RIGOROUS NUMERICS FOR MAPS AND ODEs

P. Zgliczyński

Jagiellonian University, Kraków, Poland

http://www.ii.uj.edu.pl/~zgliczyn

Interval arithmetics a cure for round-off errors

Arithmetics on closed intervals. For example:

- $[1,3] \langle + \rangle [3,17] = [4,20]$
- 1 ⟨/⟩ 3 = [0.33333, 0.33334]

diam $[a_-, a^+] = a^+ - a^-, \quad m([a_-, a^+]) = (a^+ + a^-)/2$

Rigorous interval arithmetics can be realized on the computer i.e. for each arithmetic operator $\diamondsuit \in \{+, -, \cdot, /\}$ the following is true

$$[a_{-}, a^{+}] \diamondsuit [b_{-}, b_{+}] \subset [a_{-}, a^{+}] \langle \diamondsuit \rangle [b_{-}, b_{+}]$$

For any elementary function $f: {\bf R}^n \to {\bf R}^s$ and any set $Z \subset {\bf R}^n$

$$f(Z) \subset \langle f \rangle (\langle Z \rangle)$$

Interval arithmetics - problems

wrapping

the result of evaluation of multidimensional map is product of intervals, disastrous results when considering f^n for *n*-large, ODEs

• dependency: for x = [-1, 1] holds

$$x \langle - \rangle x = [-2, 2]$$

Another example:

$$e^{-x} = \sum_{n=0}^{\infty} \frac{(-1)^n x^n}{n!}$$

 $[1 - \sinh(t), \cosh(t)] \subset \langle e^{-[0,t]} \rangle$

diam $(\langle e^{-[0,t]} \rangle) \ge e^t - 1$, diam $(e^{-[0,t]}) = 1 - e^{-t}$

Interval arithmetics - fighting the dependency problem

Let $[X] \subset \mathbf{R}^n$ - convex, $x_0 \in [X]$, $f : \mathbf{R}^n \to \mathbf{R}^k$ C^1 -function, then

 $f([X]) \subset f(x_0) + [df([X])]_I \cdot ([X] - x_0) \quad (1)$ where $[df([X])]_I$ is the interval enclosure of df([X])

$$[df(Z)]_{I} = \left\{ M \in \mathbf{R}^{k \times n}, \\ M_{ij} \in \left[\inf_{z \in Z} \frac{\partial f_{i}}{\partial x_{j}}(z), \sup_{z \in Z} \frac{\partial f_{i}}{\partial x_{j}}(z) \right] \right\}$$

Mean value form: Let $x_0 = m([X_0])$, then we set

$$\langle f \rangle ([X]) = \langle f \rangle (x_0) + \langle [df([X])]_I \cdot ([X] - x_0) \rangle$$

Interval arithmetics - fighting the dependency problem, Examples

• evaluation of f(x) = x - x, will give zero

• evaluation of $f(x) = x^2 - x^2$ on [-1, 1]< $f([-1, 1]) \ge 0 + (2x - 2x)[-1, 1] = [-4, 4]$ rather bad result

• evaluation of
$$f(x) = e^{-x}$$

$$< e^{-[0,t]} > = e^{-t/2} + \left(-e^{-[0,t]}\right) \cdot \left[-\frac{t}{2}, \frac{t}{2}\right] = e^{-t/2} + t/2 \cdot e^{-[0,t]} \cdot \left[-1, 1\right] = e^{-t/2} + t \cosh(t)/2 \cdot \left[-1, 1\right]$$

Hence

diam($\langle e^{-[0,t]} \rangle$) = $t \cosh t = t + \frac{t^3}{2!} + \frac{t^5}{4!} + \dots$, for small t we have improvement, for t large it is worse.

