Preconditioning Methods
in the Taylor Model ODE Integrator

— As an Introduction to Nedialkov’s Talk —

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Taylor Model Integration of ODEs

Goal: Determine a Taylor model, consisting of a Taylor Polynomial and an interval bound for the remainder, for the flow of the differential equation

$$\frac{d}{dt}\vec{r}(t) = \vec{F}(\vec{r}(t), t)$$

where $\vec{F}$ is sufficiently differentiable. The Remainder Bound should be fully rigorous for all initial conditions $\vec{r}_0$ and times $t$ that satisfy

$$\vec{r}_0 \in [\vec{r}_{01}, \vec{r}_{02}] = \vec{B}$$
$$t \in [t_0, t_1].$$

In particular, $\vec{r}_0$ itself may be a Taylor model, as long as its range is known to lie in $\vec{B}$. 
Key Features and Algorithms of COSY-VI

• High order expansion not only in time $t$ but also in transversal variables $\vec{x}$.

• Capability of weighted order computation, allowing to suppress the expansion order in transversal variables $\vec{x}$.

• Shrink wrapping algorithm including blunting to control ill-conditioned cases.

• Pre-conditioning algorithms based on the Curvilinear, QR decomposition, and blunting pre-conditioners.

• Resulting data is available in various levels including graphics output.
The Volterra Equation

Describe dynamics of two conflicting populations

\[
\frac{dx_1}{dt} = 2x_1(1 - x_2), \quad \frac{dx_2}{dt} = -x_2(1 - x_1)
\]

Interested in initial condition

\[x_{01} \in 1 + [-0.05, 0.05], \quad x_{02} \in 3 + [-0.05, 0.05] \text{ at } t = 0.\]

Satisfies constraint condition

\[C(x_1, x_2) = x_1x_2^2e^{-x_1-2x_2} = \text{Constant}\]
Integration of the Volterra eq. COSY-VI and AWA
**Shrink Wrapping I**

A method to remove the remainder bound of a Taylor model by increasing the polynomial part.

**Theorem (Shrink Wrapping)** Let $M = I + S(\bar{x})$, where $I$ is the identity. Let $\bar{I} = d \cdot [-1, 1]^v$, and

$$R = \bar{I} + \bigcup_{\bar{x} \in \bar{B}} M(\bar{x})$$

be the set sum of the interval $\bar{I} = [-d, d]^v$ and the range of $M$ over the original domain box $\bar{B}$. So $R$ is the range enclosure of the flow of the ODE over the interval $\bar{B}$ provided by the Taylor model. Let $q$ be the shrink wrap factor of $M$; then we have

$$R \subset \bigcup_{\bar{x} \in \bar{B}} (qM)(\bar{x}),$$

and hence multiplying $M$ with the number $q$ allows to set the remainder bound to zero.
**Shrink Wrapping**

Define the **shrink wrap factor** $q$ as

$$q = 1 + d \cdot \frac{1}{(1 - (v - 1)t) \cdot (1 - s)}.$$ 

The bounds $s = |S_i|$ and $t = |\partial S_i/\partial x_j|$ can be computed by interval evaluation.

**Remark (Typical values for $q$)** In the case of the verified integration of the Asteroid 1997 XF11, we typically have $d = 10^{-7}$, $s = 10^{-4}$, $t = 10^{-4}$, and thus $q \approx 1 + 10^{-7}$. The values for $s$ and $t$ are determined by the nonlinearity in the problem at hand, while in the absence of “noise” terms in the ODEs described by intervals, the value of $d$ is determined mostly by the accuracy of the arithmetic.
Shrink Wrapping II

Remark (Limitations of shrink wrapping)

1. The measures of nonlinearities \( s \) and \( t \) must not become too large.

2. The application of the inverse of the linear part should not lead to large increases in the size of remainder bounds.

The first requirement limits the domain size that can be covered by the TM, and it will thus happen only in extreme cases. In practice the case of large \( s \) and \( t \) is connected to also having accumulated a large remainder bound. Since the remainder bounds are calculated from the bounds of the various orders of \( S \), not much additional harm is done by removing \( S \) into the remainder bound and create a linearized Taylor model.
Blunting

Definition (Blunting of an Ill-Conditioned Matrix)
Let \( \hat{A} \) be a regular matrix that is potentially ill-conditioned and \( \vec{q} = (q_1, \ldots, q_n) \) with \( q_i > 0 \). Arrange the column vectors \( \vec{a}_i \) of \( \hat{A} \) by size. Let \( \vec{e}_i \) be the orthonormal vectors obtained through the Gram-Schmidt procedure;

\[
\vec{e}_i = \frac{\vec{a}_i - \sum_{k=1}^{i-1} \vec{e}_k (\vec{a}_i \cdot \vec{e}_k)}{\left| \vec{a}_i - \sum_{k=1}^{i-1} \vec{e}_k (\vec{a}_i \cdot \vec{e}_k) \right|}.
\]

We form vectors \( \vec{b}_i \) via

\[
\vec{b}_i = \vec{a}_i + q_i \vec{e}_i
\]

and assemble them columnwise into the matrix \( \hat{B} \). We call \( \hat{B} \) the \( \vec{q} \)-blunted matrix belonging to \( \hat{A} \).

