Constraint Satisfaction Using High-Order Taylor Models and Applications

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Assume you look for solutions of a given problem in a set D. The solutions often need to satisfy additional conditions.

$$\begin{aligned} g_j(x) &\leq 0 \text{ for } j = 1, ..., c_{\leq}, \; x \in D \\ h_j(x) &= 0 \text{ for } j = 1, ..., c_{=}, \; x \in D \end{aligned} \tag{1}$$

Typical examples are

- in optimization: find the global minimum of a function in a domain box D under aditional constraints (1)
- in Hamiltonian dynamics: solutions to Hamiltonian systems need to conserve certain invariants, e.g. energy

In particular it is hard to find *validated* solutions solving the problem *and* satisfying the constraint conditions.

A traditional approach is to subdivide D, throw away boxes which can be shown to violate the constraints (1) and attempt the minimization of f only on the remaining boxes. The problems are:

- subdivision is always expensive
- box rejection might be extra-slow because of overestimation in interval arithmetic

The general idea using Taylor Model methods:

- first represent the set F of feasible points in D which satisfy the conditions (1) by a high-order Taylor Model
$\Longrightarrow$ typically F is very small, usually a low-dimensional submanifolds
- then look for solutions only on these feasible boxes
$\Longrightarrow$ a much faster enclosure of the solutions is expected

Generally we formulate the problem as follows: Let

$$f_i(x_1, ..., x_n) = 0 \text{ for } i \in \{1, ..., m\} \tag{2}$$

be m constraint conditions, where the $f_i : \mathbb{R}^n \supset D \longrightarrow \mathbb{R}^n$ are sufficiently smooth. Assume nom that there is a point $\mathbf{x}^0$ in D satisfying the constraints (2),

$$f_i(x_1^0, ..., x_n^0) = 0 \; \forall \; i \in \{1, ..., m\}$$

We want to represent the feasible points in D by a Taylor Model expanded around $\mathbf{x}^0$. In the following we assome w.l.o.g. that $\mathbf{x}^0 = 0$.

m constraints $\Longrightarrow$ the feasible set can be parameterized by $n-m$ variables.
Assume the first $n-m$ variables can be used to do this.
Then we construct the function $\psi : D \longrightarrow \mathbb{R}^n$ by

$$\psi(x_1, \ldots, x_n) := \begin{pmatrix} x_1 \\ \vdots \\ x_{n-m} \\ f_1(x_1, \ldots, x_n) \\ \vdots \\ f_m(x_1, \ldots, x_n) \end{pmatrix}$$

Note that for a feasible point $\mathbf{x}^f \in F$ we have

$$\psi(\mathbf{x}^f) = (x_1^f, \ldots, x_{n-m}^f, 0, \ldots, 0)^T$$

If ψ is invertible on D, then conversely we have

$$\psi^{-1}(x_1, \ldots, x_{n-m}, 0, \ldots, 0) = \psi^{-1}(\psi(x_1, \ldots, x_n)) = \mathcal{I} \qquad (3)$$

It is natural that the identities in the first $n - m$ components of ψ are also preserved by ψ^{-1}.

BUT the last m components in eq. (3) contain the dependency of the constrained variables on the unconstrained variables $x_k, k \in \{1, \ldots, n - m\}$.

Then one can replace x_k by $\psi_K^{-1}(x_1, \ldots, x_{n-m}, 0, \ldots, 0)$ for $k \in \{1, \ldots, n - m\}$ and search for solutions of the original problem in terms of only the unconstrained variables.

