A priori Enclosures for ODEs:
An Alternative to Fixed Point Iterations

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Introduction

Smooth IVP: $u' = f(t,u), \;\; u(t_0) \; = \; u_0.$

($u = (u_1, \ldots, u_n), \quad f = (f_1, \ldots, f_n)$).

Moore's enclosure method:

– Automatic computation of Taylor coefficients.

– Interval iteration: For $j := 0, 1, \ldots$:

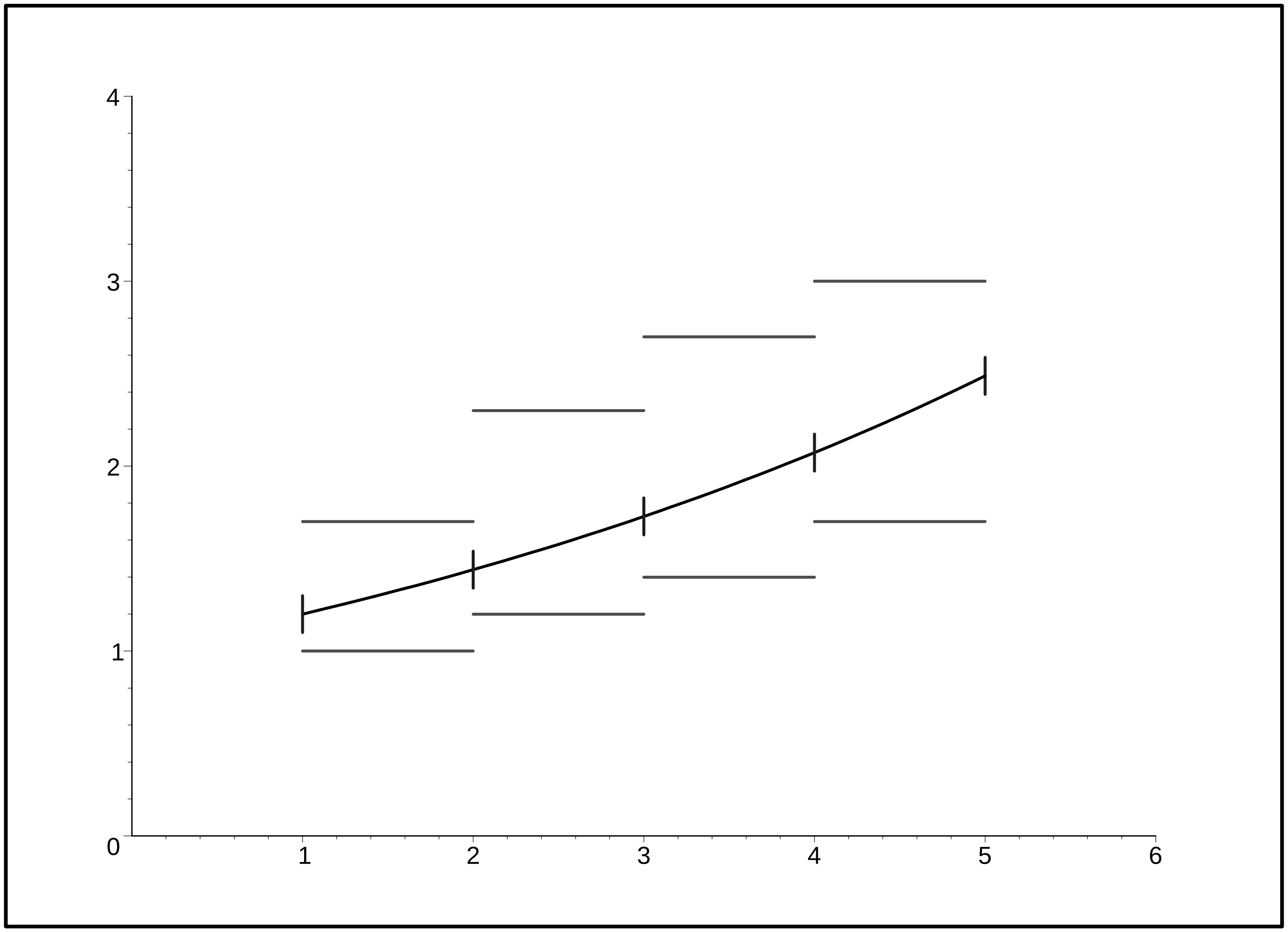
A priori enclosure: $[\widehat{u}_{j+1}] \supseteq u(t)$ for all $t \in [t_j, t_{j+1}]$ (”Algorithm I”).