Proposition (Regularity of the Blunted Matrix) The \( \vec{b}_i \) are linearly independent and thus \( \hat{B} \) is regular.

The effect of blunting is that each vector \( \vec{b}_i \) is being "pulled away" from the space spanned by the previous vectors \( \vec{b}_1, \ldots, \vec{b}_{i-1} \), and more strongly so if \( q_i \) becomes bigger and bigger.
Preconditioning the Flow

Idea: write the Taylor model of the solution as a composition of two Taylor models \((P_l + I_l)\) and \((P_r + I_r)\), and then choose \(P_l + I_l\) in such a way that in each step, the operations appearing on \(I_r\) are minimized. At the same time, \(I_l\) will be chosen as small as possible. Can be viewed as a coordinate transformation.

In the factorization, we impose that \((P_r + I_r)\) is normalized such that each of its components has a range in \([-1, 1]\), and even near the boundaries.

**Definition (Preconditioning the Flow)** Let \((P + I)\) be a Taylor model. We say that \((P_l + I_l), (P_r + I_r)\) is a factorization of \((P + I)\) if \(B(P_r + I_r) \in [-1, 1]\) and

\[
(P + I) \in (P_l + I_l) \circ (P_r + I_r)
\]

for all \(x \in D\) where \(D\) is the domain of the Taylor model \((P_r + I_r)\).
Preconditioning the Flow II

Proposition Let \((P_{l,n} + I_{l,n}) \circ (P_{r,n} + I_{r,n})\) be a factored Taylor model that encloses the flow of the ODE at time \(t_n\). Let \((P_{l,n+1}^*, I_{l,n+1}^*)\) be the result of integrating \((P_{l,n} + I_{l,n})\) from \(t_n\) to \(t_{n+1}\). Then

\[
(P_{l,n+1}^*, I_{l,n+1}^*) \circ (P_{r,n} + I_{r,n})
\]

Definition (Curvilinear Preconditioning) Let \(x^{(m)} = f(x, x', ..., x^{(m-1)}, t)\) be an \(m\)-th order ODE in \(n\) variables. Let \(x_r(t)\) be a solution of the ODE and \(x_r'(t), ..., x_r^{(k)}(t)\) its first \(k\) time derivatives. Let \(\vec{e}_1, ..., \vec{e}_l\) be the \(l\) unit vectors not in the span of \(x_r'(t), ..., x_r^{(k)}(t)\), sorted by distance from the span. Then we call the Gram-Schmidt orthonormalization of the set \(x_r'(t), ..., x_r^{(k)}(t), \vec{e}_1, ..., \vec{e}_l\) the curvilinear basis of depth \(k\).

Example (Curvilinear Solar System and Particle Accelerators) In this case, \(n = 3\), and one usually chooses \(k = 2\). The first basis vector points in the direction of motion of the reference orbit. The second vector is perpendicular to it and points approximately to the sun or the center of the accelerator. The third vector is chosen perpendicular to the plane of the previous two.
Volterra - QR based preconditioning
needle IC(1.5,-1) - QR based preconditioning
needle IC(1.5,-1) - Curvilinear preconditioning
Natural Orthonormal Coordinates

Let $x' = A \cdot x$ be an $n$-dimensional linear system that has $n$ distinct real eigenvalues $\lambda_1 > \lambda_2 > \ldots > \lambda_n$ with eigenvectors $a_1, \ldots, a_n$. We define the natural orthonormal basis $(o_i)$ of the system to be the result of applying the Gram-Schmidt orthonormalization procedure to the vectors $a_1, \ldots, a_n$, i.e. the result of the recursive computation

$$o_i = \frac{a_i - \sum_{j=1}^{i-1} o_j \cdot (a_i \cdot o_j)}{|a_i - \sum_{j=1}^{i-1} o_j \cdot (a_i \cdot o_j)|}.$$

The Natural Coordinate System has the property that as time progresses, the components motion is pulled most strongly towards the vector $b_1$, and then towards $b_2$, and so on.
Asymptotics of Curvilinear and QR Coordinates

Let \( x' = A \cdot x \) be an \( n \)-dimensional linear system that has \( n \) distinct real eigenvalues \( \lambda_i \) with eigenvectors \( a_i \). Let \( b_i \) be the natural coordinate system of the linear system.

