# An Exit Hole method for Verified Solution of Initial Value Problems for ODEs using Linear Programming for the Search of Tight Bounds

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**Abstract**

In his survey [5], NEDIALKOV stated that "Although high-order Taylor series may be reasonably efficient for mildly stiff ODEs, we do not have an interval method suitable for stiff ODEs." This paper is an attempt to find such a method, based on building a positively invariant set in extended state space. A positively invariant set is treated as a geometric generalization of differential inequalities. We construct a positively invariant set from simpler sets which are not positively invariant, but have an exit hole instead. The exit holes of simpler sets are suppressed during the construction. This paper considers only sets which are polytopes. Linear interval forms are used to evaluate a projection of ODE velocity vectors to the normals of the polytope facets. This permits the use of Linear Programming for the search for tighter positively invariant set. The Exit Hole method is illustrated by stiff Van der Pol ODE.

## 1 Introduction

In this paper we consider an Initial Value Problem (IVP) defined as in [5]

$$\dot{x}(t) = f(x(t), t),\ x(t_0) = x_0,\ x \in \mathbb{R}^n,\ t \in \mathbb{R}. \tag{1}$$

We convert this problem into an autonomous IVP

$$\dot{y}(s) = F(y(s)) = \begin{pmatrix} f(x(s), t+s) \\ 1 \end{pmatrix}, \ y(0) = y_0 = \begin{pmatrix} x_0 \\ t_0 \end{pmatrix}, \ y \in \mathbb{R}^{n+1}, \ s \in \mathbb{R}. \quad (2)$$

We don't know the initial value $y_0$, we only know that it is contained in a known $(n+1)$-dimensional box $y_0 \in \boldsymbol{y}_0$. We want to compute rigorous bounds on the true solution of (1) which enclose both uncertainty in initial conditions and roundoff and truncation errors of numerical computation. Geometrically, we want to build a tube in $\mathbb{R}^{n+1}$ which surely contains all trajectories going forward in time from all points $y_0 \in \boldsymbol{y}_0$.

The Interval Hermite-Obreschkoff $(p, q)$ method [5] finds good bounds for non-stiff and mildly stiff ODEs. It computes the interval enclosure of the $(p+q+1)$-th derivative of trajectories passing through a box in $\mathbb{R}^{n+1}$ and uses it for bounding trajectories. However, this method has difficulties for stiff ODEs. The asymptotic trajectory of a stiff ODE may have small $y^{(p+q+1)}$, but a surrounding box of the asymptotic trajectory contains side trajectories which go quickly to the asymptotic one. The side trajectories make the enclosure of $y^{(p+q+1)}$ too pessimistic.

The other approach is to consider only points on the surface of the tube. If a trajectory starting from any surface point goes inside the tube then no trajectory starting inside the tube can leave it. We do not bother about the magnitude of $F(y)$ or its derivatives inside the tube. We only explore the direction of $F(y)$ on the surface of the tube. This approach was considered by Neumaier [1],[3],[4] and Kühn [2] and in the ValEncIA-IVP solver [6],[7]. All these methods start from some approximate solution $x^*(t)$. Each cross-section of the tube by the hyperplane $t = const$ is $x^*(t) + \Sigma_t$ where $\Sigma_t$ is an $n$-dimensional set. $\Sigma_t$ continuously depends on $t$ in these approaches. It is a scaled unit ball of some $\mathbb{R}^n$ norm in Neumaier's approach. It is an $n$-parallelotope in Kühn's approach. It is an $n$-box with some sub-boxes removed by backward consistency check in ValEncIA-IVP approach. The direction of $F(y)$ on the surface is verified by the interval Taylor expansion of $F(y)$ near the approximate solution. The Taylor expansion is shared by all surface points. This saves work, but increases overestimation when the tube becomes wide. The ValEncIA-IVP reduces overestimation by splitting the tube into subintervals.

Gennat, Tibken in [8] doesn't consider any approximate solution $x^*(t)$. They use Müller's theorem which results in a box tube. Their method verifies that trajectories go inside the box by separate interval computations for each facet of the box. They also use a linear Lyapunov-like function - a linear surface in $R^n$ which is translated to an asymptotic linear surface exponentially with respect to time. Verifying each facet and linear surface separately requires more computation, but they got excellent bounds by intersecting the results of the first two mentioned methods.

