_{n+1} - 2y_n + y_{n-1} + 4h^2 y_n = 0$$

$$\begin{aligned}
y_n &= \theta^n & \theta^2 - (2 - 4h^2)\theta + 1 &= 0 \\
\theta_1 \theta_2 &= 1 & \theta &= e^{i\alpha} \\
& & e^{i\alpha} - (2 - 4h^2) + e^{-i\alpha} &= 0 \\
& & 2(1 - \cos \alpha) &= 4h^2 & \cos \alpha &= 1 - 2\sin^2 \alpha/2 \\
& & 4\sin^2 \alpha/2 &= 4h^2 \\
& \therefore \sin^2 \alpha/2 &= h^2 & \alpha &= 2\sin^{-1} h \\
y_n &= A \cos \alpha n + B \sin \alpha n \\
y_0 &= 0 \Rightarrow A = 0 & y_N &= B \sin \alpha N = 1 \\
\therefore B &= \frac{1}{\sin(\alpha N)} \\
\therefore y_n &= \frac{\sin(2n \sin^{-1} h)}{\sin(2N \sin^{-1} h)} & \sin^{-1} h &= h + \frac{h^3}{6} + O(h^5).
\end{aligned}$$

**Eg. 2:** An eigenvalue problem

$$\begin{aligned}
y'' + \lambda^2 y &= 0 \\
y(0) &= 0 = y(1) \\
y &= A \cos \lambda x + B \sin \lambda x \\
y(0) &= A = 0 \Rightarrow y(x) = B \sin \lambda x
\end{aligned}$$

$$y(1) = 0 = B \sin \lambda \quad \Rightarrow \quad \begin{aligned} \lambda &= n\pi \text{ for nontrivial sol.} \\ n &= 1, 2, \dots \end{aligned}$$

$$\Rightarrow \boxed{y_k(x) = B \sin(k\pi x); \lambda = k\pi}$$

$$\begin{aligned} FD \Rightarrow \quad y_{n+1} - 2y_n + y_{n-1} + h^2 \lambda^2 y_n &= 0 \quad n = 1, \dots, N-1 \\ y_{n+1} - (2-r^2)y_n + y_{n-1} &= 0 \quad \leftarrow \text{discrete eigenvalue problem } r = (h\lambda) \\ y_n = \theta^n : \theta - (2-r^2) + \theta^{-1} &= 0 \quad \theta_1 \theta_2 = 1 \end{aligned}$$

$$\theta = e^{i\alpha}$$

$$2[\cos \alpha - 1] + r^2 = 0$$

$$\boxed{h^2 \lambda^2 = 4 \sin^2 \left( \frac{\alpha}{2} \right)}$$

$$y_n = A \cos(\alpha n) + B \sin(\alpha n)$$

$$y_0 = A = 0$$

$$y_N = B \sin(\alpha N) = 0 \Rightarrow \alpha = \frac{k\pi}{N} \quad k = 1, \dots, N-1$$

Aside: If we had tried:  $\theta = e^\alpha$

$$e^\alpha - (2-r^2) - e^{-\alpha} = 0$$

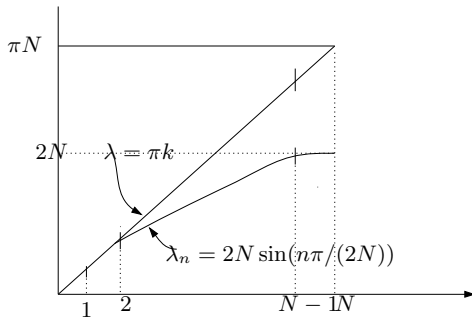
$$2 \cosh \alpha - 2 - r^2 = 0$$

$$4 \sinh^2 \frac{\alpha}{2} + r^2 = 0$$

roots unless  $\alpha \in \mathbb{C}$

Recall  $\cos \alpha - 1 = 2 \sin^2 \left( \frac{\alpha}{2} \right)$

$$\boxed{y_{k,n} = B_k \sin \left( \frac{k\pi n}{N} \right); \quad \lambda_k = \frac{2}{h} \sin \left( \frac{k\pi}{2N} \right) = 2N \sin \left( \frac{k\pi}{2N} \right)}$$



