Safety Quantification for Nonlinear and Time-Delay Systems using Occupation Measures

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Safety Example







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Safety Example (Barrier/Density Function)



Safety Example (Distance Estimate)



Safety Example

Safety Quantification 5 in

60 mph



Motivation: Epidemic



Adapted from CDC

Image credit to Mayo Clinic News Network

Problems Covered



Pose safety quantification problems

Want convex, convergent, bisection-free algorithms

Formulate using convex linear programs in measures

Increasing-quality bounds using Semidefinite Programming

Peak estimation background

- 1. Survey of Thesis Work
- 2. Peak Value-at-Risk Estimation
- 3. Time-Delay Systems

Wrap-up

Peak Estimation Background

Peak Estimation Background

Find extreme value of p(x) along trajectories



Occupation Measure

Time trajectories spend in set

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

Single trajectory: $\langle v, \mu \rangle = \int_0^T v(t, x(t \mid x_0)) dt$

Averaged trajectory: $\langle v, \mu \rangle = \int_X \left(\int_0^T v(t, x) dt \right) d\mu_0(x)$



Connection to Measures



Measures: Initial μ_0 , Peak μ_p , Occupation μ For all functions $v(t, x) \in C([0, T] \times X)$

$$\begin{split} \mu_0^* : & \langle v(0,x), \mu_0^* \rangle = v(0,x_0^*) \\ \mu_p^* : & \langle v(t,x), \mu_p^* \rangle = v(t_p^*,x_p^*) \\ \mu^* : & \langle v(t,x), \mu^* \rangle = \int_0^{t_p^*} v(t,x^*(t \mid x_0^*)) dt \end{split}$$

Lie derivative (instantaneous change along f) $\forall v \in C^1$:

$$\mathcal{L}_{f}v = \partial_{t}v(t,x) + f(t,x) \cdot \nabla_{x}v(t,x)$$
 (1a)

Conservation law: final = initial + accumulated change

$$\langle \mathbf{v}(t, \mathbf{x}), \mu_{p} \rangle = \langle \mathbf{v}(0, \mathbf{x}), \mu_{0} \rangle + \langle \mathcal{L}_{f} \mathbf{v}(t, \mathbf{x}), \mu \rangle$$
(1b)
$$\mu_{p} = \delta_{0} \otimes \mu_{0} + \mathcal{L}_{f}^{\dagger} \mu$$
(1c)

Liouville 'represents' dynamics $\dot{x}(t) = f(t, x(t))$

Infinite-dimensional Linear Program (Cho, Stockbridge, 2002)

$$p^* = \sup \langle p(x), \mu_p \rangle$$
 (2a)

$$\langle 1, \mu_0
angle = 1$$
 (2b)

$$\langle v(t,x), \mu_p \rangle = \langle v(0,x), \mu_0 \rangle + \langle \mathcal{L}_f v(t,x), \mu \rangle \quad \forall v \quad (2c)$$

$$\mu, \mu_p \in \mathcal{M}_+([0, T] \times X) \tag{2d}$$

$$\mu_0 \in \mathcal{M}_+(X_0) \tag{2e}$$

Instance of Optimal Control Program (Lewis and Vinter, 1980) $(\mu_0^*, \mu_p^*, \mu^*)$ is feasible with $P^* = \langle p(x), \mu_p^* \rangle \leq p^*$ $P^* = p^*$ if compactness, Lipschitz properties hold

Moments for Peak Estimation

Moment: $y_{\alpha} = \langle x^{\alpha}, \nu \rangle \ \forall \alpha \in \mathbb{N}^{n}$

Moment matrix $\mathbb{M}[y]_{\alpha\beta} = y_{\alpha+\beta}$ is PSD

	<i>У</i> 00	<i>Y</i> 10	<i>Y</i> 01	<i>Y</i> 20	y 11	<i>y</i> ₀₂	
$\mathbb{M}_2[y] =$	У10 У01	У ₂₀ У11	У11 У02	У ₃₀ У ₂₁	У ₂₁ У ₁₂	У ₁₂ У ₀₃	<u>≻</u> 0
	У ₂₀ У11	У ₃₀ У ₂₁	У ₂₁ У12	У ₄₀ У31	У ₃₁ У ₂₂	у ₁₁ у ₁₃	
	y ₀₂	<i>Y</i> ₁₂	<i>Y</i> 03	<i>y</i> ₂₂	<i>y</i> ₁₃	<i>y</i> ₀₄	

Liouville induces affine relation in $(\mu^0,\mu^p,\mu)
ightarrow (y^0,y^p,y)$

Peak Estimation Example Bounds



Converging bounds to min. $x_2 = -0.5734$ (moment-SOS) Box region X = [-2.5, 2.5], time $t \in [0, 5]$ Max. PSD size: $\binom{(n+1)+(d+\lfloor \deg f/2 \rfloor)}{n+1}$ (Fantuzzi, Goluskin, 2020)