Truncation error: $[z_{j+1}] := \dfrac{h^{(m+1)}}{(m+1)!} f^{(m)}([t_j, t_{j+1}], [\widehat{u}_{j+1}])$.

$$u(t_{j+1}) \in [u_{j+1}] := [u_j] + \sum_{k=1}^{m} \frac{h^k}{k!} f^{(k-1)}(t_j, [u_j]) + [z_{j+1}]$$

(”Algorithm II”).

Piecewise constant a priori enclosure



A priori Enclosures

– Moore:

Fixed point iteration with constant enclosures:
For some $h > 0$ determine interval $[\widehat{u}_1]$ such that

$$u_0 + [0, h] \cdot f([t_0, t_1], [\widehat{u}_1]) \subseteq [\widehat{u}_1]$$

$\Rightarrow$ Step size restrictions: Explicit Euler steps.

– Improvements suggested by Lohner, Corliss & Rihm, Nedialkov & Jackson, $\ldots$.

– Berz & Makino: High order TM enclosure by FP iteration

Step Size Control

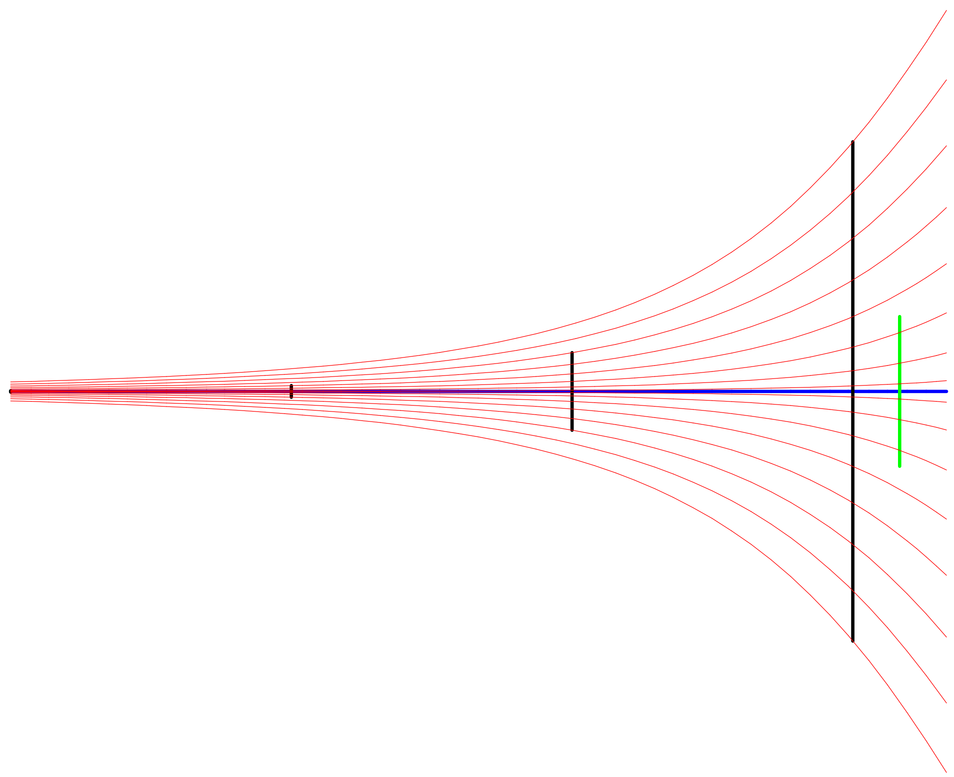
– Maximum step size for practical calculations:

  Slightly less than the radius of convergence of the Taylor series.