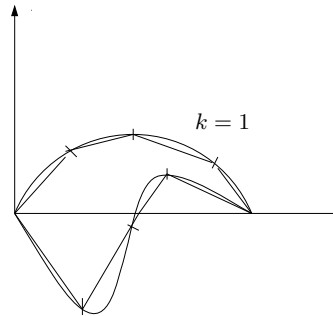
$$\begin{aligned} N \gg 1 : \quad k = 1 \\ \lambda_1 = 2N \sin \left( \frac{\pi}{2N} \right) \approx 2N \cdot \frac{\pi}{2N} = \pi \end{aligned}$$

**Asymptotic behavior of eigenvalues:**

$$\begin{aligned} \lambda_k &= 2N \left\{ \frac{k\pi}{2N} - \frac{1}{6} \left( \frac{k\pi}{2N} \right)^3 + \dots \right\} \\ &= k\pi - O \left( \frac{1}{N^2} \right) \quad k \ll N \end{aligned}$$

$$\lambda_k(N) = 2N \sin \left( \frac{k\pi}{2N} \right) = \frac{2 \sin \left( \frac{k\pi}{2N} \right)}{(1/N)} \xrightarrow{N \rightarrow \infty} \frac{2 \cos \left( \frac{k\pi}{2N} \right) \cdot \frac{k\pi}{2}}{1} \Rightarrow k\pi$$

$$y_{k,n}(N) = B_{k,n} \sin(k\pi n h)$$



**Richardson Extrapolation:**  $\lambda_k = \lambda^e + c_2h^2 + c_4h^4 + \dots$

$$\lambda_k = \lambda_k^{\text{exact}} + ch^2 \quad \lambda_k(2h) = \lambda_k^e + c4h^2 \quad \frac{4\lambda_k(h) - \lambda_k(2h)}{3} = \lambda_k^e$$

$$\lambda_1(h=1) = \frac{2}{1} \sin\left(\frac{\pi}{2}\right) = 2$$

$$\lambda_1\left(h = \frac{1}{2}\right) = \frac{2}{(1/2)} \sin\left(\frac{\pi}{4}\right) 2\sqrt{2} = 2.8284271 \quad \lambda_1\left(h = \frac{1}{4}\right) = 8 \sin\left(\frac{\pi}{8}\right) = 3.0614675$$

$$\lambda_k^e \simeq \frac{8\sqrt{2} - 2}{3} = 3.10456$$

$S$	$h_2$	$\lambda_s^0$	$\lambda_s^1$	$\lambda_s^2$	
1	1	2	3.10456	3.1414534	$\lambda_s^0 = \lambda(h_s)$
2	1/2	$2\sqrt{2}$	3.1391476		$\lambda_s^{(m)} = \lambda_{s+1}^{(m-1)} + \frac{\lambda_{s+1}^{(m-1)} - \lambda_s^{(m-1)}}{\left(\frac{h_s}{h_{s+m}}\right)^2 - 1}$
3	1/4	3.0614675			

### 1.2.2. Numerical solution of ALGEBRAIC EQUATIONS:

#### Iterative methods

Consider the solution of

$$\text{or } \sum_{j=1}^N A_{ij}x_j = b_i \quad i = 1, \dots, N \quad [A] = \begin{bmatrix} & 0 \\ L & \end{bmatrix} + \begin{bmatrix} & 0 \\ 0 & D \end{bmatrix} + \begin{bmatrix} & U \\ 0 & \end{bmatrix}$$

