Validated method for IVPs for Ordinary Differential Equations based on Chaplygin's inequalities

Dmitry Nadezhin
Sun Microsystem Laboratories
Dmitry.Nadezhin@sun.com
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Abstract

Standard numerical methods for initial value problems (IVPs) for ordinary differential equations (ODEs) return approximate solution only. Validated (also called interval) methods for IVPs for ODEs return approximate solution together with a rigorous enclosure of the true solution. A widely known validated method for IVPs for ODEs is the interval Hermite-Obreschkoff (IHO). This method meets the difficulties on stiff ODEs. The method of Chaplygin's inequalities is less known. However, it might be more suitable for problems like interval Spice simulator, because electrical circuits are described in Spice by stiff emprical ODEs which are not smooth enough. This memo describes IHO and Chaplygin validated methods and studies their stability on a simple ODE $\dot{y} = -y$.

1 Introduction

Validated (interval) methods for IVP solution return approximate solutions similar to standard (point) methods. Moreover, they return a rigorous enclosure for a true solution with a numerical proof that the true solution is inside the enclosure. The numerical proof in widely known methods is an interval calculation of approximation error inside the enclosure.

Validated methods are often obtained from corresponding standard methods by an interval calculation of the approximation error inside the enclosure. However, numerical properties of the interval variant (such as stability) may be worse than those of their point method. For example, the standard Hermite-Obreschkoff method $HO(p, q)$ is stable at negative real axis when $p \leq q$, while the interval Hermite-Obreschkoff method $IHO(p, q)$ is not stable at $z \to -\infty$ for any p and q, where $z = \lambda h$ [1]. The loss of stability is because the numerical enclosure proof considers maximum of a higher derivative of the true solution among timestep. For stiff equations, this derivative at the beginning of the timestep is much larger than its average over the entire timestep.

Chaplygin's inequality is another possible numerical proof that the true solution is inside the enclosure. This proof computes a velocity vector on the boundary of the enclosure and verifies that it is directed inward, so that there is no way for the true solution to come out from the enclosure.

This memo presents a first-order one-dimensional variant of the Chaplygin method and compares its with the first-order one-dimensional specializations of IHO.

$IHO(1,0)$ is an interval variant of the Forward Euler method, $IHO(0,1)$ is an interval variant of the Backward Euler method. Both of them are not stable at $z \to -\infty$. The Chaplygin analog of interval Backward Euler method is stable at the whole negative real axis ($\Re z < 0$, $\Im z = 0$) like its point analog.

2 The Initial Value Problem

I include here a problem formulation from [1]. The reader may refer to it for omitted details.

We consider the set of autonomous initial value problems (IVPs)

$$y'(t) = f(y) \tag{1}$$

$$y(t_0) \in [y(t_0)] \tag{2}$$

where $t \in [t_0, T]$ for some $T > t_0$. Here t_0 and $T \in \mathbb{R}$, $f \in C(D)$, $D \subseteq \mathbb{R}^n$ is open, $f : D \to \mathbb{R}^n$, and $[y_0] \subseteq D$. The condition (2) permits the initial value $y(t_0)$ to be in an interval, rather than specifying a particular value. We assume that the representation of f contains only a finite number of constants, variables, elementary operations, and standard functions.

We consider a grid $t_0, t_1, t_2, \ldots, t_m$, which is not necessarily equally spaced, and denote the stepsize from t_j to t_{j+1} by h_j ($h_j = t_{j+1} - t_j$). The step from t_j to t_{j+1} is refered to as $(j+1)$st step. We denote the solution of (1) with the initial condition y_j at t_j by

$$y(t; t_j, y_j) \tag{3}$$

For an interval $[y_j]$, we denote by $y(t; t_j, [y_j])$ the set of solutions

$$\{y(t; t_j, y_j) | y_j \in [y_j]\} \tag{4}$$

Our goal is to compute intervals, $[y_j]$, $j = 1, 2, \ldots, m$, that are guaranteed to contain the solution of (1-2) at $t_1, t_2, \ldots, t_m$. That is, $y(t_j; t_0, [y_0]) \subseteq [y_j]$, for $j = 1, 2, \ldots, m$.

The IHO and Chaplygin validated methods will be illustrated in this memo by a simple example, for which formulas (1)-(4) look like:

$$f(y) = -y,$$
$$[y_0] = [-1, 1], t_0 = 0$$
$$y(t; t_0, y_0) = y_0 e^{-(t-t_0)} = y_0 e^{-t}$$
$$y(t; t_0, [y_0]) = [-e^{-t}, e^{-t}]$$

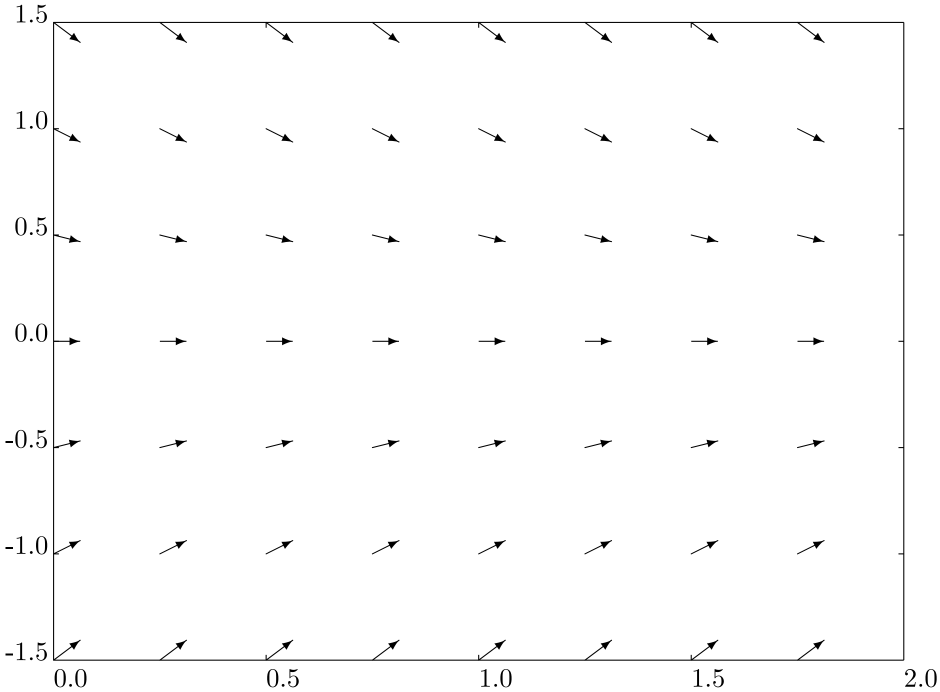

Figure 1 shows $f(y)$ as field of velocity vectors.

