
# Reachability Analysis with Approximate B-series

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# Context

## Cyber-physical systems

- Critical;
- Require safety;
- Need some planning and control solutions;
- Tainted with uncertainties (measures, inputs, etc) and approximations (modelling, algorithms).

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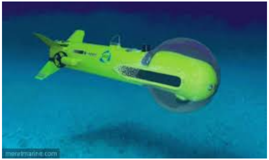


# Introduction

## The chosen approach

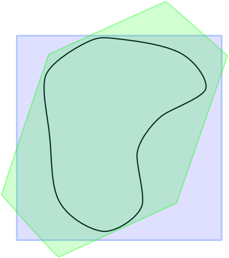
For uncertainties, set-based methods can help:

- Handle several values for measures and parameters;
- Provide some guarantees in computation with a correct-by-design abstraction.

For examples, Interval Analysis and Affine Arithmetic help to compute reliable abstractions of sets enclosed by boxes or zonotopes.

## Helpful in Robotics

- Control synthesis,
- Motion planning,
- Kinematics,
- Parameter identification, etc.



# Introduction

## Dynamical systems

Mainly interested by applications in robotics:
A robot is a dynamical system !

## Model based approaches

Need a model for dynamical systems: differential equations are suitable.

# Differential Equations

## Ordinary Differential Equation (ODE)

$$\dot{y}(t) = \frac{\partial y(t)}{\partial t} = f(y(t))$$

Solution is a function $y(t) : \mathbb{R} \mapsto \mathbb{R}^n$.

## Initial Value Problem (IVP)

From an initial value $y(0) = y_0$, solution at time $h$ can be computed by

$$y(h) = y_0 + \int_0^h f(y(s))ds$$

Hypotheses: $f$ is Lipschitz and the associated vector field is sufficiently smooth.

In general, the equation above cannot be explicitly computed due to its implicit nature.

# Differential Equations with sets

For a parametric IVP

$$\dot{y}(t) = f(y(t), p), \quad y(0) = y_0$$

## Parameters

- Constant parameters not perfectly known but bounded;
- To consider several values at once, etc.

$$p \in \mathcal{P}$$

## Initial value

- Uncertainty in measures;
- To estimate different trajectories, etc.

$$y(0) \in \mathcal{Y}_0$$

$$\dot{y}(t) \in f(y(t), \mathcal{P}), \quad y(0) \in \mathcal{Y}_0$$

# Reachability

Compute the set of states at a given time $t > 0$.

## Many names

Validated simulation, validated numerical integration, reachability analysis, guaranteed integration, etc..

## Our goal

Compute a tube enclosing all the solutions:

$$\mathcal{Y} \supset \{y(t), t \in [0, T], y(0) \in \mathcal{Y}_0, p \in \mathcal{P}\}$$

# Main tool: Interval analysis

$[x] = [\underline{x}, \overline{x}]$ stands for the set of reals $x$ s.t. $\underline{x} \leq x \leq \overline{x}$

## Arithmetic

Extension of operators $(+, -, *, /, sin, cos, ...)$, e.g. $[-1, 1] + [1, 3] = [0, 4]$
Rounding error handled $(1/3 \in 0.33333333[3, 4])$

## Extension of function

$$[f]([x]) \supset f([x]) = \{f(y) | y \in [x]\}$$

## Interval Integral

Rectangle rule: $\int_{[x]} f(x')dx' \in [f]([x]).w([x])$

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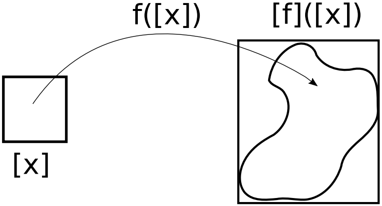


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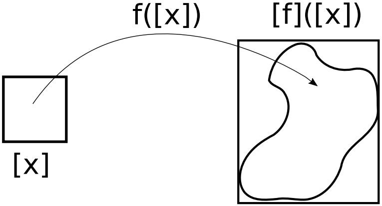


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# B-series

One formalism for numerical integration: the B-series (Cayley, Merson, Butcher, Hairer, Wanner, etc)

A B-series is a formal series of the form

$$B(a, hf, y) = a(\emptyset)y + \sum_{\tau \in \mathcal{T}} \frac{a(\tau)h^{|\tau|}}{\sigma(\tau)} F(\tau)(y),$$

with $F(.)(y)$ the elementary differentials.