5

Some methods for the reduction of the error growth

• set division: Let $S_t = \varphi(t, S)$. When S_t becomes too large, one should divide it into smaller pieces and compute further the evolution of each each piece separately

• Lohner algorithm: in order to avoid wrapping effect one should choose good coordinate frame in each step

• Taylor models (Berz, Makino):

Interval arithmetics - fighting the dependency problem, Taylor models(Berz, Makino)

All sets represented as image of polynomial maps plus small remainder term (Taylor models) - similar to symbolic computations

application of map to such that such - recomputation of the coefficient in the Taylor model

very general, flexible, virtually no dependency and wrapping problems

very slow and hard to program

One step of the Lohner algorithm

x'=f(x) induces $\varphi(t,x_0)$ - $t\text{-time},\ x_0$ - initial condition,

 $\Phi(h, x)$ - numerical method, Taylor method of order p

Input:

- t_k time, h_k time step
- $[x_k] \subset \mathbf{R}^n$, such that $\varphi(t_k, [x_0]) \subset [x_k]$

Output:

- $t_{k+1} = t_k + h_k$
- $[x_{k+1}] \subset \mathbf{R}^n$, such that $\varphi(t_{k+1}, [x_0]) \subset [x_{k+1}]$

1. Rough enclosure of $\varphi([0, h_k], [x_k])$ $[W_1] \subset \mathbf{R}^n$ compact and convex $\varphi([0, h_k], [x_k]) \subset [W_1]$

2.
$$[A_k] = \frac{\partial \Phi}{\partial x}(h_k, [x_k])$$

3. $[x_{k+1}] (m([x_k]) - \text{midpoint of } [x_k])$ $[x_{k+1}] = \Phi(h_k, m([x_k])) + [A_k]([x_k] - m([x_k])) + \text{Rem}([W_1])$

Taylor method - for rigorous integration of ODEs

x' = f(x), $x(0) = x_0$ give rise to $\varphi(t, x_0)$ [X], [Y] - interval sets - products of intervals

If $[Y] = [X] + [0, h]f([Z]) \subset int[Z]$, then $\varphi([0, h], [X]) \subset [Y]$.

Taylor expansion for $\varphi(h, x)$ for $x \in \mathbb{R}^n$, with respect to h (below n = 1), can be generated from ODE (automatic differentiation algorithm)

$$\frac{\partial}{\partial t}\varphi(0,x_0) = x^{(1)}(x_0) = f(x_0)$$
$$\frac{\partial^2}{\partial t^2}\varphi(0,x_0) = x^{(2)}(x_0) = f'(x_0)x^{(1)}$$
$$\frac{\partial^3}{\partial t^3}\varphi(0,x_0) = x^{(3)}(x_0) = f^{(2)}(x_0)(x')^2 + f'(x_0)x^{(2)}$$
...

Error term (r - the order of the Taylor method) $\frac{\partial^{r+1}}{\partial t^{r+1}}\varphi(\theta h, x_0) = \frac{\partial^{r+1}}{\partial t^{r+1}}\varphi(0, \varphi(\theta h, x_0)) \subset x^{r+1}([Y]).$

$$\varphi(h, [X_0]) \subset [X_0] + \sum_{k=1}^r x^{(k)} ([X_0]) \frac{h^k}{k!} + x^{r+1} ([Y]) \frac{h^{r+1}}{(r+1)!}.$$

Reduction of the wrapping effect

 $[x_k] = x_k + [r_k], \qquad x_k = m([x_k]), [r_k] = [x_k] - x_k$

The equation to evaluate:

$$[r_{k+1}] = [A_k][r_k] + [z_{k+1}]$$

Eventual reduction of the wrapping effect depends on how we will represent $[r_k]$

- interval set $[r_k] = \prod I_j$, I_j -interval
- \bullet parallelepiped $[r_k] = B_k[\tilde{r}_k],\ B_k$ matrix, \tilde{r}_k -interval set

 \bullet cuboid $[r_k] = Q_k[\tilde{r}_k], \; \tilde{r}_k$ -interval set, Q_k orthogonal matrix

