Numerical Methods for Differential Equations

1.- Numerical Methods for DDEs

Luis M. Abia, J. C. López Marcos, O. Angulo

abia@mac.uva.es

University of Valladolid

Valladolid, (Spain)

Delay Differential Equations

$$\mathbf{y}'(t) = \mathbf{f}(t, \mathbf{y}(t), \mathbf{y}(t - \tau(t))), \quad t_0 \le t \le T,$$
$$\mathbf{y}(t) = \phi(t), \quad t^* \le t \le t_0,$$

$f(t, \mathbf{u}, \mathbf{v})$, continuous and (locally) Lipschitz with respect its arguments $\mathbf{u}, \mathbf{v}$.

1. $\tau > 0,$ constant , $\quad t^* = \tau$, or
2. $\tau \equiv \tau(t) \ge 0, \quad t^* = \inf_{t \ge t_0}(t - \tau(t))$, and $\tau(t)$ continuous in $[t_0, T]$ or
3. $\tau \equiv \tau(t, \mathbf{y}(t)) \ge 0, \quad t^* = \inf_{t \ge t_0}(t - \tau(t, \mathbf{y}(t)))$, and $\tau(t, \mathbf{u})$ continuous and (locally) Lipschitz with respect to $\mathbf{u}$.
   (State Dependent lag function case)

$$\mathbf{y}'(t) = \mathbf{f}(t, \mathbf{y}(t), \mathbf{y}(t - \tau(t)), \mathbf{y}'(t - \sigma(t))), \quad t_0 \le t \le T,$$

(Neutral Differential Equations (NDE))

We will denote

$$\alpha(t) = t - \tau(t, \mathbf{y}(t)) \le t, \quad \beta(t) = t - \sigma(t, \mathbf{y}(t)) \le t \quad \text{delayed arguments}$$

Existence and Uniqueness of Solutions

$$y'(t) = f(t, y(t), y(t - \tau(t, y(t)))), \quad t \geq t_0, \quad y(t) = \phi(t), \quad t^* \leq t \leq t_0.$$

Under

- (H_1) There exists a $\tau_0 > 0$ such that $\alpha(t) \leq t - \tau_0$, for $t \in [t_0, T]$, or
- (H_1^*) There exists a $\tau_0 > 0$ such that $\tau(t, \mathbf{z}) \geq \tau_0$, for $t \in [t_0, T]$, and $\mathbf{z} \in \mathbb{R}^d$.

(local) existence and uniqueness are derived easily from the existence and uniqueness theory for ODEs using the **method of steps**

$$\begin{aligned}
y_1'(t) &= f(t, y_1(t), \phi(t - \tau)), \quad t_0 \leq t \leq t_1 = t_0 + \tau_0, \\
y_2'(t) &= f(t, y_2(t), y_1(t - \tau)), \quad t_1 \leq t \leq t_2 = t_1 + \tau_0, \\
&\vdots \\
y_m'(t) &= f(t, y_m(t), y_{m-1}(t - \tau)), \quad t_{m-1} \leq t \leq t_m = t_{m-1} + \tau_0,
\end{aligned}$$

Existence and Uniqueness of Solutions

$$y'(t) = f(t, y(t), y(t - \tau(t, y(t)))), \quad t \geq t_0, \quad y(t) = \phi(t), \quad t^* \leq t \leq t_0.$$

Theorem 1 (local existence) Let U and V be neighborhoods of $\Psi(t_0)$ and $\Psi(t_0 - \tau(t_0, \Psi(t_0)))$ respectively, and assume that $f(t, u, v)$ is continuous with respect to t and Lipschitz continuous with respect to u, v in $[t_0, t_0 + h] \times U \times V$, for some $h > 0$. Assume that the initial function $\Psi(t)$ is Lipschitz continuous for $t \leq t_0$ and that the delay function $\tau(t, y) \geq 0$ is continuous with respect to t and Lipschitz continuous with respect to y in $[t_0, t_0 + h] \times U$. Then there exists a unique solution in $[t_0, t_0 + \delta]$ for some $\delta > 0$ and this solution depends continuously on the initial data

R. D. Driver (1963), Hale (1986), Elsgolts and Norkin (1973)

Propagation of Discontinuities and Smoothing

Assuming a discontinuity of the first derivative of the solution at $t = t_0 = \xi_{0,1}$, and

$$\alpha(\xi_{1,i}) = t_0, \quad \alpha'(\xi_{1,i}) \neq 0 \quad \text{simple root}$$

$$f_t + f_y\, y'(\xi_{1,i}) + f_x\, y'(t_0)^+\, \alpha'(\xi_{1,i}) \neq f_t + f_y\, y'(\xi_{1,i}) + f_x\, \Psi'(t_0)^-\, \alpha'(\xi_{1,i})$$

(first level primary discontinuity of y'')

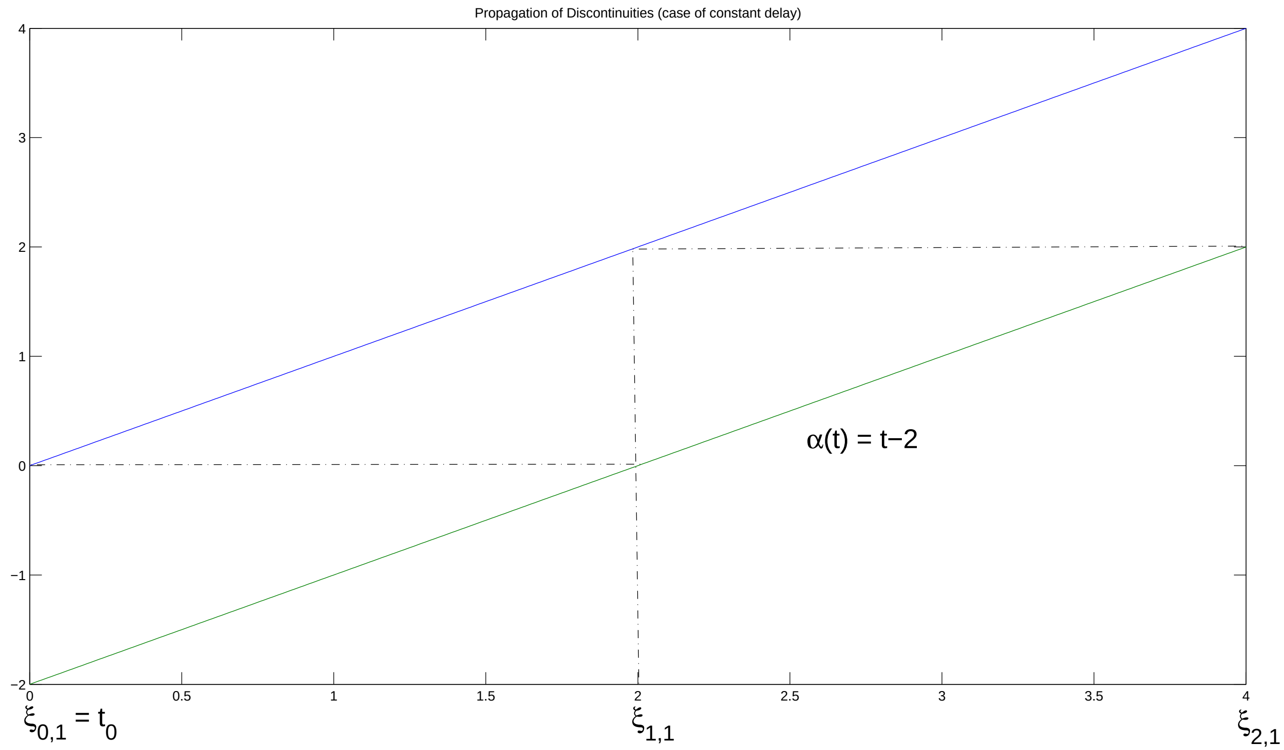
In general, solutions with odd multiplicity of