$B(a, hf, y) = a(\emptyset)y + ha(\bullet)f(y) + h^2 a($  $)(f'f)(y) + \frac{h^3}{2} a($  $)(f''(f,f))(y) + \ldots$

## Lemma (B-series and IVP)

*The exact solution of an IVP is given by a B-series*

$$y(h) = B(E, hf, y_0), \text{ with } E(\tau) = 1/\tau!$$

# B-series

A Runge-Kutta scheme approximates the solution of an ODE with a B-series:

$$y(h) \approx y_1 = B(\phi(A,b), hf, y_0),$$

if the Runge-Kutta scheme is defined as follows

$$y_1 = y_0 + b^T hf(Y), \quad Y = ey_0 + Ahf(Y),$$

Order $p$ if

$$E(\tau) = \phi(A,b)(\tau), \quad \forall \tau \in \mathcal{T}, |\tau| \leq p,$$

which means that $B(E, hf, y_0) - B(\phi(A,b), hf, y_0) \in \mathcal{O}(h^{p+1})$.

Remark: if $E(\tau) = 1/\tau!, \forall \tau \in \mathcal{T}, |\tau| \leq p$, truncated Taylor series!

# Set-based B-series

## Validated RK

$$\mathcal{Y}(h) = B(E, hf, \mathcal{Y}_0) \subset B(\phi(A,b), hf, \mathcal{Y}_0) + B(\psi(A,b), hf, \mathcal{Y}^*)$$

with $\mathcal{Y}^* \ni y(t), \forall t \in [0,h]$, and

$$\psi(A,b)(\tau) = 1/\tau! - \phi(A,b)(\tau), \forall \tau \in \mathcal{T} \text{ if } |\tau| = p+1,$$

## Picard operator

If it exists a set $\mathcal{R} \subset \mathbb{R}^n$ such that

$$B(E, [0,h]f, \mathcal{R}) \subset \mathcal{R}$$

Brouwer theorem (also proposed/studied by Picard, Poincaré and Hadamard) and Picard-Lindelöf theorem: the initial value problem has a unique solution in the set $\mathcal{R}$ (then $\mathcal{Y}^* = \mathcal{R}$). Otherwise, reduce $h$ or inflate $\mathcal{R}$.

# Truncation error

## Complexity of computation of $B(\psi(A, b), hf, \mathcal{Y}^*)$

Two methods:

- Direct form: Faà di Bruno formula (symbolic derivatives and trees[1]) or symbolic computation[4]
- Factorized (automatic differentiation and graphs[2,3])

[1] Alexandre dit Sandretto et al., "Validated explicit and implicit Runge-Kutta methods", Reliable Computing 2016
[2] Bartha et al., "Computing of B-series by automatic differentiation", Discrete and continuous dynamical systems, 2014
[3] Mullier et al., "Validated Computation of the Local Truncation Error of Runge-Kutta Methods with Automatic Differentiation", AD 2016
[4] Alexandre dit Sandretto, "Symbolic Computation of Local Truncation Error for Approximate B-Series-Based Validated Simulation", Scientific Computing and Software, Springer Proceedings in Mathematics & Statistics, 2025

# Example of symbolic approach

For one RK method and a specific ODE[(1)]

## A truncated B-series

At fourth order

$$F_f(\varnothing)+hF_f(\bullet)+\tfrac{1}{2}h^2F_f([\bullet])+\tfrac{1}{6}h^3F_f([[\bullet]])+\tfrac{1}{6}h^3F_f([\bullet,\bullet])+\tfrac{1}{24}h^4F_f([[[\bullet]]])+\tfrac{1}{24}h^4F_f([[\bullet,\bullet]])+\tfrac{1}{8}h^4F_f([\bullet,[\bullet]])+\tfrac{1}{24}h^4F_f([\bullet,\bullet,\bullet])$$

$F_f(\tau)$ are the elementary differentials.

## The selected RK method

The Kutta's method

$$\begin{array}{c|ccc} 0 & 0 & 0 & 0 \\ 0.5 & 0.5 & 0 & 0 \\ 1 & -1 & 2 & 0 \\ \hline & 1/6 & 2/3 & 1/6 \end{array}$$

(1) Obtained with the Bseries package in Julia (Ketcheson & Ranocha).

# Example of symbolic approach

The RK contribution of the B-series:

$$F_f(\varnothing)+hF_f(\bullet)+\tfrac{1}{2}h^2F_f([\bullet])+\tfrac{1}{6}h^3F_f([[\bullet]])+\tfrac{1}{6}h^3F_f([\bullet\bullet])+\tfrac{1}{24}h^4F_f([[\bullet\bullet]])+\tfrac{1}{6}h^4F_f([\bullet[\bullet]])+\tfrac{1}{24}h^4F_f([\bullet\bullet\bullet])$$

We compute the difference between the B-series and the RK:

$$\Delta = -\frac{1}{24}h^4F_f([[[\bullet]]]) + \frac{1}{24}h^4F_f([\bullet[\bullet]]).$$

Kutta is a third order scheme (well known).