• doubleton $[r_k] = C_k[r_0] + [\tilde{r}_k]$, C_k matrix, $[\tilde{r}_k]$ is either cuboid, parallelepiped or interval set

using interval sets == wrapping effect

other approaches try to minimize wrapping through choosing good coordinate frame

We choose different coordinate frame: $[r_k] = B_k[\hat{r}_k]$,

$$[r_{k+1}] = [A_k][r_k] + [z_{k+1}] = B_{k+1} \left(B_{k+1}^{-1} [A_k] B_k[\hat{r}_k] + B_{k+1}^{-1} [z_{k+1}] \right)$$

$$[r_0] = [B_0][\hat{r}_0], \quad [B_0] = \{Id\}$$
$$[\hat{r}_{k+1}] = \left([B_{k+1}^{-1}][A_k][B_k] \right) [\hat{r}_k] + [B_{k+1}^{-1}][z_{k+1}]$$
$$[r_{k+1}] = [B_{k+1}][\hat{r}_{k+1}]$$

Usually B_{k+1} is a Q-factor from QR decomposition of $U \in [A_k][B_k]$, but first we permute columns of U, so that their norms are decreasing

Even better:

$$[r_{k+1}] = C_{k+1}[r_0] + [\tilde{r}_{k+1}]$$

$$[\tilde{r}_{k+1}] = [A_k][\tilde{r}_k] + [z_{k+1}] + ([A_k]C_k - C_{k+1})[r_0],$$

$$[\tilde{r}_0] = 0$$

and $C_0 = Id, \quad C_{k+1} \in [A_k]C_k$

 $[\tilde{r}_k]$ is evaluated using previous method

When Lohner algorithm can fail?

Only the first step - the generation of the rough enclosure - is heuristic. It can happen that a solution does not exists on $[0, h_k]$.

Easy first order rough enclosure

$$x' = f(x), \quad x \in \mathbb{R}^n, \quad f \in C^1$$
 (2)
 $\varphi(t, x)$ the flow induced by (2)

Theorem: Let h > 0. Let X, Z be interval sets, $X \subset intZ$. Suppose that

 $Y := \text{interval hull}(X + [0, h]f(Z)) \subset \text{int}Z \quad (3)$ then

$$\varphi([0,h],X) \subset Y \tag{4}$$

Problem: For x' = -Lx we have a bound for the time step

$$h < \frac{1}{L}$$

Insert here an example for n = 2 with one dissipative coordinate

Improved rough enclosure for dissipative ODE

$$x'_{i} = f_{i}(x) = \lambda_{i}x_{i} + N_{i}(x), \quad i = 1, \dots, n$$
 (5)

Theorem: h > 0, $X \subset Z \subset \mathbb{R}^n$ - interval sets. Let $D \subset \{1, \ldots, n\}$ (*dissipative*(damped) directions), if $k \in D$, then

$$\lambda_k < 0$$

$$\lambda_k x_k + N_k^- < \dot{x}_k < \lambda_k x_k + N_k^+$$

where $N_k(Z) \subset (N_k^-, N_k^+)$.

For $k \in D$ we set

$$b_k^{\pm} = \frac{N_k^{\pm}}{-\lambda_k}$$

$$g_k^{\pm} = \left(X_k^{\pm} - b_k^{\pm}\right) e^{\lambda_k h} + b_k^{\pm}.$$

18

Let
$$Y = \prod_{i=1}^{n} Y_i$$
 be such that
 $Y_i = X_i + [0, h] f_i(Z), \quad i \notin D$
 $Y_i = Z_i, \quad i \in D.$

Then

$$\varphi([0,h],X) \subset Y,$$

provided the following conditions are satisfied for $i=1,\ldots,n$

1. if $i \notin D$, then

$$Y_i \subset \operatorname{int} Z_i$$

2. upper bounds for $i \in D$ if $Z_i^+ < b_i^+$, then $Z_i^+ \ge g_k^+$

3. *lower bounds* for
$$i \in D$$

$$\text{if } \quad Z_i^- > b_i^-, \quad \text{then} \quad Z_i^- \leq g_k^- \\$$

For

$$x' = -Lx, \quad L > 0$$

and X = [-1, 1] one obtains Y = [-1, 1] and no bound on h > 0.