This paper treats the tube from a geometrical point of view. The tube is built as the union of a sequence of $(n+1)$-dimensional step sets. For any step set the trajectories go inside the step set everywhere except at some part of its surface which is called the "exit hole". The exit hole of a previous step set is contained inside the next step set, so trajectories are forced to go through all step sets. The geometrical view makes it easier to build tubes which were unusual in previous approaches.

The first observation is that continuity of $\Sigma_t$ in previous approaches was too restrictive. Sometimes $\Sigma_t$ becomes instantly wider at the beginning of a time step, but at the end of the time step it becomes more tight than the continuous $\Sigma_t$ was. The search for such $\Sigma_t$ is more difficult than it was for the continuous case. Linear programming is used in this paper.

The second observation is that the tube can be built in other ways than $x^*(t) + \Sigma_t$. The integration step variable may be either $t$ or some state variable $x_i$. All we need is that the exit hole of a previous step set be inside the next step set. This gives us a solid rule to switch from one integration variable to another during the solution. The solution of Van der Pol example in this paper obtained benefits from the freedom of choice of integration variable for each step.

Section 2 contains the definition of exit hole and basic facts about it. Section 3 discusses exit holes of half-spaces. It also formulates a problem of optimal bound for scalar ODEs. This formulation helps in understanding, but it is too hard to solve it for non-linear ODEs. Section 4 explains how interval evaluation gives a simpler estimation of the exit hole condition. Section 5 tells about the exit hole of the intersection of sets. It presents trapezoid - a polytope used in this paper, and tells how to search for a tighter trapezoid using linear programming. Section 6 tells about the exit hole of the union of a sequence of sets. Section 7 contains the results of solving Van der Pol ODE.

## 2 Exit Hole

**Example IVPs** We shall illustrate definitions and theorems at three example IVPs.

Dahlquist

$$y = \begin{pmatrix} x \\ t \end{pmatrix} \in \mathbb{R}^2,\ \dot{y} = F(y) = \begin{pmatrix} -x \\ 1 \end{pmatrix},\ y_0 = \begin{pmatrix} 1 \\ 0 \end{pmatrix} \tag{3}$$

Curtiss-Hirschfelder

$$y = \begin{pmatrix} x \\ t \end{pmatrix} \in \mathbb{R}^2,\ \dot{y} = F(y) = \begin{pmatrix} 50(\cos t - x) \\ 1 \end{pmatrix},\ y_0 = \begin{pmatrix} 0 \\ 0 \end{pmatrix} \tag{4}$$

VanDerPol

$$y = \begin{pmatrix} x \\ p \\ t \end{pmatrix} \in \mathbb{R}^3,\ \dot{y} = F(y) = \begin{pmatrix} p \\ \mu(1 - x^2)p - x \\ 1 \end{pmatrix},\ y_0 = \begin{pmatrix} 2 \\ 0 \\ 0 \end{pmatrix},\ \mu = 500 \tag{5}$$

We assume that $F(y)$ is locally Lipschitz continuous in $\mathbb{R}^{n+1}$. For all $y \in \mathbb{R}^{n+1}$ there exists a neighborhood $U(y) \subseteq \mathbb{R}^{n+1}$ and a Lipschitz constant $L(y)$ such that $y_1 \in U(y), y_2 \in U(y) \Rightarrow \|F(y_1) - F(y_2)\| \leqslant L(y)\|y_1 - y_2\|$.

The Picard – Lindelöf Theorem guarantees that for any extended state $y_0 = (x_0, t_0) \in \mathbb{R}^{n+1}$ for some $\delta > 0$ there is unique solution $y(s) = (x(s), t_0 + s)$ of ODE (2) in interval $s \in [-\delta, +\delta]$. Moreover, the solution can be prolonged towards either $s \to +\infty$ or $\|x(s)\| \to \infty$. We denote the general solution of (2) stating from $y_0$ by $y(s; y_0)$.

**Definition 1.** The set $S \subseteq \mathbb{R}^{n+1}$ is said to be *positively invariant* if for any point $y_0 = (x_0, t_0) \in S$ the positive semi-orbit from $y_0$ is contained in $S$:
$\forall s \geqslant 0 \ y(s; y_0) \in S$.

The notion of positively invariant set is a global property of the set. We shall try to express it in local terms.

