SF2520 — Applied numerical methods

Lecture 6

Elliptic equations
Finite difference methods

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Today's lecture

- Summary of last lecture: introduction to PDEs
- Elliptic equations
  - Introduction
  - Theory
  - Finite difference methods, 1D

Introduction to PDE

- Parabolic
  - Model: $u_t = u_{xx}$
  - Phenomena: diffusion, "smearing"
  - Applications: heat conduction, diffusion
- Hyperbolic
  - Model: $u_t = u_x$, $u_{tt} = u_{xx}$
  - Phenomena: transport, wave propagation, advection
  - Applications: waves (electric, acoustic, elastic), fluid flow
- Elliptic
  - Model: $-(u_{xx} + u_{yy}) = f$
  - Phenomena: equilibrium, energy minization
  - Applications: electrostatics, structural mechanics, potential flow

Introduction to PDE

- A second order PDE in 2D

$$au_{xx} + 2bu_{xy} + cu_{yy} + d_1 u_x + d_2 u_y + eu = 0,$$

is classified as

$$\Delta = b^2 - ac, \qquad \begin{cases} \Delta < 0, & \text{elliptic, e.g. } u_{xx} + u_{yy} = 0, \\ \Delta = 0, & \text{parabolic, e.g. } u_x - u_{yy} = 0, \\ \Delta > 0, & \text{hyperbolic, e.g. } u_{xx} - u_{yy} = 0. \end{cases}$$

- A first order PDE system in 1D

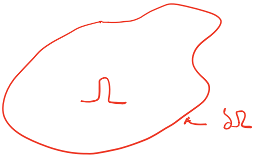
$$\boldsymbol{u}_t + A\boldsymbol{u}_x = 0,$$

is hyperbolic if A is diagonalizable with real eigenvalues.

- In physics, conservation and energy minimization principles lead to PDE models.

Elliptic equations

Model elliptic equation is the Poisson equation,



$$
\begin{aligned}
-\Delta u(\boldsymbol{x}) &= f(\boldsymbol{x}), \qquad \boldsymbol{x} \in \Omega, \\
u(\boldsymbol{x}) &= g(\boldsymbol{x}), \qquad \boldsymbol{x} \in \partial\Omega,
\end{aligned}
$$

for some given functions f, g and domain $\Omega \subset \mathbb{R}^d$.

- Partial differential equation if $d \geq 2$. E.g in 2D, $\boldsymbol{x} = (x, y)$ and

$$
u = u(x, y), \qquad \Delta u = u_{xx} + u_{yy}.
$$

- More general form

$$
\begin{aligned}
-\nabla \cdot (\kappa(\boldsymbol{x})\nabla u) + \boldsymbol{p}(\boldsymbol{x}) \cdot \nabla u + q(\boldsymbol{x})u &= f(\boldsymbol{x}), \qquad \boldsymbol{x} \in \Omega, \\
u(\boldsymbol{x}) &= g(\boldsymbol{x}), \qquad \boldsymbol{x} \in \partial\Omega,
\end{aligned}
$$

  where $\kappa(\boldsymbol{x}) \geq \kappa_0 > 0$ for all $\boldsymbol{x} \in \Omega$.
- Can also have $\kappa(\boldsymbol{x}) \in \mathbb{R}^{d \times d}$ a uniformly positive definite matrix...
- ...and/or κ, p, q depending on u and ∇u (gives nonlinear elliptic equations).

Elliptic equations, one dimension

In one dimension, $\Omega = [a, b]$ is an interval and the general form is

$$-\frac{d}{dx}\left(\kappa(x)\frac{du}{dx}\right) + p(x)\frac{du}{dx} + q(x)u = f(x), \qquad x \in (a, b),$$
$$u(a) = \alpha, \qquad u(b) = \beta.$$

- This is called a two-point boundary value problem.
- Strictly speaking not a PDE (only one independent variable) but shares many properties with the higher dimensional version.
- Compare with the initial value problem (IVP):
  - Two conditions in two different points ($u(a) = \alpha$, $u(b) = \beta$) instead of two conditions in the same point ($u(a) = \alpha$, $u'(a) = \beta$).
  - Independent variable x typically represents space, rather than time as in IVP ("$t \to x$").
- Can also have a fully nonlinear two-point boundary value problem

$$-\frac{d^2u}{dx^2} = F\left(x, u, \frac{du}{dx}\right), \qquad u(a) = \alpha, \quad u(b) = \beta.$$

