1D Boundary Value Problems: Finite Differences and Spectral Collocation

M.Sc. in Mathematical Modelling & Scientific Computing,
Practical Numerical Analysis

Michaelmas Term 2020, Lecture 5

1D Boundary Value Problem

Suppose we want to solve numerically the 2nd order linear boundary value problem

$$a(x)u'' + b(x)u' + c(x)u = f(x)$$

for $x \in (a, b)$ with Dirichlet boundary conditions

$$u(a) = u_a \quad \text{and} \quad u(b) = u_b.$$

This can be done using a finite difference scheme.

Finite Differences

One way to derive a finite difference scheme is to use Taylor series expansions. The idea is that if $u(x) \in C^4(\mathbb{R})$ then, using Taylor series expansions, we may write

$$\begin{aligned} u(x+h) &= u(x) + hu'(x) + \frac{h^2}{2}u''(x) + \frac{h^3}{6}u'''(x) + \frac{h^4}{24}u''''(\xi_+) \\ u(x-h) &= u(x) - hu'(x) + \frac{h^2}{2}u''(x) - \frac{h^3}{6}u'''(x) + \frac{h^4}{24}u''''(\xi_-) \end{aligned}$$

for some $\xi_+ \in (x, x+h)$ and $\xi_- \in (x-h, x)$.

Thus we can combine these to see

$$\frac{u(x+h) - 2u(x) + u(x-h)}{h^2} = u''(x) + \frac{h^2}{12}u''''(\xi) \qquad (1)$$

for some $\xi \in (x-h, x+h)$.

Finite Differences

Similarly, we may write

$$\begin{aligned} u(x+h) &= u(x) + hu'(x) + \frac{h^2}{2}u''(x) + \frac{h^3}{6}u'''(\eta_+) \\ u(x-h) &= u(x) - hu'(x) + \frac{h^2}{2}u''(x) - \frac{h^3}{6}u'''(\eta_-) \end{aligned}$$

for some $\eta_+ \in (x, x+h)$ and $\eta_- \in (x-h, x)$, and we can combine these to give

$$\frac{u(x+h) - u(x-h)}{2h} = u'(x) + \frac{h^2}{6}u'''(\eta) \qquad (2)$$

for some $\eta \in (x-h, x+h)$.

Finite Differences

Note that from

$$u(x+h) \quad = \quad u(x) + hu'(x) + \frac{h^2}{2}u''(x) + \frac{h^3}{6}u'''(\eta_+)$$

we could have written

$$\frac{u(x+h) - u(x)}{h} \quad = \quad u'(x) + \frac{h}{2}u''(x) + \frac{h^2}{6}u'''(\eta_+)\ . \qquad (3)$$

Similarly from

$$u(x-h) \quad = \quad u(x) - hu'(x) + \frac{h^2}{2}u''(x) - \frac{h^3}{6}u'''(\eta_-)$$

we could have written

$$\frac{u(x) - u(x-h)}{h} \quad = \quad u'(x) - \frac{h}{2}u''(x)\frac{h^2}{6}u'''(\eta_-)\ . \qquad (4)$$

Finite Differences

We can use expressions (1) and (2) as the basis for a finite difference scheme.

Let $x_i = a + ih$ for $i = 0, 1, \ldots, N$ where $h = (b-a)/N$. Then, setting $x = x_i$ in (1) and (2) (and noting $x_{i+1} = x_i + h$ and $x_{i-1} = x_i - h$) and rearranging gives

$$\begin{aligned} u''(x_i) &= \frac{u(x_{i+1}) - 2u(x_i) + u(x_{i-1})}{h^2} + \mathcal{O}(h^2) \\ u'(x_i) &= \frac{u(x_{i+1}) - u(x_{i-1})}{2h} + \mathcal{O}(h^2). \end{aligned}$$

Note that if we use (3) or (4) we have

$$\begin{aligned} u'(x_i) &= \frac{u(x_{i+1}) - u(x_i)}{h} + \mathcal{O}(h) \\ u'(x_i) &= \frac{u(x_i) - u(x_{i-1})}{h} + \mathcal{O}(h) \end{aligned}$$

so the remainder terms are larger.