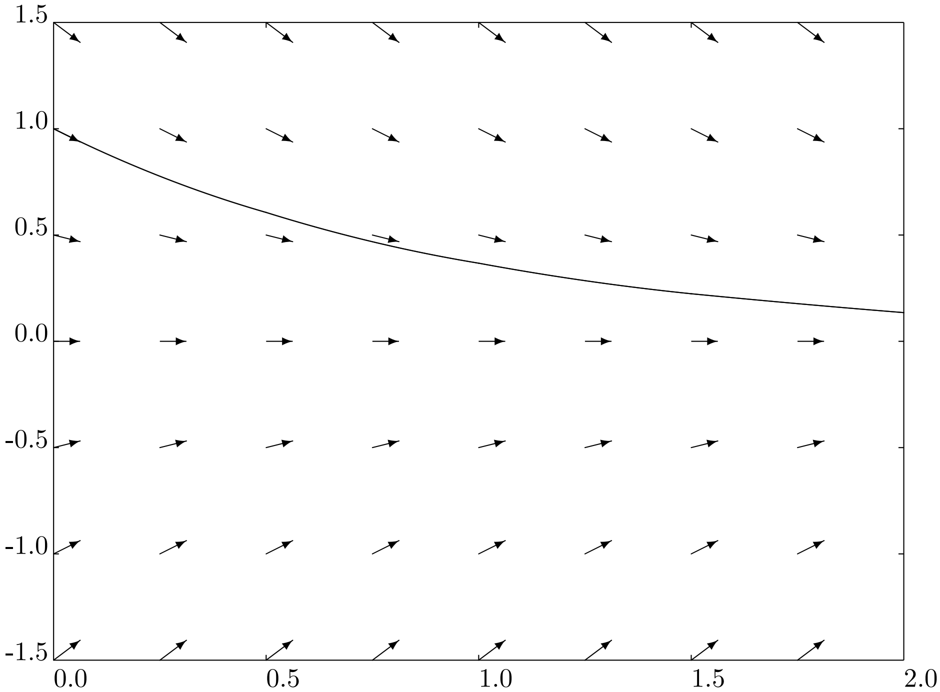

Figure 2 shows $y(t; 0, 1)$.

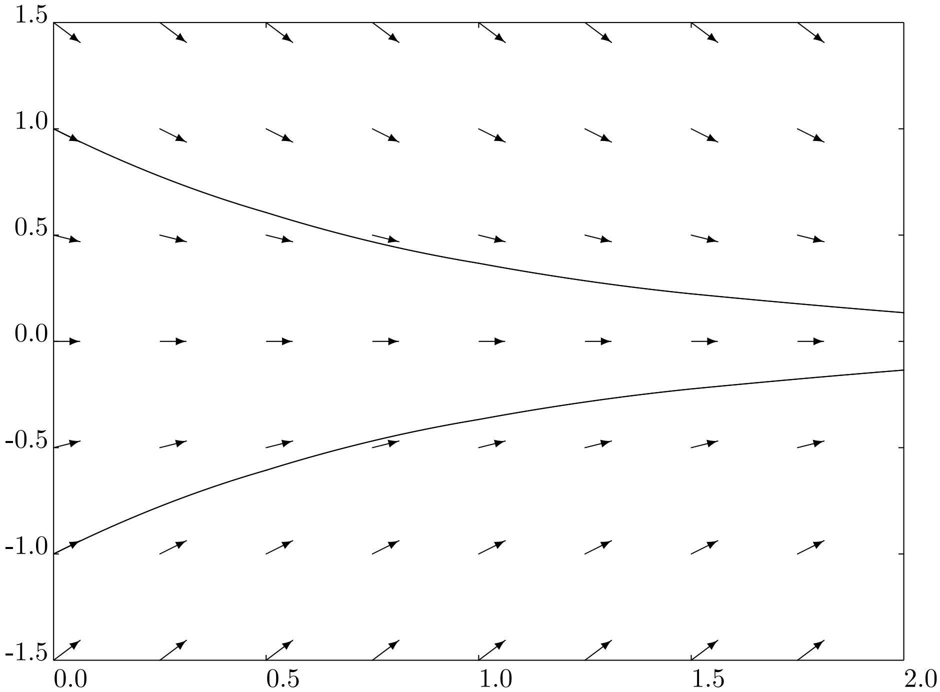

Figure 3 shows $y(t; 0, [-1, 1])$.