– Large step sizes expected to reduce overall wrapping operations.

– Helpful for tracing unstable solutions.

Tracing Unstable Solutions



Linear n–th Order ODE with Analytic Coefficient Functions

$$y^{(n)} = \sum_{i=0}^{n-1} p_i(x)\, y^{(i)} + p_{-1}(x), \quad x \in [0, r],$$

$$y^{(i)}(0) \;=\; y_{io}, \quad i = 0, 1, \ldots, n-1,$$

$$p_i(x) = \sum_{j=0}^{\infty} b_{ij}\, x^j, \quad |x| < R \;\; (R > r), \quad i = -1, 0, \ldots, n-1.$$

Power series solution: $y(x) := \sum_{k=0}^{\infty} a_k\, x^k, \quad |x| < R.$

$$a_{k+n} \;=\; \sum_{i=0}^{n-1} \sum_{j=0}^{k} \frac{P(k-j, i)\, b_{ij}}{P(k, n)}\, a_{k+i-j} \;+\; \frac{b_{-1,k}}{P(k, n)} \quad \text{for} \;\; k = 0, 1, \ldots\;,$$

where $\quad P(k, i) := (k+1) \cdots (k+i), \quad P(k, 0) := 1 \quad$ for $\; i \in \mathbb{N}, k \in \mathbb{N}_0.$

Estimation of Recurrence Relation

I. Required: $\forall i \; \exists m_i \geq i + 2$, $\exists B_i \geq 0$ so that

$$|b_{ij}| \;\leq\; \frac{B_i}{P(j - m_i, m_i) r^j} \quad \text{for all } j > m_i.$$

II. Find $K \geq mn$, $q \in [0, 1]$:

$$\frac{\max\limits_{\nu=K-m}^{K+n-1} |a_\nu r^\nu|}{\max\limits_{\nu=0}^{K+n-1} |a_\nu r^\nu|} \;\leq\; q$$

Estimation of Recurrence Relation

III. Recess condition: Find κ such that

$$q \sum_{i=0}^{n-1} \sum_{j=0}^{m_i} \frac{r^{n-i+j}\, P(\kappa - j, i)\ |b_{ij}|}{P(\kappa, n)} + \frac{B_{-1}\, r^{n+m_{-1}}}{P(\kappa - m_{-1}, m_{-1} + n)\ \max\limits_{\nu=0}^{\kappa+n-1}\ |a_\nu\, r^\nu|}$$

$$+ \sum_{i=0}^{n-1} \frac{B_i\, r^{n+m_i-i}}{P(\kappa, n)} \left(\frac{(-1)^{i+1} i!}{P(m_i - 2 - i, i+1)\, P(\kappa - m_i + 1 + i, m_i - 1 - i)} \right.$$

$$\left. + \sum_{\nu=0}^{i-1} \frac{(-1)^{i-\nu} i!(i-\nu)! P(\kappa - m_i, \nu)}{\nu! P(m_i - 2 - i + \nu, i - \nu + 1)(m_i - 1)!} + \frac{P(\kappa - m_i, i)}{(m_i - 1) m_i!} \right) \ \leq\ q$$

Enclosure Theorems

Theorem 1. *The recess condition holds for sufficiently large values of* κ*.*

Theorem 2. *If the recess condition holds, then*

$$|a_k r^k| \;\leq\; q \cdot \max_{\nu=0}^{\kappa+n-1} |a_\nu r^\nu| \;=:\; A \quad \textit{for all } k \geq \kappa + n.$$

Theorem 3. *If the recess condition holds, then for* $h = \omega r$*,* $0 \leq \omega < 1$*, and* $k \geq \kappa$*,*

$$|\, y(h) - \sum_{\nu=0}^{k-1} a_\nu \, h^\nu \,| \;=\; |\sum_{\nu=k}^{\infty} a_\nu \, r^\nu \, \omega^\nu| \;\leq\; A \sum_{\nu=k}^{\infty} \omega^\nu \;=\; \frac{A\,\omega^k}{1-\omega} \,.$$

Practical calculations

– Step size control:

Recess condition can be tested a priori for r and κ.