Finite Differences

We let U_i be the numerical approximation to the exact solution at x_i, i.e. $U_i \approx u(x_i)$. Then a finite difference scheme for

$$a(x)u'' + b(x)u' + c(x)u \;\; = \;\; f(x)$$

is

$$a(x_i)\frac{U_{i+1} - 2U_i + U_{i-1}}{h^2} + b(x_i)\frac{U_{i+1} - U_{i-1}}{2h} + c(x_i)U_i \;\; = \;\; f(x_i)$$

for $i = 1, \ldots, N-1$. The boundary conditions are imposed as

$$U_0 \; = \; u_a \quad \text{and} \quad U_N \; = \; u_b.$$

The error for this scheme is $\mathcal{O}(h^2)$.

Finite Differences — Implementation

Consider the example

$$u'' + u = 0$$

with $u(-1) = u(1) = 1$ (and exact solution $u(x) = \cos(x)/\cos(1)$).

We can re-arrange the finite difference scheme to get

$$\frac{1}{h^2} U_{i-1} + \left(-\frac{2}{h^2} + 1 \right) U_i + \frac{1}{h^2} U_{i+1} = 0$$

for $i = 1, \ldots, N-1$ with $U_0 = U_N = 1$.

Finite Differences — Implementation

We can eliminate U_0 and U_N to get a tridiagonal system of the form

$$(A + I)\mathbf{U} \quad = \quad \mathbf{b}$$

where $\mathbf{U} = (U_1, U_2, \dots U_{N-1})^T$, I is the $(N-1) \times (N-1)$ identity matrix, $\mathbf{b} = (-1/h^2, 0, \dots, 0, -1/h^2)$ and

$$A \quad = \quad \frac{1}{h^2} \begin{pmatrix} -2 & 1 & & & \\ 1 & -2 & 1 & & \\ & \ddots & \ddots & \ddots & \\ & & 1 & -2 & 1 \\ & & & 1 & -2 \end{pmatrix}.$$

Finite Differences — Implementation

`fin_diff_solve.m`

Finite Differences

An alternative derivation is via differentiating interpolants.

For example, the interpolant of $u(x)$ through x_{i-1} and x_i is

$$p(x) = u(x_{i-1})\frac{x_i - x}{x_i - x_{i-1}} + u(x_i)\frac{x - x_{i-1}}{x_i - x_{i-1}}$$

with derivative

$$p'(x_i) = \frac{u(x_i) - u(x_{i-1})}{x_i - x_{i-1}}$$

which gives a backward difference as in (4).

Similarly, differentiating the interpolant of $u(x)$ through x_i and x_{i+1} and evaluating at x_i gives a forward difference as in (3).

Finite Differences

To get higher order approximations we use higher order interpolants.

For example, the interpolant of $u(x)$ through x_{i-1}, x_i and x_{i+1} on a uniform grid is

$$\begin{aligned} p(x) &= u(x_i) + \frac{u(x_{i+1}) - u(x_{i-1})}{2h}(x - x_i) \\ &\quad + \frac{u(x_{i+1}) - 2u(x_i) + u(x_{i-1})}{2h^2}(x - x_i)^2 \end{aligned}$$

with derivatives

$$p'(x_i) = \frac{u(x_{i+1}) - u(x_{i-1})}{2h} \, ,$$

and

$$p''(x_i) = \frac{u(x_{i+1}) - 2u(x_i) + u(x_{i-1})}{h^2} \, ,$$

as we derived using (1) and (2).

Finite Differences

In the same way as for interpolation and quadrature, extending this to higher order interpolants on a uniform mesh can be disastrous.

In general using 4, 6, 8 degree polynomials is practical for finite differences on uniform meshes.

Question is how to easily work out the finite difference stencils using higher degree polynomials on non-uniform grids.

Differentiation Matrices

Recall the Lagrange form of the interpolant

$$p_n(x) \;=\; \sum_{k=0}^{n} L_{n,k}(x) u(x_k)$$

with derivatives

$$p_n'(x_i) \;=\; \sum_{k=0}^{n} L_{n,k}'(x_i) u(x_k)\ .$$

We seek the matrix D with entries $d_{i,k} = L_{n,k}'(x_i)$ so that we may write

$$p_n'(x_i) \;=\; [d_{i,0}, d_{i,1}, \ldots d_{i,n}] \begin{bmatrix} u(x_0) \\ u(x_1) \\ \vdots \\ u(x_n) \end{bmatrix}$$

Then D is the differentiation matrix for the points $\{x_i\}$.