3 First-order standard (point) methods

3.1 Forward Euler method

The standard Forward Euler method returns

$$y_{j+1} = y_j + h_j f(y_j) \tag{5}$$

The point Forward Euler method for the example returns

$$y_{j+1} = (1 - h_j) y_j$$

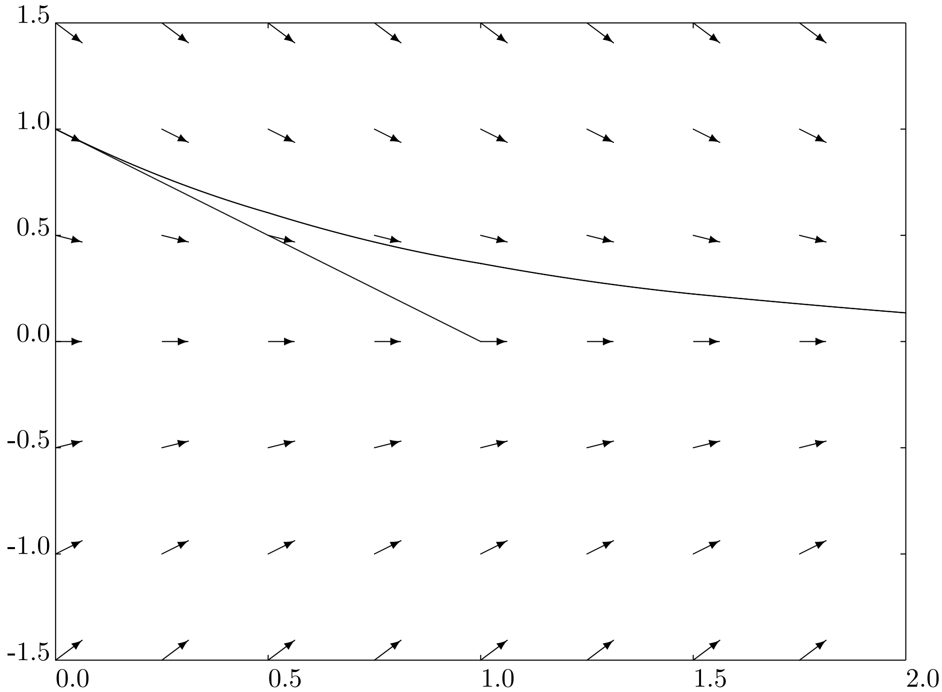

Figure 4 shows first step of Forward Euler from $y_0 = 1$ with $h_0 = h = 1$: $y_1 = (1 - h) = 0$.

The point Forward Euler is stable ($|y_{j+1}| < |y_j|$) only when $0 < h_j < 2$.

3.2 Backward Euler method

The point Backward Euler method determines y_{j+1} from the implicit equation

$$y_{j+1} - h_j f(y_{j+1}) = y_j \tag{6}$$

The point Backward Euler method for the example returns

$$y_{j+1} = \frac{y_j}{1 + h_j}$$

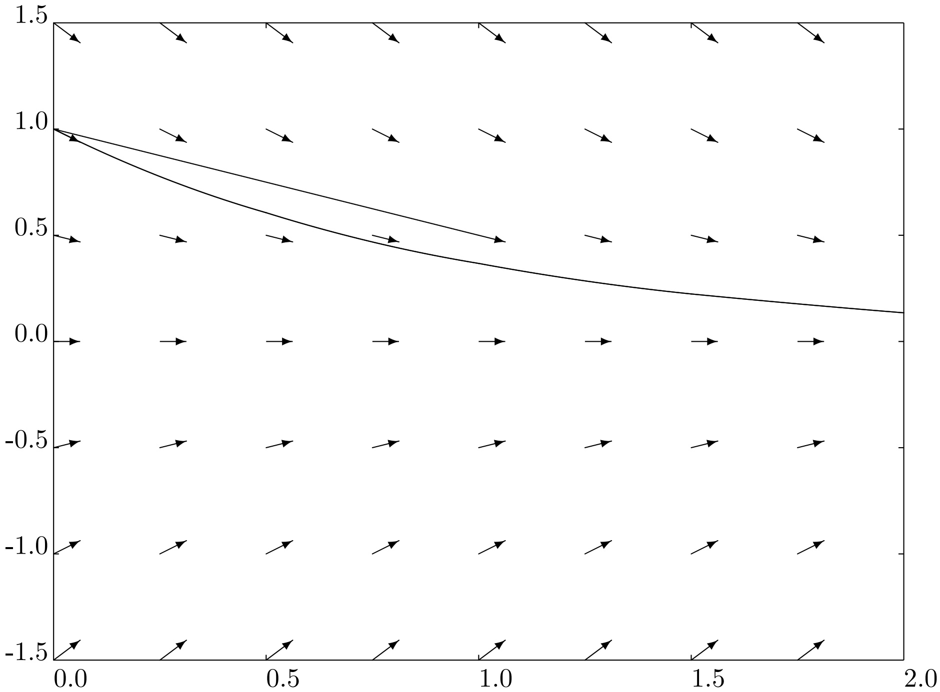

Figure 5 shows first step of the Backward Euler from $y_0 = 1$ with $h_0 = h = 1$: $y_1 = \frac{1}{1+h} = \frac{1}{2}$.

The point Backward Euler method is stable ($|y_{j+1}| < |y_j|$) for any $h_j > 0$.

4 Interval Hermite-Obreschkoff methods

Interval Hermite-Obreschkoff methods $IHO(p, q)$ consider up to p-th derivatives of true solution at the start of timestep t_j and up to q-th derivatives of true solution at the end of timestep t_{j+1}. We consider first-order methods $IHO(1, 0)$ and $IHO(0, 1)$ which are analogs of the Forward Euler and Backward Euler point methods.

Each Hermite-Obreschkoff method uses expressions for derivatieves of the true solution $y(t)$ by t.

$$\dot{y}(t) = f(y(t)) \tag{7}$$

$$\ddot{y}(t) = \frac{d}{dt}f(y(t)) = \frac{\partial f(y(t))}{\partial y}\dot{y}(t) = \frac{\partial f(y(t))}{\partial y}f(y(t)) \tag{8}$$

Formulas (7) and (8) in our example become

$$\dot{y}(t) = f(y(t)) = -y(t)$$

$$\ddot{y}(t) = \frac{\partial(-y)}{\partial y}(-y(t)) = y(t)$$

The first phase of the Interval-Obreschkoff method at each step finds a rough estimate of the solution - an interval $[\tilde{y}_j]$ such that for all $y_j \in [y_j]$, $t \in [t_j, t_{j+1}]$

$$y(t; t_j, y_j) \in [\tilde{y}_j] \tag{9}$$

We don't consider the first estimate in details here. In our example the rough estimate will be

$$[\tilde{y}_j] = [y_j]$$

because $0 \in [y_j]$ and absolute value of true solutions decrease with time.

