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DEPARTAMENTO DE FISICA TEORICA I

Física computacional

Example of computation of local error and absolute stability domain for multistep implicit numerical schemes.

Consider the two-step implicit Adams-Boulton scheme for inital value problems

$$y_{n+1} = y_n + \frac{h}{12}\left[\,5\,f\big(t_{n+1},\, y_{n+1}\big) + 8\,f\big(t_n,\, y_n\big) - f\big(t_{n-1}, y_{n-1}\big)\,\right]. \tag{7}$$

Estimate its local error and study its absolute stability for real $\partial f/\partial y$.

This scheme is implicit since it provides an equation for y_{n+1} that must be solved in terms of y_{n-1} and y_n at every step. The computation of the local error for implicit schemes is abit more involved than for explicit ones, so we will do this case in full detail.

Computation of the local error.

By definition, the local error of a numerical scheme is the difference

$$e_{n+1} = y_{n+1} - y\,(t_{n+1})$$

bewteen the numerical solution y_{n+1} provided by the scheme and the true solution $y(t_{n+1})$ under the assumption that they agree at all previous steps, so that

$$e_k = 0 \quad\Leftrightarrow\quad y'_k := y'(t_k) = f(t_k, y_k) \qquad k \le n\,. \tag{8}$$

Using eq. (8), for the scheme (7), we have

$$e_{n+1} = y_n + \frac{5h}{12} f\big(t_{n+1}, y_{n+1}\big) + \frac{2h}{3}\,y'(t_n) - \frac{h}{12}\,y'(t_{n-1}) - y\,(t_{n+1})\,. \tag{9}$$

We are want to expand the right-hand side of this equation up to a sufficiently high order in h, say order h^4. The quantities $y\,(t_{n+1})$ and $y^{'}(t_{n-1})$ are the exact solution and its derivative at t_{n+1} and t_{n-1}, so they can be power expanded in h:

$$\begin{aligned} y\,(t_{n+1}) &= y_n + h\,y'_n + \frac{h^2}{2}\,y''_n + \frac{h^3}{6}\,y'''_n + \frac{h^4}{24}\,y''''_n + O(h^5) \\ y'(t_{n-1}) &= y'_n - h\,y''_n + \frac{h^2}{2}\,y'''_n - \frac{h^3}{6}\,y''''_n + O(h^4)\,. \end{aligned}$$

Substituting these expression in the equation for e_{n+1} gives

$$e_{n+1} = \frac{5h}{12}\, f\big(t_{n+1},\, y_{n+1}\big) - \frac{5h}{12}\, y'_n - \frac{5h^2}{12}\, y''_n - \frac{5h^3}{24}\, y'''_n - \frac{h^4}{36}\, y''''_n + O(h^5)\,. \tag{10}$$

The difference with explicit schemes is that the right-hand side in eq. (10) depends on the numerical solution y_{n+1} through $f\big(t_{n+1},\, y_{n+1}\big)$ and, being a numerical solution, y_{n+1} does not have a Taylor expansion in powers of h. To compute $f\big(t_{n+1},\, y_{n+1}\big)$ to order h^3, we ***first*** iterate eq. (7) three times, ***next*** expand the result in powers of h and ***finally*** group terms of the same order in h using that

$$\begin{aligned}
y'_n &= f\big|_n \\
y''_n &= f_t\big|_n + f_y\big|_n\, y'_n \\
y'''_n &= f_{tt}\big|_n + 2\, f_{ty}\big|_n\, y'_n + f_{yy}\big|_n\, \big(y'_n\big)^2 + f_y\big|_n\, y''_n \\
y''''_n &= f_{ttt}\big|_n + 3\, f_{tty}\big|_n\, y'_n + 3\, f_{tyy}\big|_n \big(y'_n\big)^2 + 3\, f_{ty}\big|_n\, y''_n + f_{yyy}\big|_n\, \big(y'_n\big)^3 + 3\, f_{yy}\big|_n\, y'_n\, y''_n + f_y\big|_n\, y'''_n \\
&\ \vdots
\end{aligned}$$

Let us do so.