Taylor inversion of ψ

We obtain the Taylor polynomial of ψ^{-1} from the Taylor polynomial of ψ:

- write $\psi(\mathbf{x}) = L\,\mathbf{x} + N(\mathbf{x})$, where L is linear and N is purely nonlinear
- note that $\psi(\mathbf{0}) = \mathbf{0}$
- $$\begin{aligned} \psi \circ \psi^{-1} &= \mathcal{I} \\ \Longrightarrow \quad L \circ \psi^{-1} &= \mathcal{I} - N \circ \psi^{-1} \\ \Longrightarrow \quad \psi^{-1} &= L^{-1} \circ (\mathcal{I} - N \circ \psi^{-1}) \end{aligned}$$
- define the contracting operator $\mathcal{O}(.) := L^{-1} \circ (\mathcal{I} - N \circ .)$ and apply a fixed point theorem: repeated iteration (beginning with the identity $\mathcal{I}$) yields ψ^{-1} in finitely many steps

After the polynomial part of ψ^{-1} has been obtained, we can immediately extract the polynomial parts of the parametrization of the constrained variables $x_{n-m+1}, \ldots, x_n$ in terms of the unconstrained variables $x_1, \ldots, x_{n-m}$.

Let P_i be the polynomial part of the constrained x_i, then outfit P_i heuristically with a remainder bound

$$I_i := [-\epsilon_l^i, \epsilon_u^i] \ \forall \ i \in \{1, \ldots, m\}$$

An educated guess for the magnitude of the $\epsilon_{l,u}^i$ would be to evaluate $f_i(x_1 + [0,0], \ldots, x_{n-m} + [0,0], P_1 + [0,0], \ldots, P_m + [0,0])$.

The validity of the attempted remainder bound I_i can be checked by scanning the complement of $P_i(D) + I_i$ in D and for a violation of the constraint f_i.

We can inplement this scanning procedure by expressing the $(n - m) + i$-th variable $x_{(n-m)+i}$ by the auxiliary variables $y_i \in [-1, 1]$

$$\begin{aligned} x^+_{n-m+i} &= (P_i + \epsilon^i_u)(1 + y_i)/2 + x^{max}_{(n-m)+i}(1 - y_i)/2 \\ x^-_{n-m+i} &= (P_i - \epsilon^i_l)(1 + y_i)/2 + x^{min}_{(n-m)+1}(1 - y_i)/2 \end{aligned}$$

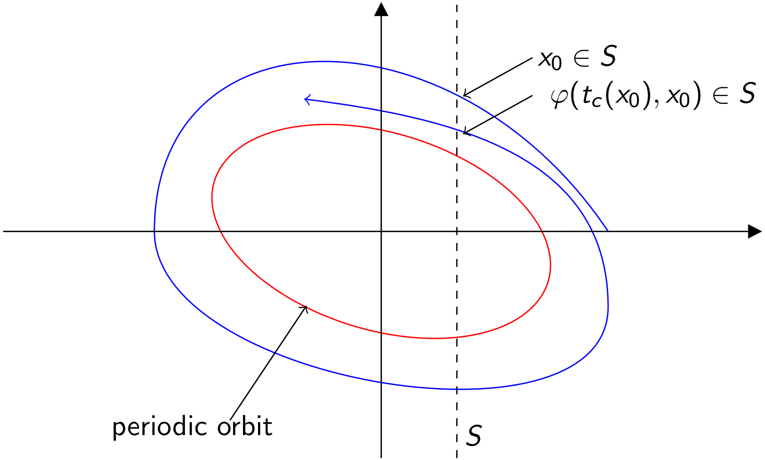
If it can be ascertained that

$$\begin{aligned} 0 &\notin f_i(x_1, ..., x^+_{n-m+i}(y_i), ...x_n) \text{ for } x_j, y_i \in [-1, 1] \\ 0 &\notin f_i(x_1, ..., x^-_{n-m+i}(y_i), ...x_n) \text{ for } x_j, y_i \in [-1, 1] \end{aligned}$$

using a rigorous range bounding scheme, then it is shown that the i-th constraint is violated everywhere outside $P_i + I_i$

$\Longrightarrow P_i + I_i$ forms a rigorous enclosure of the feasible set satisfying f_i.

Review: Definition of a Poincaré map



The construction of the Poincaré map $\mathcal{P}(x_0)$ can thus be reduced the the construction of the crossing time t_c.