**Definition 2.** The point $y_e = (x_e, t_e) \in \mathbb{R}^{n+1}$ is an *exit point* of ODE (2) from a set $\Omega \subseteq \mathbb{R}^{n+1}$ if $y_e \in \overline{\Omega}$ and no starting segment of its positive semi-orbit is contained in $\Omega$: $\forall h > 0 \ \exists s \in [0, h[ \ y(s; y_e) \notin \Omega$. The exit point from a set necessarily belongs to the border of the set $y_e \in \partial\Omega$.

**Definition 3.** The *exit hole* $E\Omega$ is a set of all exit points of ODE from a set $\Omega$. It follows from the definition that $E\emptyset = \emptyset$ and $E\mathbb{R}^{n+1} = \emptyset$.

Let $\Omega = \{(x,t) |\ x \geqslant a,\ t \in \mathbb{R}\}$. Then
for Dahlquist ODE
$$E\Omega = \begin{cases} \emptyset, & \text{for } a \leqslant 0 \\ \{(a,t) |\ t \in \mathbb{R}\}, & \text{for } a > 0 \end{cases}$$
for Curtiss-Hirschfelder ODE
$$E\Omega = \begin{cases} \emptyset, & \text{for } a \leqslant -1 \\ \{(a,t) |\ -\arccos a + 2\pi k < t \leqslant \arccos a + 2\pi k\}, & \text{for } -1 < a < 1\,. \\ \{(a,t) |\ t \in \mathbb{R}\}, & \text{for } a \geqslant 1 \end{cases}$$
Let $\Omega = \{(x,p,t) | x \geqslant a,\ p \in \mathbb{R},\ t \in \mathbb{R}\}$. Then for VanDerPol example
$$E\Omega = \begin{cases} \{(a,p,t) |\ p < 0,\ t \in \mathbb{R}\}, & \text{for } a \leqslant 0 \\ \{(a,p,t) |\ p \leqslant 0,\ t \in \mathbb{R}\}, & \text{for } a > 0 \end{cases}.$$
The next proposition says that each solution of ODE which starts inside $\Omega$ and reachs outside $\Omega$ crosses boundary $\partial\Omega$ in an exit point.

**Proposition 1.** Let $y_0 \in \Omega,\ s_{out} > 0,\ y(s_{out}; y_0) \notin \Omega$. Then exists $s_e \in [0, s_{out}]$ such that $y_e = y(s_e; y_0)$ is an exit point of ODE from $\Omega$.

Proof. Let $s_e = \inf\{s \in [0, s_{out}] | y(s; y_0) \notin \Omega\}$. Let $y_e = y(s_e; y_0)$. If $s_e = 0$ then $y_e = y_0 \in \Omega$. If $s_e > 0$ then $y(s; y_0) \in \Omega$ for all $s \in [0, s_e[$. $y(s; y_0)$ as function of $s$ is continuous,so $y_e \in \overline{\Omega}$.

The curve $y(s; y_e) = y(s_e + s; y_0)$ is a solution of ODE (2) within a range $[0, s_{out} - s_e]$ starting from $y_e$. Suppose that $y_e$ is not an exit point. Then $\exists \delta > 0 \ \forall s \in [0, \delta[ \ y(s; y_e) \in \Omega$ and $\inf\{s \geqslant 0 | y(s; y_0) \notin \Omega\} \geqslant s_e + \delta$ that contradicts definition of $s_e$ $\blacksquare$.

**Proposition 2.** If exit hole of ODE from a set $\Omega$ is empty, then the set is positively invariant set.

Proof. Suppose that $\Omega$ is not positively invariant set. So there is a point $y_0 = (x_0, t_0) \in \Omega$, and $s > 0$ so that $y(s; y_0) \notin \Omega$. By proposition 1 there is an exit point $y_e = y(s_e; y_0)$ for some $s_e$ that contradicts to emptiness of $E\Omega$ $\blacksquare$.

# 3 Half spaces

We consider how to find exit holes of ODE from closed half space

$$\Omega = \{y | c^T y \geqslant a\}$$

with inward-pointing normal $c \in \mathbb{R}^{n+1}$, $c \neq 0$. Let $y_0$ is a point on the boundary of $\Omega$ that is hyperplane $c^T y_0 = a$. The first-order expansion of general ODE solution near $y_0$ is

$$y(s; y_0) = y_0 + F(y_0)s + o(s).$$

So

$$c^T y(s; y_0) = c^T y_0 + c^T F(y_0)s + o(s) = a + c^T F(y_0)s + o(s).$$

If $c^T F(y_0) > 0$ then $y_0$ is not an exit point.
If $c^T F(y_0) < 0$ then $y_0$ is an exit point.
If $c^T F(y_0) = 0$ then we don't know whether $y_0$ is an exit point. In this case the second-order expansion gives us similar conditions based on sign of $c^T \frac{\partial F(y_0)}{\partial y} F(y_0)$.