Computation of the Poincaré map

•One needs a procedure which gives a rigorous estimates between time steps for *x*-variable for ODE - rough enclosure ok

• we need to come very close to section

•the section error is minimized for sections perpendicular to the flow

Lohner algorithm

 $[x_k] = x_k + [r_k],$ where $[r_k] = Q_k[\tilde{r}_k]$ or $[r_k] = C_k[r_0] + Q_k[\tilde{r}_k]$

1. Finding rough enclosure [W] of $\varphi([0, h_k], [x_k])$

2.
$$[A_k] = \frac{\partial \Phi}{\partial x}(h, [x_k])$$

3.
$$x_{k+1} = m(\Phi(h_k, x_k)),$$

 $[z_{k+1}] = Rem([W]) + \Phi(h_k, x_k) - x_{k+1}$

4. $[r_{k+1}] = [A_k] \cdot [r_{k+1}] + [z_{k+1}]$ - the rearangement computations

Step 2 - the most time consuming part (we practically solve variational equation)

 $Cost(Step 2) \approx n^{?}Cost(Step 3)$

Cost(Step3) >> Cost(Step1 + Step4)

Very slow compared to nonrigorous computations by factor of order 10n.

Reasons:

the interval arithmetics is at least two times slower than nonrigorous one

The Lohner algorithm is a C^0 -algorithm, but internally is in fact C^1

Question: Can one do better with C^0 algorithm?

C^0 - algorithm

 $[x_k] = x_k + B(0, r_k)$, where $r \in \mathbb{R}$, B(0, r) - the ball of radius r. The choice of the good norm is an important parameter of algorithm.

- **1.** Find rough enclosures $\varphi([0, h_k], [x_k]) \subset [W]$ of and $\varphi([0, h_k], x_k) \subset [W_1]$
- **2.** compute l = l(df([W]))

3.
$$x_{k+1} = m(\Phi(h_k, x_k) + Rem([W_1])), z_{k+1} = \Phi(h_k, x_k) + Rem([W_1]) - x_{k+1}$$

4.
$$r_{k+1} = r_k e^{lh_k} + ||z_{k+1}||$$

Question: what is l(df([W]))?

Propagation of errors according to the typical numerical analysis textbook:

$$x' = f(x)$$

$$|f(x) - f(y)| \le L|x - y|.$$
(6)

Let $\varphi(t, x_0)$ be a solution of (6) with an initial condition $x(0) = x_0$. Then

$$|\varphi(t,x) - \varphi(t,y)| \le e^{Lt}|x-y|, \qquad t \ge 0$$

This is very bad estimate

Examples:

 $\bullet \, x' = -10 x$, predicts error-growth: e^{10t}

• for the Lorenz attractor (from the proof by Galias and P. Z.), gives an estimate for Lipschitz constant for the Poincare map $L > 10^9$, while from simulations it is clear that $L \approx 5-6$

• in the proof for Rössler system (P.Z.), gives an estimate for the Lipschitz constant of Poincare map $L > 5 \cdot 10^{41}$, while from simulations $L \approx$ 2-3 cosmic computation time

Logarithmic norms

Logarithmic norm: $Q \in R^{n \times n}$ $\mu(Q) = \lim_{h>0, h \to 0} \frac{\|I + hQ\| - 1}{h}$ can be negative !!!

