Notes on Karr, Integrators and Stiff Systems

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Stiff Systems

Stiff equations are equations where certain implicit methods perform better, usually tremendously better, than explicit ones. Curtiss & Hirschfelder (1952)

If a numerical method with a finite region of absolute stability, applied to a system with any initial conditions, is forced to use in a certain interval of integration a steplength which is excessively small in relation to the smoothness of the exact solution in that interval, then the system is said to be stiff in that interval. Lambert (1992)

Dahlquist's test

Dahlquist's test equation:

$$y' = \lambda y, \qquad \lambda \in \mathbb{C}, \Re(\lambda) < 0 \tag{1}$$

Doing Euler's forward (explicit) method on this,

$$y_{n+1} = y_n + hy'_n = (1 + h\lambda)y_n \tag{2}$$

if $h > \frac{2}{||\lambda||}$ then $\lim_{n\to\infty} ||y_n|| = \infty$ even though $\lim_{x\to\infty} y(x) = 0$.

Euler's backward (implicit) method doesn't have this problem,

$$y_{n+1} = y_n + hy'_{n+1} = \frac{y_n}{1 - h\lambda} \tag{3}$$

Linear Stability

Define $z = h\lambda$ and then consider the stability function R,

$$y_{n+1} = R(z)y_n \tag{4}$$

The absolute stability region of a method is the region where,

$$||R(z)|| < 1 \tag{5}$$

when it is applied to Dahlquist's test equation.

More generally, we look at the eigenvalues of the Jacobian matrix $\partial \mathbf{y}'/\partial \mathbf{y}$ of a problem (just λ for Dahlquist's equation) and the largest negative one governs minimum step size.

Stiff Systems – Textbook Examples

- Curtiss & Hirschfelder (1952)

$$y'(x) = -50\,(y(x) - \cos(x)) \tag{6}$$

- Robertson (1966)

$$\begin{aligned} A &\xrightarrow{0.04} B \\ 2B &\xrightarrow{3\cdot 10^7} C + B \\ B + C &\xrightarrow{10^4} A + C \end{aligned} \tag{7}$$

- Gear (1971)

$$\begin{aligned} u' &= 998u + 1998v & \qquad u &= 2e^{-x} - e^{-1000x} \\ v' &= -999u - 1999v & \qquad v &= -e^{-x} + e^{-1000x} \end{aligned} \tag{8}$$

Testing Karr: a very simple linear system

Bucher's example from his M.Sc thesis (just Dahlquist again):

$$y' = \alpha y + \beta y \tag{9}$$

With $\alpha < 0$ and $\beta < 0$, which has the exact integrator:

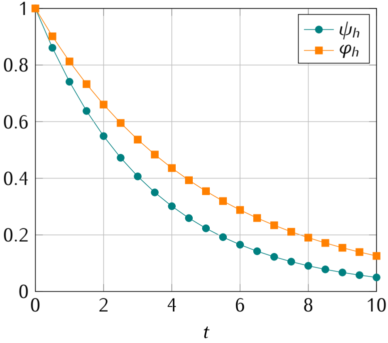
$$\psi_h = e^{(\alpha+\beta)h} \tag{10}$$

Split it in two parts:

$$f^{[1]} = \alpha y \qquad f^{[2]} = \beta y \tag{11}$$

$$\varphi_h^{[1]} = e^{\alpha h} \qquad \varphi_h^{[2]} = e^{\beta h} \tag{12}$$

Exact solution vs. Karr's method



$\alpha = -0.05$
$\beta = -0.25$
$h = 0.5$

Karr says to adjust the inputs according to consumption,

$$\delta_h^{[1]} = \frac{e^{\alpha h} - 1}{e^{\alpha h} + e^{\beta h} - 2} \tag{13}$$

to make the combined integrator,

$$\varphi_h = \varphi_h^{[1]} \circ \delta_h^{[1]} + \varphi_h^{[2]} \circ \delta_h^{[2]} \tag{14}$$

This underestimates the change.