Elliptic equations, boundary conditions

Other boundary conditions also possible. For $\boldsymbol{x} \in \partial\Omega$,

- "Dirichlet"-conditions

$$u(\boldsymbol{x}) = g(\boldsymbol{x}).$$

- "Neumann"-conditions

$$\frac{\partial u(\boldsymbol{x})}{\partial n} = \hat{n}(\boldsymbol{x}) \cdot \nabla u(\boldsymbol{x}) = g(\boldsymbol{x}).$$

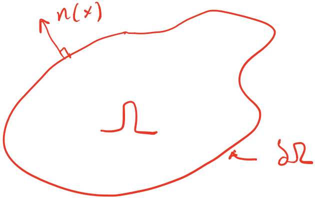
- "Robin"-conditions.

$$\frac{\partial u(\boldsymbol{x})}{\partial n} = g_1(\boldsymbol{x})u(\boldsymbol{x}) + g_2(\boldsymbol{x}).$$

- "Periodic" conditions

$$u(a) = u(b), \qquad u_x(a) = u_x(b),$$

(in one dimension).



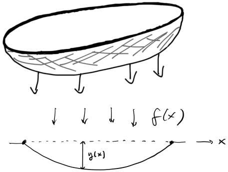
Elliptic equations, examples

Elliptic equations describe equilibrium phenomena. (Energy minimization.)

- Membrane deflection

$$-\nabla \cdot (\kappa \nabla u) = f, \quad \boldsymbol{x} \in \Omega \qquad u = 0, \quad \boldsymbol{x} \in \partial\Omega,$$

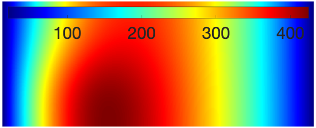
u — displacement of membrane
κ — membrane tensile stress
f — load distribution



- Steady heat flow in a metal block,

$$-\nabla \cdot (\kappa \nabla u) = f, \quad \boldsymbol{x} \in \Omega \qquad u = 20 \text{ (left/right)}, \qquad u_y = 0 \text{ (top/bottom)}$$

u — temperature
κ — heat conductivity
f — heat source
$u = 20$ is temperature of boundary
$u_y = 0$ for insulated boundary

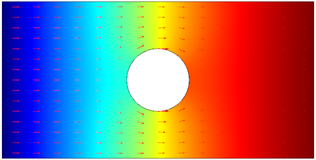


Elliptic equations, examples

- Stationary (DC) current in resistor

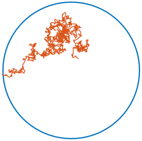
$$-\nabla\cdot(\kappa\nabla u) = 0, \quad \boldsymbol{x}\in\Omega \qquad u = V_0 \text{ (left)}, \quad u = 0 \text{ (right)}, \quad u_y = 0 \text{ (top/bottom)}$$

u — electric potential
κ — conductivity
$-\kappa\nabla u$ — electric current
V_0 — potential on left side
$u = 0$ for grounded boundary
$u_y = 0$ for insulated boundary



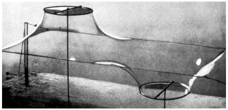
- Expected escape time of Brownian motion

$$-\Delta u = 2, \quad \boldsymbol{x}\in\Omega$$
$$u = 0, \quad \boldsymbol{x}\in\partial\Omega.$$



- Minimal surfaces (soap bubbles on wireframes)

$$-\nabla\cdot\left(\frac{\nabla u}{\sqrt{1+|\nabla u|^2}}\right) = 0, \quad \boldsymbol{x}\in\Omega,$$
$$u(\boldsymbol{x}) = g(\boldsymbol{x}), \quad \boldsymbol{x}\in\partial\Omega.$$



Elliptic equations, theory

- Existence and uniqueness question more subtle than for initial value problem.
  Example in 1D:

  $$u_{xx} + u = 0, \qquad u(0) = 0, \quad u(b) = \beta.$$

  General (ODE) solution is:

  $$u(x) = c_0 \cos(x) + c_1 \sin(x).$$

  But $u(0) = 0$ means $c_0 = 0\dots$
  $\dots$and $u(b) = \beta$ then means $c_1 = \beta/\sin(b)$.
  This gives three possibilties:
    - Unique solution if $\sin(b) \neq 0$, i.e. $b \neq n\pi$, with n integer.
    - No solution if $b = n\pi$ and $\beta \neq 0$.
    - Infinitely many solutions if $b = n\pi$ and $\beta = 0$.
  - Note, in IVP we have $u'(0)$ given instead of $u(b)$. Then a unique solution always exists.
- Even simple linear problems can fail to have a unique solution!