Let \( B \) be a box with nonzero volume, and \( x_r = \sum_{i=1}^{n} X_i a_i \in B \) such that \( X_i \neq 0 \). If \( x_r \) is used as the reference orbit to define the curvilinear coordinates \( c_i \), then the curvilinear coordinates converge to the natural orthonormal coordinates, i.e. we have

\[
  c_i \to o_i \text{ for all } i \text{ as } t \to \infty.
\]

Similarly, let \( q_i \) denote the coordinates obtained from the QR procedure; then the curvilinear coordinates converge to the natural orthonormal coordinates, i.e.

\[
  q_i \to o_i \text{ for all } i \text{ as } t \to \infty
\]

Hence the dynamics expressed in \textbf{curvilinear and QR coordinates} has the same asymptotic behavior.
Natural Blunted Coordinates, Asymptotics

Let $x' = A \cdot x$ be an $n$-dimensional linear system that has $n$ distinct real eigenvalues $\lambda_1 > \lambda_2 > \ldots > \lambda_n$ with normalized eigenvectors $a_1, \ldots, a_n$. Let $o_i$ be the natural orthogonal coordinates belonging to $a_i$, and let $q_i \geq 0$ be the parameters from the blunting operation. We define the natural blunted basis $(b_i)$ via

$$b_i = \frac{a_i + q_i o_i}{|a_i + q_i o_i|}.$$  

Note that for $q_i \neq 0$, the matrix $(b_i)$ is well-conditioned. Let $c_i$ be the blunted coordinates of the dynamics, then we observe

$$c_i \to b_i \text{ for all } i \text{ as } t \to \infty.$$  

We see $b_1 = o_1$. Now consider entire motion expressed in $b_i$ coordinates; in these coordinates, $b_i$ is the orthonormal basis $o_i$, and so the dynamics expressed in blunted and QR coordinates has the same asymptotic behavior.
Random Matrices - Discrete

Select 1000 twodimensional random matrices with coefficients in $[-1, 1]$. Sort according to eigenvalues into seven sub-cases.

Perform iteration in the following ways:

- Naive Interval
- Naive Taylormodel
- Parallelepiped-preconditioned Taylormodel
- QR-preconditioned Taylormodel
- Blunted preconditioned TM, various blunting factors
- Set of four floating point corner points for volume estimation

Perform the following tasks:

- Iterations through matrix
325 Conjugate EVs Random Matrices

![Graph showing log_10(Mean) vs. Step Number for various matrices: VE, IN, TMN, TMP, TMQ, TMB.](image-url)
520 Real EVs (ratio < 5) Random Matrices

The graph shows the logarithm (base 10) of the mean values across different step numbers for various matrices. The x-axis represents the step number, ranging from 0 to 250, and the y-axis represents the log_{10}(Mean), which ranges from 0 to -80.

The different lines on the graph correspond to different matrices:
- VE
- IN
- TMN
- TMP
- TMQ
- TMB

Each line represents the mean values of the respective matrix over the range of step numbers, illustrating how their values decrease as the step number increases.
80 Real EVs (5 ≤ ratio < 10) Random Matrices
40 Real EVs (10 <= ratio < 20) Random Matrices

log_{10}(Mean) vs Step Number

- VE
- IN
- TMN
- TMP
- TMQ
- TMB
18 Real EVs (20 <= ratio < 50) Random Matrices
Random Matrices - Discrete

Select 1000 twodimensional random matrices with coefficients in $[-1, 1]$. Sort according to eigenvalues into seven sub-cases.

Perform iteration in the following ways:

- ...
- ...
- ...
- ...
- ...
- ...
- ...

Perform the following tasks:

- ...

- Sets of iterations through matrix and its inverse
325 Conjugate EVs Random Matrices

log_{10}(Mean)

Step Number

VE
IN
TMN
TMP
TMQ
TMB
80 Real EVs (5 <= ratio < 10) Random Matrices

log_{10}(Mean)

Step Number

VE
IN
TMN
TMP
TMQ
TMB
40 Real EVs (10 <= ratio < 20) Random Matrices

log_{10}(Mean)

Step Number

VE
IN
TMN
TMP
TMQ
TMB
18 Real EVs (20 ≤ ratio < 50) Random Matrices
325 Conjugate EVs Random Matrices

log_10(Mean)

Step Number (showing every 20th step)
520 Real EVs (ratio < 5) Random Matrices
80 Real EVs (5 ≤ ratio < 10) Random Matrices
40 Real EVs (10 <= ratio < 20) Random Matrices

Step Number (showing every 20th step)
18 Real EVs (20 <= ratio < 50) Random Matrices

Step Number (showing every 20th step)
COSY-VI Integration of the Roessler eqs.
AWA Integration of the Roessler eqs.
COSY-VI Integration of the Roessler eqs.
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