$$\alpha(\xi_{k,j}) = \xi_{k-1,i}, \quad \text{for some } \xi_{k-1,i}$$

(k-level primary discontinuity of $y^{(k+1)}$).
Other discontinuities in the derivatives with respecto to t in the functions $\alpha(t)$, $\mathbf{f}$, and ϕ are called secondary discontinuities.

Propagation of Discontinuities and Smoothing

Case of Constant Delay

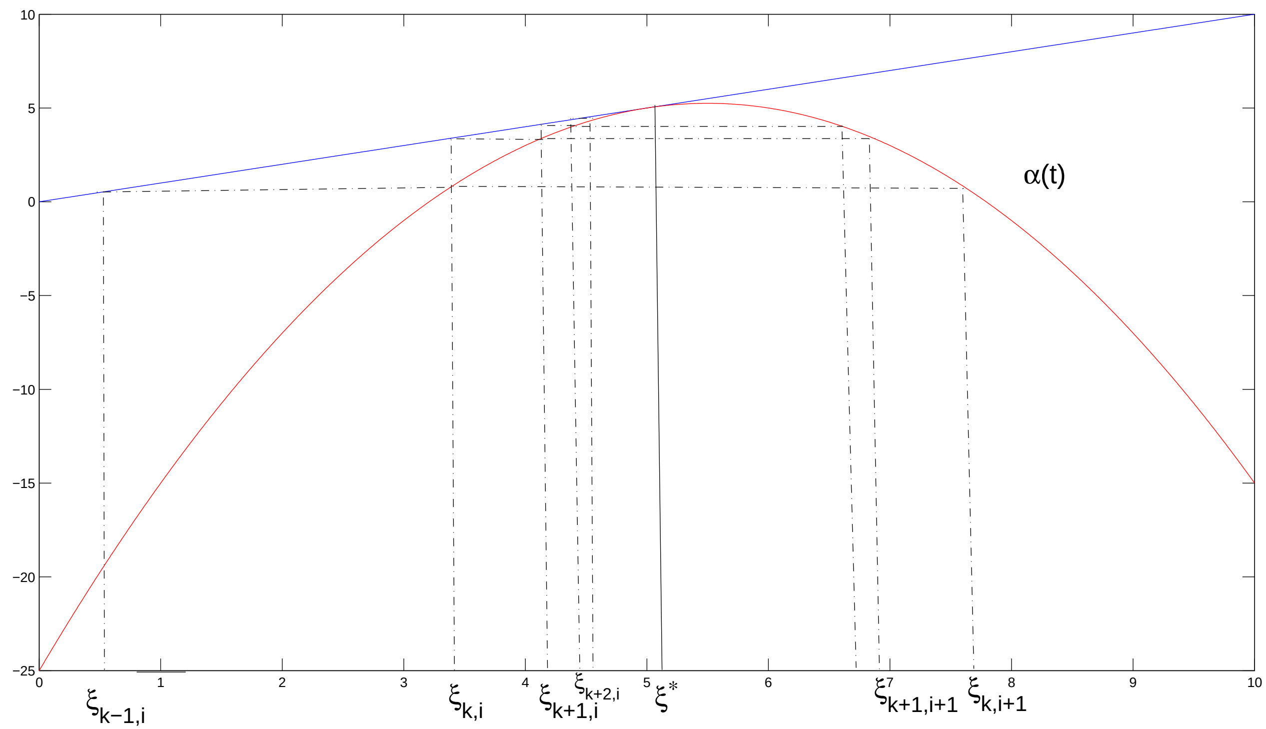


$$\xi_{0,1} < \xi_{1,1} < \cdots < \xi_{k,1} < \cdots$$

This is also the case when $\alpha(t)$ is an strictly increasing function.

Propagation of Discontinuities and Smoothing

Case of vanishing discontinuity



For general DDE, we will assume

- (H_1) There exists a $\tau_0 > 0$ such that $\alpha(t) \leq t - \tau_0$, for $t \in [t_0, T]$,

We replace $[t_i, t_{i+1}]$ with $[\xi_i, \xi_{i+1}]$, $i = 0, 1, 2, \ldots$, where $\xi_0 = t_0$, and for $i \geq 0$, ξ_{i+1} is the minimum root with odd multiplicity of $\alpha(t) = \xi_i$. (set of principal discontinuity points).

Propagation of Discontinuities

- The extension of these ideas to general systems was developped by Willé and Baker (1992). In a system of DDEs discontinuities tracking can be complicated by discontinuities being propagated between solution components. This fact gives rise to the concept of strong and weak coupling and network dependency graphs. Strong coupling describes the propagation of discontinuities between different solution components by an ODE term. Weak coupling describes the propagation of discontinuities within the same solution component and between different solution components by a DDE term.
  For example, for the system

$$
\begin{aligned}
y_1'(t) &= f_1(y_2(t), y_3(t-1)), \\
y_2'(t) &= f_2(y_3(t)), \qquad\qquad t \geq 0 \\
y_3'(t) &= f_3(y_1(t), y_2(t-1))
\end{aligned}
$$

  y_2 is strongly connected with y_1, y_3 is strongly connected with y_2, and y_1 is strongly connected with y_3. However, y_3 is weakly connected with y_1, and y_2 is weakly connected with y_3.

The Numerical Approach

$$y'(t) = f(t, y(t), y(t-\tau(t))), \quad t \geq t_0, \quad y(t) = \phi(t), \quad t^* \leq t \leq t_0.$$

- Variable step-size codes (with dense output) to solve for the y in the method of steps. .
- In the Method of Steps (constant lag scalar DDE)

$$\begin{aligned}
y_1'(t) &= f(t, y_1(t), \Psi(t-\tau)), \quad t_0 \leq t \leq t_1 = t_0 + \tau, \quad \rightarrow \tilde{y}_1(t) \\
y_2'(t) &= f(t, y_2(t), \tilde{y}_1(t-\tau)), \quad t_1 \leq t \leq t_2 = t_1 + \tau, \quad \rightarrow \tilde{y}_2(t) \\
&\vdots \\
y_m'(t) &= f(t, y_m(t), \tilde{y}_{m-1}(t-\tau)), \quad t_{m-1} \leq t \leq t_m = t_{m-1} + \tau, \quad \rightarrow \tilde{y}_m(t)
\end{aligned}$$

Issues to consider for DDE

1. Dense Output to evaluate delayed solution values
2. The tracking of discontinuities in the solution
3. Vanishing lag delays and overlapping.