Let us rewrite the first-order condition in terms of $f(x, t)$ with $c = (c_x, c_t)$

$$c^T F(y) = c_x^T f(x, t) + c_t \tag{6}$$

**Example: Normal parallel to time** Let normal is $c = (0, c_t)$. Then $c^T F(y) = c_t$ for any ODE. For positive half space $\Omega_+ = \{(x, t) | t \geqslant a,\ x \in \mathbb{R}^n\}$ exit hole is empty $E\Omega_+ = \emptyset$. For negative half space $\Omega_- = \{(x, t) | t \leqslant a,\ x \in \mathbb{R}^n\}$ exit hole is entire boundary $E\Omega_- = \partial\Omega_- = \{(x, a) |\ x \in \mathbb{R}^n\}$.

**Scalar ODEs** Now consider scalar ODE ($n = 1$) and $c_x \neq 0$. Let $k = -c_t/c_x$. The equation of half-plane whose boundary contains given point $y_0 = (x_0, t_0)$ is

$$c_x(x - x_0 - k(t - t_0)) \geqslant 0$$

The first-order condition is

$$c^T F(y) = c_x(f(x, t) - k).$$

When $c_x > 0$ the equation of half space is $x \geqslant x_0 + \underline{k}(t - t_0)$. If $f(x_0 + \underline{k}(t - t_0), t) > \underline{k}$ for $t \in [t_0, t_1]$ then this half-plane doesn't have exit points with $t \in [t_0, t_1]$.
When $c_x < 0$ the equation of half space is $x \leqslant x_0 + \overline{k}(t - t_0)$. If $f(x_0 + \overline{k}(t - t_0), t) < \overline{k}$ for $t \in [t_0, t_1]$ then this half-plane doesn't have exit points with $t \in [t_0, t_1]$.

**Dahlquist ODE** Let $x_0 > 0$.
The half-plane $x \leqslant x_0 + \overline{k}t$ doesn't have exit points with $t \in [0, h)$ when $\forall t \in [0, h)\ -(x_0 + \overline{k}t) < \overline{k}$ i.e. when $\overline{k} \geqslant -\frac{x_0}{1+h}$.
The half-plane $x \geqslant x_0 + \underline{k}t$ doesn't have exit points with $t \in (0, h)$ when $\forall t \in (0, h)\ -(x_0 + \underline{k}t) > \underline{k}$ for $t \in (0, h)$ i.e. when $\underline{k} \leqslant -x_0$. Second-order condition proves that $(x_0, 0)$ isn't exit point too.

We have bounds

$$x_0(1-t) \leqslant x(t; x_0) \leqslant x_0\left(1 - \frac{t}{1+h}\right)$$

$$x_0(1-h) \leqslant x(h; x_0) \leqslant x_0 \frac{h}{1+h}.$$

For this ODE the lower bound is the same as forward-Euler point integration method returns, the upper bound is the same as backward-Euler point integration method returns.

When we bound $x(t; 1)$ by half-planes with $x_0 = 1$ the bounds are $1 - h \leqslant x(h; 1) \leqslant \frac{h}{1+h}$. The upper bound is asymptotically tight at $h \to +\infty$, the lower bound is not. However, we can try half-planes with $x_0 < 1$ for large $h$. The half-plane $x \geqslant 0 + 0t$ is better lower bound for $h > 1$.

So for each $h$ the tightest enclosure of the solution of Dahlqusit ODE $x(h; 1)$ by two half-planes is

$$x(h; 1) \in \begin{cases} [1-h, \frac{1}{1+h}], & \text{for } h \in [0, 1] \\ [0, \frac{1}{1+h}], & \text{for } h \in [1, +\infty) \end{cases}.$$

In general the tightest lower bound is obtained by following semi-infinite programming problem (the problem for upper bound is similar)

$$\begin{gathered} b + \underline{k} \to \max \\ b \leqslant x_0 \\ f(b + \underline{k}t, t) \geqslant \underline{k},\ \forall t \in [t_0, t_1] \end{gathered}$$

We don't solve semi-infinite problem in non-linear case. Instead we enclose $f(x, t)$ by piece-wise linear bounds. In this case the semi-infinite problem becomes linear programming problem. The next section is about piece-wise linear enclosure by interval techniques.