- the crossing time for trajectories starting at $x_0 \in D$ exists and is uniquely determined
- it is contained implicitly in the vectorfield of the RHS of the ODE and the geometry of the surface S
- a polynomial approximation of $t_c(x_0)$ yields a polynomial approximation of $\mathcal{P}(x_0)$ by insertion into the flow $\varphi(t, x_0)$

$$\mathcal{P}(x_0) := \varphi(t_c(x_0), x_0)$$

- a Taylor model of $t_c(x_0) + I_{t_c}$ yields a Taylor model of $\mathcal{P}(x_0) + I_{\mathcal{P}}$ by insertion into the flow $\varphi(t, x_0) + I_\varphi$

$$\mathcal{P}(x_0) + I_{\mathcal{P}} := \varphi(t_c(x_0) + I_{t_c}, x_0 + [0, 0]) + I_\varphi$$

Treatable types of Poincaré sections

The method is able to model Poincaré sections S of the form $S := \{x \in \mathbb{R}^n : \sigma(x) = 0\}$ for some C^k-function $\sigma : \mathbb{R}^n \longrightarrow \mathbb{R}$.

- typically σ is $C^\infty \Longrightarrow S$ is smooth
- the case where S is a plane is the most common in applications: $S := \{x \in \mathbb{R}^n : x_1 = c\}$ for some $c \in \mathbb{R}$. Here $\sigma(x) := x_1 - c$

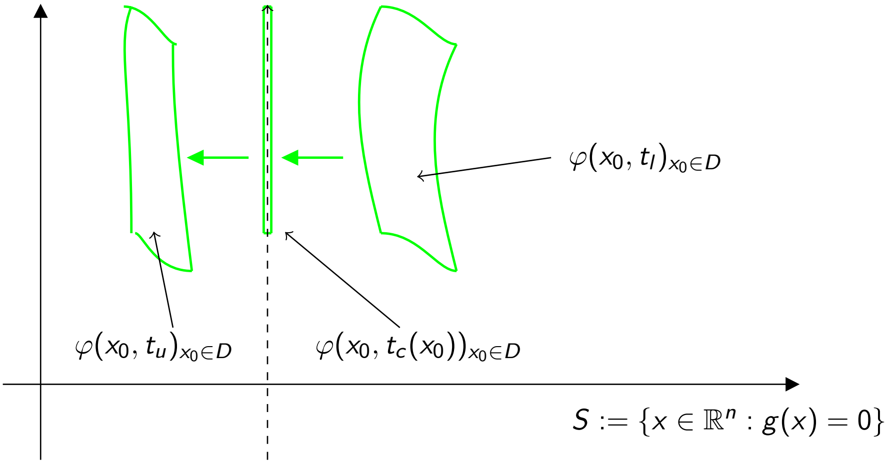
An additional condition is that the flow is 'sufficiently' transverse to the section.

Assume that we have performed a validated Taylor model integration from the initial condition $x(t=0) = X_0 + D$ until the last timestep before we cross the Poincaré section, at time t_l.

The interesting part happens in the final timestep, i.e. there is a time interval $I_t = [0, t_u]$ sucht that for the reference orbit:

$$\exists \tau \in I_t : \varphi(x_0, \tau) \in S$$

This allows us to use the machinery from the last section and formulate the finding of the Poincaré map as a constraint satisfaction problem.