Continuous ODE Method

- ODE method $$y'(t) = g(t, y(t)), \quad t \geq t_0, \quad y(t_0) = y_0.$$

$$y_{n+1} = \alpha_{n,1} y_n + \cdots + \alpha_{n,k} y_{n-k+1} + h_{n+1} \Phi(y_n, \ldots, y_{n-k+1}; g, \Delta_n), \quad n \geq k-1,$$
$$y_0, \ldots, y_{k-1} \quad \text{given ,}$$

with $\Delta_n = \{t_{n-k+1}, \ldots, t_n, t_{n+1}\}$

- Interpolation in $[t_n, t_{n+1}]$,

$$\begin{aligned} \eta(t_n + \theta h_{n+1}) \quad &= \quad \beta_{n,1}(\theta) y_{n+j_n} + \cdots + \beta_{n,j_n+i_n+1}(\theta) y_{n-i_n} \\ &\quad + h_{n+1} \Psi(y_{n+j_n}, \ldots, y_{n-i_n}; \theta, g, \Delta'_n), \quad 0 \leq \theta \leq 1, \end{aligned}$$

with $\Delta'_n = \{t_{n-i_n}, \ldots, t_{n+j_n}, t_{n+j_n+1}\}$.

- $\eta(t_n) = y_n, \quad \eta(t_{n+1}) = y_{n+1}$ (continuity conditions).
- There existe an $\Omega > 0$, such that

$$\Omega^{-1} h_{n+1+i} \leq h_{n+1} \leq \Omega h_{n+1+i}, \quad i = -k+1, \ldots, 1,$$
$$\Omega^{-1} h_{n+1+i} \leq h_{n+1} \leq \Omega h_{n+1+i}, \quad i = -i_n+1, \ldots, j_n,$$

Continuous ODE Method

We assume

- The increment functions Φ and Ψ in the continuous ODE method are Lipschitz continuous with respect their y arguments, and

$$\|\Phi(y_n, \ldots, y_{n-k+1}; \tilde{g}, \Delta_n) - \Phi(y_n, \ldots, y_{n-k+1}; g, \Delta_n)\|$$
$$\leq \gamma_g \sup_{t_{n-k+1} \leq t \leq t_{n+1}, y} \|\tilde{g}(t, y) - g(t, y)\|, \quad \forall \tilde{g} \in C^0$$
$$\|\Psi(y_{n+j_n}, \ldots, y_{n-i_n}; \theta, \tilde{g}, \Delta_n') - \Psi(y_{n+j_n}, \ldots, y_{n-i_n}; \theta, g, \Delta_n')\|$$
$$\leq \gamma_g' \sup_{t_{n-i_n} \leq t \leq t_{n+j_n+1}, y} \|\tilde{g}(t, y) - g(t, y)\|, \quad \forall \tilde{g} \in C^0$$

Let

$$C_n = \begin{bmatrix} \alpha_{n,1} & \alpha_{n,2} & \cdots & \alpha_{n,k-1} & \alpha_{n,k} \\ 1 & 0 & \cdots & 0 & 0 \\ 0 & 1 & \cdots & 0 & 0 \\ \vdots & \vdots & & \vdots & \vdots \\ 0 & 0 & \cdots & 1 & 0 \end{bmatrix}$$

be the companion matrix of the polynomial $p_n(\lambda) = \lambda^k - \alpha_{n,1}\lambda^{k-1} - \cdots \alpha_{n,0}$.

Continuous ODE Method

$$y'(t) = g(t, y(t)), \quad t \geq t_0, \quad y(t_0) = y_0.$$

- The ODE method is consistent of order p, when p is the largest integer such that for all C^q-continuous right-hand-side functions g and for all mesh points, we have

$$\|u_{n+1}(t_{n+1}) - \tilde{y}_{n+1}\| = O(h_{n+1}^{p+1}), \quad (h \to 0)$$

uniformly with respect to y_n^* varying in bounded subsets, for $n = 0, \ldots, N-1$, where $u_{n+1}(t)$ is the local solution given by the solution of

$$\begin{cases} u'_{n+1}(t) = g(t, u_{n+1}(t)), & t_n \leq t \leq t_{n+1}, \\ u_{n+1}(t_n) = y_n^* \end{cases}$$

and

$$\begin{aligned} \tilde{y}_{n+1} \quad &= \quad \alpha_{n,1} u_{n+1}(t_n) + \cdots + \alpha_{n,k} u_{n+1}(t_{n-k+1}) \\ & \quad\quad + h_{n+1} \Phi(u_{n+1}(t_n), \ldots, u_{n+1}(t_{n-k+1}); g, \Delta_n), \end{aligned}$$

Continuous ODE Method

$$y'(t) = g(t, y(t)), \quad t \geq t_0, \quad y(t_0) = y_0.$$

- The interpolant is consistent of uniform norm q, if q is the largest integer such that for all C^q-continuous right-hand-side functions g and for all mesh points,

$$\max_{t_n \leq t \leq t_{n+1}} \|u_{n+1}(t) - \tilde{\eta}(t)\| = O(h_{n+1}^{p+1}), \quad (h \to 0)$$

uniformly with respect to y_n^* varying in bounded subsets, for $n = 0, \ldots, N-1$, where $u_{n+1}(t)$ is the local solution given by the solution of

$$\begin{cases} u'_{n+1}(t) = g(t, u_{n+1}(t)), \quad t_n \leq t \leq t_{n+1}, \\ u_{n+1}(t_n) = y_n^* \end{cases}$$

and

$$\begin{aligned} \tilde{\eta}(t_n + \theta h_{n+1}) \quad = \quad & \beta_{n,1}(\theta) u_{n+1}(t_{n+j_n}) + \cdots + \beta_{n,j_n+i_n+1}(\theta) u_{n+1}(t_{n-i_n}) \\ & + h_{n+1} \Psi(u_{n+1}(t_{n+j_n}), \ldots, u_{n+1}(t_{n-i_n}); \theta, g, \Delta'_n). \end{aligned}$$