#### Jacobi Iteration:

$$\sum_{j=1}^{i-1} A_{ij}x_j + A_{ii}x_i + \sum_{j=i+1}^N A_{ij}x_j = b_i$$

$$\text{or } Lx + Dx + Ux = b$$

Iteration Procedure:

$$x_i^{(k+1)} = \left( b_i - \sum_{j=1}^{i-1} A_{ij}x_j^{(k)} - \sum_{j=i+1}^N A_{ij}x_j^{(k)} \right) / A_{ii} \iff \mathbf{x}^{(k+1)} = D^{-1} (\mathbf{b} - L\mathbf{x}^{(k)} - U\mathbf{x}^{(k)})$$

$$\text{or } x_i^{(k+1)} = x_i^{(k)} + \left( b_i - \sum_{j=1}^{i-1} A_{ij}x_j^{(k)} - A_{ii}x_i^{(k)} - \sum_{j=i+1}^N A_{ij}x_j^{(k)} \right) / A_{ii} \iff \mathbf{x}^{(k+1)} = \mathbf{x}^{(k)} + D^{-1} (\mathbf{b} - A\mathbf{x}^{(k)})$$

$$x^{(k+1)} = x^{(k)} + D^{-1} (\mathbf{b} - A\mathbf{x}^{(k)})$$

Let  $r^{(k)} = b - Ax^{(k)}$  define the residual vector  
 $= A((x^* - x)^{(k)})$   
 $= Ae^k$  which is a measure of the error.

$$\boxed{x^{(k+1)} = x^{(k)} + \omega D^{-1} r^{(k)}} \text{ where } \omega \text{ is an acceleration parameter.}$$

## Jacobi iteration

Eg. 1

$$\begin{aligned} u'' &= 0 & u_{ex} &= 1 - x \\ u(0) &= 1 & u(1) &= 0 \\ \frac{u_{n+1} - 2u_n + u_{n-1}}{h^2} &= 0 & u_0 &= 1 & u_N &= 0 \end{aligned}$$

$$A u = b$$

$$\begin{bmatrix} -2 & 1 & & & \\ 1 & -2 & 1 & & \\ & \ddots & & & \\ & & 0 & \ddots & 1 \\ & & & & 1 & -2 \end{bmatrix} \begin{bmatrix} u_1 \\ \vdots \\ u_{N-1} \end{bmatrix} = \begin{bmatrix} -1 \\ 0 \\ \vdots \\ \vdots \\ 0 \end{bmatrix}$$

$$u_n^{(k+1)} = \frac{u_{n+1}^{(k)} + u_{n-1}^{(k)}}{2}$$

Let  $u_0^{(0)} = 1$     $u_1^{(0)} = 0$     $u_2^{(0)} = 0$     $u_3^{(0)} = 0 \Leftarrow$  BC

$$u_1^{(1)} = (0 + 1)/2 = 1/2$$

$$u_2^{(1)} = (0 + 0)/2 = 0$$

$$u_1^{(2)} = (0 + 1)/2 = 1/2$$

$$u_2^{(2)} = (0 + 1/2)/2 = 1/4$$

$$u_1^{(3)} = (1/4 + 1)/2 = 5/8$$

$$u_2^{(3)} = (0 + 1/2)/2 = 1/4$$

$$u_1^{(4)} = (1/4 + 1)/2 = 5/8 = 0.625$$

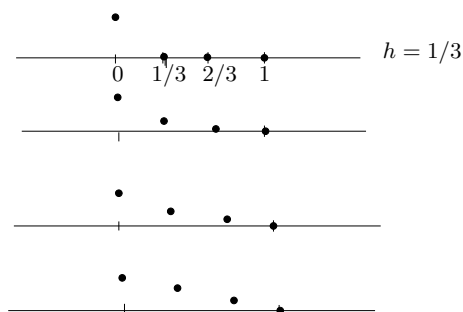
$$u_2^{(4)} = (0 + 5/8)/2 = 5/16 = 0.3125$$