Elliptic equations, theory, cont.

Theorem

For the Poisson equation with Dirichlet boundary conditions,

$$\begin{aligned} -\Delta u(\boldsymbol{x}) &= f(\boldsymbol{x}), \qquad \boldsymbol{x} \in \Omega, \\ u(\boldsymbol{x}) &= g(\boldsymbol{x}), \qquad \boldsymbol{x} \in \partial\Omega, \end{aligned}$$

there is a unique (strong) solution $u \in C^2(\Omega)$ if $f \in C^1(\bar{\Omega})$, $g \in C(\partial\Omega)$ and Ω is an open bounded set in $\mathbb{R}^d$ with smooth boundary.

- Condition on $\partial\Omega$ can be relaxed to include also e.g. a square. (Should satisfy the "exterior sphere condition".)
- For the weak form of Poisson one can have less smooth f.

Theorem

If $f \in L^2(\Omega)$, $g \in H^{1/2}(\partial\Omega)$ and $\partial\Omega$ is Lipschitz, there exists a unique weak solution $u \in H^1(\Omega)$.

Elliptic equations, theory, one dimension

Theorem

For the two-point boundary value problem with Dirichlet boundary conditions,

$$-\frac{d}{dx}\left(\kappa(x)\frac{du}{dx}\right) + p(x)\frac{du}{dx} + q(x)u = f(x), \qquad x \in (a, b),$$
$$u(a) = \alpha, \qquad u(b) = \beta$$

there is a unique (strong) solution $u \in C^2(a, b)$ if $\kappa(x) > 0$, $q(x) \geq 0$ for all $x \in [a, b]$, and $\kappa \in C^1(a, b)$, $\kappa, p, q, f \in C([a, b])$.

Remarks:

- For IVP the conditions in red are not needed.
- There may exist unique solutions even if the red conditions are violated.

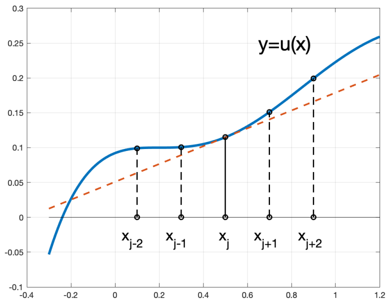
Difference approximations of derivatives

Consider discrete points $x_j = jh$ with $h \ll 1$. In numerical methods for PDEs we need to approximate $u'(x_j)$, $u''(x_j)$, ... given function values in nearby points,

$$\ldots, u(x_{j-2}),\ u(x_{j-1}),\ u(x_j),$$

$$u(x_{j+1}),\ u(x_{j+2}), \ldots,$$

Simple examples: (Let $u_j := u(x_j)$.)



$$u'(x_j) \approx \frac{u_{j+1} - u_j}{h},$$ "forward difference", error = $O(h)$

$$u'(x_j) \approx \frac{u_j - u_{j-1}}{h},$$ "backward difference", error = $O(h)$

$$u'(x_j) \approx \frac{u_{j+1} - u_{j-1}}{2h},$$ "central difference", error = $O(h^2)$

$$u''(x_j) \approx \frac{u_{j+1} - 2u_j + u_{j-1}}{h^2},$$ "central difference", error = $O(h^2)$

Difference approximations of derivatives

- Errors determined by Taylor expansion around $x = x_j$.

  (New formulae can also be derived via operator calculus; see Appendix A.3 in Edsberg.)
- Skewed (asymmetric) formulae use only points on one side of x_j (useful for boundary conditions). E.g.

$$u'(x_j) = \frac{-3u_j + 4u_{j+1} - u_{j+2}}{2h} + O(h^2).$$

- The common expression $(\kappa(x)u_x(x))_x$ approximated as

$$\frac{d}{dx}\left(\kappa(x)\frac{du}{dx}\right)\Bigg|_{x=x_j} = \frac{\kappa_{j+\frac{1}{2}}u_{j+1} - (\kappa_{j+\frac{1}{2}} + \kappa_{j-\frac{1}{2}})u_j + \kappa_{j-\frac{1}{2}}u_{j-1}}{h^2} + O(h^2),$$

  where $\kappa_{j\pm\frac{1}{2}} := \kappa(x_j \pm \frac{h}{2})$. (Rather than expanding to $\kappa u_{xx} + \kappa_x u_x$ and approximating these derivatives.)
- Higher order approximations require function values in more points.