• for Euclidean norm $\mu(Q) = \text{the largest eigenvalue of} \quad 1/2(Q+Q^T).$

• for max norm $||x|| = \max_k |x_k|$ $\mu(Q) = \max_k (q_{kk} + \sum_{i \neq k} |q_{ki}|)$

• for norm
$$||x|| = \sum_k |x_k|$$

$$\mu(Q) = \max_i (q_{ii} + \sum_{k \neq i} |q_{ki}|)$$

Logarithmic norms - Fundamental lemma

Lemma: Let $\phi(t, x)$ be a flow induced by

x' = f(x).

Assume that Z is a convex set,

$$y([0,T]), \varphi([0,T], x_0) \in Z$$
$$\mu\left(\frac{\partial f}{\partial x}(\eta)\right) \leq l, \quad \text{for } \eta \in Z$$
$$\left\|\frac{dy}{dt}(t) - f(y(t))\right\| \leq \delta.$$

Then for $0 \leq t \leq T$ we have

 $\|\varphi(t,x_0)-y(t)\| \le e^{lt}\|y(0)-x_0\|+\delta \frac{e^{lt}-1}{l}, \quad \text{if } l \ne 0.$

For l = 0 we have

$$\|\varphi(t,x_0)-y(t)\|\leq \rho+\delta t.$$

In particular: e^{lT} is a Lipschitz constant for $\phi(t, \cdot)$ in Z (if Z is forward invariant).

Examples:

 $\bullet \, x' = -10 x$, predicts error-growth: $e^{-10t} \, \mathrm{very}$ good

• in the proof for Rössler system (P.Z.) logaritmic norm based on the euclidian norm was used, the estimate for the Lipschitz constant of Poincare map in some region was $L > 2 \cdot 10^4$, while from simulations $L \approx 2-3$ this is doable. Using Lohner algorithm with cuboids one get Lipschitz constant around 60 and using doubletons something like 6-10.

Lohner-type algorithm for differential inclusion

$$x'(t) \in f(x(t)) + [\delta]$$
 (7)
 $x \in \mathbf{R}^n$, $[\delta] \subset \mathbf{R}^n$
Find a rigorous enclosure for $x(t)$.

We compare the solutions of two ODEs

$$x_1' = f(x_1), (8)$$

$$x'_2 = f(x_2) + y(t)$$
 (9)

$$x_1(t_0) = x_2(t_0) = x_0 \tag{10}$$

where $y(t) \in [\delta]$ is given (but unknown) function.

Lohner-type algorithm for differential inclusion - Fundamental Lemma

Lemma: Let: $[W_1] \subset [W_2] \subset \mathbb{R}^n$ - convex and compact. $x_1([t_0, t_0+h]) \subset [W_1], x_2([t_0, t_0+h]) \subset [W_2]$ for any continuous function $y : [t_0, t_0+h] \rightarrow [\delta]$.

Then the following inequality holds for $t \in [t_0, t_0 + h]$ and for $i = 1, ..., n_1$

$$|x_{1,i}(t) - x_{2,i}(t)| \le \left(\int_{t_0}^t e^{J(t-s)}C\,ds\right)_i, \quad (11)$$

where

$$C_{i} \geq \sup |[\delta_{i}]|, \quad i = 1, ..., n_{1}$$

$$J_{ij} \geq \sup \frac{\partial f_{i}}{\partial x_{j}}([W_{2}]) \text{ if } i = j,$$

$$J_{ij} \geq \sup \left| \frac{\partial f_{i}}{\partial x_{j}}([W_{2}]) \right| \text{ if } i \neq j.$$

31

Lohner-type algorithm for differential inclusion - one step

 $\varphi(t, x_0, [\delta])$ - a solution of $x' \in f(x) + [\delta], x(0) = x_0$. $\overline{\varphi}(t, x_0)$ - a solution of $x' = f(x), x(0) = x_0$.

Input data: t_k , h_k - a time step, $[x_k] \subset \mathbf{R}^n$, such that $\varphi(t_k, [x_0], [\delta]) \subset [x_k]$.

