Data driven peak and reachability set estimation

Jared Miller, Mario Sznaier
SIAM DS MS112, May 25, 2021
Main Ideas

$L_\infty$ bounded noise setting yields polytopic constraints

Use polytopic structure to simplify nonpositivity

Apply to Peak and Reachable Set Estimation
Peak Estimation Background
Peak Estimation Problem

Find maximum value of $p(x)$ along trajectories

$$P^* = \max_{t, \, x_0 \in X_0} p(x(t))$$

$$\dot{x}(t) = f(t, x(t)) \quad t \in [0, T]$$

$$x(0) = x_0 \in X_0$$

$$\dot{x} = [x_2, -x_1 - x_2 + x_1^3/3]$$
Infinite dimensional linear program (Fantuzzi, Goluskin, 2020)

Uses auxiliary function $v(t, x)$

\[
d^* = \min_{\gamma \in \mathbb{R}} \gamma
\]

\[
\begin{align*}
\gamma & \geq v(0, x) \quad \forall x \in X_0 \\
\mathcal{L}_f v(t, x) & \leq 0 \quad \forall (t, x) \in [0, T] \times X \\
v(t, x) & \geq p(x) \quad \forall (t, x) \in [0, T] \times X \\
v & \in C^1([0, T] \times X)
\end{align*}
\]

$P^* = d^*$ holds if $[0, T] \times X$ is compact, $f$ Lipschitz
Optimal $v(t, x)$ should be constant until peak is achieved
\[ \dot{x} = [x_2, -x_1 w - x_2 + x_1^3 / 3] \]

\[ w \in [0.5, 1.5], \quad x_0 = [1; 0] \]
Peak Estimation with Uncertainty

Dynamics $\dot{x} = f(t, x(t), w(t))$

Uncertain process $w(t) \in W$, $\forall t \in [0, T]$

Time-dependent $w$

$$\mathcal{L}_f v(t, x) \leq 0 \quad \forall (t, x, w) \in [0, T] \times X \times W$$

Time-independent $w$ ($\frac{dw}{dt} = 0$)

$$\mathcal{L}_f v(t, x, w) \leq 0 \quad \forall (t, x, w) \in [0, T] \times X \times W$$
Data Driven Setting
Noise Model

Ground truth $\dot{x} = F(t, x)$

Corrupted observations of system $F$ in $t \in [0, T]$

$(t_j, x_j, \dot{x}_j) \quad \forall j = 1, \ldots, N_s$

Assumption of $L_\infty$ bounded noise

$\|F(t_j, x_j) - \dot{x}_j\|_\infty \leq \epsilon \quad \forall j = 1, \ldots, N_s$
Sampling: Flow System

\[ \dot{x} = [x_2, -x_1 - x_2 + x_1^3/3] \]
Parameterize unknown $F$ by functions in dictionary:

$$\dot{x}(t) = f(t, x, w) = f_0(t, x) + \sum_{\ell=1}^{L} w_{\ell} f_{\ell}(t, x)$$

Affine in uncertainties $w$

Bounded noise constraint $\epsilon$

$$\| F(t_j, x_j) - \dot{x}_j \|_\infty \leq \epsilon \quad \forall j = 1, \ldots, N_s$$
$$\| f(t_j, x_j, w) - \dot{x}_j \|_\infty \leq \epsilon \quad \forall j = 1, \ldots, N_s$$
2 linear constraints for each coordinate $i$, sample $j$

$$-\epsilon \leq f_0(t_j, x_j)_i + \sum_{\ell=1}^{L} w_\ell f_\ell(t_j, x_j)_i - (\dot{x}_j)_i \leq \epsilon$$

Polytopic region $W = \{ w \in \mathbb{R}^L \mid Aw \leq b \}$ with $b \in \mathbb{R}^{2N_xN_s}$
Prior Work

Data Driven Solving Methods:

- Interval Analysis
- Koopman Operators
- Infinite LPs
- SVM/Deep Learning

Data Driven Polytopic Framework:

- Safety Verification
- Stabilizing and Safe Control (barrier/density)
Summary of Assumptions

Set \([0, T] \times X\) is compact

Dynamics \(f(t, x, w)\) are Lipschitz, affine in \(w\)

Uncertainty \(W\) is a compact polytope \(\{w \mid Aw \leq b\}\)