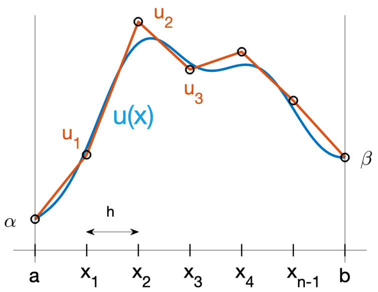
Numerical methods in 1D – finite difference method

Consider the two-point boundary value problem:

$$-\frac{d}{dx}\left(\kappa(x)\frac{du}{dx}\right) + p(x)\frac{du}{dx} + q(x)u = f(x),$$

for $a < x < b$, with boundary conditions

$$u(a) = \alpha, \qquad u(b) = \beta$$



Split finite difference method into several steps:

1. Discretize

   Introduce the discrete points $x_j = a + jh$, where $h = \frac{b-a}{n}$.

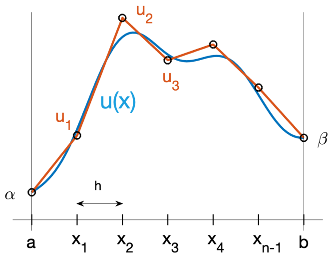
   Approximate exact solution in x_j by u_j,

   $$u_j \approx u(x_j).$$

   Also let $p_j = p(x_j)$, $q_j = q(x_j)$ and $\kappa_{j\pm1/2} = \kappa(x_j \pm h/2)$.

Consider the two-point boundary value problem:

$$-\frac{d}{dx}\left(\kappa(x)\frac{du}{dx}\right) + p(x)\frac{du}{dx} + q(x)u = f(x),$$



2. Approximate derivatives with (second order) differences

For every inner point, $j = 1, \ldots, n-1$,

$$\frac{d}{dx}\left(\kappa\frac{du}{dx}\right)\bigg|_{x=x_j} = \frac{\kappa_{j+\frac{1}{2}}u(x_{j+1}) - (\kappa_{j+\frac{1}{2}} + \kappa_{j-\frac{1}{2}})u(x_j) + \kappa_{j-\frac{1}{2}}u(x_{j-1})}{h^2} + O(h^2),$$

and

$$\frac{du(x_j)}{dx} = \frac{u(x_{j+1}) - u(x_{j-1})}{2h} + O(h^2).$$

This gives for $j = 1, \ldots, n-1$ (upon entering it into the equation)

$$-\frac{\kappa_{j+\frac{1}{2}}u(x_{j+1}) - (\kappa_{j+\frac{1}{2}} + \kappa_{j-\frac{1}{2}})u(x_j) + \kappa_{j-\frac{1}{2}}u(x_{j-1})}{h^2} + p_j\frac{u(x_{j+1}) - u(x_{j-1})}{2h} + q_j u(x_j) = f_j + O(h^2).$$

3. Define the approximation

Given

$$-\frac{\kappa_{j+\frac{1}{2}}u(x_{j+1})-(\kappa_{j+\frac{1}{2}}+\kappa_{j-\frac{1}{2}})u(x_j)+\kappa_{j-\frac{1}{2}}u(x_{j-1})}{h^2}+p_j\frac{u(x_{j+1})-u(x_{j-1})}{2h}+q_ju(x_j)=f_j+O(h^2).$$

Neglect $O(h^2)$ and replace $u(x_j)\mapsto u_j$,

$$-\frac{\kappa_{j+\frac{1}{2}}u_{j+1}-(\kappa_{j+\frac{1}{2}}+\kappa_{j-\frac{1}{2}})u_j+\kappa_{j-\frac{1}{2}}u_{j-1}}{h^2}+p_j\frac{u_{j+1}-u_{j-1}}{2h}+q_ju_j=f_j.$$