Karr-splitting linear equations

Forget α and β, let's split into n parts using k_i instead:

$$\varphi_h = \frac{\sum_{i=1}^{n} e^{k_i h}\left(e^{k_i h} - 1\right)}{\sum_{i=1}^{n} e^{k_i h} - 1} \tag{15}$$

Theorem

For a Karr-splitting φ_h of a linear system in one dimension (cf. Eq 15) with has the exact integrator $\psi_h = e^{kh}$ where $k = \sum_i k_i$, if $k_i < 0 \ \forall i \in [1 \ldots n]$ then φ_h is absolutely stable, and furthermore,

$$\frac{\varphi_h}{\psi_h} > 1$$

Equal splitting

Suppose that the Karr-splitting is equal i.e. that it has all k_i equal to $\frac{k}{n}$ for some k. Then we get the integrator,

$$\varphi_h = \frac{\sum_{i=1}^{n} e^{\frac{k}{n}h}\left(e^{\frac{k}{n}h} - 1\right)}{\sum_{i=1}^{n}\left(e^{\frac{k}{n}h} - 1\right)} = e^{\frac{k}{n}h} < 1 \tag{16}$$

and

$$\frac{\varphi_h}{\psi_h} = e^{\left(\frac{1}{n}-1\right)kh} > 1 \tag{17}$$

Equal splitting – doubling n

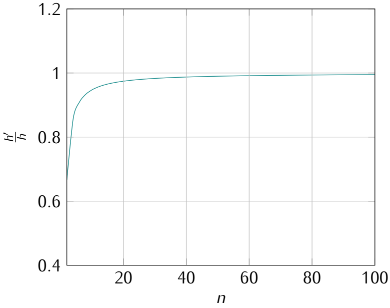
What happens if we double n? What time-step do we need to keep the answer the same?

Setting,

$$e^{\left(\frac{1}{2n}-1\right)kh'} = e^{\left(\frac{1}{n}-1\right)kh} \qquad (18)$$

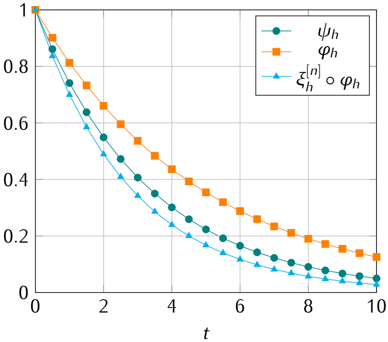
and solving for h',

$$h' = \frac{2n-2}{2n-1}h \qquad (19)$$



$\Rightarrow$ splitting matters most for smaller n. After that, the damage has already been done...

Correction!



Karr has *metabolism* that corrects splitting, we do not.

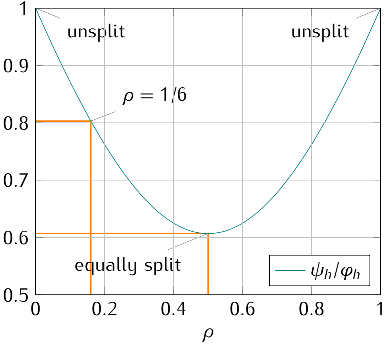
Let's try a corrector made for an equally split system,

$$\xi_h^{[n]} = \frac{\psi_h}{\varphi_h} = e^{\left(1-\frac{1}{n}\right)kh} \qquad (20)$$

$$\ldots = e^{\frac{\alpha+\beta}{2}h}$$

This is better, but it overshoots the mark!

ρ–SPLITTING



In this plot we have set $\lambda = -1$.