Convergence

Theorem 2 Let the ODE method be consistent of order $p \geq 1$. If

- There exists a norm $\| \cdot \|_*$, independent of both n and Δ, such that $\|C_n\|_* \leq 1$.
- g is C^p-continuous.
- $y_0, \ldots, y_{k-1}$ approximate the exact solution to the order p;

then the ODE method is convergent of order p on any bounded interval $[t_0, T]$, that is,

$$\max_{1 \leq n \leq N} \|y(t_n) - y_n\| = O(h^p), \quad (h \to 0).$$

Moreover, if the interpolant is consistent of uniform order q, then the continuous ODE method is uniformly convergent of order $q' = \min(p, q+1)$, that is

$$\max_{t_0 \leq t \leq T} \|y(t) - \eta(t)\| = O(h^{q'}).$$

The Standard Approach to DDEs

$$\mathbf{y}'(t) = \mathbf{f}(t, \mathbf{y}(t), \mathbf{y}(t - \tau(t, \mathbf{y}(t)))), \quad t_0 \le t \le T,$$
$$\mathbf{y}(t) = \phi(t), \quad t^* \le t \le t_0,$$

is solved step by step throught the local problems

$$\begin{cases} \omega'_{n+1}(t) = f(t, \omega_{n+1}(t), x(t - \tau(t, \omega_{n+1}(t)))), & t_n \le t \le t_{n+1} \\ \omega_{n+1}(t_n) = y_n, \end{cases}$$

where

$$x(s) = \begin{cases} \Psi(s), & s \le t_0, \\ \eta(s), & t_0 \le s \le t_n, \\ \omega_{n+1}(s), & t_n \le s \le t_{n+1} \end{cases}$$

and $\eta(t)$ is the interpolant associated to the continuous ODE method.

The Standard Approach to DDEs

$$y'(t) = f(t, y(t), y(t-\tau(t))), \quad t_0 \le t \le T, \quad y(t) = \phi(t), \quad t \le t_0$$

- We assume a non-vanishing time dependent delay, and stepsizes small enough to avoid overlapping. (H_1 hypothesis).
- The mesh Δ include the principal discontinuity points as well discontinuity points of order $\le p$.

$$\xi_0 = t_0 < \xi_1 < \cdots < \xi_r < T$$

- The ODE method is consistent of order p, satisfies the stability condition and, for $k > 1$, is restarted after each discontinuity point $\xi, i = 0, \ldots, s$ by a method of order $\ge p - 1$.
- The interpolant is consistent of uniform order q.
- $[t_{n-i_n}, t_{n+j_n+1}] \subset [\xi_i, \xi_{i+1}]$ for some index $0 \le i \le s$.

Then the resulting method of steps, through recursive integration of ODEs accross the intervals $[\xi_{i-1}, \xi_i]$, is convergent with discrete global order and uniform global order $q' = \text{mín}(p, q+1)$.

The Standard Approach to DDEs

$$y'(t) = f(t, y(t), y(t - \tau(t))), \quad t_0 \leq t \leq T, \quad y(t) = \phi(t), \quad t \leq t_0$$

- For a general time dependent delay, assuming that overlapping occurs, we need to solve for $\eta(t)$,

$$\begin{aligned}\eta(t_n + \theta h_{n+1}) \quad &= \quad \beta_{n,1}(\theta) y_n + \cdots + \beta_{n,1+i_n} y_{n-i_n} \\ &\quad + h_{n+1} \Psi(y_n, \ldots, y_{n-i_n}; \theta, g_\eta, \Delta'_n), \quad 0 \leq \theta \leq 1,\end{aligned}$$

  where $g_\eta(t, y) = f(t, y, \eta(t - \tau(t)))$.
  This is a well-posed problem if h_{n+1} is enough small, by the contractivity of

$$\begin{aligned}\mathcal{F}(\eta)(s) \quad &= \quad \beta_{n,1}(\theta) y_n + \cdots + \beta_{n,1+i_n} y_{n-i_n} \\ &\quad + h_{n+1} \Psi(y_n, \ldots, y_{n-i_n}; \theta, g_\eta, \Delta'_n), \quad \theta = \frac{s - t_n}{h_{n+1}}\end{aligned}$$

Then the resulting method of steps, through recursive integration of ODEs accross the intervals $[\xi_{i-1}, \xi_i]$, is convergent with discrete global order and uniform global order $q' = \text{mín}(p, q+1)$.

Example

For the problem $y'(t) = f(t, y(t), y(t/2)), t \geq 0$, and $y(0) = y_0$,

- The use of the backward Euler method with linear interpolation, provides for the first step

$$y_1 = y_0 + hf(h, y_1, \eta(h/2))$$
$$\eta(\theta h) = (1-\theta)y_0 + \theta y_1.$$

With $X = \eta(h/2)$ and $Y = y_1$ and $K = f(h, Y, X)$, the system reduces to

$$K = f(h, y_0 + hK, y_0 + K/2).$$

- For the Heun method with linear interpolation,

$$y_1 = y_0 + h/2(f(0, y_0, y_0) + f(h, y_0 + hf(0, y_0, y_0), \eta(h/2)))$$
$$\eta(\theta h) = (1-\theta)y_0 + \theta y_1.$$

the step reduces to solve, for $X = \eta(h/2)$,

$$X = y_0 + h/4(f(0, y_0, y_0) + f(h, y_0 + hf(0, y_0, y_0), X)).$$

The Algorithm for State Dependent Delays

We consider the algorihm for the BDF formulae

$$y_{n+1} = \alpha_{n,1} y_n + \cdots \alpha_{n,k} y_{n-k+1} + h_{n+1}\beta_{n,0} f(t_{n+1}, y_{n+1}, \eta(t_{n+1} - \tau(t_{n+1}, y_{n+1}))),$$

with the continuous extension

$$\begin{aligned} \eta(t_n + \theta h_{n+1}) &= \beta_{n,1}(\theta) y_n + \cdots + \beta_{n,1+i_n}(\theta) y_{n-i_n} + \\ &\quad h_{n+1}\beta_{n,0}(\theta) f(t_{n+1}, y_{n+1}, \eta(t_{n+1} - \tau(t_{n+1}, y_{n+1}))). \end{aligned}$$

- Predictor: Set $y^0_{n+1} = \eta(t_n)$,
- For $\nu = 0$ to $m - 1$,
  - Evaluation:

    1. Compute the argument $s = t_{n+1} - \tau(t_{n+1}, y^\nu_{n+1})$.
    2. If $s \le t_n$, then set $X = \eta(s)$; else set $\theta^\nu = \dfrac{s - t_n}{h_{n+1}}$ and solve for X

    $$X = \beta_{n,1}(\theta^\nu) + \cdots + \beta_{n,1+i_n}(\theta^\nu) y_{n-y_n} + h_{n+1}\beta_{n,0}(\theta^\nu) f(t_{n+1}, y^\nu_{n+1}, X).$$

    3. Evaluate $f(t_{n+1}, y^\nu_{n+1}, X)$;
  - Correction: $y^{\nu+1}_{n+1} = \alpha_{n,1} y_n + \cdots + \alpha_{n,k} y_{n-k+1} + h_{n+1} f(t_{n+1}, y^\nu_{n+1}, X)$.
- End

Continuous Extensions of RK Methods

$$y'(t) = g(t, y(t)), \quad t \geq t_0, \quad y(t_0) = y_0.$$

- Given a continuous RK method of s-stages

$$\begin{aligned} \mathbf{y}_{n+1} &= \mathbf{y}_n + h_{n+1} \sum_{i=1}^{s} b_i \mathbf{g}(t_n + c_i h_{n+1}, \mathbf{Y}_i), \\ \mathbf{Y}_i &= \mathbf{y}_n + h_{n+1} \sum_{j=1}^{s} a_{ij} \mathbf{g}(t_n + c_j h_{n+1}, \mathbf{Y}_j), \quad i = 1, \ldots, s, \end{aligned}$$

  we consider

$$\eta(t_n + \theta h_{n+1}) = \mathbf{y}_n + h_{n+1} \sum_{i=1}^{s} b_i(\theta) \mathbf{g}(t_n + c_i h_{n+1}, \mathbf{Y}_i), \quad 0 \leq \theta \leq 1,$$

- The coefficients $b_i(\theta), i = 1, \ldots, s$ are polynomials of degree $\leq \delta$, satisfying

$$b_i(0) = 0, \quad b_i(1) = b_i, \quad i = 1, \ldots, s, \quad \text{(continuity conditions)}$$

- If $a_{ij} = 0, j \geq i$, the method is an explicit continuous RK method of first class.

