MATH 408: Computational Methods for Differential Equations

Higher-Order Methods for Two-Point BVPs

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Outline

Higher-Order Methods for Second-Order BVPs

We will now return to our simple model problem

$$u''(x) = f(x)$$
$$u'(0) = \sigma, \quad u(1) = \beta$$

with mixed Dirichlet–Neumann BCs.

We focus on approximating the derivatives with higher-order accuracy (see Section 2.20 of [2]).

Our earlier discretizations were second-order accurate, using a three-point symmetric stencil for the ODE, i.e.,

$$u''(x_j) \approx \frac{U_{j-1} - 2U_j + U_{j+1}}{h^2},$$

and the one-sided three-point stencil for the Neumann BC at $x = 0$, i.e.,

$$u'(0) \approx \frac{-3U_0 + 4U_1 - U_2}{2h}.$$

How do we get approximations to $u''(x_j)$ and $u'(0)$ that are better than second-order accurate?

Recall what we did in `Notes408_01_FiniteDifferences`: perform polynomial interpolation at more points and then use the appropriate derivative of the polynomial to approximate the derivatives of u.

Fortunately, we can also use the MATLAB function `fdcoeffF.m`.

Example

Fourth-order accurate approximations can be obtained with

- five-point symmetric stencil for the ODE: `12*fdcoeffF(2,0,-2:2)`, or

$$u''(x_j) \approx \frac{-U_{j-2} + 16U_{j-1} - 30U_j + 16U_{j+1} - U_{j+2}}{12h^2}.$$

- one-sided five-point stencil for $u'(0)$: `12*fdcoeffF(1,0,0:4)`, or

$$u'(0) \approx \frac{-25U_0 + 48U_1 - 36U_2 + 16U_3 - 3U_4}{12h}.$$

Let's take another look at the approximation of $u''(x_j)$

$$u''(x_j) \approx \frac{-U_{j-2} + 16U_{j-1} - 30U_j + 16U_{j+1} - U_{j+2}}{12h^2}.$$

We can apply this only for $j = 2, 3, \ldots, m-2, m-1$.
This leaves us without an approximation of $u''(x_1)$ and $u''(x_m)$.
We need additional FD formulas for those:

- $u''(x_1)$ with `12*fdcoeffF(2,1,0:5)`, or

$$u''(x_1) \approx \frac{10U_0 - 15U_1 - 4U_2 + 14U_3 - 6U_4 + U_5}{12h^2},$$

- $u''(x_m)$, analogously, with `12*fdcoeffF(2,4,0:5)`, or

$$u''(x_m) \approx \frac{U_{m-4} - 6U_{m-3} + 14U_{m-2} - 4U_{m-1} - 15U_m + 10U_{m+1}}{12h^2}.$$

Both of these approximations are also fourth-order accurate, but require six terms to achieve this.

A fourth-order FD discretization of the BVP

$$u''(x) = f(x)$$
$$u'(0) = \sigma, \quad u(1) = \beta$$

now becomes $AU = F$ with $U = [U_0, U_1, \ldots, U_m, U_{m+1}]^T$ and

$$A = \frac{1}{12h^2}\begin{bmatrix} -25h & 48h & -36h & 16h & -3h & 0 & \ldots & 0 \\ 10 & -15 & -4 & 14 & -6 & 1 & \ldots & 0 \\ -1 & 16 & -30 & 16 & -1 & 0 & \ldots & \vdots \\ \vdots & \ddots & \ddots & \ddots & \ddots & \ddots & \ddots & \vdots \\ \vdots & \ldots & 0 & -1 & 16 & -30 & 16 & -1 \\ 0 & \ldots & 1 & -6 & 14 & -4 & -15 & 10 \\ 0 & 0 & \ldots & \ldots & \ldots & 0 & 0 & 12h^2 \end{bmatrix} \text{ and } F = \begin{bmatrix} \sigma \\ f(x_1) \\ f(x_2) \\ \vdots \\ f(x_{m-1}) \\ f(x_m) \\ \beta \end{bmatrix}.$$

Note that the $(m+2) \times (m+2)$ matrix A is essentially pentadiagonal (except for rows 1, 2 and $m+1$).

