

1D Boundary Value Problems: Finite Differences and Spectral Collocation

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

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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

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

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

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

Thus we can combine these to see

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

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

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

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

Finite Differences

Note that from

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

we could have written

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

Similarly from

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

we could have written

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

Finite Differences

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

Let $x_i = a + ih$ for $i = 0, 1, \dots, N$ 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

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

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

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

so error 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 $i = 1, \dots, N - 1$. The boundary conditions are imposed as

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

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

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

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

$$p'_n(x_i) = [d_{i,0}, d_{i,1}, \dots, d_{i,n}] \begin{bmatrix} u(x_0) \\ u(x_1) \\ \vdots \\ u(x_n) \end{bmatrix}.$$

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

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

Differentiation Matrices

From this we get

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

Let

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

Then

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

Finally

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

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

$$\omega_0 = [(-2h - (-h))(-2h)(-2h - h)(-2h - 2h)]^{-1} = \frac{1}{24h^4} = \omega_4$$

$$\omega_1 = [(-h) - (-2h)](-h)(-h - h)(-h - 2h)]^{-1} = -\frac{1}{6h^4} = \omega_3$$

$$\omega_2 = \frac{1}{4h^4}.$$

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

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

- ▶ 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 construct 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

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

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

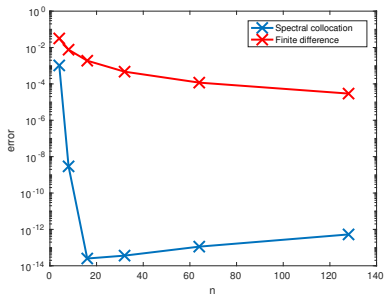
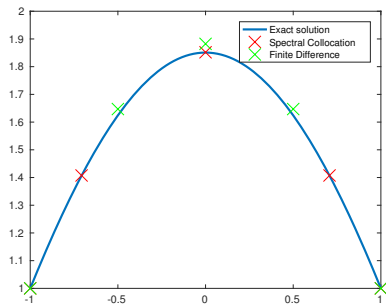
Of course since we are looking at a second order ODE, we need two boundary conditions. If we use $u(-1) = u(1) = 1$ then we can rewrite the first and last rows as

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

The exact solution to this BVP is

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

Boundary Value Problems



Boundary Value Problems

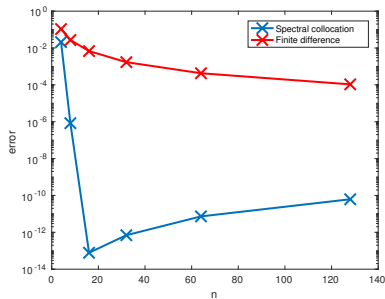
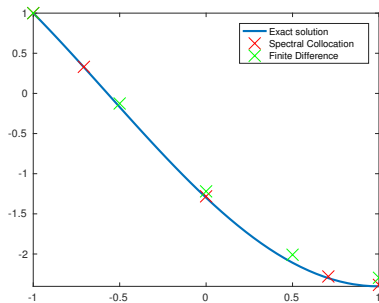
Alternatively we could use $u(-1) = 1$ and $u'(1) = 0$. We then use the final row of D to replace the last row of $D^2 + I$ so we have

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

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

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

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/>.