Differentiation Matrices

Recall the second barycentric interpolation formula from lecture 1:

$$p_n(x) \;=\; \frac{\sum_{l=0}^{n} \frac{\omega_l}{x-x_l} u(x_l)}{\sum_{l=0}^{n} \frac{\omega_l}{x-x_l}} \,,$$

where the ω_l are given by

$$\omega_l \;=\; \frac{1}{\prod_{j\neq l}(x_l - x_j)} \,.$$

This allows us to write

$$L_{n,k}(x) \;=\; \frac{\sum_{l=0}^{n} \frac{\omega_l}{x-x_l} L_{n,k}(x_l)}{\sum_{l=0}^{n} \frac{\omega_l}{x-x_l}} \;=\; \frac{\frac{\omega_k}{x-x_k} 1}{\sum_{l=0}^{n} \frac{\omega_l}{x-x_l}}$$

Differentiation Matrices

From this we get

$$L_{n,k}(x) \sum_{l=0}^{n} \frac{\omega_l}{x - x_l} \quad = \quad \frac{\omega_k}{x - x_k} \; .$$

Let

$$s_i(x) \quad = \quad \sum_{l=0}^{n} \frac{\omega_l (x - x_i)}{x - x_l} \; = \; \sum_{l \neq i} \frac{\omega_l (x - x_i)}{x - x_l} + \omega_i \; .$$

Then

$$L_{n,k}(x) s_i(x) \; = \; L_{n,k}(x) \sum_{l=0}^{n} \frac{\omega_l (x - x_i)}{x - x_l} \quad = \quad \frac{\omega_k (x - x_i)}{x - x_k} \; ,$$

Finally

$$L'_{n,k}(x) s_i(x) + L_{n,k}(x) s'_i(x) \quad = \quad \omega_k \left(\frac{x - x_i}{x - x_k} \right)' \; = \; \omega_k \frac{x_i - x_k}{(x - x_k)^2} \; .$$

Differentiation Matrices

For $x = x_i$ where $i \neq k$

$$L'_{n,k}(x_i)s_i(x_i) + L_{n,k}(x_i)s'_i(x_i) \;=\; \omega_k \frac{x_i - x_k}{(x_i - x_k)^2} \;=\; \frac{\omega_k}{x_i - x_k}\,.$$

Since $s_i(x_i) = \omega_i$ and $L_{n,k}(x_i) = 0$ we have

$$L'_{n,k}(x_i)\omega_i \;=\; \frac{\omega_k}{x_i - x_k}$$

and so

$$d_{i,k} \;=\; L'_{n,k}(x_i) \;=\; \frac{\omega_k/\omega_i}{x_i - x_k}$$

for $i \neq k$.

Differentiation Matrices

For $i = k$ we use the fact that we know p_n interpolates constants exactly and that the derivative of a constant is zero so

$$\sum_{k=0}^{n} d_{i,k} \;\; = \;\; 0$$

which means that

$$d_{i,i} \;\; = \;\; -\sum_{\substack{k=0 \\ k \neq i}}^{n} d_{i,k} \; .$$

This means that if we know the barycentric weights we can compute the differentiation stencil. Note these formulae work for any set of points.

Differentiation Matrix: Example

Let $x_0 = -2h$, $x_1 = -h$, $x_2 = 0$, $x_3 = h$ and $x_4 = 2h$.

Then with

$$\omega_k = \prod_{j \neq k} (x_k - x_j)^{-1}$$

we have

$$\begin{aligned}
\omega_0 &= [(-2h-(-h))(-2h)(-2h-h)(-2h-2h)]^{-1} = \frac{1}{24h^4} = \omega_4 \\
\omega_1 &= [(-h)-(-2h))(-h)(-h-h)(-h-2h)]^{-1} = -\frac{1}{6h^4} = \omega_3 \\
\omega_2 &= \frac{1}{4h^4} \,.
\end{aligned}$$

Hence, with $d_{i,k} = (\omega_k/\omega_i)/(x_i - x_k)$, we get

$$d_{2,0} = \frac{1}{12h} = -d_{2,4}, \quad d_{2,1} = -\frac{2}{3h} = -d_{2,3}\,,$$

and $d_{2,2} = -(d_{2,0} + d_{2,1} + d_{2,3} + d_{2,4}) = 0$.