After rewriting and reordering terms we have,

$$\underbrace{\left(-\frac{\kappa_{j-\frac{1}{2}}}{h^2}-\frac{p_j}{2h}\right)}_{a_j}u_{j-1}+\underbrace{\left(\frac{\kappa_{j-\frac{1}{2}}+\kappa_{j+\frac{1}{2}}}{h^2}+q_j\right)}_{b_j}u_j+\underbrace{\left(-\frac{\kappa_{j+\frac{1}{2}}}{h^2}+\frac{p_j}{2h}\right)}_{c_j}u_{j+1}=f_j.$$

$$a_ju_{j-1}+b_ju_j+c_ju_{j+1}=f_j,\quad j=1,\dots,n-1.$$

$$a_j=-\frac{\kappa_{j-\frac{1}{2}}}{h^2}-\frac{p_j}{2h},\qquad b_j=\frac{\kappa_{j-\frac{1}{2}}+\kappa_{j+\frac{1}{2}}}{h^2}+q_j,\qquad c_j=-\frac{\kappa_{j+\frac{1}{2}}}{h^2}+\frac{p_j}{2h}.$$

Numerical methods in 1D – finite difference method

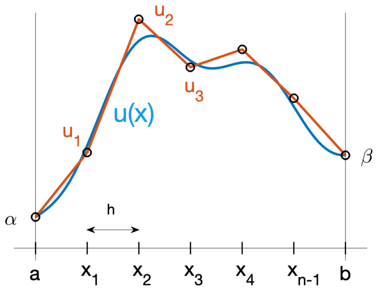
Given $n-1$ equations:

$$a_j u_{j-1} + b_j u_j + c_j u_{j+1} = f_j,$$

för $j = 1, \ldots, n-1$, where

$$u_0, u_1, \ldots, u_{n-1}, u_n$$

are included ($n+1$ values).



4. **Apply boundary conditions**

   At $j = 1$ we use the fact that $u_0 = \alpha$,

$$a_1 \color{red}{\alpha} + b_1 u_1 + c_1 u_2 = f_1 \quad \Rightarrow \quad b_1 u_1 + c_1 u_2 = f_1 - a_1 \alpha.$$

   At $j = n-1$ we use the fact that $u_n = \beta$,

$$a_{n-1} u_{n-2} + b_{n-1} u_{n-1} + c_{n-1} \color{red}{\beta} = f_{n-1} \quad \Rightarrow \quad a_{n-1} u_{n-2} + b_{n-1} u_{n-1} = f_{n-1} - c_{n-1} \beta.$$

   Gives $n-1$ unknowns and $n-1$ equations!

Numerical methods in 1D – finite difference method

Given the equations:

$$
\begin{aligned}
b_1 u_1 + c_1 u_2 &= f_1 - a_1\alpha, \\
a_j u_{j-1} + b_j u_j + c_j u_{j+1} &= f_j, \qquad\qquad j = 2, \ldots, n-2, \\
a_{n-1} u_{n-2} + b_{n-1} u_{n-1} &= f_{n-1} - c_{n-1}\beta.
\end{aligned}
$$

This is a linear system of equations for $\{u_j\}$!

5. Formulate as matrix equation

   With

$$
\boldsymbol{u} = \begin{pmatrix} u_1 \\ u_2 \\ \vdots \\ u_{n-2} \\ u_{n-1} \end{pmatrix}, \quad A = \begin{pmatrix} b_1 & c_1 & & & \\ a_2 & b_2 & c_2 & & \\ & \ddots & \ddots & \ddots & \\ & & a_{n-2} & b_{n-2} & c_{n-2} \\ & & & a_{n-1} & b_{n-1} \end{pmatrix} \quad \boldsymbol{f} = \begin{pmatrix} f_1 - a_1\alpha \\ f_2 \\ \vdots \\ f_{n-2} \\ f_{n-1} - c_{n-1}\beta \end{pmatrix},
$$

   the equations can be written $A\boldsymbol{u} = \boldsymbol{f}$, where $\boldsymbol{u}, \boldsymbol{f} \in \mathbb{R}^{n-1}$ and $A \in \mathbb{R}^{(n-1)\times(n-1)}$.

