1.2 Differences, Derivatives, Boundary Conditions

\begin{align*}
\begin{array}{c}
u(0) = 0, \ u(1) = 0 \\
u'(0) = 0, \ u'(1) = 0
\end{array} & \quad \text{K has } u_0 = u_{n+1} = 0 \\
\begin{array}{c}
u'(0) = 0, \ u(1) = 0 \\
u(0) = u(1), \ u'(0) = u'(1)
\end{array} & \quad \text{B has } u_0 = u_1, \ u_n = u_{n+1}
\end{align*}

An infinite tridiagonal matrix, with no boundary, maintains 1, −2, 1 down its infinitely long diagonals. Chopping off the infinite matrix would be the same as pretending that \( u_0 \) and \( u_{n+1} \) are both zero. That leaves \( K_n \), which has 2's in the corners.

**Problem Set 1.2**

1. What are the second derivative \( u''(x) \) and the second difference \( \Delta^2 U_n \)? Use \( \delta(x) \).

\[
u(x) = \begin{cases} Ax & \text{if } x \leq 0 \\ Bx & \text{if } x \geq 0 \end{cases} \quad U_n = \begin{cases} An & \text{if } n \leq 0 \\ Bn & \text{if } n \geq 0 \end{cases} = \begin{bmatrix} -2A \\ -A \\ 0 \\ B \\ 2B \end{bmatrix}
\]

\( u(x) \) and \( U \) are piecewise linear with a corner at 0.

2. Solve the differential equation \( -u''(x) = \delta(x) \) with \( u(-2) = 0 \) and \( u(3) = 0 \). The pieces \( u = A(x + 2) \) and \( u = B(x - 3) \) meet at \( x = 0 \). Show that the vector \( U = (u(-1), u(0), u(1), u(2)) \) solves the corresponding matrix problem \( KU = F = (0, 1, 0, 0) \).

Problems 3–12 are about the “local accuracy” of finite differences.

3. The \( h^2 \) term in the error for a centered difference \( (u(x + h) - u(x - h))/2h \) is \( \frac{1}{6} h^2 u'''(x) \). Test by computing that difference for \( u(x) = x^3 \) and \( x^4 \).

4. Verify that the inverse of the backward difference matrix \( \Delta_- \) in (28) is the sum matrix in (29). But the centered difference matrix \( \Delta_0 = (\Delta_+ + \Delta_-)/2 \) might not be invertible! Solve \( \Delta_0 u = 0 \) for \( n = 3 \) and \( n = 5 \).

5. In the Taylor series (2), find the number \( a \) in the next term \( ah^4 u'''(x) \) by testing \( u(x) = x^4 \) at \( x = 0 \).

6. For \( u(x) = x^4 \), compute the second derivative and second difference \( \Delta^2 u/(\Delta x)^2 \). From the answers, predict \( c \) in the leading error in equation (9).

7. Four samples of \( u \) can give fourth-order accuracy for \( du/dx \) at the center:

\[
\frac{-u_2 + 8u_1 - 8u_{-1} + u_{-2}}{12h} = \frac{du}{dx} + bh^4 \frac{d^5 u}{dx^5} + \ldots
\]

1. Check that this is correct for \( u = 1 \) and \( u = x^2 \) and \( u = x^4 \).
2. Expand \(u_2, u_1, u_{-1}, u_{-2}\) as in equation (2). Combine the four Taylor series to discover the coefficient \(b\) in the \(h^4\) leading error term.

8 Question Why didn’t I square the centered difference for a good \(\Delta^2\)?

Answer A centered difference of a centered difference stretches too far:

\[
\frac{\Delta_0 \Delta_0}{2h} u_n = \frac{u_{n+2} - 2u_n + u_{n-2}}{(2h)^2}
\]

The second difference matrix now has \(1, 0, -2, 0, 1\) on a typical row. The accuracy is no better and we have trouble with \(u_{n+2}\) at the boundaries.