# 4 Enclosure of function in a surface

In previous section we used analytical calculations to prove that there are no exit holes in some part $S$ of a surface. We checked that condition $c^T F(y) > 0$ is valid in $S$. In other words we checked that $m = \min_{y \in S} c^T F(y) > 0$.

Analytical calculations are possible for simple examples only. We use interval arithmetic to estimate minimum of a $c^T F(y)$ defined by an expression $c^T \mathsf{F}(y)$ in a set $S$.

The simplest way is natural interval evaluation. Let the interval hull of a set $\square S = \boldsymbol{s}$. Then $m \geqslant \inf \mathsf{F}(\boldsymbol{s})$. Sometimes the result of the calculation is tight enough.

**Estimation of Autonomous scalar ODE.** Let $F(y) = (f(x), 1)^T$ and $n = 1$. Let $f(x)$ is defined by such expression that $\mathsf{f}(\boldsymbol{x}) = \mathrm{range}_{x \in \boldsymbol{x}} f(x)$. Let $\square S = \boldsymbol{s} = \boldsymbol{x} \times [t_0, t_1]$. Then

$$\mathrm{range}_{y \in S} c^T F(y) = \mathrm{range}_{y=(x,t)^T \in S}(c_x f(x) + c_t) =$$
$$c_x \mathrm{range}_{x \in \boldsymbol{x}} f(x) + c_t = c_x \mathsf{f}(\boldsymbol{x}) + c_t = c^T \mathsf{F}(\boldsymbol{x}).$$

**Estimation of Curtiss-Hirschfelder ODE.** We use the expression $\mathsf{F}(y) = 50(\cos(t) - x)$. Let us consider a surface

$$S = \{y = (x,t)^T \mid c_x(x - x_0) + c_t(t - t_0) = 0, t \in [t_0, t_1]\} =$$
$$\{y = (x,t)^T \mid x = x_0 + k(t - t_0), t \in [t_0, t_1]\}$$

where $k = -\frac{c_t}{c_x}, x_1 = x_0 + k(t_1 - t_0), 0 \leqslant t_0 < t_1 \leqslant \frac{\pi}{2}$.

Suppose $k < 0$.

$$\square S = \boldsymbol{s} = ([x_1, x_0], [t_0, t_1])^T$$
$$c^T \mathsf{F}(\boldsymbol{s}) = c_x \mathsf{f}([x_0, x_1], [t_0, t_1]) + c_t =$$
$$c_x 50(\cos[t_0, t_1] - [x_1, x_0]) + c_t =$$
$$c_x 50[\cos(t_1) - x_0, cos(t_0) - x_1] + c_t \supset$$
$$\mathrm{range}_{t \in [t_0, t_1]} 50(cos(t) - x_0 - k(t - t_0)) = \mathrm{range}_{y \in S} c^T F(y)$$

Simple interval extension doesn't give us exact estimation.

**Mean value form** We use a mean value form interval extension with the center $y^* \in S$ to obtain a better estimation than simple interval calculation.

$$c^T F(y) \in \boldsymbol{F}_{c,y^*}(y) = c^T \mathsf{F}(y^*) + \boldsymbol{l}^T (y - y^*), \tag{7}$$

where $\boldsymbol{l}^T = c^T \mathsf{F}'(\boldsymbol{s})$. Suppose that $S$ is a convex hull of some number of boxes or points $S = \mathrm{ch}\left(\bigcup_{i \in I} \boldsymbol{s}_i\right)$. The real functions $\underline{F}_{c,y^*}$ and $\overline{F}_{c,y^*}$ are respectively concave and convex functions of $y$. So they achive their minimum and maximum respectively at boxes - arguments of convex hull. Then

$$\mathrm{range}_{y \in S} c^T F(y) \subseteq c^T \mathsf{F}(y^*) + \square \bigcup_{i \in I} \boldsymbol{l}^T (\boldsymbol{s}_i - y^*)$$

.

We want to choose $y^* \in S$ to obtain tighter lower bound. The choice will use only $\boldsymbol{l} = c^T \mathsf{F}'(\boldsymbol{s})$ and no other information about $F(y)$. We can choose $\underline{y}^* = \mathrm{argmax}_{y^* \in \boldsymbol{s}} \min_{y \in \boldsymbol{s}} (y - y^*)^T \boldsymbol{l}$.