4.1 Forward $IHO(1, 0)$ method

The $IHO(1, 0)$ method expands the true solution near t_j by a Taylor series of power 1.

$$y(t; t_j, y_j) = y_j + (t - t_j)f(y_j) + \frac{(t - t_j)^2}{2}\ddot{y}(\tau), t_j \le \tau \le t \tag{10}$$

The Taylor remainder is contained in the result of the interval computation of (8) on a rough estimate (9)

$$\frac{(t - t_j)^2}{2}\ddot{y}(\tau) \in \frac{h_j^2}{2}\frac{\partial f([\tilde{y}])}{\partial y}f([\tilde{y}]) \tag{11}$$

The accurate $IHO(1.0)$ estimation of $y(t_{j+1}; t_j, y_j)$ is

$$y(t_{j+1}; t_j, y_j) \in y_j + h_j f(y_j) + \frac{h_j^2}{2}\frac{\partial f([\tilde{y}])}{\partial y}f([\tilde{y}]) \tag{12}$$

For our example

$$y(t_{j+1}; t_j, y_j) \in (1 - h_j)y_j + \frac{h_j^2}{2}[\tilde{y}_j]$$

$$[y_{j+1}] = (|1 - h_j| + \frac{h_j^2}{2})[y_j]$$

The $IHO(1,0)$ is stable $(|[y_{j+1}]| < |[y_j]|$ only when $0 < h_j < \sqrt{5} - 1$.

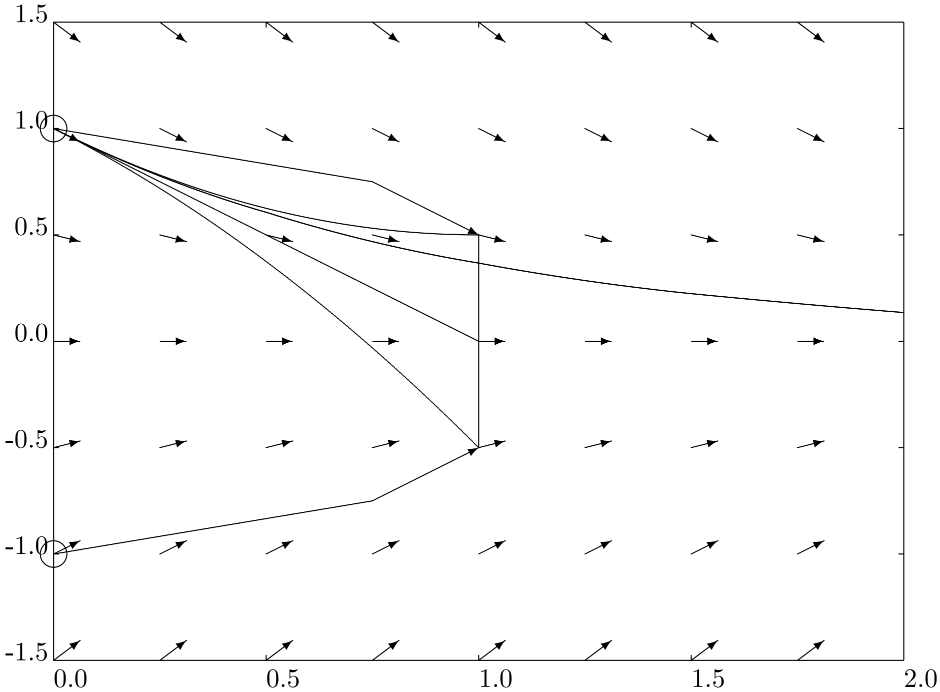

Figure 6 shows the interval Taylor expansion of $y(t; 0, 1)$. It consists of the middle line $y = 1 - t$ surrounded by a remainder interval $\frac{t^2}{2}[-1, 1]$. Arrows from small circles to the remainder interval show that the minimum and maximum of the remainder interval are determined by the second derivative of the true solution at ends of the rought estimate $[\tilde{y}] = [-1, 1]$.

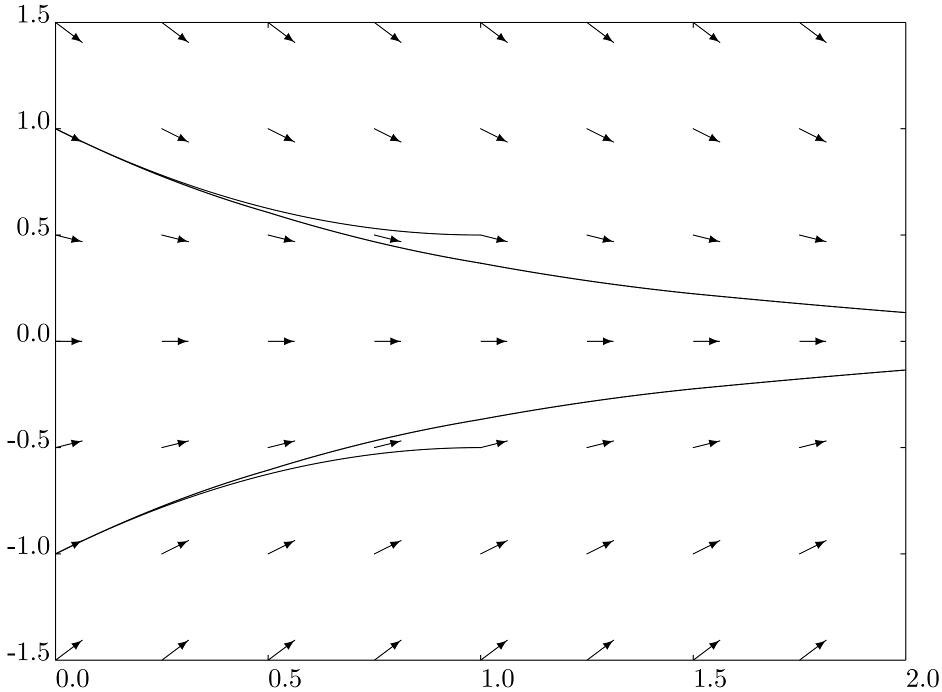

Figure 7 shows $IHO(1,0)$ bounds of $y(t;0,[-1,1])$. For $t=1$ they are $[-\frac{1}{2},\frac{1}{2}]$.