Continuous Extensions of RK Methods

$$y'(t) = g(t, y(t)), \quad t \geq t_0, \quad y(t_0) = y_0.$$

- It is possible to construct the interpolatory formulae using $s^* - s$ aditional new stages

$$\begin{aligned}
\eta(t_n + \theta h_{n+1}) &= \mathbf{y}_n + h_{n+1} \sum_{i=1}^{s^*} b_i(\theta) \mathbf{g}(t_n + c_i h_{n+1}, \mathbf{Y}_i), \quad 0 \leq \theta \leq 1, \\
\mathbf{Y}_i &= \mathbf{y}_n + h_{n+1} \sum_{j=1}^{s^*} a_{ij} \mathbf{g}(t_n + c_j h_{n+1}, \mathbf{Y}_j), \quad i = s+1, \ldots, s^*,
\end{aligned}$$

- This are call second class CRK methods. The coefficients $b_i(\theta)$ are polynomials of degree $\leq \delta$ satisfying

$$b_i(0) = 0, \quad i = 1, \ldots s, \quad b_i(1) = b_i, \quad i = 1, \ldots, s, \quad b_i(1) = 0, \quad i = s+1, \ldots, s^*$$

(continuity conditions)

- Cubic Hermite interpolation
  Given the approximations $y_n, y_{n+1}, f_n, f_{n+1}$, we construct the cubic polynomial interpolation.

$$p_3(\theta) = (1-\theta)y_n + \theta y_{n+1} + \theta(\theta-1)\left((1-2\theta)(y_{n+1} - y_n) + (\theta - 1)h_n f_n + \theta h_n f_{n+1}\right).$$

  For methos of order $p \geq 3$ the formula gives a continuous extension of order 3.

Continuous Extensions of RK Methods

$$y'(t) = g(t, y(t)), \quad t \geq t_0, \quad y(t_0) = y_0.$$

$$\begin{array}{c|cccccc}
c_1 & a_{11} & \cdots & a_{1s} & 0 & \cdots & 0 \\
\vdots & \vdots & \ddots & \vdots & \vdots & \ddots & \vdots \\
c_s & a_{s1} & \cdots & a_{ss} & 0 & \cdots & 0 \\
c_{s+1} & a_{s+1,1} & \cdots & a_{s+1,s} & a_{s+1,s+1} & \cdots & a_{s+1,s^*} \\
\vdots & \vdots & \ddots & \vdots & \vdots & \ddots & \vdots \\
c_{s^*} & a_{s^*,1} & \cdots & a_{s^*,s} & a_{s^*,s+1} & \cdots & a_{s^*,s^*} \\
\hline
 & b_1(\theta) & \cdots & b_s(\theta) & b_{s+1}(\theta) & \cdots & b_{s^*}(\theta)
\end{array},$$

$$\mathbf{c} = [c_1, \ldots, c_s, \ldots, c_{s^*}]^T, (abscisae)$$

$$\mathbf{b} = [b_1(\theta), \ldots, b_s(\theta), \ldots b_{s^*}(\theta)]^T, (weights)$$

$$A = (a_{ij})_{i,j=1}^{s}, \quad \sum_{j=1}^{s} a_{ij} = c_i, i = 1, \ldots, s^*$$

Natural Continuous Extensions of RK

- (Zennaro, 1986) The interpolant $\eta(t)$ of order and degree q is a natural continuous extension of the RK method of order p,if

$$\int_{t_n}^{t_{n+1}} G(t)[u'_{n+1}(t) - \eta'(t)]dt\| = O(h_{n+1}^{p+1})$$

  for every sufficiently smooth matrix-valued function G, uniform with respect to $n = 0, \ldots, N-1$, where $u_{n+1}(t)$ denotes the local solution.

- The natural continuous extension of minimal order $q = \left\lfloor \dfrac{p+1}{2} \right\rfloor$ is given by the conditions

$$b_i(0) = 0, \quad \int_0^1 \theta^r b'_i(\theta) d\theta = b_i c_i^r, \quad r = 0, \ldots, q-1.$$

Some Examples of CERK Methods

- One-stage ERK of order $p = 1$ (Euler method)
  - $q = 1$: $b_1(\theta) = \theta$,
- Two-stage ERK of order $p = 2$
  - $q = 1$: $b_i(\theta) = b_i\,\theta, i = 1, 2$,
  - $q = 2$: $b_1(\theta) = (b_1 - 1)\,\theta^2 + \theta, \quad b_2(\theta) = b_2\theta^2$,
- Three-stage ERK methods of order $p = 3$ ($c_2, c_3 \neq 0$)
  - $q = 2$: $b_i(\theta) = w_i\theta^2 + (b_i - w_i)\theta, i = 1, 2, 3$, where

    $$w_1 = -\frac{1}{2c_3} - (c_3 - c_2)\lambda, \quad w_2 = c_3\,\lambda, \quad w_3 = \frac{1}{2c_3} - c_\lambda$$

    with λ real.
  - There is no NCE of order $q = 3$.
- Four-stage ERK methods of order $p = 4$:
  - $q = 2$: $b_i(\theta) = 3(2c_i - 1)b_i\theta^2 + 2(2 - 3c_i)b_i\theta, \quad i = 1, 2, 3, 4$.
  - $q = 3$: $b_1(\theta) = 2(1 - 4b_1)\theta^3 + 3(3b_1 - 1)\theta^2 + \theta$,

    $$b_i(\theta) = 4(3c_i - 2)b_i\theta^3 + 3(3 - 4c_i)b_i\theta^2, \quad i = 2, 3, 4$$
  - $q = 4$: There is no NCE of order $q = 4$.