Differentiation Matrix: Example

Thus

$$p_4'(0) \;=\; \frac{1}{h}\left[\frac{1}{12}, -\frac{2}{3}, 0, \frac{2}{3}, -\frac{1}{12}\right] p_4(\mathbf{x})$$

Let $u(x) = \sin(x)$ then

$$p_4(\mathbf{x}) \;=\; \begin{pmatrix} \sin(-2h) \\ \sin(-h) \\ \sin(0) \\ \sin(h) \\ \sin(2h) \end{pmatrix}$$

and with $h = 0.1$ we get $\frac{1}{h}\left[\frac{1}{12}, -\frac{2}{3}, 0, \frac{2}{3}, -\frac{1}{12}\right] p_4(\mathbf{x}) = 0.99999667.$

Differentiation Matrices on Uniform Grids

On uniform grids, the stencils have generally already been worked out. See, for example https://en.wikipedia.org/wiki/Finite_difference_coefficient

Central finite difference [edit]

This table contains the coefficients of the central differences, for several orders of accuracy:[1]

Derivative	Accuracy	−4	−3	−2	−1	0	1	2	3	4
1	2				−1/2	0	1/2			
	4			1/12	−2/3	0	2/3	−1/12		
	6		−1/60	3/20	−3/4	0	3/4	−3/20	1/60	
	8	1/280	−4/105	1/5	−4/5	0	4/5	−1/5	4/105	−1/280
2	2				1	−2	1			
	4			−1/12	4/3	−5/2	4/3	−1/12		
	6		1/90	−3/20	3/2	−49/18	3/2	−3/20	1/90	
	8	−1/560	8/315	−1/5	8/5	−205/72	8/5	−1/5	8/315	−1/560
3	2			−1/2	1	0	−1	1/2		
	4		1/8	−1	13/8	0	−13/8	1	−1/8	
	6	−7/240	3/10	−169/120	61/30	0	−61/30	169/120	−3/10	7/240
4	2			1	−4	6	−4	1		
	4		−1/6	2	−13/2	28/3	−13/2	2	−1/6	
	6	7/240	−2/5	169/60	−122/15	91/8	−122/15	169/60	−2/5	7/240
5	2		−1/2	2	−5/2	0	5/2	−2	1/2	
6	2		1	−6	15	−20	15	−6	1	

Higher Derivatives

To get second derivatives we could

- Compute

$$L''_{n,k}(x_j) = d^{[2]}_{k,j} \quad = \quad \begin{cases} 2d^{[1]}_{k,j}(d^{[1]}_{j,j} - 1/(x_j - x_k)), & j \neq k \\ -\sum_{l \neq j} d^{[2]}_{j,l} & j = k \end{cases}$$

- Use $u'' \approx D(Dp_n)$

In general the two approaches are not equivalent.

Spectral Collocation

- Here the idea is to use the above methods to contrstruct global differentiation matrices for high degree global interpolants.
- On equispaced points this will be bad, but for Chebyshev or Legendre grids it will work well!
- Global interpolants lead to geometric convergence but dense matrices.
- Here $D^2 = D^{[2]}$.

Boundary Value Problems

Suppose we want to solve an ODE of the form

$$u'' + u = 0$$

then we can write

$$D^2 u + u = (D^2 + I)u = 0$$

where D is the differentiation matrix. This leads to (using a Chebyshev grid with five points)

$$\begin{pmatrix} 18.000 & -28.485 & 18.000 & -11.515 & 5.0000 \\ 9.2426 & -13.000 & 6.0000 & -2.0000 & 0.7574 \\ -1.0000 & 4.0000 & -5.0000 & 4.0000 & -1.0000 \\ 0.7574 & -2.0000 & 6.0000 & -13.000 & 9.2426 \\ 5.0000 & -11.515 & 18.000 & -28.485 & 18.000 \end{pmatrix} \begin{pmatrix} u_0 \\ u_1 \\ u_2 \\ u_3 \\ u_4 \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ 0 \\ 0 \\ 0 \end{pmatrix}$$