The result after each iteration is:

<u>*After 1 iteration.*</u> The function $f(t_{n+1}, y_{n+1})$ up to order one in h is:

$$\begin{aligned}
f_{[1]}\big(t_{n+1}, y_{n+1}\big) &= f\Big(t_{n+1},\ y_n - \frac{h}{12}\, y'_{n-1} + \frac{2h}{3}\, y'_n + \frac{5h}{12}\, f\big(t_{n+1},\ y_{n+1}\big)\Big) \\
&= f\Big(t_n + h,\ y_n - \frac{h}{12}\,\big[\, y'_n + O(h)\,\big] + \frac{2h}{3}\, y'_n + \frac{5h}{12}\, f\big(t_n + O(h),\, y_n + O(h)\big)\Big) \\
&= \Big[\ \text{Note that}\ \ f\big(t_n + O(h),\, y_n + O(h)\big) = f(t_n, y_n) + O(h) = y'_n + O(h)\ \Big] \\
&= f\Big(t_n + h,\ y_n + h\, y'_n + O\big(h^2\big)\Big) \\
&= f\big|_n + h\, \Big(f_t\big|_n + f_y\big|_n\, y'_n\Big) + O\big(h^2\big) \\
&= y'_n + h\, y''_n + O\big(h^2\big)
\end{aligned}$$

<u>*After 2 iterations.*</u> Up to order 2, we have

$$\begin{aligned}
f_{[2]}\big(t_{n+1}, y_{n+1}\big) &= f\Big(t_{n+1},\ y_n - \frac{h}{12}\, y'_{n-1} + \frac{2h}{3}\, y'_n + \frac{5h}{12}\, f_{[1]}\big(t_{n+1}, y_{n+1}\big)\Big) \\
&= f\Big(t_n + h,\ y_n - \frac{h}{12}\,\big[\, y'_n - h\, y''_n + O(h^2)\,\big] + \frac{2h}{3}\, y'_n + \frac{5h}{12}\,\big[\, y'_n + h\, y''_n + O(h^2)\,\big]\Big) \\
&= f\Big(t_n + h,\ y_n + h y'_n + \frac{h^2}{2}\, y''_n + O\big(h^3\big)\Big) \\
&= y'_n + h\, y''_n + \frac{h^2}{2}\,\Big[\, f_{tt}\big|_n + 2\, f_{ty}\big|_n\, y'_n + f_{yy}\big|_n\, \big(y'_n\big)^2 + f_y\big|_n\, y''_n\,\Big] + O\big(h^3\big) \\
&= y'_n + h\, y''_n + \frac{h^2}{2}\, y'''_n + O\big(h^3\big)
\end{aligned}$$

After 3 iterations. Iterating once morw, we get the third order contribution:

$$
\begin{aligned}
f_{[3]}\big(t_{n+1},\, y_{n+1}\big) &= f\Big(t_{n+1},\; y_n - \frac{h}{12}\, y'_{n-1} + \frac{2h}{3}\, y'_n + \frac{5h}{12}\, f_{[2]}\big(t_{n+1}, y_{n+1}\big)\Big) \\
&= f\Big(t_n + h,\; y_n - \frac{h}{12}\,\big[\, y'_n - h\, y''_n + \frac{h^2}{2}\, h'''_n + O(h^3)\,\big] + \frac{2h}{3}\, y'_n \\
&\qquad + \frac{5h}{12}\,\big[\, y'_n + h\, y''_n + \frac{h^2}{2}\, y'''_n + O(h^3)\,\big]\Big) \\
&= f\Big(t_n + h,\; y_n + h\, y'_n + \frac{h^2}{2}\, y''_n + \frac{h^3}{6}\, y'''_n + O\big(h^4\big)\Big) \\
&= y'_n + h\, y''_n + \frac{h^2}{2}\, y'''_n \\
&+ \frac{h^3}{6}\,\Big[\, f_{ttt}\big|_n + 3\, f_{tty}\big|_n\, y'_n + 3\, f_{tyy}\big|_n \big(y'_n\big)^2 \\
&\qquad + 3\, f_{ty}\big|_n\, y''_n + f_{yyy}\big|_n\, \big(y'_n\big)^3 + 3\, f_{yy}\big|_n\, y'_n\, y''_n + f_y\big|_n\, y'''_n\,\Big] \\
&+ O\big(h^4\big) \\
&= y'_n + h\, y''_n + \frac{h^2}{2}\, y'''_n + \frac{h^3}{6}\, y''''_n + O\big(h^4\big)\,.
\end{aligned}
$$

Substituting in eq. (10), we arrive at the following local error

$$
\big|e_{n+1}\big| = \frac{h^4}{24}\, y''''_n + O\big(h^5\big)\,.
$$

Absolute stability.

Stability studies the propagation in the scheme of a deviation δ_n from a solution y_n. Let y_{n+1} denote the solution at $n+1$ computed with eq. (7) from y_{n-1} and y_n. Replace now y_{n-1} and y_n with $y_{n-1}+\delta_{n-1}$ and $y_n+\delta_n$, and write $y_{n+1}+\delta_{n+1}$ for the solution at $n+1$. We want to study δ_{n+1} in terms of δ_n and δ_{n-1}.