– Very large step sizes:

Multiple precision arithmetic required.

Computation of B_i

Analytic function: $p(z) = \sum_{j=0}^{\infty} b_j z^j, \quad z \in \mathbb{C}, \quad |z| \leq r.$

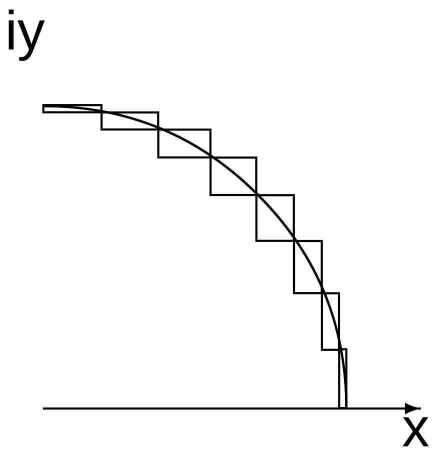
Cauchy's estimate: $|b_j| \; \leq \; \frac{M(r)}{r^j}, \quad j \in \mathbb{N},$ $M(r) := \max_{|z|=r} |p(z)|$.

CE of m–th derivative: $p^{(m)}(z) \; = \; \sum_{j=0}^{m} P(j,m) b_{j+m} z^j$

$$\Rightarrow \; |P(j,m) b_{j+m}| \; \leq \; \frac{N(r)}{r^j}, \quad N(r) := \max_{|z|=r} |p^{(m)}(z)| \, .$$

$$\Leftrightarrow \; |b_j| \; \leq \; \frac{B}{P(j-m,m) r^j}, \quad B = N(r) r^m, \quad \text{for } j \geq m.$$

Interval Computation of M



Cover C with complex intervals

$$Z_k, \quad k = 1, \ldots, k_{\max}.$$

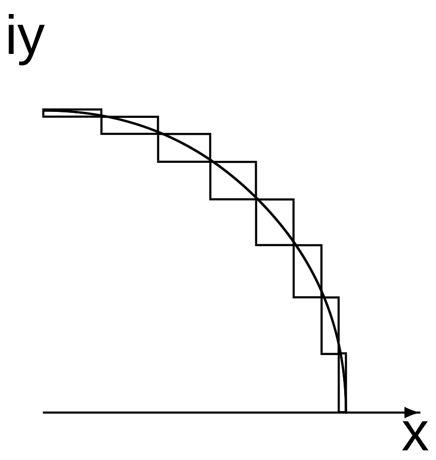
Use complex interval functions to compute

$$[\underline{F}_k, \overline{F}_k] \supseteq |f(Z_k)| \text{ for all } k.$$

$$\Rightarrow M(r) \leq \max_k \overline{F}_k.$$

Adaptive refinement of Z_k with branch and bound algorithm.

Interval Computation of M



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Adaptive refinement of Z_k with branch and bound algorithm.

Example 1: $y'' = y,\, y(0) = 1,\; y'(0) = -1$.

Exact Solution: $y(x) = e^{-x}$.

h	$[y](h)$	L	κ	Time
20	$2.061\,153\,622\,438\,55_{7}^{9}$ E-009	3	97	0.11
40	$4.248\,354\,255\,291\,5_{88}^{91}$ E-018	4	170	0.39
100	$3.720\,075\,976\,020\,83_{5}^{7}$ E-044	7	386	2.47
200	$1.383\,896\,526\,736\,73_{7}^{8}$ E-087	12	745	12.74
300	$5.148\,200\,222\,412\,01_{2}^{6}$ E-131	18	1104	37.19

AWA:

h	$[y](h)$	Degree	No. of steps	Time
10	$4.539\,99_{28}^{32}$ E-05	20	33	0.11
15	3.0_{57}^{61} E-07	20	50	0.17
20	${}_{-2.724}^{3.136}$ E-08	20	69	0.28
40	${}_{-1.422}^{1.422}$ E+01	20	101	0.39