Nonempty interior: \(\exists w \in \mathbb{R}^L \mid Aw < b\)
Constraint Decomposition
Setting of time-dependent uncertainty $w(t) \in W$

Problem is Feasible

$$\mathcal{L}_{f(t,x,w)} v(t, x) \leq 0 \quad \forall (t, x, w) \in [0, T] \times X \times W$$

Problem is Infeasible

$$\mathcal{L}_{f(t,x,w)} v(t, x) > 0 \quad \exists (t, x, w) \in [0, T] \times X \times W$$

Pair of Strong Alternatives
Inequalities and Multipliers

One strict inequality, $m$ non-strict inequalities

$$R = \{ w \mid H(w) > 0, h_1(w) \geq 0, \ldots, h_m(w) \geq 0 \}$$

Define weighted sum with multipliers $\zeta \geq 0$

$$S(w; \zeta) = H(w) + \sum_{k=1}^{m} \zeta_k h_k(w)$$

$S$ is positive for all $w \in R, \ zeta \geq 0$
Lagrange dual function $g$

$$g(\zeta) = \sup_{w \in \mathbb{R}^L} S(w; \zeta) = \sup_{w \in \mathbb{R}^L} H(w) + \sum_{k=1}^{m} \zeta_k h_k(w)$$

Certificate $\zeta$ that $R$ is empty:

$$g(\zeta) \leq 0 \quad \forall \zeta \geq 0$$

Weak alternative $g(\zeta) \leq 0$ is strong if:

- $H(w), \ \forall \ h_k(w)$ convex in $w$
- Exists a point $w : \forall \ h_k(w) > 0$ (Slater)
Region $R = \{ w \mid \mathcal{L}_f v(t, x) > 0, \; Aw \leq b \}$

Form Lagrange dual $g(\zeta; v) = \sup_{w \in \mathbb{R}^L} S(w; \zeta, t, x)$:

$$g(\zeta; v) = \begin{cases} 
\mathcal{L}_{f_0} v + b^T \zeta & (A^T)\ell \zeta - f_\ell \cdot \nabla_x v = 0 \quad \forall \ell \\
\infty & \text{else}
\end{cases}$$

Bounded $g$ requires equality constraints over $[0, T] \times X$
Lie Polytopic Decomposition

Original

\[ \mathcal{L}_f v(t, x) \leq 0 \quad \forall (t, x, w) \in [0, T] \times X \times W \]

Decomposed

\[ \mathcal{L}_{f_0} v(t, x) + b^T \zeta(t, x) \leq 0 \quad \forall (t, x) \in [0, T] \times X \]

\[ (A^T)_{\ell} \zeta(t, x) = f_{\ell} \cdot \nabla_x v(t, x) \quad \forall \ell = 1, \ldots, L \]

\[ \zeta_k(t, x) \in C_+([0, T] \times X) \quad \forall k = 1, \ldots, m \]

Strong equivalence (given convexity in \( w \))
Summary of Relaxations

Time-independent to time-dependent uncertainty

Nonnegativity to Sum of Squares

Sum of Squares at finite degree
Peak Estimation (revisited)
Include time-varying uncertainty $w(t) \in \mathcal{W}$

$$d^* = \min_{\gamma \in \mathbb{R}} \gamma$$

$$\gamma \geq v(0, x) \quad \forall x \in X_0$$

$$\mathcal{L}_f v(t, x) \leq 0 \quad \forall (t, x, w) \in [0, T] \times X \times \mathcal{W}$$

$$v(t, x) \geq p(x) \quad \forall (t, x) \in [0, T] \times X$$

$$v \in C^1([0, T] \times X)$$
Only the Lie Derivative constraint changes

\[ d^* = \min_{\gamma \in \mathbb{R}} \gamma \]
\[ \gamma \geq v(0, x) \quad \forall x \in X_0 \]
\[ \mathcal{L}_{f_0} v(t, x) + b^T \zeta(t, x) \leq 0 \quad \forall (t, x) \in [0, T] \times X \]
\[ (A^T)_{\ell} \zeta(t, x) = (f_{\ell} \cdot \nabla_x) v(t, x) \quad \forall \ell = 1, \ldots, L \]
\[ v(t, x) \geq p(x) \quad \forall (t, x) \in [0, T] \times X \]
\[ v(t, x) \in C^1([0, T] \times X) \]
\[ \zeta_k(t) \in C_+([0, T] \times X) \quad \forall k = 1, \ldots, m \]
Peak Estimation Example (Flow)