$$u_1^{(5)} = (5/16 + 1)/2 = 21/32 = 0.6563$$

$$u_2^{(5)} = (0 + 5/8)/2 = 5/16 = 0.3125$$

$$u_1^{(6)} = (5/16 + 1)/2 = 21/32 = 0.6563$$

$$u_2^{(6)} = (0 + 21/32)/2 = 21/64 = 0.3281.$$





**Gauss Seidel:**

↓ since these are known

$$x_i^{(k+1)} = \left( b_i - \sum_{j=1}^{i-1} A_{ij}x_j^{(k+1)} - \sum_{j=i+1}^N A_{ij}x_j^{(k)} \right) / A_{ii}$$

$$\Leftrightarrow \boxed{x^{(k+1)} = D^{-1} \left( b - Lx^{(k+1)} - ux^{(k)} \right)} \text{ or } \boxed{x^{(k+1)} = x^{(k)} + D^{-1} \left( b - Lx^{(k+1)} - Dx^{(k)} - ux^{(k)} \right)}$$

$$(D + L)x^{(k+1)} = Dx^{(k)} + \left( b - Dx^{(k)} - ux^{(k)} \right)$$

$$= (D + L)x^{(k)} + \left( b - Lx^{(k)} - Dx^{(k)} - ux^{(k)} \right)$$

$$\therefore x^{(k+1)} = x^{(k)} + (D + L)^{-1} \left( b - Ax^{(k)} \right)$$

$$\boxed{x^{(k+1)} = x^{(k)} + (D + L)^{-1}r^{(k)}} \Leftarrow \text{Interpretation.}$$

**Successive-over-Relaxation (SOR):**

$$x^{(k+1)} = x^{(k)} + \omega D^{-1} \left( b - Lx^{(k+1)} - Dx^{(k)} - Ux^{(k)} \right). \quad \begin{array}{l} \omega \text{ acceleration parameter} \\ \omega = 1 \Rightarrow GS. \end{array}$$

**Interpretation:**

$$(\omega^{-1}D + L)x^{(k+1)} = (\omega^{-1}D + L)x^{(k)} + \left( b - Lx^{(k)} - Dx^{(k)} - ux^{(k)} \right)$$

$$\therefore x^{(k+1)} = x^{(k)} + (\omega^{-1}D + L)^{-1} \left( b - Ax^{(k)} \right)$$

$$\boxed{x^{(k+1)} = x^{(k)} + (\omega^{-1}D + L)^{-1}r^{(k)}}.$$

**Gauss Seidel Iteration**

Eg:

$$\begin{aligned} u'' &= 0 & u &= 1 - x \\ u(0) &= 1; & u(1) &= 0 \\ \frac{u_{n+1} - 2u_n + u_{n-1}}{h^2} &= 0 \end{aligned}$$

$$\begin{bmatrix} -2 & 1 & & & \\ 1 & -2 & 1 & & \\ & 0 & 1 & -2 & 1 \\ & & & & & 0 & 1 & -2 \end{bmatrix} \begin{bmatrix} u_1 \\ \vdots \\ u_{N-1} \end{bmatrix} = \begin{bmatrix} -1 \\ 0 \\ \vdots \\ 0 \end{bmatrix}$$

$$Au = b$$

$$u_n^{(k+1)} = \frac{\left( u_{n+1}^{(k)} + u_{n-1}^{(k+1)} \right)}{2}$$

Let

$$\begin{aligned}
u_0^{(0)} &= 1 & u_1^{(0)} &= 0 & u_2^{(0)} &= 0 & u_3^{(0)} &= 0 \Leftarrow BC \\
u_1^{(1)} &= (0 + 1)/2 = 1/2 = 0.5 \\
u_2^{(1)} &= (0 + 1/2)/2 = 1/4 = 0.25
\end{aligned}$$