Boundary Value Problems

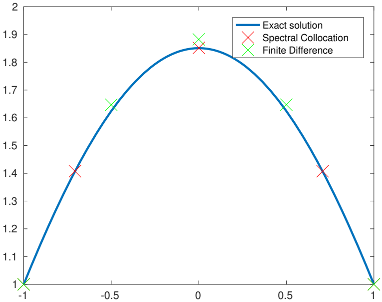
Of course since we are looking at a second order ODE, we need two boundary conditions. If we use $u(-1) = u(1) = 1$ then we can rewrite the first and last rows as

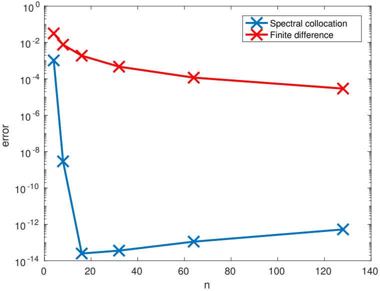
$$\begin{pmatrix} 1 & 0 & 0 & 0 & 0 \\ 9.2426 & -13.000 & 6.0000 & -2.0000 & 0.7574 \\ -1.0000 & 4.0000 & -5.0000 & 4.0000 & -1.0000 \\ 0.7574 & -2.0000 & 6.0000 & -13.000 & 9.2426 \\ 0 & 0 & 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} u_0 \\ u_1 \\ u_2 \\ u_3 \\ u_4 \end{pmatrix} = \begin{pmatrix} 1 \\ 0 \\ 0 \\ 0 \\ 1 \end{pmatrix}$$

The exact solution to this BVP is

$$u(x) = \frac{\cos(x)}{\cos(1)} .$$

Boundary Value Problems





Boundary Value Problems

`spec_colloc_solve.m`

Boundary Value Problems

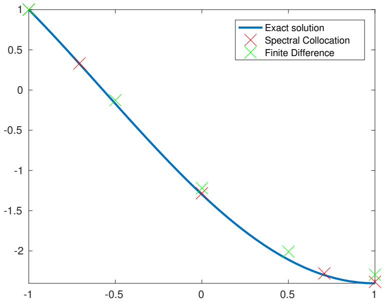
Alternatively we could use $u(-1) = 1$ and $u'(1) = 0$. We then use the final row of D to replace the last row of $D^2 + I$ so we have

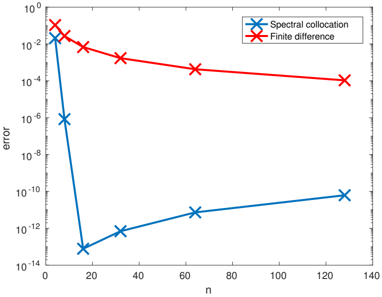
$$\begin{pmatrix} 1 & 0 & 0 & 0 & 0 \\ 9.2426 & -13.000 & 6.0000 & -2.0000 & 0.7574 \\ -1.0000 & 4.0000 & -5.0000 & 4.0000 & -1.0000 \\ 0.7574 & -2.0000 & 6.0000 & -13.000 & 9.2426 \\ 0.5000 & -1.1716 & 2.0000 & -6.8284 & 5.5000 \end{pmatrix} \begin{pmatrix} u_0 \\ u_1 \\ u_2 \\ u_3 \\ u_4 \end{pmatrix} = \begin{pmatrix} 1 \\ 0 \\ 0 \\ 0 \\ 0 \end{pmatrix}$$

The exact solution to this BVP is

$$u(x) = \frac{\cos(x-1)}{\cos(2)} .$$

Boundary Value Problems





More Boundary Value Problems

Now consider the problem

$$\begin{aligned} u'' + \sin(x) u &= 0 \\ u(-1) &= 1 \\ u'(1) &= 0 \,. \end{aligned}$$

We can write this as

$$(D^2 + \mathrm{diag}(\sin(x)))u = 0$$

with the boundary conditions enforced as before.

What Else?

This methodology:

- can easily be adapted to other intervals than $[-1, 1]$;
- extends easily to higher order differential equations;
- extends easily to systems of equations;
- can be extended with Newton's method to solve nonlinear problems;
- is the basis for some of the ODE methods within the Chebfun system — see http://www.chebfun.org/.