4.2 Backward $IHO(0,1)$ method

The $IHO(0,1)$ method expands the true solution near t_{j+1} by a Taylor series of power 1.

$$y(t; t_{j+1}, y_{j+1}) = y_{j+1} + (t - t_{j+1}) f(y_{j+1}) + \frac{(t - t_{j+1})^2}{2} \ddot{y}(\tau), t \leq \tau \leq t_j \quad (13)$$

The Taylor remainder is contained in the result of the interval computation of (8) on a rough estimate (9)

$$\frac{(t - t_{j+1})^2}{2} \ddot{y}(\tau) \in \frac{h_j^2}{2} \frac{\partial f([\tilde{y}])}{\partial y} f([\tilde{y}]) \quad (14)$$

For our example

$$y(t; t_{j+1}, y_{j+1}) = y_{j+1} - (t - t_{j+1}) y_{j+1} + \frac{(t - t_{j+1})^2}{2} [\tilde{y}]$$

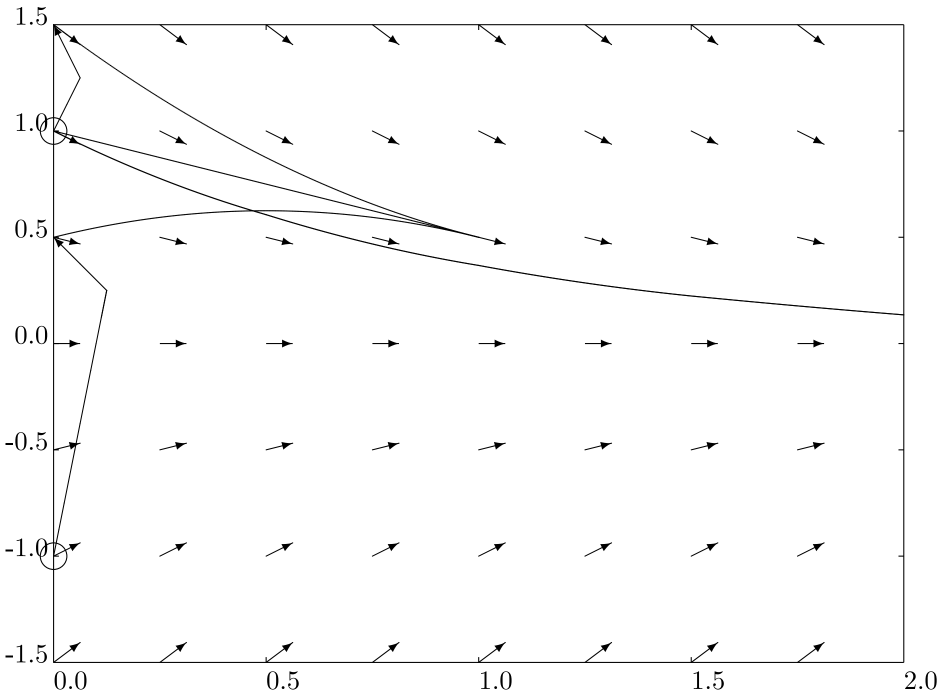

Figure 8 shows the interval Taylor expansion of $y(t; 1, \frac{1}{2})$. It consists of the middle line $y = \frac{1}{2} - \frac{1}{2}(t-1) = 1 - \frac{1}{2}t$ surrounded by a remainder interval $\frac{(t-1)^2}{2}[-1, 1]$. Arrows from small circles to the remainder interval show that the minimum and maximum of the remainder interval are determined by the second derivative of the true solution at ends of the rought estimate $[\tilde{y}] = [-1, 1]$.

The $IHO(0,1)$ method considers that the interval bound of $y(t_{j+1}; t_j, y_j)$ consists of all y_{j+1} for which

$$y_j \in y_{j+1} - h_j f(y_{j+1}) + \frac{h_j^2}{2} \frac{\partial f([\tilde{y}])}{\partial y} f([\tilde{y}]) \tag{15}$$

For our example

$$y_j \in (1 + h_j) y_{j+1} + \frac{h_j^2}{2} [\tilde{y}_j]$$

$$[y_{j+1}] = \frac{1 + \frac{h_j^2}{2}}{1 + h_j} [y_j]$$

The $IHO(1,0)$ is stable ($|[y_{j+1}]| < |[y_j]|$ only when $0 < h_j < 2$.

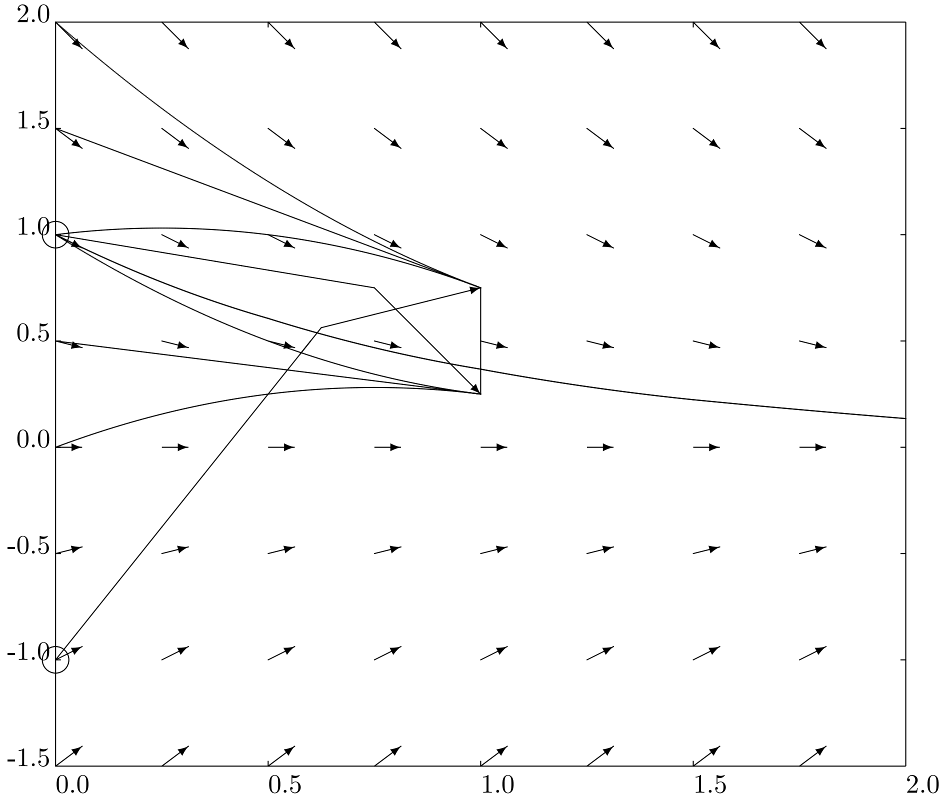

Figure 9 shows minimal $y_1 = \frac{1}{4}$ and maximal $y_1 = \frac{3}{4}$ such that $y_0 = 1$ is in the interval Taylor expansion of $y(t; 1, y_1)$.