Can you construct a fourth-order accurate centered difference for \(d^2u/dx^2\), choosing the right coefficients to multiply \(u_2, u_1, u_0, u_{-1}, u_{-2}\)?

9 Show that the fourth difference \(\Delta^4 u/(\Delta x)^4\) with coefficients \(1, -4, 6, -4, 1\) approximates \(d^4u/dx^4\) by testing on \(u = x, x^2, x^3, \) and \(x^4\):

\[
\frac{\Delta^4 u}{\Delta x^4} = \frac{u_{2} - 4u_1 + 6u_0 - 4u_{-1} + u_{-2}}{(\Delta x)^4} = \frac{d^4u}{dx^4} + \text{(which leading error?)}
\]

10 Multiply the first difference matrices in the order \(\Delta_+ \Delta_-\), instead of \(\Delta_- \Delta_+\) in equation (27). Which boundary row, first or last, corresponds to the boundary condition \(u = 0\)? Where is the approximation to \(u' = 0\)?

11 Suppose we want a one-sided approximation to \(du/dx\) with second order accuracy:

\[
\frac{ru(x) + su(x - \Delta x) + tu(x - 2\Delta x)}{\Delta x} = \frac{du}{dx} \quad \text{for} \quad u = 1, x, x^2.
\]

Substitute \(u = 1, x, x^2\) to find and solve three equations for \(r, s, t\). The corresponding difference matrix will be lower triangular. The formula is “causal.”

12 Equation (7) shows the “first difference of the first difference.” Why is the left side within \(O(h^2)\) of \(\frac{1}{h} \left[ u'_{i+\frac{1}{2}} - u'_{i-\frac{1}{2}} \right]\)? Why is this within \(O(h^2)\) of \(u''\)?

Problems 13–19 solve differential equations to test global accuracy.

13 Graph the free-fixed solution \(u_0, \ldots, u_8\) with \(n = 7\) in Figure 1.4, in place of the existing graph with \(n = 3\). You can use formula (30) or solve the 7 by 7 system. The \(O(h)\) error should be cut in half, from \(h = \frac{1}{4}\) to \(\frac{1}{8}\).

14 (a) Solve \(-u'' = 12x^2\) with free-fixed conditions \(u'(0) = 0\) and \(u(1) = 0\). The complete solution involves integrating \(f(x) = 12x^2\) twice, plus \(Cx + D\).
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(b) With \( h = \frac{1}{n+1} \) and \( n = 3, 7, 15 \), compute the discrete \( u_1, \ldots, u_n \) using \( T_n \):

\[
\frac{u_{i+1} - 2u_i + u_{i-1}}{h^2} = 3(ih)^2 \quad \text{with} \quad u_0 = 0 \quad \text{and} \quad u_{n+1} = 0.
\]

Compare \( u_i \) with the exact answer at the center point \( x = ih = \frac{1}{2} \). Is the error proportional to \( h \) or \( h^2 \)?

15 \hspace{1cm} \text{Plot the} \ u = \cos 4\pi x \ \text{for} \ 0 \leq x < 1 \ \text{and the discrete values} \ u_i = \cos 4\pi ih \ \text{at the meshpoints} \ x = ih = \frac{i}{n+1}. \ \text{For small} \ n \ \text{these values will not catch the oscillations of} \ \cos \pi x. \ \text{How large is a good} \ n? \ \text{How many mesh points per oscillation?}

16 \hspace{1cm} \text{Solve} \ -u'' = \cos 4\pi x \ \text{with fixed-fixed conditions} \ u(0) = u(1) = 0. \ \text{Use} \ K_4 \ \text{and} \ K_8 \ \text{to compute} \ u_1, \ldots, u_n \ \text{and plot on the same graph with} \ u(x):}

\[
\frac{u_{i+1} - 2u_i + u_{i-1}}{h^2} = \cos 4\pi ih \quad \text{with} \quad u_0 = u_{n+1} = 0.
\]