Survey of Thesis Work

Distance Estimation Problem

Unsafe set X_{μ} , point-set distance $c(x; X_{\mu}) = \inf_{y \in X_{\mu}} c(x, y)$ $P^* = \inf_{t, x_0 \in X_0} c(x(t \mid x_0); X_u)$ $\dot{x}(t) = f(t, x(t))$ $\forall t \in [0, T], x(0) = x_0.$

L₂ bound of 0.2831

Distance Program (Measures)

Infinite Dimensional Linear Program (Convergent)

$$p^* = \inf \langle c(x,y), \eta(x,y) \rangle$$
 (3a)

$$\langle 1, \mu_0 \rangle = 1$$
 (3b)

$$\langle \mathbf{v}(t,x), \mu_p \rangle = \langle \mathbf{v}(0,x), \mu_0 \rangle + \langle \mathcal{L}_f \mathbf{v}(t,x), \mu \rangle \quad \forall \mathbf{v} \quad (3c)$$

$$\langle w(x), \eta(x, y) \rangle = \langle w(x), \mu_{P}(t, x) \rangle$$
 $\forall w$ (3d)

$$\eta \in \mathcal{M}_+(X \times X_u) \tag{3e}$$

$$\mu_{\rho}, \ \mu \in \mathcal{M}_{+}([0, T] \times X)$$
(3f)

$$\mu_0 \in \mathcal{M}_+(X_0) \tag{3g}$$

Probability measures: (μ_0, μ_p, η)

Near-optimal trajectories if moment-matrix pprox rank-1

Distance Example (Flow Moon)



Collision if X_u was a half-circle

Distance Example (Flow Moon)



 L_2 bound of 0.1592

Safety of Shapes

Points on shape S with orientation ω (e.g., rigid body motion)



 L_2 bound of 0.1465, rotating square

Distance with Bounded Uncertainty

Dynamics $\dot{x}(t) = f(t, x(t), w(t))$ with $w(t) \in W$ Young measure $\mu(t, x, w)$, Liouville term $\langle \mathcal{L}_f v(t, x, w), \mu \rangle$



 L_2 bound of 0.1691, $w(t) \in [-1, 1]$

Hybrid Systems

Continuous dynamics with discrete jumps/transitions



 $R_{\text{left} \rightarrow \text{bottom}} = [1 - x_2; x_1], \qquad R_{\text{right} \rightarrow \text{top}} = [x_2; x_1]$

Sampling: Flow System

Data $\mathcal{D} = \{(t_j, x_j, \dot{x}_j)\}_j$ under mixed L_∞ -bounded noise



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

Given data \mathcal{D} , budget ϵ , system model $\{f_0, f_\ell\}$ Parameterize ground truth F by functions in dictionary

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

Ground truth satisfies corruption $J(w^*) \leq \epsilon$

$$L_\infty$$
 example: $J(w) = \max_j \|f(t_j, x_j, w) - \dot{x}_j\|_\infty$

Distance Estimation Example (Flow)

Input-affine + Semidefinite Representable uncertainty

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

PSD Size $8568 \rightarrow 56$ (L = 10) using robust counterparts



How much data corruption is needed to crash?

$$Q^{*} = \inf_{t^{*}, x_{0}, w} \left[\sup_{t \in [0, t^{*}]} J(w(t)) \right]$$
$$\dot{x}(t) = f(t, x(t), w(t)) \qquad \forall t \in [0, t^{*}]$$
$$x(t \mid x_{0}, w(\cdot)) \in X_{u}$$
$$w(\cdot) \in W, \ t^{*} \in [0, T], \ x_{0} \in X_{0}$$

Model safe if $Q^* > \epsilon$

Example Crash-Bounds

Two trajectories have same distance, different crash-bounds



Green-Top $Q^* = 0.316$, Yellow-Bottom $Q^* = 0.622$

Peak-Minimizing Control

Add state $\dot{z} = 0$ (Molina, Rapaport, Ramírez 2022)

$$Q_{z}^{*} = \inf_{t^{*}, x_{0}, z, w} z$$
(4a)

$$\dot{x}(t) = f(t, x(t), w(t)) \quad \forall t \in [0, t^{*}]$$
(4b)

$$\dot{z}(t) = 0 \quad \forall t \in [0, t^{*}]$$
(4c)

$$J(w(t)) \leq z \quad \forall t \in [0, t^{*}]$$
(4d)

$$x(t^{*} \mid x_{0}, w(\cdot)) \in X_{u}$$
(4e)

$$w(\cdot) \in W, t^{*} \in [0, T]$$
(4f)

$$x_{0} \in X_{0}, z \in [0, J_{max}]$$
(4g)