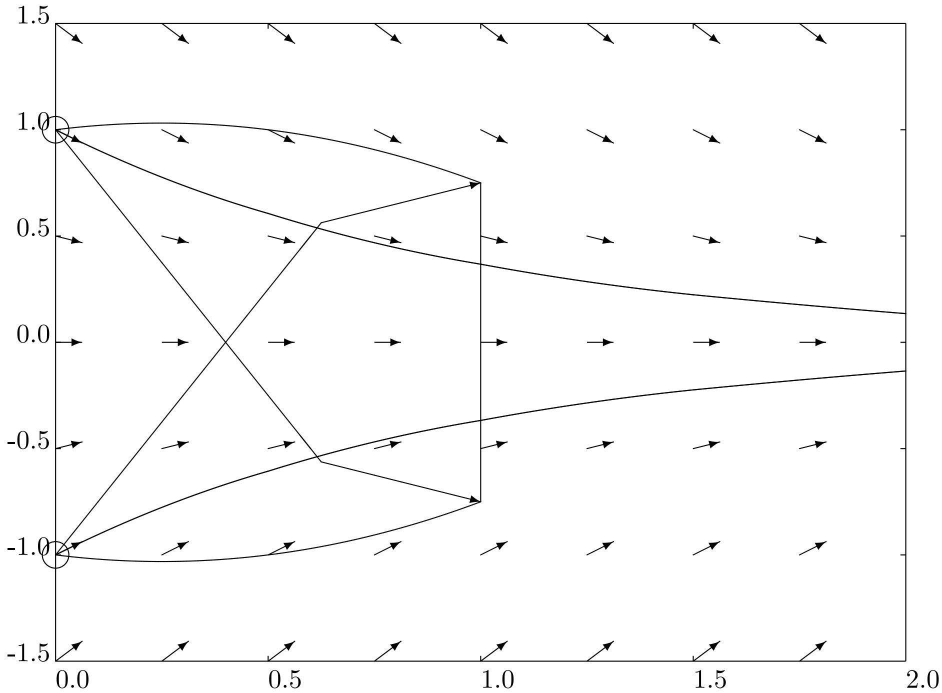

Figure 10 shows $IHO(0,1)$ bounds of $y(1;0,[-1,1])$. They are $[-\frac{3}{4},\frac{3}{4}]$.

This figure shows the interval analog $IHO(0,1)$ of the point Backward Euler is not as stable as the point method.

1) The curvatives of the upper and the lower bounds are derived from $\ddot{y}(0)$ and this is larger than the average absolute value of $\ddot{y}(t)$ over the entire timestep;

2) The curvative of the upper bound of solutions is derived from the $\ddot{y}(t)$ at the lower end of initial interval and the curvative of the lower bound of solutions is derived from the $\ddot{y}(t)$ at the higher end of initial interval;

The Chaplygin method is free from these issues.

5 Chaplygin method

Let $\hat{y}(t)$ is a smooth function considered as approximate solution of (1). The defect of $\hat{y}(t)$ is defined as $\delta(t) = \frac{d\hat{y}}{dt} - f(\hat{y}(t))$. Here is Chaplygin's theorem about differential inequalities. Suppose that $\underline{y}(t)$ and $\overline{y}(t)$ are smooth functions such that their defects are respectively negative and positive at timestep and that their values at begin of timestep bound the intitial value of y_j:

$$\dot{\underline{y}}(t) - f(\underline{y}(t)) < 0 \tag{16}$$

$$\dot{\overline{y}}(t) - f(\overline{y}(t) > 0 \tag{17}$$

$$\underline{y}(t_j) \leq y_j \leq \overline{y}(t_j) \tag{18}$$

when $t_j \leq t \leq t_{j+1}$. Then for all $t_j < t \leq t_{j+1}$

$$\underline{y}(t) < y(t; t_j, y_j) < \overline{y}(t) \tag{19}$$

Graphically, inequalities (16) and (17) means that the velocity vectors on curves $\underline{y}(t)$ and $\overline{y}(t)$ are derected inward the region between the curves. Anylitically, we can verify (16) and (17) by interval algorithm of search of roots of defect expressions in the interval $[t_j, t_{j+1}]$. Such algorithms are described for example in [2].

The difficulty of Chaplygin's method is to guess $\underline{y}(t)$ and $\overline{y}(t)$. For any $\epsilon > 0$ we could choose such a pair in our example

$$\underline{y}(t) = e^{-t} - \epsilon$$

$$\overline{y}(t) = e^{-t} + \epsilon$$

The conditions (16-18) are satisfied

$$\dot{\underline{y}}(t) - f(\underline{y}(t)) = -e^{-t} + (e^{-t} - \epsilon) = -\epsilon < 0$$

$$\dot{\overline{y}}(t) - f(\overline{y}(t)) = -e^{-t} + (e^{-t} + \epsilon) = \epsilon > 0$$

$$\underline{y}(0) <= 1 <= \overline{y}(0)$$

So $y(t; 0, 1) \in [e^{-t} - \epsilon, e^{-t} + \epsilon]$ and the width of this interval can be made arbitrarily small for any given t. However, this is not "honest", because guessing these bounds is as hard as finding the exact solution. We should restrict $\underline{y}(t)$ and $\overline{y}(t)$ to some simple class of functions.