Example 2

$$y^{(4)} = (x^2+10x+26)\,y^{(3)} + (-20x-99.5)\,y'' + (x^2+10x+25)\,y' + (-2x^2-4x+29.5)\,y$$

$$y(0)=5,\ y'(0)=4,\ y''(0)=3,\ y^{(3)}(0)=2. \qquad (y(x)=(5-x)\,e^x.)$$

h	ε_{abs}	$[y](h)$	L	κ	Time
1	—	$1.087\ldots61^9_7$E+01	2	58	0.11
1.25	—	$1.308\ldots19^1_0$E+01	2	72	0.17
1.5	—	$1.568\ldots32^3_2$E+01	2	88	0.22
4	—	$5.459\ldots42^6_2$E+01	7	364	2.25
5	1E–050	$^{4.951}_{-4.951}$ E–065	12	548	5.28

AWA:

h	$[y](h)$	Degree	No. of steps	Time
1	$1.087\,312\,^{77}_{68}$E+01	20	61	2.42
1.25	1.30^{91}_{86}E+01	20	81	3.13
1.5	$^{34.960}_{-6.183}$	20	101	3.95

Example 3

$$y'' = \alpha e^x y + e^{-x} - \alpha,\ y(0) = 1,\ y'(0) = -1. \qquad (y(x) = e^{-x}.)$$

α	x	$[y](x)$	Prec.	Steps	k_{max}
0.01	5	$6.737\ldots46_6^9$E–03	2	1	105
0.01	7.5	$5.530\ 843\ 701\ 4_{75}^{84}$E–04	2	2	105
0.01	10	$^{6.250}_{2.846}$E–05	2	3	161
10	4	$1.831\ldots41_7^9$E–02	3	1	201
250	2.25	$1.053\ldots64_4^4$E–01	3	1	181

AWA:

α	x	$[y](x)$	Order	Steps
0.01	5	$6.737\ 946\ 999\ _{067}^{109}$E–03	20	10
0.01	7.5	$5.530\ 843\ _{661}^{753}$E–04	20	22
0.01	10	$^{4.336}_{-3.294}$E–03	20	67
10	4	$^{1.070}_{-0.688}$E+02	20	84
250	1.5	$^{1.341}_{-0.451}$E+00	20	78

Nonlinear ODEs

$$y' = f(p(x), y), \quad y(0) \;=\; \eta.$$

$$f_i(x) = \sum_{j=1}^{J} p_{ij}(x) \prod_{l=1}^{n} y_l^{\alpha_{ijl}}, \qquad p_{ij}(x) = \sum_{k=0}^{\infty} b_{ijk}\, x^k,$$

$$\alpha_{ijl} \in \mathbb{N}_0, \;\; b_{ijk} \in \mathbb{R}, \;\; |b_{ijk}| \;\leq\; \frac{B_{ij}}{R^k}.$$

(f_i is a polynomial in y, with analytic coefficient functions $p_{ij}(x)$).

Power series solution:

$$y_i(x) := \sum_{k=0}^{\infty} a_{ik}\, x^k, \quad |x| < r \text{ for some } r > 0.$$

Estimation: For $i = 1, \ldots, n$ compute $A_i > 0$ and $r > 0$, so that

$$|a_{ik}| \;\leq\; \frac{A_i}{r^k} \quad \text{for all } i = 1, \ldots, n \text{ and all } k \in \mathbb{N}.$$

Example 4: Lorenz Equations

$$\begin{aligned}
\dot{x} &= -\sigma x + \sigma y, & x(0) &= 0; & \sigma &= 10 \\
\dot{y} &= rx - y - xz, & y(0) &= 1; & r &= 28 \\
\dot{z} &= -bz + xy, & z(0) &= 0; & b &= \frac{8}{3}\,.
\end{aligned}$$

Comparison of step sizes:

t	Steps	AWA
0.25	6	12
0.5	13	31
1.0	26	64