The formula for of $y^*$ is provided by BAUMANN [12].

$$y^* = \begin{cases} \overline{s}_i, & \text{for } \underline{l}_i \leqslant 0 \\ \underline{s}_i, & \text{for } \overline{l}_i \geqslant 0 \\ (\overline{l}_i \underline{x}_i - \underline{l}_i \overline{x}_i)/(\overline{l}_i - \underline{l}_i), & \text{otherwise,} \end{cases}.$$

He showed that this value is optimal for estimation in $\boldsymbol{s}$. For all $y \in \boldsymbol{s}$

$$\inf \boldsymbol{F}_{c,y} \leqslant \boldsymbol{F}_{c,y^*}.$$

We choose for estimation in $S$ by analogy

$$y^* = \operatorname*{argmax}_{y^* \in S} \min_{y \in S} (y - y^*)^T \boldsymbol{l}.$$

When the set is a convex hull of two boxes $S = \mathrm{ch}\,(\boldsymbol{s}_0 \cup \boldsymbol{s}_1)$, the choice of $y^*$ is a linear programming problem. It has $3n+1$ variables $y_i^*$, $p_{0i}$, $p1i$, $\alpha$, $m$:

$$\begin{gathered} m \to \max \\ m \leqslant p_{01} + p_{02} + \cdots + p_{0n} \\ p_{0i} \leqslant \underline{\boldsymbol{l}}_i(\underline{\boldsymbol{s}}_{0i} - y_i^*),\ p_{0i} \leqslant \overline{\boldsymbol{l}}_i(\underline{\boldsymbol{s}}_{0i} - y_i^*),\ p_{0i} \leqslant \underline{\boldsymbol{l}}_i(\overline{\boldsymbol{s}}_{0i} - y_i^*),\ p_{0i} \leqslant \overline{\boldsymbol{l}}_i(\overline{\boldsymbol{s}}_{0i} - y_i^*) \\ m \leqslant p_{11} + p_{12} + \cdots + p_{1n} \\ p_{1i} \leqslant \underline{\boldsymbol{l}}_i(\underline{\boldsymbol{s}}_{1i} - y_i^*),\ p_{1i} \leqslant \overline{\boldsymbol{l}}_i(\underline{\boldsymbol{s}}_{1i} - y_i^*),\ p_{1i} \leqslant \underline{\boldsymbol{l}}_i(\overline{\boldsymbol{s}}_{1i} - y_i^*),\ p_{1i} \leqslant \overline{\boldsymbol{l}}_i(\overline{\boldsymbol{s}}_{1i} - y_i^*) \\ 0 \leqslant \alpha \leqslant 1 \\ \alpha \underline{\boldsymbol{s}}_{0i} + (1-\alpha)\underline{\boldsymbol{s}}_{1i} \leqslant y_i^* \\ y_i^* \leqslant \alpha \overline{\boldsymbol{s}}_{0i} + (1-\alpha)\overline{\boldsymbol{s}}_{1i} \end{gathered}$$

These real equations emulate interval evaluation $\max_{y^* \in S} \min(\boldsymbol{l}(\boldsymbol{s}_0 - y^*) \cup \boldsymbol{l}(\boldsymbol{s}_1 - y^*))$

This estimation is heuristic. The $y^*$ may be suboptimal if $S$ isn't a box. Nevertheless, the mean-value form remains correct for any $y^* \in \boldsymbol{S}$. So we don't bother about rigorous solution of the LP problem. We use point LP solver like [14] and we don't bother about interval LP solver.

# 5 Trapezoid

**Proposition 3.** Let $S$ is the intersection of finite number of sets $S = \bigcap_{i \in I} S_i$. Then $ES = \bigcup_{i \in I}(ES_i \cap \overline{S})$.

In this paper we shall apply this proposition to a trapezoid of dimension $n+1$. It has two parallel facets which are boxes of dimension $n$. Parallel facets are orthogonal either to time axis or to one of state axis. We can consider this axis as integration variable. Such trapezoid is an intersection of $2(n+1)$ half spaces.