Output data: $t_{k+1} = t_k + h_k$, $[x_{k+1}] \subset \mathbb{R}^{n_1}$, such that $\varphi(t_{k+1}, [x_0], [\delta]) \subset [x_{k+1}]$. Lohner-type algorithm for differential inclusion - one step - details

1. Generation of a priori bounds for φ . Find a convex and compact set $[W_2] \subset \mathbf{R}^n$, such that

$$\varphi([0, h_k], [x_k], [\delta]) \subset [W_2].$$
(12)

2. Computation of $\overline{\varphi}$. We use Lohner algorithm to obtain $[\overline{x}_{k+1}] \subset \mathbf{R}^n$ and a convex and compact set $[W_1] \subset \mathbf{R}^n$, such that

$$\overline{\varphi}(h_k, [x_k]) \subset [\overline{x}_{k+1}]$$

$$\overline{\varphi}([0, h_k], [x_k]) \subset [W_1]$$

Lohner-type algorithm for differential inclusion - one step - details continued

3. Computation of perturbation. Using Fundamental Lemma we find a set $[\Delta] \subset \mathbf{R}^n$, such that

$$\varphi(t_{k+1}, [x_0], [\delta]) \subset \overline{\varphi}(h_k, [x_k]) + [\Delta].$$
 (13)
Hence

$$\varphi(t_{k+1}, [x_0], [y_0]) \subset [x_{k+1}] = [\overline{x}_{k+1}] + [\Delta]$$
(14)

Lohner-type .. - details and comments

Part 3 - details

1. We set

$$C_{i} = \operatorname{right} \left(\left| \begin{bmatrix} \delta_{i} \end{bmatrix} \right| \right), \quad i = 1, \dots, n_{1}$$
$$J_{ij} = \operatorname{right} \left(\frac{\partial f_{i}}{\partial x_{i}} (\begin{bmatrix} W_{2} \end{bmatrix}) \right) \text{ if } i = j,$$
$$J_{ij} = \operatorname{right} \left(\left| \frac{\partial f_{i}}{\partial x_{j}} (\begin{bmatrix} W_{2} \end{bmatrix}) \right| \right), \text{ if } i \neq j.$$
$$2.D = \int_{0}^{h} e^{J(h-s)} C \, ds$$

3. $[\Delta_i] = [-D_i, D_i]$, for $i = 1, ..., n_1$

Lohner-type ... - Computation of $\int_0^t e^{A(t-s)} C \, ds.$

$$\int_{0}^{t} e^{A(t-s)} C \, ds = t \left(\sum_{n=0}^{\infty} \frac{(At)^{n}}{(n+1)!} \right) \cdot C. \quad (15)$$

We fix any norm $\|\cdot\|$, preferably the L^{∞} -norm, $(\|x\|_{\infty} = \max_{i} |x_{i}|).$

$$\tilde{A} = At, \qquad A_n = \frac{\tilde{A}^n}{(n+1)!},$$
$$\sum_{n=0}^{\infty} \frac{(At)^n}{(n+1)!} = \sum_{n=0}^{\infty} A_n$$
$$A_0 = \mathrm{Id}, \qquad A_{n+1} = A_n \cdot \frac{\tilde{A}}{n+2}$$

Remainder: $||A_{N+k}|| \le ||A_N|| \cdot \left\|\frac{\tilde{A}}{N+2}\right\|^k$. If $\left\|\frac{\tilde{A}}{N+2}\right\| < 1$, then

$$\left\|\sum_{n>N} A_n\right\| \le \|A_N\| \cdot \left\|\frac{\tilde{A}}{N+2}\right\| \cdot \left(1 - \left\|\frac{\tilde{A}}{N+2}\right\|\right)^{-1}$$

Lohner-type .. - Representation of sets and rearrangement.

Lohner's approach.