17 \hspace{1cm} \text{Test the differences} \ \Delta_0 u = (u_{i+1} - u_{i-1}) \ \text{and} \ \Delta^2 u = u_{i+1} - 2u_i + u_{i-1} \ \text{on} \ u(x) = e^{ax}. \ \text{Factor out} \ e^{ax} \ \text{this is why exponentials are so useful}. \ \text{Expand} \ e^{a\Delta x} = 1 + a\Delta x + (a\Delta x)^2/2 + \cdots \ \text{to find the leading error terms.}

18 \hspace{1cm} \text{Write a finite difference approximation (using} \ K \ \text{with} \ n = 4 \ \text{unknowns to}}

\[
\frac{d^2 u}{dx^2} = x \quad \text{with boundary conditions} \ u(0) = 0 \ \text{and} \ u(1) = 0.
\]

\text{Solve for} \ u_1, u_2, u_3, u_4. \ \text{Compare them to the true solution.}

19 \hspace{1cm} \text{Construct a centered finite difference approximation} \ K/ h^2 \ \text{and} \ \Delta_0/2h \ \text{to}

\[
-\frac{d^2 u}{dx^2} + \frac{du}{dx} = 1 \quad \text{with} \ u(0) = 0 \ \text{and} \ u(1) = 0.
\]

\text{Separately use a forward difference} \ \Delta_+ U / h \ \text{for} \ du/ dx. \ \text{Notice} \ \Delta_0 = (\Delta_+ + \Delta_-)/2. \ \text{Solve for the centered} \ u \ \text{and uncentered} \ U \ \text{with} \ h = 1/5. \ \text{The true} \ u(x) \ \text{is the particular solution}

\text{function} \ \text{of} \ \text{any} \ A + Be^x. \ \text{Which} \ A \ \text{and} \ B \ \text{satisfy the boundary conditions? How close are \ u \ \text{and} \ U \ \text{to} \ u(x) ?}

20 \hspace{1cm} \text{The transpose of the centered difference} \ \Delta_0 \ \text{is} \ -\Delta_0 \ (\text{antisymmetric}). \ \text{That is like the minus sign in integration by parts, when} \ f(x)g(x) \ \text{drops to zero at} \ \pm \infty:

\begin{align*}
\text{Integration by parts} & \quad \int_{-\infty}^{\infty} f(x) \frac{dg}{dx} \ dx = - \int_{-\infty}^{\infty} \frac{df}{dx} \ g(x) \ dx. \\
\text{Verify the summation by parts} & \quad \sum_{i=-\infty}^{\infty} f_i \ (g_{i+1} - g_{i-1}) = - \sum_{i=-\infty}^{\infty} (f_{i+1} - f_{i-1}) \ g_i.
\end{align*}

\text{Hint: Change} \ i + 1 \ \text{to} \ i \ \text{in} \ \sum f_i \ g_{i+1}, \ \text{and change} \ i - 1 \ \text{to} \ i \ \text{in} \ \sum f_i g_{i-1}.\]
21  Use the expansion \( u(h) = u(0) + hu'(0) + \frac{1}{2} h^2 u''(0) + \cdots \) with zero slope \( u'(0) = 0 \) and \( -u'' = f(x) \) to derive the top boundary equation \( u_0 - u_1 = \frac{1}{2} h^2 f(0) \). This factor \( \frac{1}{2} \) removes the \( O(h) \) error from Figure 1.4: good.

22  (added in 2012) Solve \( -\frac{d^2 u}{dx^2} = f(x) \) with \( u(0) = 0 \) and \( u'(1) = 0 \) (free end) when \( f(x) = 1 \) for \( x \leq a \), \( f(x) = 0 \) for \( x > a \). Does \( du/dx \) jump at \( x = a \)? You could start with complete solutions and determine constants.

With \( a = \frac{1}{2} \), what would be a reasonable finite difference approximation to this problem?