40 observations with $\epsilon=[0, 0.5]$

$\dot{x} = [x_2, -x_1 - x_2 + x_1^3/3], \ T = 5$

Ground Truth
Noisy Data
Peak Estimation Example (Flow)

\[ \dot{x} = [x_2, -wx_1 - x_2 + x_1^3 / 3] \]

\[ L = 1, \ m = 80 \ (2 \ \text{nonredundant}) \]
Peak Estimation Example (Flow)

\[ \dot{x} = \left[ x_2, \text{cubic}(x_1, x_2) \right] \]

Order 4 bound = 0.841

\[ L = 10, \quad m = 80 \quad (33 \text{ nonredundant}) \]
Peak Estimation Example (Flow)

\[ \dot{x} = [x_2, \text{cubic}(x_1, x_2)] \]

\[ X_0 = \{ x \mid (x_1 - 1.5)^2 + x_2 \leq 0.4^2 \} \]
Dynamics model:

\[ S' = -\beta SI \]
\[ I' = \beta SI - \gamma I \]

Truth: \( \beta = 0.4 \), \( \gamma = 0.1 \)

\( m = 400 \) constraints
Peak Estimation Example (Epidemic)

$T = 40$, Unknown $(\beta, \gamma)$

$L = 2$, $m = 400$ (5 nonredundant)
Peak Estimation Example (Twist)

Dynamics model:

\[ \dot{x}_i = A_{ij}x_j - B_{ij}(4x_j^3 - 3x_j) \]

\[ A = \begin{bmatrix} -1 & 1 & 1 \\ -1 & 0 & -1 \\ 0 & 1 & -2 \end{bmatrix} \]

\[ B = \begin{bmatrix} -1/2 & 0 & -1/2 \\ 0 & 1/2 & 1/2 \\ 1/2 & 1/2 & 0 \end{bmatrix} \]

\[ X_0 = [-1, 0, 0], \quad T = 8 \]

Order 3 bound = 0.753
Peak Estimation Example (Twist)

100 Noisy Observations with $\epsilon=0.5$

$m = 2N_sN_x = 600$ constraints
Peak Estimation Example (Twist)

Order 3 bound = 0.819

Unknown $A$, Known $B$

$L = 9$, $m = 600$ (34 nonredundant)
Peak Estimation Example (Twist)

Known $A$, Unknown $B$

$L = 9$, $m = 600$ (30 nonredundant)
Peak Estimation Example (Twist)

Order 2 bound = 0.97

Unknown A, Unknown B

$L = 18, \ m = 600$ (70 nonredundant)
Reachable Set Estimation
Reachable Set Estimation

Find set of states reachable from $x_0 \in X_0$ at time $t = T$

$$P^* = \max_{X_T \subseteq X} \operatorname{vol}(X_T)$$

$$X_T : \exists x(t \mid x_h) :$$

$$\dot{x}(t) = f(t, x(t), w(t)) \quad \forall t \in [0, T]$$

$$w(t) \in W \quad \forall t \in [0, T]$$

$$x(0) \in X_0, \ x(T) \in X_T$$
Reachability indicator function $\chi_T$

$$\chi_T(x) = \begin{cases} 1 & x \in X_T \\ 0 & x \notin X_T \end{cases}$$

Create upper bound approximant $\omega(x) \in C(X)$:

$$\omega(x) \geq 1 \quad \forall x \in X_T \subseteq X$$

$$\omega(x) \geq 0 \quad \forall x \in X$$

Stone-Weierstrass: $\omega(x)$ is polynomial
Determine quality by comparing $\int_X \omega(x)dx$ vs $\text{vol}(X_T)$

$X_T = [0.1, 0.5] \cup [0.8, 0.9]$
Reachable Set Standard Program

Infinite dimensional linear program (Henrion, Korda, 2012)

\[
\begin{align*}
 d^* &= \min \int_X \omega(x) dx \\
 v(0, x) &\leq 0 \quad \forall x \in X_0 \\
 \mathcal{L}_f(t, x, w) v(t, x) &\leq 0 \quad \forall (t, x, w) \in [0, T] \times X \times W \\
 v(T, x) + \omega(x) &\geq 1 \quad \forall x \in X \\
 v(t, x) &\in C^1([0, T] \times X) \\
 \omega(x) &\in C_+(X)
\end{align*}
\]

