Finite difference approximations converge study and solver

Recall the finite difference method. Let interval \((a, b)\) be (equidistantly) divided into points \(a = x_1, x_2, \ldots, x_{N-1}, x_N = b\), where \(x_{k+1} - x_k = h\) and \(k \in \{1, \ldots, N - 1\}\). The difference approximations of the \(n'\)th order derivative can be generally written as

\[
f^{(n)}(x_k) = \sum_{j \in \omega_k} \alpha_j f(x_j) + O(h^p),
\]

where \(\omega\) is the set of indexes (defining the points, where \(f\) is evaluated) and \(\alpha_j\)'s are the corresponding weights.

For example, the central difference approximation of the derivative is

\[
f'(x_k) = \frac{f(x_{k+1}) - f(x_{k-1})}{2h} + O(h^2),
\]

i.e., \(\omega_k := \{k-1, k+1\}\), \(\alpha_1 := -\frac{1}{2h}\) and \(\alpha_2 := \frac{1}{2h}\).

Convergence study

Obviously the central difference scheme cannot be used at points \(x_1\) and \(x_N\), since \(x_0\) and \(x_{N+1}\) are unknown. The tempting alternative is to apply forward and backward difference schemes, respectively. However, then the second order convergence is ruined.

1. Select a differentiable function \(f\) and compute \(f'\) analytically.
2. Compute the approximation \(f'_h\) the way described above.
3. Observe the first order convergence by plotting the error

\[
e_h := \max_{k \in \{1, \ldots, N\}} |f'(x_k) - f'_h(x_k)|
\]

as a function of \(N\) in loglog-scale together with the curves \(y = (1/N)\) and \(y = (1/N)^2\).

In order to recover the second order convergence, one must derive difference scheme that exploits the values at points \(x_k, x_{k+1}\), and \(x_{k+2}\) to approximate \(f'(x_k)\). For the end points one needs the scheme that uses \(x_k, x_{k-1}\), and \(x_{k-2}\).
1. Derive the desired scheme (hint: Write Taylor series at developed at point \( x \) and evaluate it at \( x - 2h, \ x - h, \ x + h, \) and \( x + 2h \), i.e.,

\[
\begin{align*}
f(x - 2h) &= f(x) - f'(x)2h + \frac{1}{3}f''(x)h^2 - \frac{5}{3}f'''(x)h^3 + O(h^4) \\
f(x - h) &= f(x) - f'(x)h + \frac{1}{3}f''(x)h^2 - \frac{1}{3}f'''(x)h^3 + O(h^4) \\
f(x + h) &= f(x) + f'(x)h + \frac{1}{3}f''(x)h^2 + \frac{1}{3}f'''(x)h^3 + O(h^4) \\
f(x + 2h) &= f(x) + 2f'(x)h + \frac{4}{3}f''(x)h^2 + \frac{8}{3}f'''(x)h^3 + O(h^4)
\end{align*}
\]

Then sum these expressions with proper weights to cancel out the unwanted terms.

2. Repeat the earlier numerical experiment and observe the improved convergence.

One dimensional solver

Use the finite difference scheme to generate approximate solution to the problem

\[-u''(x) = f(x), \quad x \in (0, 1)\]

\[u(0) = 0,\]

\[u'(1) = 0.\]

Use the second order accurate scheme to take into account the Neumann boundary condition at \( x = 1 \).

1. Write the solver, you can use the example code at the webpage as a starting point.

2. Observe the convergence rates when \( f(x) = 1 \) and when

\[
f(x) = \begin{cases} 
-1, & \text{if } x \in [0, \frac{1}{2}) \\
1, & \text{if } x \in \left[\frac{1}{2}, 1\right]
\end{cases}
\]

It is recommended to select such grids that \( x_k = \frac{k}{2} \) for some \( k \).