In part 3:

$$[x_{k+1}] = [\overline{x}_{k+1}] + [\Delta]$$
(16)

Evaluations 2 and 3. In this representation

$$[x_k] = x_k + [B_k][\tilde{r}_k].$$
(17)

In the context of our algorithm in part 3 we obtain

$$[\overline{x}_{k+1}] = \overline{x}_{k+1} + [B_{k+1}][\overline{r}_{k+1}].$$
(18)

We set

$$\begin{aligned} x_{k+1} &= m(\overline{x}_{k+1} + [\Delta]) \\ [\tilde{r}_{k+1}] &= [\overline{r}_{k+1}] + [B_{k+1}^{-1}] \left(\overline{x}_{k+1} + [\Delta] - x_{k+1} \right). \end{aligned}$$

Lohner-type .. - Representation of sets and rearrangement II

Evaluation 4. In this representation

$$[x_k] = x_k + C_k[r_0] + [B_k][\tilde{r}_k].$$
(19)

In the context of our algorithm in part 3 we obtain

$$[\overline{x}_{k+1}] = \overline{x}_{k+1} + C_{k+1}[r_0] + [B_{k+1}][\overline{r}_{k+1}].$$
(20)

Equation (16) is taken into account exactly in the same way as in previous evaluations, i.e. we use equations (19) and (19).

Variational equations, C^n -computations

Let

$$\frac{\partial \varphi_i}{\partial x_j}(t, x_0) = V_{i,j}(t),$$
$$\frac{\partial^2 \varphi_i}{\partial x_j \partial x_k}(t, x_0) = H_{ijk}(t).$$

It is well known that

$$x' = f(x), \qquad (21)$$

$$\frac{d}{dt}V_{ij}(t) = \sum_{s=1}^{n} \frac{\partial f_i}{\partial x_s}(x)V_{sj}(t) \qquad (22)$$

$$\frac{d}{dt}H_{ijk}(t) = \sum_{s,r=1}^{n} \frac{\partial^2 f_i}{\partial x_s \partial x_r}(x)V_{rk}(t)V_{sj}(t) + \sum_{s,r=1}^{n} \frac{\partial f_i}{\partial x_s \partial x_r}(x)V_{sj}(t) + \sum_{s,r=1}^{n} \frac{\partial f_i}{\partial x_s \partial x}(x)V_{sj}(t) + \sum_{s,r=1}^{n} \frac{\partial f_i}{\partial x_s \partial x}(x)V_{sj}(t) + \sum_{s,r=1}^{n} \frac{\partial f_i}{\partial x}(x)V_{sj}(t) + \sum_{s,r=1}^{n} \frac{\partial f_i}{\partial x}(x)V_{sj}(t) + \sum_{s,r=1}^{n} \frac{\partial f_i}{\partial x}(x)V_{sj}(t) + \sum_{$$

$$\sum_{s=1}^{n} \frac{\partial f_i}{\partial x_s}(x) H_{sjk}(x), \qquad (23)$$

with the initial conditions

$$x(0) = x_0, \quad V(0) = Id,$$

 $H_{ijk}(0) = 0, \quad i, j, k = 1, ..., n.$

An algorithm for C^n -computations

Simple approach: Apply C^0 -Lohner algorithm to the system of variational equations, this works rather badly

• the control of wrapping effect may for x variables may not work

 computationally ineffective because it totally ignores the structure of the system,

Let $\Phi(h, x)$ be a Taylor expansion for $\varphi(h, x)$ of order p, then $V(h, x) = \frac{\partial \Phi}{\partial x}(h, x) + h^{p+1}$

Observe that $\frac{\partial \Phi}{\partial x}(h, [W])$ is already computed in step 2 of C^0 algorithm

An effective C^n -algorithm

•takes into account the structure of the system variational equations

• the rearrangement is done separately which partial derivatives of given order

• implemented in CAPD library, we did some computer assisted proofs involving C^5 computations for ODE n=2,3