Instead of n parts, how about just 2 parts,

$$
\begin{aligned}
f^{[1]} &= \rho\lambda y \\
f^{[2]} &= (1-\rho)\,\lambda y
\end{aligned}
\tag{21}
$$

$$
\begin{aligned}
\varphi_h^{[1]} &= e^{\rho\lambda h} \\
\varphi_h^{[2]} &= e^{(1-\rho)\lambda h}
\end{aligned}
\tag{22}
$$

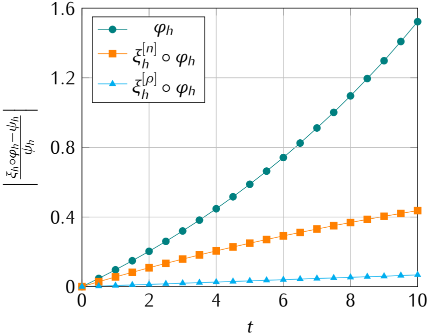
and we allow the proportion to vary $\rho \in [0 \ldots 1]$.

A better correction

We can use the ρ-splitting to make a corrector (Eq 23).

It's ugly, but does the trick.

The plot shows relative error for various strategies.



$$\xi_h^{[\rho]} = \frac{\psi_h}{\varphi_h} = \frac{e^{\lambda h}\left[e^{\rho\lambda h} + e^{(1-\rho)\lambda h} - 2\right]}{e^{2\rho\lambda h} + e^{2(1-\rho)\lambda h} - e^{\rho\lambda h} - e^{(1-\rho)\lambda h}} \qquad (23)$$

Splitting and parallelism

$$
\begin{array}{ccc}
\mathbb{P}^n \ni & \begin{bmatrix} \mathbf{y}^{[1]} \\ \mathbf{y}^{[2]} \\ \vdots \\ \mathbf{y}^{[n]} \end{bmatrix} \xrightarrow{\quad\varphi_h\quad} \begin{bmatrix} \varphi_h^{[1]}\mathbf{y}^{[1]} \\ \varphi_h^{[2]}\mathbf{y}^{[2]} \\ \vdots \\ \varphi_h^{[n]}\mathbf{y}^{[n]} \end{bmatrix} & \\
& S = \pi_1 \uparrow \qquad\qquad\qquad\qquad \downarrow F = \xi_h \pi_2 & \\
\mathbb{Y} \ni & \mathbf{y_n} \xrightarrow[\quad\psi_h\quad]{} \mathbf{y}_{n+1} &
\end{array}
$$

Degree of sequentialism

Sequentialism: relative error per unit time

$$\mathrm{Seq}(\varphi, \mathbf{y}) \equiv \lim_{h \to 0} \frac{||\psi_h \mathbf{y} - \pi_2 \varphi_h \pi_1 \mathbf{y}||}{h||\psi_h \mathbf{y}||} \tag{24}$$

If $\mathrm{Seq}(\varphi_h, \mathbf{y}) = 0$ then the necessary corrector $\xi_h = Id$ and $\pi_2 \varphi_h \pi_1$ is a “normal” parallel process.

We could then sensibly define parallelism as,

$$\mathrm{Par}(\varphi, \mathbf{y}) \equiv \frac{1}{\mathrm{Seq}(\varphi, \mathbf{y})} \tag{25}$$

Karr in real life

Karr's method only des this kind of parallel splitting some variables. It is a straight composition method in others.

$$\hat{\varphi}_h^{[i]} \circ \begin{bmatrix} \mathbf{y}^{[1]} \\ \vdots \\ \mathbf{y}^{[i]} \\ \vdots \\ \mathbf{y}^{[n]} \\ \hline \mathbf{y} \end{bmatrix} = \begin{bmatrix} \mathbf{y}^{[1]} \\ \vdots \\ \varphi_h^{[i]+} \mathbf{y}^{[i]} \\ \vdots \\ \mathbf{y}^{[n]} \\ \hline \varphi_h^{[i]\circ} \mathbf{y} \end{bmatrix} \tag{26}$$

And the actual integrator is a composition of these,

$$\varphi_h = \hat{\varphi}_h^{[n]} \circ \hat{\varphi}_h^{[n-1]} \circ \cdots \circ \hat{\varphi}_h^{[2]} \circ \hat{\varphi}_h^{[1]} \tag{27}$$