We can restrict $\underline{y}(t)$ and $\overline{y}(t)$ by polynomials.
For our example we could choose

$$\underline{y}(t) = 1 - t$$
$$\overline{y}(t) = 1 - t + \frac{1}{2}t^2$$

The conditions (16-18) are satisfied when $t > t_0 = 0$

$$\dot{\underline{y}}(t) - f(\underline{y}(t)) = (-1) + (1 - t) = -t < 0$$
$$\dot{\overline{y}}(t) - f(\overline{y}(t)) = (-1 + t) + (1 - t + \frac{1}{2}t^2) = \frac{1}{2}t^2 > 0$$
$$\underline{y}(0) <= 1 <= \overline{y}(0)$$

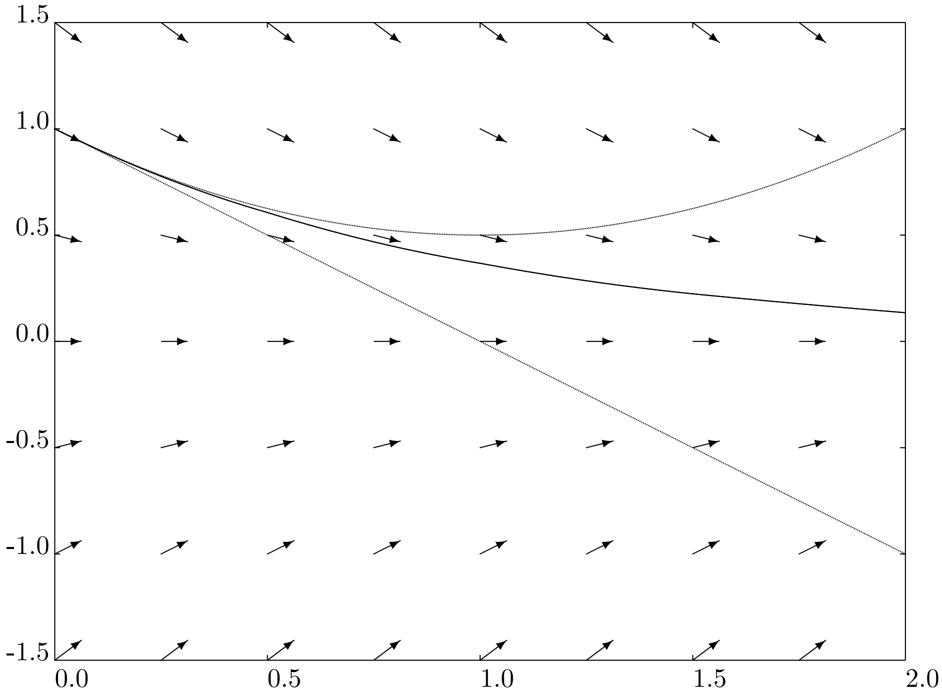

Figure 11 shows a pair of bound functions $y(t; 0, 1) \in [\underline{y}, \overline{y}] = [1-t, 1-t+\frac{1}{2}t^2]$

6 First-order Chaplygin method

We can further restrict Chaplygin bound functions $\underline{y}(t)$ and $\overline{y}(t)$ to be linear.

$$\underline{y}(t) = \underline{a} + \underline{k}(t - t_j) \tag{20}$$

$$\overline{y}(t) = \overline{a} + \overline{k}(t - t_j) \tag{21}$$

Then conditions (16-18) for any $t_j <= t <= t_{j+1}$

$$\underline{k} - f(\underline{a} + \underline{k}(t - t_j)) < 0 \tag{22}$$

$$\overline{k} - f(\overline{a} + \overline{k}(t - t_j)) > 0 \tag{23}$$

$$\underline{a} <= y_j <= \overline{a} \tag{24}$$

If $\frac{\partial f(y)}{\partial y} < \frac{1}{h_j}$ then the left sides of (22-23) are monotonic by $\underline{k}$ and $\overline{k}$. Hence there are $\underline{k}^*(t)$ and $\overline{k}^*(t)$ such that

$$\underline{k}^*(t) - f(\underline{a} + \underline{k}^*(t)(t - t_j)) = 0 \tag{25}$$

$$\overline{k}^*(t) - f(\overline{a} + \overline{k}^*(t)(t - t_j)) = 0 \tag{26}$$

and (22)-(23) are equivalent to

$$\underline{k} < \min_{t \in [t_j, t_{j+1}]} \underline{k}^*(t) \tag{27}$$

$$\overline{k} > \max_{t \in [t_j, t_{j+1}]} \overline{k}^*(t) \tag{28}$$

For our example

$$\underline{k}^*(t) = \frac{-\underline{a}}{1 + (t - t_j)}$$

$$\underline{k} = -\underline{a} \qquad \text{when } \underline{a} >= 0$$

$$\underline{k} = \frac{-\underline{a}}{1 + h_j} \qquad \text{when } \underline{a} <= 0$$

$$\overline{k}^*(t) = \frac{-\overline{a}}{1 + (t - t_j)}$$

$$\overline{k} = -\overline{a} \qquad \text{when } \overline{a} <= 0$$

$$\overline{k} = \frac{-\overline{a}}{1 + h_j} \qquad \text{when } \overline{a} >= 0$$

So if we choose $[\underline{a}, \overline{a}] = [y_0] = [-1, 1]$

$$[y_1] = y(h; 0, [-1, 1]) = [-1 + \frac{1}{1+h}h, 1 - \frac{1}{1+h}h] = [-\frac{1}{1+h}, \frac{1}{1+h}]$$