Numerical methods – finite difference method

Summary

- Finite difference method leads to linear system of equations $A\boldsymbol{u} = \boldsymbol{f}$.

$$\boldsymbol{u} = \begin{pmatrix} u_1 \\ u_2 \\ \vdots \\ u_{n-2} \\ u_{n-1} \end{pmatrix}, \quad A = \begin{pmatrix} b_1 & c_1 & & & \\ a_2 & b_2 & c_2 & & \\ & \ddots & \ddots & \ddots & \\ & & a_{n-2} & b_{n-2} & c_{n-2} \\ & & & a_{n-1} & b_{n-1} \end{pmatrix} \quad \boldsymbol{f} = \begin{pmatrix} f_1 - a_1\alpha \\ f_2 \\ \vdots \\ f_{n-2} \\ f_{n-1} - c_{n-1}\beta \end{pmatrix},$$

  Note: Elements are not constant along diagonals if κ, p, q vary with x.
- Matrix A is always sparse (here tridiagonal). Higher order and higher dimensions lead to more diagonals. Use methods for sparse matrices (`sparse` format) when solving system in Matlab.
- When $p \equiv 0$ (no u_x term) the matrix A is symmetric positive definite.
- Method is second order accurate when second order difference approximations are used for the derivatives,

$$\max_{0\leq j\leq n} |u_j - u(x_j)| \leq Ch^2, \qquad (C \text{ independent of } h).$$

- Condition number of A grows as $O(h^{-2})$ when $h \to 0$.

Numerical methods in 1D – nonlinear problems

Finite differences for a nonlinear equation

Want to solve

$$-u_{xx} = F(x,u), \qquad u(a) = \alpha, \qquad u(b) = \beta.$$

Steps 1-4 gives as before:

$$\begin{aligned} b_1 u_1 + c_1 u_2 &= F(x_1, u_1) - a_1\alpha, \\ a_j u_{j-1} + b_j u_j + c_j u_{j+1} &= F(x_j, u_j), \qquad\qquad j = 2, \ldots, n-2, \\ a_{n-1} u_{n-2} + b_{n-1} u_{n-1} &= F(x_{n-1}, u_{n-1}) - c_{n-1}\beta. \end{aligned}$$

This is a nonlinear system of equations!

5. Write as nonlinear system

   We get $\boldsymbol{F}(\boldsymbol{u}) = 0$ where

$$\boldsymbol{F}(\boldsymbol{u}) = \begin{pmatrix} b_1 & c_1 & & & \\ a_2 & b_2 & c_2 & & \\ & \ddots & \ddots & \ddots & \\ & & a_{n-2} & b_{n-2} & c_{n-2} \\ & & & a_{n-1} & b_{n-1} \end{pmatrix} \boldsymbol{u} - \begin{pmatrix} F(x_1, u_1) - a_1\alpha \\ F(x_2, u_2) \\ \vdots \\ F(x_{n-2}, u_{n-2}) \\ F(x_{n-1}, u_{n-1}) - c_{n-1}\beta \end{pmatrix}.$$

Numerical methods in 1D – nonlinear problems

Need to solve $\boldsymbol{F}(\boldsymbol{u}) = 0$, where

$$\boldsymbol{F}(\boldsymbol{u}) = \underbrace{\begin{pmatrix} b_1 & c_1 & & & \\ a_2 & b_2 & c_2 & & \\ & \ddots & \ddots & \ddots & \\ & & a_{n-2} & b_{n-2} & c_{n-2} \\ & & & a_{n-1} & b_{n-1} \end{pmatrix}}_{A} \boldsymbol{u} - \begin{pmatrix} F(x_1, u_1) - a_1\alpha \\ F(x_2, u_2) \\ \vdots \\ F(x_{n-2}, u_{n-2}) \\ F(x_{n-1}, u_{n-1}) - c_{n-1}\beta \end{pmatrix}.$$

- Use Newton's method
$$\boldsymbol{u}^{k+1} = \boldsymbol{u}^k - J(\boldsymbol{u}^k)^{-1}\boldsymbol{F}(\boldsymbol{u}^k).$$
- Note that the Jacobian matrix J is tridiagonal,
$$J(\boldsymbol{u}) = A - \begin{pmatrix} F_u(x_1, u_1) & & & \\ & F_u(x_2, u_2) & & \\ & & \ddots & \\ & & & F_u(x_{n-1}, u_{n-1}) \end{pmatrix}.$$
  $\Rightarrow$ Each iteration is cheap if a `sparse` solver is used.
- Starting guess for iteration needed.
- The shooting method can also be used for 1D problems. (See Edsberg.)