Let us write inequalities describing a trapezoid with integration variable $t$ and with parallel facets $(\boldsymbol{x}_0, t_0)$ and $(\boldsymbol{x}_1, t_1)$.

$$S = S^L \cap \boldsymbol{S}^R \cap \bigcap_{1 \leqslant i \leqslant n} (S^{il} \cap S^{iu})$$
$$S^L = \{y = (x, t) \mid t \geqslant t_0\}$$
$$S^R = \{y = (x, t) \mid t \leqslant t_1\}$$
$$S^{il} = \{y = (x, t) \mid x_i \geqslant \underline{\boldsymbol{x}}_{0i} + \frac{\underline{\boldsymbol{x}}_{1i} - \underline{x}_{0i}}{t_1 - t_0}(t - t_0)\}$$
$$S^{ir} = \{y = (x, t) \mid x_i \geqslant \overline{\boldsymbol{x}}_{0i} + \frac{\overline{\boldsymbol{x}}_{1i} - \overline{x}_{0i}}{t_1 - t_0}(t - t_0)\}$$
$$F^L = S \cap \partial \boldsymbol{S}^L$$
$$F^R = S \cap \partial \boldsymbol{S}^R$$
$$F^{il} = S \cap \partial \boldsymbol{S}^{il}$$
$$F^{ir} = S \cap \partial \boldsymbol{S}^{ir}$$

We want that exit hole of trapezoid is located only at the surface $F^R$. The proposition guarantees this if exit holes of other surfaces doesn't intersect with $S$. So we have a strong variant of Müller theorem. Let

$$f_i(x, t) > \frac{\underline{\boldsymbol{x}}_{1i} - \underline{\boldsymbol{x}}_{0i}}{t_1 - t_0}(t - t_0) \qquad \text{if } y = (x, t) \in F^{il} \tag{8}$$
$$f_i(y, t) < \frac{\overline{\boldsymbol{x}}_{1i} - \overline{\boldsymbol{x}}_{0i}}{t_1 - t_0}(t - t_0) \qquad \text{if } y = (x, t) \in F^{iu} \tag{9}$$

then $ES \subseteq F^R$. If we replace strong inequalities $>$ and $<$ by weak inequalities $\geqslant$ and $\leqslant$ the theorem is still correct, but its prove is more complicated.

The trapezoid with integration variable $x_k$ is described in similar way. Müller theorem for such trapezoid will use $\frac{f_i(x,t)}{f_k(x,t)}$ instead of $f_i(x, t)$. The trapezoid will have a pair of side facets related to time. Müller theorem will use $\frac{1}{f_k(x,t)}$ for them.

Suppose that we want to build a trapezoid $S$ with specified $t_0$ and $t_1$ which contains specified box $\boldsymbol{y}_{entry}$ such that $ES \subseteq F^R$. Also we want to obtain $F^R$ as narrow as possible. We can
- guess a priory enclosures for each future surface $\boldsymbol{a}^{il}$ and $\boldsymbol{a}^{iu}$,
- evaluate $\boldsymbol{l}^{il} = \mathsf{f}'_i(\boldsymbol{a}^{il})$ and $\boldsymbol{l}^{iu} = \mathsf{f}'_i(\boldsymbol{a}^{iu})$,
- guess center points for each side facet $y^{il*} \in \boldsymbol{a}^{il}$ and $y^{ir*} \in \boldsymbol{a}^{ir}$,
- choose weights $w_i$ of component width - and solve such a linear programming

(written in macro style)

$$\sum_{i=1}^{i=n} w_i(\overline{x}_{1i} - \underline{x}_{1i}) \to \min$$

$$\min(\boldsymbol{l}^{il}(\boldsymbol{s}^{ilL} - y^{il*}), \boldsymbol{l}^{il}(\boldsymbol{s}^{ilR} - y^{il*})) \geq \frac{\underline{\boldsymbol{x}}_{1i} - \underline{x}_{0i}}{t_1 - t_0}(t - t_0)$$

$$\max(\boldsymbol{l}^{iu}(\boldsymbol{s}^{iuL} - y^{iu*}), \boldsymbol{l}^{iu}(\boldsymbol{s}^{iuR} - y^{iu*})) \geq \frac{\overline{\boldsymbol{x}}_{1i} - \overline{x}_{0i}}{t_1 - t_0}(t - t_0)$$