Remark

- *The MATLAB codes* `FDApproximationRates2.m` *and* `BVP4Demo.m` *illustrate the accuracy of a few one-sided FD approximations and the BVP discretization, respectively.*
- *If we want an even higher-order method we could use, e.g., sixth-order approximations.*
- *But then we need to implement separate formulas for BCs as well as for $u''(x_j)$, where $j = 1, 2, m-1, m$.*
- *Instead, it is actually easier to just* **use all points** *for* **all** *derivative approximations. This gives rise to so-called spectral methods, which we discuss next.*

Spectral Methods—A Motivating Example

Another class of very accurate numerical methods for BVPs (as well as many time-dependent PDEs) are the so-called spectral methods.

The basic idea is similar to FD methods. However, now we use **all** grid points to obtain our derivative approximations.

Some basics are provided in Section 2.21 of LeVeque's book [2]. Much more detail can be found in [3] by Trefethen.

Example (Motivation for study of spectral methods)

Compare

- `BVP4Demo.m`: fourth-order accurate
- `BVPSpectralDemo.m`: spectrally accurate

Spectral accuracy gives us a **much smaller error with significantly fewer grid points**.

Differentiation Matrices

The main ingredient for spectral methods is the concept of a differentiation matrix D (which you can also view as a first-order, but dense, FD matrix).

This matrix maps a vector U of approximate function values

$$U = [U_1, \ldots, U_m]^T$$

at the grid points $x_1, \ldots, x_m$ to a vector U' of approximate derivative values, i.e.,

$$U' = \mathsf{D}U.$$

We can think of the matrix D as a discrete differential operator.

What does such a differentiation matrix look like?

Let's assume

- the grid points are uniformly spaced with spacing $h = x_{j+1} - x_j$ for all j,
- the vector of approximate function values U comes from a periodic function.

Thus we can add the two auxiliary values

$$U_0 = U_m \quad \text{and} \quad U_{m+1} = U_1 .$$

To approximate $u'(x_j)$ we start with another look at the FD approach.

We first use symmetric (second-order accurate) FDs

$$u'(x_j) \approx U_j' = \frac{U_{j+1} - U_{j-1}}{2h}, \quad j = 1, \ldots, m.$$

Remark

This formula also holds at both ends ($j = 1$ and $j = m$) since u is assumed to be periodic.

We can collect this in matrix-vector form as $U' = \mathrm{D}U$ with U and U' as above and

$$\mathrm{D} = \frac{1}{h} \begin{bmatrix} 0 & \frac{1}{2} & & & -\frac{1}{2} \\ -\frac{1}{2} & 0 & \frac{1}{2} & & \\ & \ddots & \ddots & \ddots & \\ & & -\frac{1}{2} & 0 & \frac{1}{2} \\ \frac{1}{2} & & & -\frac{1}{2} & 0 \end{bmatrix}.$$

Remark

1. *The matrix* D *has a very special structure. It is both*
   - *Toeplitz, i.e., the entries in each diagonal are constant, and*
   - *circulant, i.e., generated by a single row vector whose entries are shifted by one (in a circulant manner) each time a new row is generated.*
2. *As we will see later, the fast Fourier transform (FFT) can deal with such matrices in a particularly efficient manner.*

As we saw earlier, there is a close connection between FD approximations of derivatives and polynomial interpolation.

Example

Symmetric 2nd-order accurate approximation of first-order derivative:

- differentiate the polynomial p of degree two that interpolates the data $\{(x_{j-1}, U_{j-1}), (x_j, U_j), (x_{j+1}, U_{j+1})\}$,
- and evaluate at $x = x_j$.

Example

Degree four polynomial that interpolates the five (symmetric) pieces of data $\{(x_{j-2}, U_{j-2}), (x_{j-1}, U_{j-1}), (x_j, U_j), (x_{j+1}, U_{j+1}), (x_{j+2}, U_{j+2})\}$.
This leads to

$$u'(x_j) \approx U_j' = \frac{U_{j-2} - 8U_{j-1} + 8U_{j+1} - U_{j+2}}{12h}, \quad j = 1, \ldots, m,$$

which can be obtained with `12*fdcoeffF(1,0,-2:2)`.