FIGURE

$$\begin{aligned}
u_1^{(2)} &= (1 + 1/4)/2 = 5/8 = 0.625 \\
u_2^{(2)} &= (0 + 5/8)/2 = 5/16 = 0.3125
\end{aligned}$$

$$\begin{aligned}
u_1^{(1)} &= \frac{u_2^{(0)} + u_0^{(1)}}{2} \\
u_2^{(1)} &= \frac{u_1^{(0)} + u_1^{(1)}}{2}
\end{aligned}$$

$$\begin{aligned}
u_1^{(3)} &= (1 + 5/16)/2 = 21/32 = 0.6563 \\
u_2^{(3)} &= (0 + 21/32)/2 = 21/64 = 0.3281
\end{aligned}$$

$$\begin{aligned}
u_1^{(4)} &= (1 + 21/64)/2 = 85/128 = 0.6641 \\
u_2^{(4)} &= (0 + 85/128)/2 = 85/256 = 0.3320
\end{aligned}$$

$$\begin{aligned}
u_1^{(5)} &= (1 + 85/256)/2 = 341/512 = 0.6660 \\
u_2^{(5)} &= (0 + 341/512)/2 = 341/1024 = 0.3330.
\end{aligned}$$

**General iterative method:**

$$x^{(k+1)} = x^{(k)} + \alpha_k B^{-1} r^{(k)} \text{ where } r^k = b - Ax^k.$$

$$\alpha_k \equiv 1 \quad B^{-1} = D^{-1} \Rightarrow \text{Jacobi}$$

$$\alpha_k = 1 \quad B^{-1} = (\omega^{-1}D + L) \Rightarrow \text{SOR and Gauss Seidel.}$$

$$\alpha_k = 1 \quad B^{-1} = A^{-1} \Rightarrow \text{Newton's method (vacuous in this case).}$$

$$\begin{aligned}
r^{(k+1)} &= b - Ax^{k+1} \\
&= b - A \left( x^{(k)} + \alpha_k B^{-1} r^{(k)} \right) \\
&= r^{(k)} - \alpha_k AB^{-1} r^{(k)} \\
&= (I - \alpha_k AB^{-1}) r^{(k)} \\
&= (I - \alpha_k AB^{-1}) (I - \alpha_{k-1} AB^{-1}) r^{(k-1)}
\end{aligned}$$

$$r^{(k+1)} = \prod_{s=1}^k (I - \alpha_s AB^{-1}) r^{(1)} = P_k(AB^{-1}) r^{(1)}$$

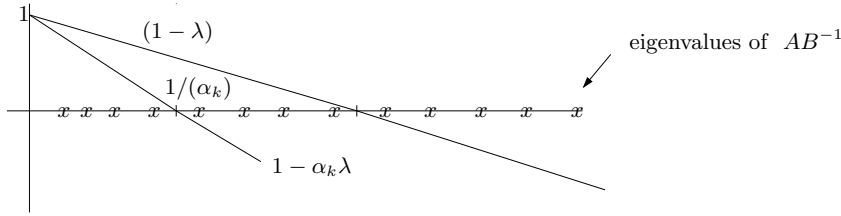
where  $P_k(\hat{A}) = \prod_{s=1}^k (I - \alpha_s \hat{A})$  is a polynomial of degree  $k$  in  $\hat{A}$ .

Let  $\{\lambda_j\}$  be the eigenvalues and  $\{v_j\}$  be the corresponding eigenvectors of  $\hat{A} = AB^{-1}$ : i.e.  $\hat{A}v_j = \lambda_j v_j$ . Then expanding  $r^1$  and  $r^{(k+1)}$  in terms of  $\{v_j\}$ :

$$r^{(1)} = \sum_{j=1}^N \hat{r}_j^{(1)} v_j \quad \text{and} \quad r^{(k+1)} = \sum_{j=1}^N \hat{r}_j^{(k+1)} v_j$$

we obtain:

$$\hat{r}_j^{(k+1)} = \prod_{s=1}^k (1 - \alpha_s \lambda_j) \hat{r}_j^{(1)} = P_k(\lambda_j) \hat{r}_j^{(1)}$$