$\varphi(x_0, t_l)_{x_0 \in D}$
$\varphi(x_0, t_u)_{x_0 \in D}$
$\varphi(x_0, t_c(x_0))_{x_0 \in D}$
$S := \{x \in \mathbb{R}^n : g(x) = 0\}$

Consider the domain box $D \times I_t$, where $I_t = [t_l, t_u]$. For the crossing time $t_c(x_0)$ we have to satisfy

$$\sigma(\varphi(x_0, t_c(x_0))) = 0 \,\forall\, x_0 \in D$$

whence we construct

$$\psi(x_0, t) = \begin{pmatrix} x_{0,1} \\ \vdots \\ x_{0,n} \\ \sigma(\varphi(x_0, t)) \end{pmatrix}, \; (x_0, t) \in D \times I_t$$

and after that we perform the inversion using DA-arithmetic and obtain ψ^{-1}.
Then we can evaluate $\psi^{-1}(x_{0,1}, ..., x_{0,n}, 0)$ and extract

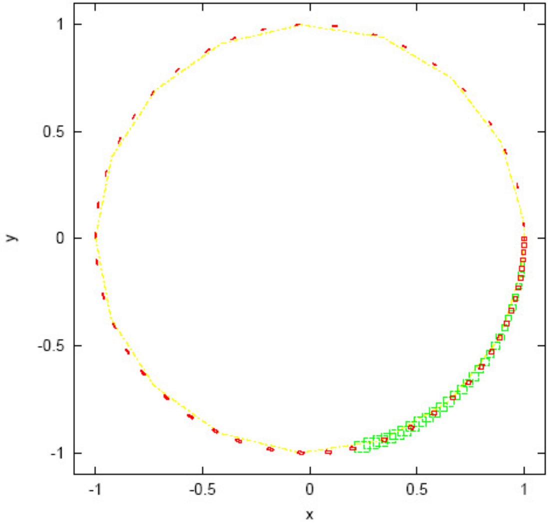
$$t_c(x_0) := \psi^{-1}_{n+1}(x_{0,1}, ..., x_{0,n}, 0)$$

An example: a muon cooling ring

$$\begin{aligned}
\dot{x_1} &= x_3 \\
\dot{x_2} &= x_4 - \frac{\alpha}{\sqrt{x_3^2 + x_4^2}} \cdot x_3 + \frac{\alpha}{\sqrt{x_1^2 + x_2^2}} \cdot x_2 \\
\dot{x_3} &= x_4 \\
\dot{x_4} &= -x_3 - \frac{\alpha}{\sqrt{x_3^2 + x_4^2}} \cdot x_4 - \frac{\alpha}{\sqrt{x_1^2 + x_2^2}} \cdot x_1
\end{aligned}$$

- $\alpha \in [0, 1]$ is the damping parameter, $\alpha = 1$ being the strongest damping

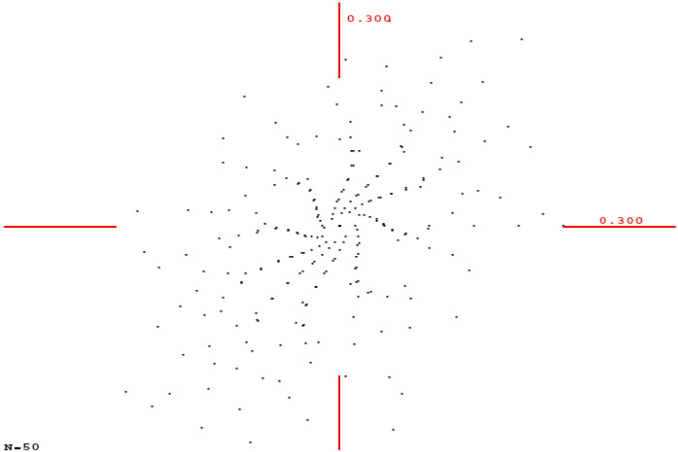
Muon cooler: action in x_1-x_2-plane



Muon cooler: example settings

- we consider the initial conditions $x(0) = X_0 + x_0$ where $X_0 = (0, 1, 1, 0)^T$ and $D = [-10^{-4}, 10^{-4}]$
- trajectories close to $\varphi(0, t)$ are 'pulled' towards the reference orbit $\Longrightarrow$ 'cooling' in transverse coordinates
- we consider the surface where $x_1 = 0$
- an 16th order computation was performed using COSY Infinity [3]

Muon cooler:Tracking picture in x_2-x_4- coordinates



References

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