The resulting differentiation matrix is

$$D = \frac{1}{h} \begin{bmatrix} 0 & \frac{2}{3} & -\frac{1}{12} & & & \frac{1}{12} & -\frac{2}{3} \\ -\frac{2}{3} & 0 & \frac{2}{3} & -\frac{1}{12} & & & \frac{1}{12} \\ & \ddots & \ddots & \ddots & \ddots & \ddots & \\ -\frac{1}{12} & & & \frac{1}{12} & -\frac{2}{3} & 0 & \frac{2}{3} \\ \frac{2}{3} & -\frac{1}{12} & & & \frac{1}{12} & -\frac{2}{3} & 0 \end{bmatrix}.$$

This matrix is again a circulant Toeplitz matrix (since the data is assumed to be periodic). However, now there are five diagonals, instead of the three for the second-order example above.

Example

The fourth-order convergence of this FD approximation is illustrated in `FD4Demo.m`.

It should now be clear that—in order to increase the accuracy of the FD derivative approximation to spectral order—we want to keep on increasing the polynomial degree so that more and more grid points are being used, and the differentiation matrix becomes a dense matrix.

Thus, we can think of spectral methods as FD methods based on **global** polynomial interpolants instead of local ones.

For an infinite interval with infinitely many grid points spaced a distance h apart we will show in `Notes408_16_UnboundedGrids` that the resulting differentiation matrix is given by the circulant Toeplitz matrix

$$\mathsf{D} = \frac{1}{h}\begin{bmatrix} & \vdots & \\ \ddots & \frac{1}{3} & \\ \ddots & -\frac{1}{2} & \\ \ddots & 1 & \\ & 0 & \\ & -1 & \ddots \\ & \frac{1}{2} & \ddots \\ & -\frac{1}{3} & \ddots \\ & \vdots & \end{bmatrix}.$$

For a finite (even) m and periodic data we will show later that the differentiation matrix is given by

$$D_m = \begin{bmatrix} & \vdots & \\ \ddots & \frac{1}{2}\cot\frac{3h}{2} & \\ \ddots & -\frac{1}{2}\cot\frac{2h}{2} & \\ \ddots & \frac{1}{2}\cot\frac{1h}{2} & \\ & 0 & \\ & -\frac{1}{2}\cot\frac{1h}{2} & \ddots \\ & \frac{1}{2}\cot\frac{2h}{2} & \ddots \\ & -\frac{1}{2}\cot\frac{3h}{2} & \ddots \\ & \vdots & \end{bmatrix}. \tag{1}$$

Example

If $m = 4$, then we have

$$\mathsf{D}_4 = \begin{bmatrix} 0 & -\frac{1}{2}\cot\frac{3h}{2} & \frac{1}{2}\cot\frac{2h}{2} & -\frac{1}{2}\cot\frac{1h}{2} \\ -\frac{1}{2}\cot\frac{1h}{2} & 0 & -\frac{1}{2}\cot\frac{3h}{2} & \frac{1}{2}\cot\frac{2h}{2} \\ \frac{1}{2}\cot\frac{2h}{2} & -\frac{1}{2}\cot\frac{1h}{2} & 0 & -\frac{1}{2}\cot\frac{3h}{2} \\ -\frac{1}{2}\cot\frac{3h}{2} & \frac{1}{2}\cot\frac{2h}{2} & -\frac{1}{2}\cot\frac{1h}{2} & 0 \end{bmatrix}.$$

Remark

- *The* MATLAB *script* `PSDemo.m` *illustrates the spectral convergence obtained with the matrix* D_m *for various values of m.*
- *The output should be compared with that of the previous example* `FD4Demo.m`*.*

References I

- U. Ascher, R. Mattheij and R. Russell.
  Numerical Solution of Boundary Value Problems for Ordinary Differential Equations.
  SIAM, Philadelphia, 1995.
- R. LeVeque.
  Finite Difference Methods for Ordinary and Partial Differential Equations.
  SIAM, Philadelphia, 2007.
- L. N. Trefethen.
  Spectral Methods in MATLAB.
  SIAM, Philadelphia, 2000.