High Order Continuous Extensions of RK

- Continuous Extensions of RK of second class.
- (Sarafyan, 1972) Construct high order approximations of $y(t)$ at some interior points, followed by the construction of the Hermite-Birkhoff interpolant at those points and the extreme of the interval.
  - CERK of eight stages with order 6, and uniform order 4.
  - CERK of ten stages with order 6, and uniform order 5: Used in DKLAG6 Code of Corwin, Sarafyan and Thomson.
- For DOPRI54 there is an embedded continuous extension with 7 stages of order 4, and a C^1 fifth order Hermite interpolatory with 9 stages. For example,

$$
\begin{aligned}
b_1(\theta) &= \theta(1+\theta(-1337/480+\theta(1039/360+\theta(-1163/1152)))),\\
b_2(\theta) &= 0,\\
b_3(\theta) &= 100\theta^2(1054/9275+\theta(-4682/27825+\theta(379/5565)))/3,\\
b_4(\theta) &= -5\theta^2(27/40+\theta(-9/5+\theta(83/96)))/2,\\
b_5(\theta) &= 18225\theta^2(-3/250+\theta(22/375+\theta(-37/600)))/848,\\
b_6(\theta) &= -22\theta^2(-3/10+\theta(29/30+\theta(-17/24)))/7,
\end{aligned}
$$

Collocation Methods

- Given distinct abscissae $c_1, \ldots, c_s$ in $[0,1]$, we construct the interpolant $\eta(t)$ of degree s defined by

$$\eta(t_n) = y_n, \quad \eta'(t_n + c_i h_{n+1}) = g(t_n + c_i h_{n+1}, \eta(t_n + c_i h_{n+1})), \quad i = 1, \ldots, s$$

- The collocation method is equivalent to the s-stage implicit CRK method wiht coefficients

$$a_{ij} = \int_0^{c_i} \ell_j(t)dt, \quad b_i(\theta) = \int_0^{\theta} \ell_i(t)dt, \quad i = 1, \ldots, s.$$

where $\ell_i(t) = \prod_{k \neq i} \dfrac{t - c_k}{c_i - c_k}$, are the Lagrange polynomials.

- The collocation method is a continuous RK method wiht order $p \geq s$ and uniform order $q = s$.
- If $M(t) = \prod_{i=1}^{s}(t - c_i)$ is orthogonal in $[0,1]$ to polynomials of degree $r-1$, then the collocation method has order $p = s + r$.

Examples of Collocation Methods

- Gaussian methods (order $p = 2s$, $q = s$)
  - $s = q = 1$ (Midpoint rule): $b_1(\theta) = \theta$, $c_1 = a_{11} = \dfrac{1}{2}$.
  - $s = q = 2$ (Hammer-Hollingsworth method):

$$\begin{array}{c|cc} \frac{1}{2} - \frac{\sqrt{3}}{6} & \frac{1}{4} & \frac{1}{4} - \frac{\sqrt{3}}{6} \\ \frac{1}{2} + \frac{\sqrt{3}}{6} & \frac{1}{4} + \frac{\sqrt{3}}{6} & \frac{1}{4} \\ \hline & 1/2 & 1/2 \end{array}, \qquad \begin{aligned} b_1(\theta) &= -\frac{\sqrt{3}}{2}\theta(\theta - 1 - \frac{\sqrt{3}}{3}), \\ b_2(\theta) &= \frac{\sqrt{3}}{2}\theta(\theta - 1 + \frac{\sqrt{3}}{3}), \end{aligned}$$

- Radau IIA methods (order $p = 2s - 1$, $q = s$)
  - $s = q = 1$ (Backward Euler): $b_1(\theta) = \theta$, $b_1 = c_1 = a_{11} = 1$.
  - $s = q = 2$ (Ehle Method):

$$b_1(\theta) = -\frac{3}{4}\theta(\theta - 2), \quad b_2(\theta) = \frac{3}{4}\theta(\theta - \frac{2}{3}), \quad A = \begin{bmatrix} \frac{5}{12} & \frac{-1}{12} \\ \frac{3}{4} & \frac{1}{4} \end{bmatrix}.$$

Examples of Collocation Methods

- Lobatto IIIA methods (order $p = 2s - 2$, $q = s$)
  - $s = q = 2$ (Trapezoidal rule): $b_1(\theta) = -\frac{1}{2}\theta(\theta - 2)$, $b_2(\theta) = \frac{1}{2}\theta^2$, $A = \begin{bmatrix} 0 & 0 \\ \frac{1}{2} & \frac{1}{2} \end{bmatrix}$.
  - $s = q = 3$ (Ehle Method):

$$\begin{array}{c|ccc} 0 & 0 & 0 & 0 \\ 1/2 & 5/24 & 1/3 & -1/24 \\ 1 & 1/6 & 2/3 & 1/6 \\ \hline & 1/6 & 2/3 & 1/6 \end{array}, \qquad \begin{aligned} b_1(\theta) &= 2\theta(\frac{1}{3}\theta^2 - \frac{3}{4}\theta + \frac{1}{2}), \\ b_2(\theta) &= -4\theta^2(\frac{1}{3}\theta - \frac{1}{2}), \\ b_3(\theta) &= 2\theta^2(\frac{1}{3}\theta - \frac{1}{4}). \end{aligned}$$

Continuous RK methods. Direct method

- Order conditions

$$
\begin{aligned}
\textstyle\sum_{i=1}^s b_i(\theta) &= \theta, \\
\textstyle\sum_{i=1}^s b_i(\theta)c_i &= \frac{1}{2}\theta^2, \\
\textstyle\sum_{i=1}^s b_i(\theta)c_i^2 &= \frac{1}{3}\theta^3, \\
\textstyle\sum_{i=1}^s b_i(\theta)a_{ij}c_j &= \frac{1}{6}\theta^3, \\
\textstyle\sum_{i=1}^s b_i(\theta)c_i^3 &= \frac{1}{4}\theta^4, \\
\textstyle\sum_{i=1}^s b_i(\theta)c_i a_{ij}c_j &= \frac{1}{8}\theta^4, \\
\textstyle\sum_{i=1}^s b_i(\theta)c_i a_{ij}c_j^2 &= \frac{1}{12}\theta^4, \\
\textstyle\sum_{i=1}^s b_i(\theta)a_{ij}a_{jk}c_k &= \frac{1}{24}\theta^4
\end{aligned}
$$