$$\boldsymbol{y}_{entry} \subseteq S$$

where $\boldsymbol{s}^{ilL} = F^{il} \cap F^{L}$, $\boldsymbol{s}^{iuL} = F^{iu} \cap F^{L}$, $\boldsymbol{s}^{ilR} = F^{il} \cap F^{R}$, $\boldsymbol{s}^{iuR} = F^{iu} \cap F^{R}$ are ridges of dimension $n-1$. The exact size of linear program depends on number $n_J$ of non-zero items in system Jacobian
- $4n$ variables describing trapezoid $\boldsymbol{x}_0$ and $\boldsymbol{x}_1$;
- $4n_J$ variables for partial interval products;
- $16n_J$ constraints simulating partial interval products;
- $4n$ constrains simulating min and max;
- $2n$ or $4n$ constraints to cover $\boldsymbol{y}_{entry}$;
- Total $4(n + n_J)$ variables and $8(n + 2n_J)$ constraints.

This procedure can be applied in iterative manner. In this case previous facets give us are blunted to get a priory enclosure. Also previous facets are used to get center points by a procedure described in the previous section.

# 6 Union of a sequence

**Proposition 4.** Let $S$ is the union of finite number of sets $S = \bigcup_{i=1}^{i=n} S_i$. Then $ES \subseteq \bigcup_{i\in I} ES_i$.

**Proposition 5.** Let $S$ is the union of finite number of sets $S = \bigcup_{i=1}^{i=n} S_i$. Let exit hole of each set is contained in the next sets $\forall 1 \leqslant i < n$ $ES_i \subseteq \bigcup_{j=i+1}^{j=n} S_j$. Then $ES \subseteq ES_n$.

**Corollary** Let in previous proposition $T = \min_t(x,t) \in ES_n$. Then $S \cup \{(x,t) \mid \boldsymbol{t} \geqslant T, x \in \mathbb{R}^n\}$ is a positively invariant set.

These propositions explain how steps with different integration variables are glued together.

# 7 Experimental result

These schema was applied to the Van der Pol example in time interval $[0, 500]$. The first simulation started with exact initial value and the second one had an uncertainty in $x$: $\boldsymbol{y}_0 = \begin{pmatrix}[2] & [0] & [0]\end{pmatrix}^T$ and $\boldsymbol{y}_0 = \begin{pmatrix}[1.999, 2.001] & [0] & [0]\end{pmatrix}^T$. A sequence of 448 integration steps was specified manually. Each step had predefined integration variable and the value of the integration variable at the end of the step was specified. The integration variable was alternatively $x$ or $p$ at most steps. Integration variable was $t$ only at a few final steps to make results comparable with VNODELP solver. We ran VNODELP solver with the default integration order $order = 20$, with zero relative tolerance $RTol = 0$ and with different absolute tolerance $ATol$. VNODELP returns excellent accuracy starting from exact initial value for small $ATol$ and breaks when $ATol \geqslant 3.7302E-6$. It breaks always (at least when $ATol \geqslant 1E-30$) starting from uncertain initial point.

| Simulation | $x(500)$ | $p(500)$ |
|---|---|---|
| ExitHole | [-1.90962,-1.82260] | [0.00144430,0.00156996] |
| ExitHole from uncertain | [-1.90982,-1.82117] | [0.00144271,0.00157226] |
| VNODE ATol=1E-6 | [-1.86426,-1.86383] | [0.00150619,0.00150682] |
| VNODE ATol=3.73E-6 | [-1.89020,-1.83789] | [0.00110276,0.00191025] |

| Simulation | Steps | CPU(sec) |
|---|---|---|
| ExitHole | 448 | 17.13 |
| ExitHole from uncertain | 448 | 17.17 |
| VNODE ATol=1E-6 | 76878 | 205.25 |
| VNODE ATol=3.73E-6 | 81101 | 217.13 |

# 8 Conclusions and Outlook on Future Work

The first-order version of the Exit Hole method described in this paper can't compete with VNODELP high-order method when we need extremely tight bounds on a trajectory from an exact initial point. However, it can build low-accuracy bounds with less work than the high-order method. Also, it can bound trajectories when the initial point is uncertain.

An evident enhancement of the Exit Hole method for bounding a single trajectory is to use the high-order approximate solution $y^*(s)$. Here $s$ is not necessary $t$. The first-order method will bound difference between exact and approximate trajectories. The KÜHN's approach [2] may be helpful to suppress wrapping effect.

The possible enhancement of the Exit Hole method for bounding a set of trajectories with uncertain initial values and uncertain ODE parameters is to consider step sets that are more complicated than trapezoids but are still tractable.

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