Butcher: the difference of the two Lagrangian remainders is the error of the RK method (for short).

# Example of symbolic approach

We consider the coupled Van der Pol:

$$\begin{cases} \dot{x}_1 & = y_1 \\ \dot{y}_1 & = \mu(1 - x_1^2)y_1 + b(x_2 - x_1) - x_1 \\ \dot{x}_2 & = y_2 \\ \dot{y}_2 & = \mu(1 - x_2^2)y_2 - b(x_2 - x_1) - x_2 \\ \dot{b} & = 0 \end{cases} \tag{1}$$

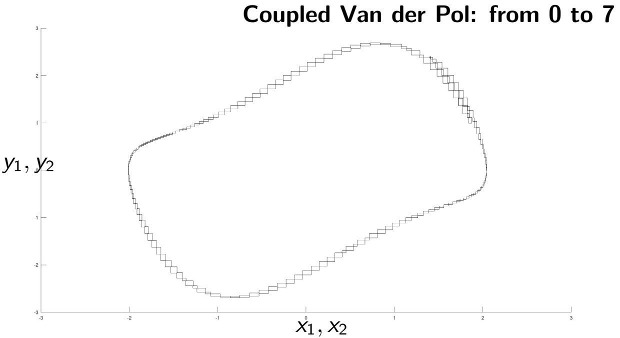
with $\mu = 1$.

The code can be generated (and optimized) for computation with sets:

$x_1(h) - \tilde{x}_1 = -0.0416666666666667 * h^4 * (b * (-x_2 + y_2 * (1.0 - x_2^2) + b * (x_1 - x_2)) + (1.0 - x_1^2) * (y_1 * (-2 * x_1 * y_1 - b - 1) + y_2 * b + (1.0 - x_1^2) * (-x_1 + y_1 * (1.0 - x_1^2) + b * (-x_1 + x_2))) + (-x_1 + y_1 * (1.0 - x_1^2) + b * (-x_1 + x_2)) * (-2 * x_1 * y_1 - b - 1)) - 1.11022302462516e - 16 * h * y_1$

# Example of symbolic approach

The initial conditions are $x_{1,2}(0) = 1.4$, $y_{1,2}(0) = 2.4$ and $b(0) = 1$



# Approximate B-series

What happends if the order of $\Delta$ is different than the expected one ?

Example:

| | | | |
|---|---|---|---|
| 0 | 0 | 0 | 0 |
| 0.5 | **0.6** | 0 | 0 |
| 1 | −1 | 2 | 0 |
| | 1/6 | 2/3 | 1/6 |

$\Delta \Rightarrow$

$-1.1102230246251565e{-16}h^1 F_f(\bullet) + 0.06666666666666665 h^2 F_f($$) + 0.03333333333333326 h^3 F_f($$) +$
$0.03666666666666665 h^3 F_f($$) - 0.04166666666666664 h^4 F_f($$) + 0.01833333333333333 h^4 F_f($$) +$
$0.07499999999999998 h^4 F_f($$) + 0.01011111111111107 h^4 F_f($$)$

Numerical errors and false order (weak order?),
but RK+$\Delta$ = exact $(p+1)$ B-series !

We propose to call this object “Approximate B-series”.

# Parametrized AB-series

We consider the RK:

| | | | |
|---|---|---|---|
| 0 | 0 | 0 | 0 |
| $0.5-k$ | $0.5-k$ | 0 | 0 |
| 0.6 | $-0.2$ | 0.8 | 0 |
| | 0.2 | 0.4 | 0.4 |

$\Delta = h^2(-0.4k - 0.0599999999999)\,F_f($  $) + h^3(-0.32k - 0.00666666666666)\,F_f($  $)+$

$h^3\left(0.2(0.5-k)^2 - 0.0946666666666\right)F_f($  $) + \frac{-h^4}{24}F_f($  $)+$

$h^4\left(0.16(0.5-k)^2 - \frac{1}{24}\right)F_f($  $) + h^4(-0.192k - 0.029)\,F_f($  $)+$

$h^4\left(0.0666666666666(0.5-k)^3 - 0.0272666666666\right)F_f($  $)$

First remarks: second order is feasible if $k=-0.15$; third order cannot be obtained...

# How to select $k$ ?

Several ideas may come:

- Order 2 by chosing $k = -0.15$;
- Delete the largest elementary differential;
- Minimize $\Delta$;
- Randomly;
- etc...