Finite differences for a nonlinear equation

One can also consider

$$-u_{xx} = F(x, u, u_x), \qquad u(a) = \alpha, \qquad u(b) = \beta.$$

- Upon approximating u_x with central differences, we get $\boldsymbol{F}(\boldsymbol{u}) = 0$ as before, where

$$\boldsymbol{F}(\boldsymbol{u}) = \begin{pmatrix} b_1 & c_1 & & & \\ a_2 & b_2 & c_2 & & \\ & \ddots & \ddots & \ddots & \\ & & a_{n-2} & b_{n-2} & c_{n-2} \\ & & & a_{n-1} & b_{n-1} \end{pmatrix} \boldsymbol{u} - \begin{pmatrix} F\left(x_1, u_1, \frac{u_2-\alpha}{2h}\right) - a_1\alpha \\ F\left(x_2, u_2, \frac{u_3-u_1}{2h}\right) \\ \vdots \\ F\left(x_{n-2}, u_{n-2}, \frac{u_{n-1}-u_{n-3}}{2h}\right) \\ F\left(x_{n-1}, u_{n-1}, \frac{\beta-u_{n-2}}{2h}\right) - c_{n-1}\beta \end{pmatrix}.$$

- This can again be solved by Newton's method.
- Jacobian matrix is still tridiagonal, since F only depends on u_{j-1}, u_j and u_{j+1} in equation j.

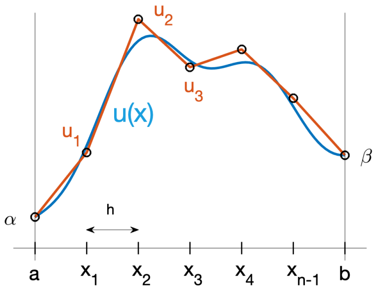
Numerical methods in 1D – other boundary conditions

Finite difference method for:

$$-\frac{d}{dx}\left(\kappa(x)\frac{du}{dx}\right) + p(x)\frac{du}{dx} + q(x)u = f(x),$$

when $a < x < b$, and a Robin condition at $x = a$,

$$\frac{du(a)}{dx} = \alpha_0 u(a) + \alpha_1, \qquad u(b) = \beta.$$



Need to change step 4:

4. Apply boundary conditions
   To eliminate u_0 in the equation for $j = 1$,
   $$a_1 u_0 + b_1 u_1 + c_1 u_2 = f_1,$$
   we must now also discretize the boundary condition
   $$\frac{du(a)}{dx} = \alpha_0 u(a) + \alpha_1.$$

Numerical methods in 1D – boundary conditions

$$\frac{du(a)}{dx} = \alpha_0 u(a) + \alpha_1.$$

Forward difference

- Approximate derivative

$$\frac{u(a+h) - u(a)}{h} = \alpha_0 u(a) + \alpha_1 + O(h).$$

- Neglect $O(h)$ and replace $u(x_j) \mapsto u_j$

$$\frac{u_1 - u_0}{h} = \alpha_0 u_0 + \alpha_1 \quad \Rightarrow \quad u_0 = d_0 + d_1 u_1, \quad d_0 = \frac{-h\alpha_1}{1 + h\alpha_0}, \quad d_1 = \frac{1}{1 + h\alpha_0}.$$

- Insert in equation for $j = 1$

$$a_1 \color{red}{(d_0 + d_1 u_1)} \color{black}{} + b_1 u_1 + c_1 u_2 = f_1 \quad \Rightarrow \quad (a_1 d_1 + b_1) u_1 + c_1 u_2 = f_1 - a_1 d_0.$$

- Matrix form changes only in first row:

$$A = \begin{pmatrix} b_1 & c_1 & & \\ a_2 & b_2 & c_2 & \\ & \ddots & \ddots & \ddots \end{pmatrix}, \; \boldsymbol{f} = \begin{pmatrix} f_1 - a_1 \alpha \\ f_2 \\ \vdots \end{pmatrix} \quad \Rightarrow \quad \begin{pmatrix} b_1 + a_1 d_1 & c_1 & & \\ a_2 & b_2 & c_2 & \\ & \ddots & \ddots & \ddots \end{pmatrix}, \; \begin{pmatrix} f_1 - a_1 d_0 \\ f_2 \\ \vdots \end{pmatrix}.$$

- Total method only first order accurate! (Forward difference is first order.)