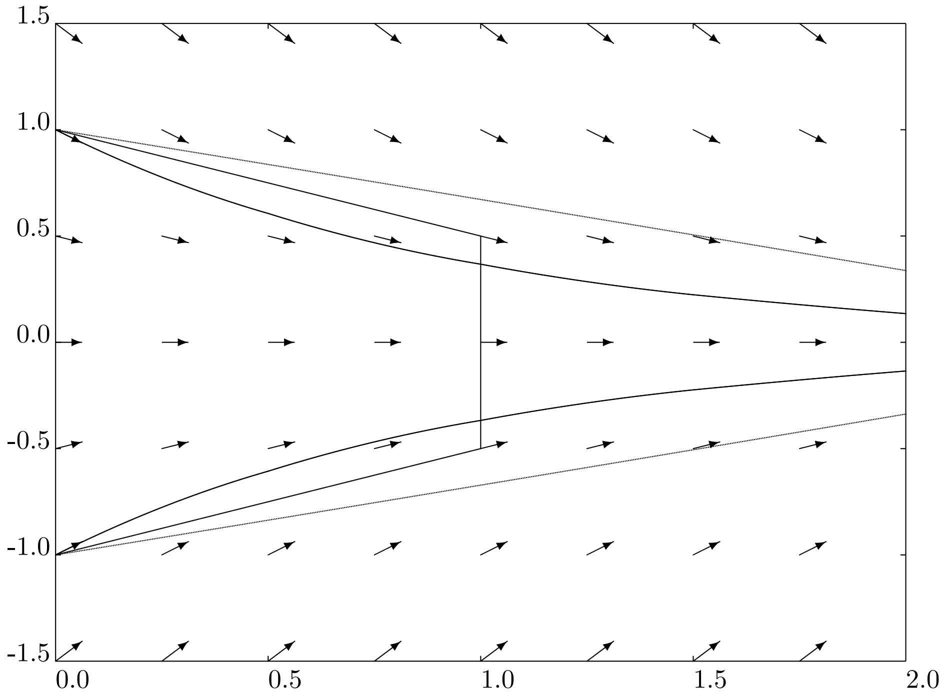

Figure 12 shows intervals returned by first order Chaplygin method for $h = 1$ and $h = 2$.

$$y(1; 0, [-1, 1]) \subset [y_1] = [-\frac{1}{2}, \frac{1}{2}]$$
$$y(2; 0, [-1, 1]) \subset [y_1] = [-\frac{1}{3}, \frac{1}{3}]$$

The method is stable ($|[y_1]| < |[y_0]|$) for any $h > 0$.

Let us make bounds $y(h;0,1)$. If we choose $[\underline{a},\overline{a}] = [1,1]$ then the method will give us

$$y(h;0,1) \in [1-h, 1-\frac{1}{1+h}h] = [1-h, \frac{1}{1+h}]$$

When $h > 1$ the lower bound of the interval becomes negative. The interval becomes too wide. However, if we choose $[\underline{a},\overline{a}] = [0,1]$ then the method will give us

$$y(h;0,1) \in [0, 1-\frac{1}{1+h}h] = [0, \frac{1}{1+h}]$$

which is better. We see that in the Chaplygin method, a wider initial interval may give a narrower final interval for large timesteps.

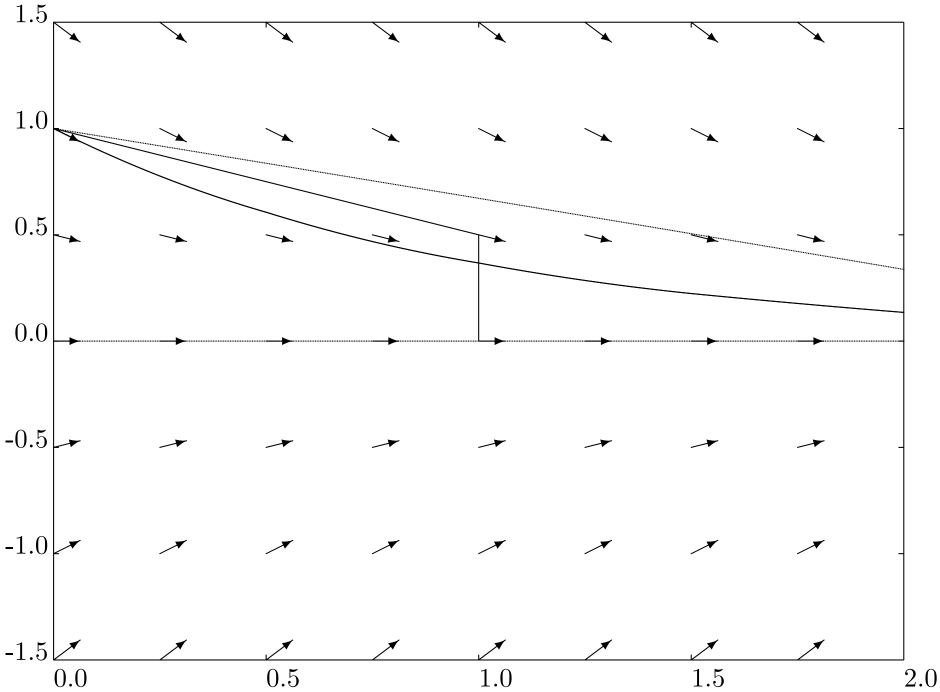

Figure 13 shows intervals returned by first order Chaplygin method for $h = 1$ and $h = 2$.

$$y(1;0,[1,1]) \subset [y_1] = [0, \frac{1}{2}]$$
$$y(2;0,[1,1]) \subset [y_1] = [0, \frac{1}{3}]$$

7 Conclusion

The Chaplygin validated method for IVP solutions seems more stable than IHO methods on stiff problems, Also it doesn't require interval computation of higher derivatives of right-hand side $f(y)$. This method seems attractive for Interval Spice simulation, where parasitics make IVP stiff, and empirical device models may not be smooth enough.

However, this will be possible only after developing automatic methods for choosing Chaplygin's bound functions $\underline{y}(t)$ and $\overline{y}(t)$

8 References

[1] Computing Rigorous Bounds on the Solution of an Initial Value Problem for an Ordinary Differential Equation, Nedialko (Ned) Stoyanov Nedialkov, Ph.D. Thesis, Computer Science Dept., Univ. of Toronto, 1999. http://www.cs.toronto.edu/pub/reports/na/ned-99-phd.ps.gz

[2]Global Optimization using Interval Anaylysis: Second Edition, Eldon Hansen, G.William Walster, Marcel Dekker, Inc, 2004.