A work in progress...any remark or idea is welcome !

# Delete the largest derivative

Van der Pol is (theoretically) bounded, due to limit cycle, in $([-2,2],[-3,3])$, so we can bound $\Delta$ on the whole space.

 $: -0.4k - 0.0599999999999 = 0 \implies k = -0.15$

 $: -0.32k - 0.00666666666666 \implies k = -0.0208333$

 $: 0.2\,(0.5-k)^2 - 0.0946666666666 = 0 \implies k = -0.187992$

 : cannot be cancelled

 $: 0.16\,(0.5-k)^2 - \frac{1}{24} \implies k = -0.010310$

 $: -0.192k - 0.029 = 0 \implies k = -0.15104166$

 $: 0.0666666666666\,(0.5-k)^3 - 0.0272666666666 = 0 \implies k = -0.242291$

# Delete the largest derivative

$max(\Delta)$ for different $k$:

| | |
|---|---|
| $-0.15$ | $880.462$ |
| $-0.0208333$ | $791.599$ |
| $-0.187992$ | $908.228$ |
| $-\mathbf{0.01031}$ | $784.727$ |
| $-0.151042$ | $881.213$ |
| $-0.242291$ | $949.239$ |

Remark: second order does not provide the minimal value...

# Optimization

From the last results, trying to cancel (reduce) at the same time

 : $-0.32k - 0.00666666666666$

 : $0.16\,(0.5-k)^2 - \frac{1}{24}$

could be interesting.

$$g(k) = (0.16(0.5-k)^2 - 1/24)^2 + (-0.32k - 0.00666666666666)^2$$

$$\Rightarrow k = -0.01861703$$

# Experimentation

Let's try these values (and a few others) !

## Procedure

- Validated simulation till $t = 7$
- First part of the AB-series computed with parametrized RK
- Second part ($\Delta$) with generated code
- Comparison regarding several values: diameters of $x$ and $y$; number of steps; minimal stepsize; maximal stepsize; maximal tolerance

# Results

Sort by $max(\Delta)$

| k | -0.01031 | -0.0208333 | -0.15 | -0.151042 | -0.187992 | -0.242291 |
|---|---|---|---|---|---|---|
| diam(x) | 0.011645 | 0.00688322 | 0.0385362 | 0.0259102 | 0.0205072 | 0.0133194 |
| diam(y) | 0.0283198 | 0.0211882 | 0.104743 | 0.0764496 | 0.0557753 | 0.0335257 |
| nb steps | 2281 | 2207 | 2011 | 1902 | 1957 | 2126 |
| min(h) | 7.25E-05 | 0.00125 | 0.000337384 | 0.00112955 | 0.00132966 | 0.00109533 |
| max (h) | 0.00734451 | 0.0073282 | 0.00702523 | 0.00702005 | 0.0070519 | 0.00706827 |
| tol | 3.18E-06 | 3.18E-06 | 3.21E-06 | 3.21E-06 | 3.19E-06 | 3.18E-06 |

For the "optimal" value:

| | | | | | | |
|---|---|---|---|---|---|---|
| -0.01861703 | 0.0118101 | 0.0283495 | 2240 | 0.00125 | 0.00732893 | 3.18E-06 |

Remarks: as expected, first and second value provide good results, but not the best everywhere...Optimal value follows. Second order method gives the worst result. To conclude, the results are ambiguous...

# Intersection ?

We obtained 6 reachable sets with the 6 different values for $k$, so we can intersect them

Diameters: 0.00688 and 0.008828

Remark: of course the best result, huge gain on $y$ but neglectable on $x$ (for 12000 steps !).

This technique can be interesting for difficult problems (such as chaotic) and easily parallelized.

# Interval for $k$ ?

## Opposite idea

Let's try with the interval $[-0.020833, -0.01031]$

Diameters: 0.0134956 and 0.0381649, not so far than best results...

The use of intervals in RK coefficients has an acceptable impact.

# Random values

## 50 random values

$k$ between -0.3 and 0, and intersection.

Diameters: 0.00665 and 0.00929, interesting to think instead of random (second worst, even if first better).

Remark: whatever the value of $k$, the intersection of the reachable sets is not empty because each set is guaranteed.

# Conclusion

## Another possible use of AB-series

Design of a RK method to vanish some derivatives. Some ideas have been tested.

## Need some works to

- Define problems that require this approach (chaos ?);
- Find the optimal AB-series for such problems (intersection for specific values seems the best idea);
- Develop the tool and release.

## Future

Mix RK and Taylor expansion in AB-series...

# Questions?