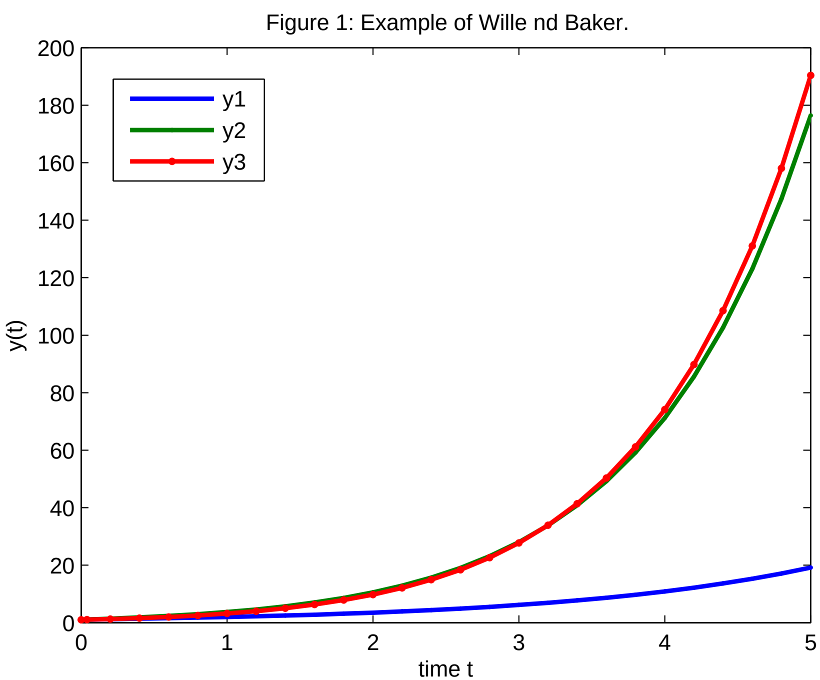
-

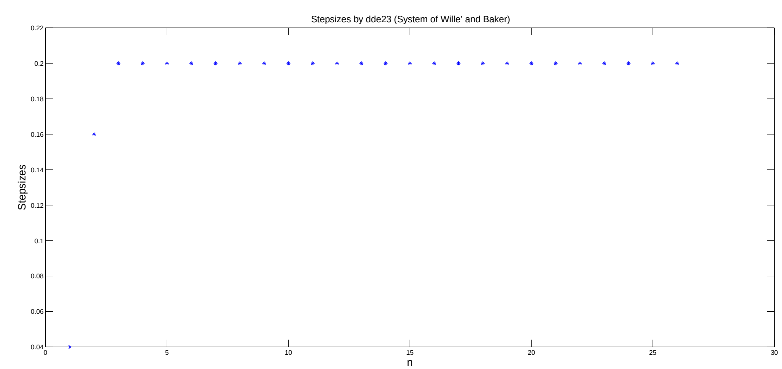
order q	1	2	3	4	5	6	7	8	$r \geq 9$
n. of stages in CERK(q)	1	2	4	6	8	11	≥ 12	≥ 14	≥ 16
n. of stages in ERK(q)	1	2	3	4	6	7	9	11	$\geq r+3$

Examples of some codes

1. RETARD : DOPRI54 with dense output by Shampine (Hermite) by E. Hairer and G. Wanner (1993), easy to use, (you can download from the webb page of Prof. Hairer). Constant delays.
2. RADAR5 : RADAU-IIA (collocation RK method,implicit of s stages), Order $s+1$, stiff problems, by E. Hairer and N. Guglielmi (also from webb page of E. Hairer), University of Geneve.
3. ARCHI : DOPRI54 with fifth order Hermite interpolant by Shampine, tracking the propagation of the discontinuities of the derivative, ARCHI-L and ARCHI-N adapted for solving parameter estimation problems, by C.A.H. Paul (Univ. Manchester).(1997).
4. DKLAG5 $\rightarrow$ DKLAG6 : Embedded RK-Sarafyan 6(5), state-dependent delays, handle vanishing delays, by S. P. Corwin (Radford Univ), D. Sarafyan (New Orleans Univ.), S. Thompson (Radford Univ.)
5. DDE-STRIDE : Singly implicit RK method adapted to DDEs, by Prof. Butcher (1992), University of Auckland.
6. DD23 by Shampine and Thompson. This uses the imbedded RK pair of order 2(3) with continuous extension based on cubic Hermite interpolation for solving DDEs with many constant delays. Is the method for DDEs in MatLab.

$$
\begin{aligned}
y_1'(t) &= y_1(t-1),\\
y_2'(t) &= y_1(t-1) + y_2(t-0{,}2), \quad 0 \le t \le 5\\
y_3'(t) &= y_2(t),\\
y_1(t) &= y_2(t) = y_3(t) = 1, \quad t \le 0
\end{aligned}
$$





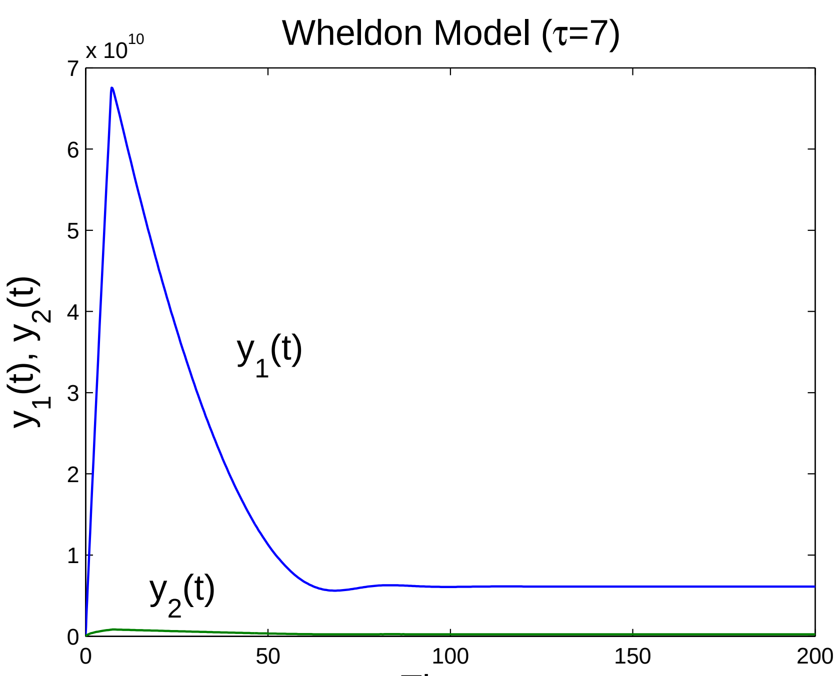
dde23 Statistics: number of steps 26, failed steps = 0, number of evaluations = 118

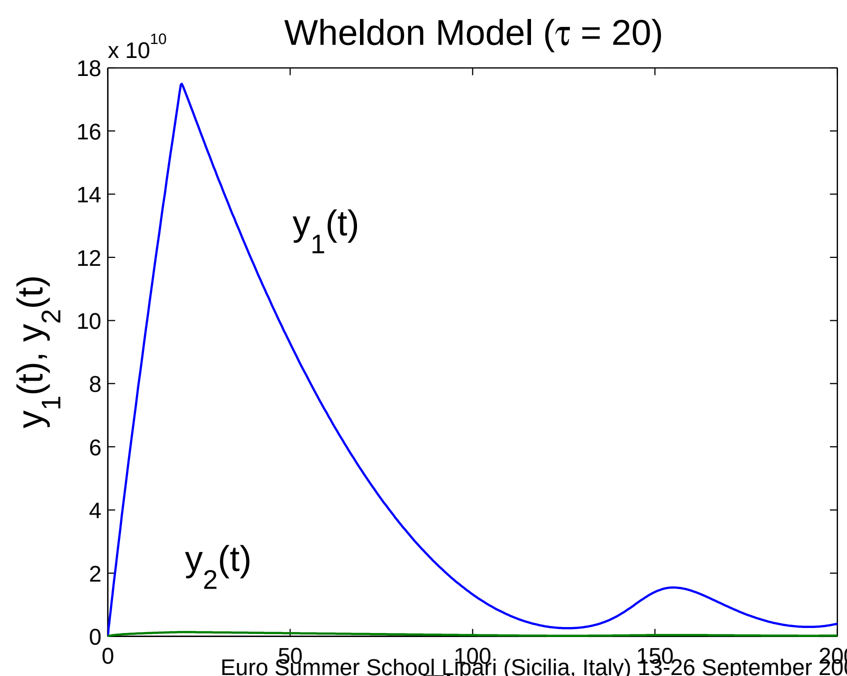
- Wheldon model of cronic granulotic leukemia (N. MacDonald, '*Time Lags in Biological Systems*' (1978)):