**Note:** For Jacobi and SOR  $\alpha_k \equiv 1$  so that  $P_k(\lambda) = (1 - \lambda)^k$

$$\begin{aligned} |r^{(k+1)}|^2 &= \left| \sum_i (1 - \lambda_j) \hat{r}_j^{(k)} v_j \right|^2 \\ &\leq |1 - \hat{\lambda}|^2 \left| \sum_j \hat{r}_j^{(k)} v_j \right|^2 \quad \hat{\lambda} : |1 - \hat{\lambda}| = \max \{ |1 - \lambda_1|, |1 - \lambda_N| \} \end{aligned}$$

$$\boxed{|r^{k+1}| \leq \rho |r^{(k)}|} \text{ where } \rho = \max \{ |1 - \lambda_1|, |1 - \lambda_N| \}.$$

**Example of degredation of Jacobi with mesh refinement.**

$$\begin{aligned} -u'' &= f \\ A \cdot u_n &= -u_{n-1} + 2u_n - u_{n+1} = h^2 f_n \\ \lambda_k &= 4 \sin^2 \left( \frac{k\pi}{2N} \right) \quad \text{are the eigenvalues of } A \\ AD^{-1} &= \frac{-E^{-1} + 2 - E}{2} \Rightarrow \mu_1 = 2 \sin^2 \left( \frac{\pi}{2N} \right) \stackrel{N \gg 1}{\approx} \frac{\pi^2}{2N^2} \\ \therefore \rho &\stackrel{N \gg 1}{\approx} 1 - \frac{\pi^2}{2N^2}. \end{aligned}$$

We can expect poor performance as  $N$  increases. Look for the number of iterations it will take to achieve a tolerance  $\varepsilon$ :

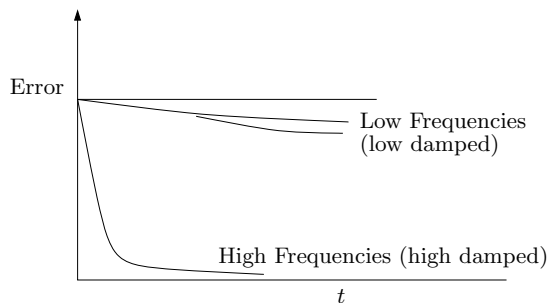
$$\begin{aligned} \rho^r &= \varepsilon \\ r &= \frac{\ln \varepsilon}{\ln \rho} = \frac{\ln \varepsilon}{\ln \left( 1 - \frac{\pi^2}{2N^2} \right)} = \frac{\ln \varepsilon}{-\frac{\pi^2}{2N^2} \left( 1 + \frac{1}{2} \left( \frac{\pi^2}{2N^2} \right) + \dots \right)} \sim -\frac{2N^2}{\pi^2} \ln \varepsilon \end{aligned}$$

**Physical interpretation of Jacobi's method as a diffusion process:**

$$\begin{aligned} u_n^{(k+1)} &= \frac{u_{n+1}^{(k)} + u_{n-1}^{(k)}}{2} \\ \therefore u_n^{(k+1)} - u_n^{(k)} &= \frac{u_{n+1}^{(k)} - 2u_n^{(k)} + u_{n-1}^{(k)}}{2} \\ \therefore \frac{u_n^{(k+1)} - u_n^{(k)}}{\Delta t} &= \left( \frac{h^2}{2\Delta t} \right) \frac{u_{n+1}^{(k)} - 2u_n^{(k)} + u_{n-1}^{(k)}}{h^2} \stackrel{h, \Delta t \rightarrow 0}{\longleftrightarrow} \boxed{\frac{\partial u}{\partial t} = \frac{D \partial^2 u}{\partial x^2}} \end{aligned}$$