The new solution at $n+1$ is given by

$$
\begin{aligned}
y_{n+1} + \delta_{n+1} = y_n + \delta_n + \frac{h}{12}\,\big[\, & 5\, f\big(t_{n+1},\, y_{n+1} + \delta_{n+1}\big) + 8\, f\big(t_n,\, y_n + \delta_n\big) \\
& - f\big(t_{n-1}, y_{n-1} + \delta_{n-1}\big)\,\big]\,.
\end{aligned}
$$

Assuming that δ_n and δ_{n-1} are samll enough, the right hand side can be expanded in powes of δ_n and δ_{n-1}. After retaining linear terms, this gives

$$
\begin{aligned}
y_{n+1} + \delta_{n+1} = y_n + \delta_n + \frac{h}{12}\,\big[\, & 5\, f\big(t_{n+1},\, y_{n+1}\big) + 5 f_y\big(t_{n+1},\, y_{n+1}\big)\, \delta_{n+1} + 8\, f\big(t_n,\, y_n\big) \\
& + 8 f_y\big(t_n,\, y_n\big)\, \delta_n - f\big(t_{n-1},\, y_{n-1}\big) - f_y\big(t_{n-1},\, y_{n-1}\big)\, \delta_{n-1}\,\big]\,.
\end{aligned}
\tag{11}
$$

Since y_{n-1}, y_n, y_{n+1} satisfy eq. (7), eq. (11) becomes

$$
\delta_{n+1} = \delta_n + \frac{h}{12}\,\big(\, 5 f_y\big|_{n+1}\, \delta_{n+1} + 8 f_y\big|_n\, \delta_n - f_y\big|_{n-1}\,\big)\,. \tag{12}
$$

Introduce now g connecting e_{k+1} and e_k for all k through

$$\delta_{k+1} = \rho\, \delta_k\,. \tag{13}$$

Eq. (12) then implies

$$\rho^2 = \rho + \frac{5}{12}\, z_{n+1}\, \rho^2 + \frac{2}{3}\, z_n\, \rho - \frac{1}{12}\, z_{n-1}\,, \tag{14}$$

where z_n has been defined as

$$z_n := h\, f_y\big|_n = h\, \frac{\partial f}{\partial y}\, (t_n, y_n)\,.$$

Eq. (14) is a quadratic equation in ρ whose coefficients depend on z_{n-1}, z_n and z_{n+1}. To ensure stability, we require $|\delta_{k+1}| \leq |\delta_k|$, so that the solutions $\rho_\pm$ to eq. (14) must satisify

$$|\rho_\pm| \leq 1\,. \tag{15}$$

Note that condition (15) guarantees that the deviation δ_k remains bounded from above by the initial deviation δ_0 for all k.

As it stands, eq. (14) must be solved at every step, since the coefficients involve z_{n-1}, z_n, z_{n+1} and these depend on n. To study absolute stability, we take z_n independnet of n. That is, $z_n = z$ for all n. If in addition we assume z_n to be real, eq. (14) reduces to

$$\rho^2 \left(1 - \frac{5z}{12}\right) - \rho \left(1 + \frac{2z}{3}\right) + \frac{z}{12} = 0\,. \tag{16}$$

This is the characterisitc equation for the scheme (7). Its solutions

$$\rho_\pm = \frac{6}{12 - 5z} \left(1 + \frac{2z}{3} \pm \sqrt{1 - z + \frac{7z^2}{12}}\,\right)$$

must satisfy eq. (15). Writing the latter as $-1 \leq \rho_\pm \leq 1$, we have

$$-\Big(2 - \frac{5z}{6}\Big) \;\leq\; 1 + \frac{2z}{3} \pm \sqrt{1 - z + \frac{7z^2}{12}} \;\leq\; 2 - \frac{5z}{6}$$

It follows that z must be less or equal than $\frac{12}{5}$ and that it must satisfy the conditions:

$$u_\mp(z) := -3 + \frac{z}{6} \mp \sqrt{1 - z + \frac{7z^2}{12}} \;\leq\; 0 \qquad 0 \;\leq\; 1 - \frac{3z}{2} \mp \sqrt{1 - z + \frac{7z^2}{12}} =: v_\mp(z)\,.$$

Since

$$u_-(z) \leq 0 \;\text{ for all }\; z \qquad\qquad v_-(z) \leq 0 \;\text{ for }\; z \geq 0$$

$$u_+(z) \leq 0 \;\text{ for }\; |z| \leq 6\sqrt{\frac{2}{5}} \qquad\qquad v_+(z) \leq 0 \;\text{ for }\; z \geq \frac{6}{5}\,,$$

we conclude that the method is stable for

$$\frac{6}{5} \leq z \leq 6\sqrt{\frac{2}{5}}\,.$$

The definition of stability given here goes in the literature under the name of absolute stability. It requires that, for a given z, the roots g_r of the characteristic equation of a numerical scheme must have $|g_r| < 1$.