Numerical methods in 1D – boundary conditions

$$\frac{du(a)}{dx} = \alpha_0 u(a) + \alpha_1.$$

Skewed approximation

- Approximate derivative with skewed (asymmetric) formula

$$\frac{-3u(a) + 4u(a+h) - u(a+2h)}{2h} = \alpha_0 u(a) + \alpha_1 + O(h^2).$$

- Neglect $O(h^2)$ and replace $u(x_j) \mapsto u_j$

$$\frac{-3u_0 + 4u_1 - u_2}{2h} = \alpha_0 u_0 + \alpha_1 \quad \Rightarrow \quad u_0 = d_0 + d_1 u_1 + d_2 u_2, \quad d_0 = \frac{-2h\alpha_1}{3 + 2h\alpha_0}, \ldots$$

- Inserting in equation $j = 1$ gives the change in matrix form

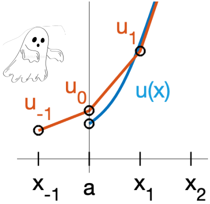
$$A = \begin{pmatrix} b_1 & c_1 & & \\ a_2 & b_2 & c_2 & \\ & \ddots & \ddots & \ddots \end{pmatrix}, \quad \boldsymbol{f} = \begin{pmatrix} f_1 - a_1\alpha \\ f_2 \\ \vdots \end{pmatrix} \quad \Rightarrow \quad \begin{pmatrix} b_1 + a_1 d_1 & c_1 + a_1 d_2 & & \\ a_2 & b_2 & c_2 & \\ & \ddots & \ddots & \ddots \end{pmatrix}, \quad \begin{pmatrix} f_1 - a_1 d_0 \\ f_2 \\ \vdots \end{pmatrix}.$$

- Total method second order accurate.
- To recover value of u_0 one can use $u_0 = d_0 + d_1 u_1 + d_2 u_2$.

Numerical methods in 1D – boundary conditions

$$\frac{du(a)}{dx} = \alpha_0 u(a) + \alpha_1 .$$

Ghost point and central difference



- Add a new grid point at $x_{-1} = a - h$ outside domain and a new unknown u_{-1}. Keep equation for $j = 0$,
$$a_0 \color{red}{u_{-1}} + b_0 u_0 + c_0 u_1 = f_0 .$$
- Approximate derivative with central difference and neglect $O(h^2)$,
$$\frac{u(a+h) - u(a-h)}{2h} = \alpha_0 u(a) + \alpha_1 + O(h^2) \quad \Rightarrow \quad \frac{u_1 - u_{-1}}{2h} = \alpha_0 u_0 + \alpha_1 ,$$
$$\Rightarrow \quad u_{-1} = d_{-1} + d_0 u_0 + d_1 u_1 , \quad d_{-1} = -2h\alpha_1 , \quad d_0 = -2h\alpha_0 , \quad d_1 = 1 .$$
- Inserting in equation $j = 0$ gives the change in matrix form

$$A = \begin{pmatrix} b_1 & c_1 & & \\ a_2 & b_2 & c_2 & \\ & \ddots & \ddots & \ddots \\ & & & \end{pmatrix}, \quad \boldsymbol{f} = \begin{pmatrix} f_1 - a_1 \alpha \\ f_2 \\ \vdots \end{pmatrix} \quad \Rightarrow \quad \begin{pmatrix} b_0 + a_0 d_0 & c_0 + a_0 d_1 & & \\ a_1 & b_1 & c_1 & \\ & \ddots & \ddots & \ddots \\ & & & \end{pmatrix}, \quad \begin{pmatrix} f_0 - a_0 d_{-1} \\ f_1 \\ \vdots \end{pmatrix} .$$

- Total method second order accurate.
- Value of u_0 computed, no need to recover. Note: n unknowns, not $n - 1$!

Numerical methods in 1D – boundary conditions

Remarks

- Skewed approximations and ghost point methods retains second order. (Forward difference only first order.)
- Change in boundary condition only affects the first row in the matrix equation. (But gives of course big change in solution!)
- One more unknown is used in the ghost point method so A is one row/column larger.
- A is not necessarily symmetric even if $p \equiv 0$.
- Boundary condition can also always be added as a separate new equation to the system. E.g. for skewed approximation one could simply add

  $$u_0 = d_0 + d_1 u_1 + d_2 u_2,$$

  and include this in matrix form. However, then A is only pentadiagonal. Also, this approach does not work for parabolic equations.