Fourier analysis:

$$\begin{aligned}\frac{\partial \hat{u}}{\partial t} &= -D\omega^2 \hat{u} \\ \hat{u} &= \hat{u}_0 e^{-D\omega^2 t}\end{aligned}$$



**Minimization approach to solving linear equations:**

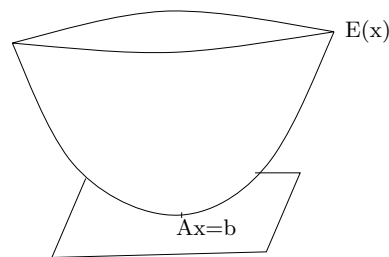
Instead of solving  $Ax = b$ , consider the equivalent problem of minimizing the quadratic form

$$E(x) = \frac{1}{2}x^T Ax - x^T b.$$

For a minimum we have the necessary conditions

$$0 = \frac{\partial E}{\partial x} = Ax - b.$$

Let  $A$  be symmetric and positive definite, then the eigenvalues  $\lambda_k$  of  $A$  are all real and positive. So  $E(x)$  can be viewed as a parabolic surface with elliptic cross sections.

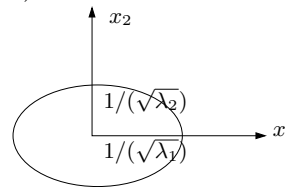


**2D Example:**

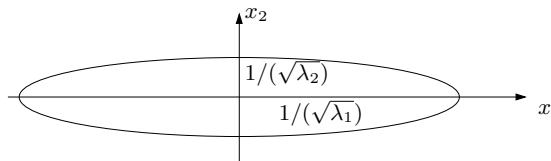
$$A = \begin{pmatrix} \lambda_1 & 0 \\ 0 & \lambda_2 \end{pmatrix}$$

$$E = \frac{1}{2}x^T Ax - x^T b = \frac{1}{2}(\lambda_1 x_1^2 + \lambda_2 x_2^2) - (x_1 b_1 + x_2 b_2)$$

Level sets of  $E$  are ellipses

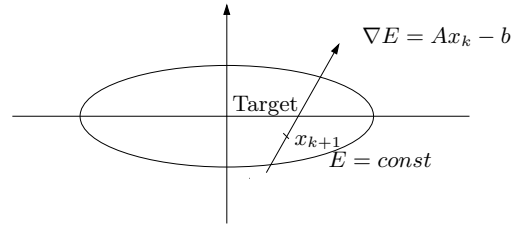


What happens if  $\lambda_2 \gg \lambda_1$



Steepest descent algorithm:

Idea: Search for a minimum along the path defined by  $\nabla E = Ax - b$



Consider the so-called Richardson Scheme:

$$x_{k+1} = x_k + \alpha_k(b - Ax_k). \quad \text{We must look in the steepest descent direction } -\nabla E.$$

Choose  $\alpha_k$  to minimize  $E$  :

$$\begin{aligned} E(x_{k+1}) &= x_{k+1}^T A x_{k+1} \\ &= (x_k + \alpha r_k)^T A (x_k + \alpha r_k) \\ 0 = \frac{\partial E}{\partial \alpha} &= 2r_k^T A (x_k + \alpha r_k) \Rightarrow \alpha_k = -\frac{r_k^T A x_k}{r_k^T A r_k}. \end{aligned}$$

**Algorithm:** Steepest descents.

$$x_{k+1} = x_k + \alpha_k r_k \quad \text{where} \quad \alpha_k = -\frac{r_k^T A x_k}{r_k^T A r_k}.$$

**Notice:**

- The similarity to the general iterative method, in this case  $B = I$ .
- The role of the preconditioner is to try to make all the eigenvalues of  $AB^{-1}$  as close as possible to 1. In this case the ellipses  $\sim$  circles and the steepest descent method will converge rapidly.