$$
\begin{aligned}
y_1'(t) &= \frac{\alpha}{1+\beta y_1(t-\tau)^{\gamma}} - \frac{\lambda y_1(t)}{1.+\mu y_2(t)^{\delta}},\\
y_2'(t) &= \frac{\lambda y_1(t)}{1+\mu y_2(t)^{\delta}} - \omega y_2(t) \quad 0 \le t \le 200\\
y_1(t) &= y_2(t) = 100, \quad t \le 0.
\end{aligned}
$$

Parameters:

$\alpha = 1{,}1e10, \beta = 10e-12, \gamma = 1{,}25, \delta = 1., \lambda = 10, \mu = 4{,}0e-8, \omega = 2{,}43$





Vanishing lags DDEs

- Only a question to consider for explicit high order methods.
- A delay vanishes at a point Ξ_a if $\tau(\xi_a, y(\xi_a)) = 0$. Assuming continuity, $t - \tau(t, y(t)) \rightarrow \xi_a$ as $t \rightarrow \xi_a$. When this happens the RK equations become **implicit.** This also happens when the step-size is greater then the lag.
- Two simple solutions:
  1. Reduce the stepsize until the problem no longer occurs;
  2. Extrapolate from a previous interpolant.
  3a. To define an initial interpolant $\hat{\eta}(t_n + \theta h) = \hat{\eta}(t_n)$,
  3b. Solve the RK equations,
  3c. Interpolate the numerical solution.
  3d repeat (3b) and (3c) (a finite number of times or until the convergence).

Stability Concepts

$$y'(x) = \lambda y(x) + \mu y(x-\tau), \quad x \geq 0, \quad \lambda, \mu \in C.$$

Trying solutions of the form $y(x) = e^{\zeta x}$, $\zeta \in C$, we obtain the characteristic equation

$$\zeta = \lambda + \mu e^{-\zeta\tau}$$

The right half plane $\Re\zeta \geq 0$ ia mapped under the right hand side onto a circle centered at a with radius b. If this circle lies completely in the open left half-plane (LHP), it is clear that then the characteristic equation can have no solutions in the RHP. This occurs whenever

$$\Re(\lambda) + |\mu| < 0.$$

This is a sufficient condition for stability of the zero solution of the DDE test problem. In fact, this stability is independent of the delay τ.

Definition: A numerical method for DDEs is said P-stable if $\text{lím}_{n\to\infty} y_n = 0$ holds for all constant delays τ and all initial functions $\phi(x)$ when the method is applied to the test equation subject to the condition above and with uniform stepsize $h_n = h$ satisfying $h = \tau/r$ for some positive integer r. If we dropp the restriction that $h = \tau/r$ we say that the method is GP-stable.

P-estabilidad de θ-métodos

As an illustration we consider el θ-método

$$y_{n+1} = y_n + \theta h f(t_{n+1}, y_{n+1}) + h(1-\theta) f(t_n, y_n),$$

with piecewise linear interpolation for the value $y_{n-m+\delta}$, where $(m-\delta)h = \tau$, and $0 \le \delta < 1$. Then, with $\hat{\lambda} = h\lambda; \hat{\nu} = h\mu$,

$$\begin{aligned}(1-\theta\hat{\lambda})y_{n+1} \quad &= \quad (1+(1-\theta)\hat{\lambda})y_n + \theta\hat{\mu}(\delta y_{n+2-m} + (1-\delta)y_{n+1-m}) \\ &\quad\quad +(1-\theta\hat{\mu}(\delta y_{n+1-m} + (1-\delta)y_{n-m})\end{aligned}$$

To investigate its numerical stability, we substitute y_n with z^n, to get $p_m(z) = q(z)z^m - p(z,\delta)$, with

$$\begin{aligned} q(z) \quad &= \quad z - \frac{1+(1-\theta)\hat{\lambda}}{1-\theta\hat{\lambda}}, \\ p(z,\delta) \quad &= \quad \frac{(\delta z + (1-\delta))(\theta z + (1-\theta))m\hat{u}}{1-\theta\hat{\lambda}}. \end{aligned}$$

El θ-método es GP-estable si y sólo si $1/2 \le \theta \le 1$.

Theorem (Zennaro (1986), Watanabe and Roth (1985))
For a certain class of RK methods including collocation A-stability implies P-stability if a suitable interpolation is used. This is also true for multistep methods.

Linear Stability Analysis

- We will assume that when advancing from $x = nh$, a RK method produces a full-step approximation $y_{n+1} \approx y(((n+1)h)$, a continuous approximate solution $u_n(nh+\theta h) \approx y(nh+\theta h)$ with $u_n((n+1)h) = y((n+1)h)$ and possibly low order approximations $Y_{n,i} \approx y(nh+c_r h)$.

$$\begin{aligned} u_n(nh+\theta h) &= u_n(nh) + h\sum_{i=1}^{s} b_i(\theta)Y'_{n,i}, \\ Y'_{n,i} &= \lambda Y_{n,i} + \mu u_{m_i}(nh+c_i h-\tau), \end{aligned}$$

where $nh + c_i h - \tau \in [m_i h, (m_i+1)h]$. for some $m_i < n$. (We will assume $\tau = Nh$ and then $m_i = m = n - N$).
A tedious calculus gives a recurrence of the form

$$y_{n+1} = [1 + \lambda h \mathbf{b}^T (I - \lambda h A)^{-1} \mathbf{e}] y_n + \mu h \mathbf{b}^T (I - \lambda h \mathbf{A})^{-1} \mathbf{u}_{n-N},$$

An example

The improved Euler method with the continuous extension of order 2.

- With $\tau = h$; that is, $N = 1$, is posible an analytical solution. This result

$$\lambda h = \frac{1}{2}\mu h - 1 - \frac{1}{2}\sqrt{(\mu h - 6)(\mu h + 2)}, \quad \mu h(1 + \lambda h) = -2,$$
$$\lambda h = \frac{1}{2}\mu h - 1 + \frac{1}{2}\sqrt{(\mu h - 6)(\mu h + 2)}, \quad \lambda h = -\mu h$$
$$\lambda h = 2$$

- With $\tau = 5{,}25h$, we must solve numerically:
  1. Boundary locus stability plot.
  2. Discrete grid search.
  3. A mixture of both