Approximation \( X_T \subset \{ x \in X \mid \omega(x) \geq 1 \} \)
Reachable Set Decomposed Program

Approximation $X_T \subset \{ x \in X \mid \omega(x) \geq 1 \}$

$$d^* = \min \int_X \omega(x) \, dx$$

$$v(0, x) \leq 0 \quad \forall x \in X_0$$

$$\mathcal{L}_{f_0} v(t, x) + b^T \zeta(t, x) \leq 0 \quad \forall (t, x) \in [0, T] \times X$$

$$(A^T)_{\ell} \zeta(t, x) = (f_\ell \cdot \nabla_x)v(t, x) \quad \forall \ell = 1, \ldots, L$$

$$v(T, x) + \omega(x) \geq 1 \quad \forall x \in X$$

$$v(t, x) \in C^1([0, T] \times X)$$

$$\omega(x) \in C_+(X)$$

$$\zeta_k(t) \in C_+([0, T] \times X) \quad \forall k = 1, \ldots, m$$
Reachable Set Estimation Example (Flow)

Order 6 area = 0.129

\[ L = 1, \ m = 80 \ (2 \ \text{nonredundant}) \]
Reachable Set Estimation Example (Flow)

Order 4 area = 2.7

$L = 10, \ m = 80$ (33 nonredundant)
Reachable Set Estimation Example (Flow)

Order 4 volume = 0.756

Unknown A, Known B

$L = 9, m = 600$ (34 nonredundant)
Take-aways
Exploit polytopic structure of $L_\infty$-bounded noise

More SOS constraints in fewer variables

Tractable optimization problems (after preprocessing)
Future Work

- Streaming data and warm starts
- Time-space partitioning
- Maximum positively invariant sets
- Optimal control and extraction
- Hybrid systems
- Compatibility with structure (e.g. sparsity)
Acknowledgements

LAAS-CNRS: Didier Henrion

Robust Systems Lab: Tianyu Dai

Chateaubriand Fellowship of the Office for Science Technology of the Embassy of France in the United States.

National Science Foundation

Air Force Office of Scientific Research
Thank you for your attention
Extra Material
Preprocessing: Centering

Chebyshev center $c$: center of sphere with largest radius in $W$

Find through linear programming

$$\max r$$
$$A_k c + r \| A_k \|_2 \leq b_k \quad \forall k$$
$$r \geq 0, \ c \in \mathbb{R}^L$$

Shifted dynamics $f_0 \leftarrow f_0 + \sum_{\ell=1}^{L} c_{\ell} f_{\ell}$
Preprocessing: Redundancy

Majority of $m = 2N_x N_s$ constraints are often redundant

Convex hull of dual polytope:
Time: $\Omega(m \log m + m^{[L/2]})$

Linear program per constraint:
Time: $m \times \tilde{O}(mL + L^3)$
(Jan van den Brand et al. 2020)
Variations: Nonnegative Control

Control set is $W = \{ w \mid Aw \leq b, \ w \geq 0 \}$

\[
\mathcal{L}_{f_0} v(t, x) + b^T \zeta(t, x) \leq 0 \quad \forall (t, x) \in [0, T] \times X
\]
\[
(A^T)_{\ell} \zeta(t, x) \geq f_{\ell} \cdot \nabla_x v(t, x) \quad \forall (t, x) \in [0, T] \times X, \forall \ell
\]
\[
\zeta_k(t, x) \in C_+([0, T] \times X) \quad \forall k = 1, \ldots, m
\]

Mix $\geq$ and $=$ depending on input structure
Variations: Centrally Symmetric Control Set

If \( w \in W \), then \( -w \in W \)

Control set is \( W = \{ w | -b \leq Aw \leq b \} \)

\[
\mathcal{L}_0 v(t, x) + b^T \zeta(t, x) \leq 0 \quad \forall (t, x) \in [0, T] \times X \\
(A^T) \ell \zeta(t, x) \geq |f_\ell \cdot \nabla_x v(t, x)| \quad \forall (t, x) \in [0, T] \times X, \forall \ell \\
\zeta_k(t, x) \in C_+([0, T] \times X) \quad \forall k = 1, \ldots, m
\]

Generalization of ”Convex Optimization of Nonlinear Feedback Controllers via Occupation Measures” by Majumdar et. al.  
\((A = I, b = 1)\)