Equivalent formulation, $Q^* = Q_z^*$

Data-Driven Flow Crash-Bound

CasADi matches degree-4 moment-SOS crash bound



Terminal measure $\mu_p \in \mathcal{M}_+([0, T] \times X_u)$

True $\epsilon = 0.5 < 0.5499$, distance ≈ 0.2014

Flow Crash-Subvalue

Piecewise-polynomial subvalue for crash-safety

Based on Joint+Marginal optimization (Lasserre, 2010)



Bound of 0.3399 \leq 0.5499, but valid everywhere in X

Peak Value-at-Risk Estimation

with M. Tacchi, M. Sznaier, A. Jasour

Stochastic Differential Equation

Multivariate SDE dx = f(t, x)dt + g(t, x)dw (Itô)

Drift f and Diffusion g



Geometric Brownian Motion

Value-at-Risk (Quantile)

 ϵ -VaR of univariate measure $\omega(q)$ is unique number with



VaR = 1.282 for unit normal distribution at $\epsilon = 10\%$
Maximal Value at Risk



Red + Black areas = 10% probability

Value-at-Risk Example (Monte Carlo)

50,000 samples with T = 5, $\Delta t = 10^{-3}$



Maximize VaR of p(x) along SDE trajectories

 $p_{\#}\mu_{t^*}$: distribution of p(x(t)) at time t^*

$$P^* = \sup_{t^* \in [0,T]} VaR_{\epsilon}(p_{\#}\mu_{t^*})$$
(5a)
$$dx = f(t,x)dt + g(t,x)dw$$
(5b)
$$stopping time of min(t^*, exit from X)$$
(5c)

stopping time of min(t^{\prime} , exit from X) (5c) $x(0) \sim \mu_0.$ (5d) Concentration inequalities can upper-bound VaR

$$VaR_{\epsilon}(\omega) \leq \operatorname{stdev}(\omega)r + \operatorname{mean}(\omega)$$



Coherent Risk Measures (e.g., CVaR) can also bound VaR

Apply concentration inequalities to get upper bound $P_r^* \ge P^*$ Objective upper-bounds VaR w.r.t. time- t^* distribution μ_{t^*}

$$P_{r}^{*} = \sup_{t^{*} \in [0,T]} r \sqrt{\langle p^{2}, \mu_{t^{*}} \rangle - \langle p, \mu_{t^{*}} \rangle^{2}} + \langle p, \mu_{t^{*}} \rangle$$
(6a)
$$dx = f(t,x)dt + g(t,x)dw$$
(6b)
$$stopping time of min(t^{*}, exit from X)$$
(6c)
$$x(0) \sim \mu_{0}.$$
(6d)

Max-Mean: $\epsilon = 0.5$, r = 0 (Cho, Stockbridge, 2002)

Occupation measure μ , terminal measure $\mu_{ au}$

Second-Order Cone Program in measures (3d SOC)

$$p_r^* = \sup r \sqrt{\langle p^2, \mu_\tau \rangle - \langle p, \mu_\tau \rangle^2} + \langle p, \mu_\tau \rangle$$
 (7a)

$$\mu_{\tau} = \delta_0 \otimes \mu_0 + \mathcal{L}^{\dagger} \mu \tag{7b}$$

$$\mu_{ au}, \ \mu \in \mathcal{M}_+([0, T] imes X)$$
 (7c)

Generator $\mathcal{L}v = \partial_t v + f \cdot \nabla_x v + g^T (\nabla^2_{xx} v)g/2$ (Dynkin's) Results in upper-bound $p_r^* \ge P_r^* \ge P^*$, use moments

Chance-Peak Examples

Two-State

Stochastic Flow system from Prajna, Rantzer with T = 5

$$dx = \begin{bmatrix} x_2 \\ -x_1 - x_2 - \frac{1}{2}x_1^3 \end{bmatrix} dt + \begin{bmatrix} 0 \\ 0.1 \end{bmatrix} dw.$$



Maximize $-x_2$ with d = 6 (dashed=50%, solid=85% [ours])

Three-State

Stochasic Twist system with T = 5

$$dx = \begin{bmatrix} -2.5x_1 + x_2 - 0.5x_3 + 2x_1^3 + 2x_3^3 \\ -x_1 + 1.5x_2 + 0.5x_3 - 2x_2^3 - 2x_3^3 \\ 1.5x_1 + 2.5x_2 - 2x_3 - 2x_1^3 - 2x_2^3 \end{bmatrix} dt + \begin{bmatrix} 0 \\ 0 \\ 0.1 \end{bmatrix} dw.$$



Maximize x_3 with d = 6 (translucent=50%, solid=85%) 40

Two-State Switching

Switching subsystems at T = 5

$$dx = \left\{ \begin{bmatrix} -2.5x_1 - 2x_2 \\ -0.5x_1 - x_2 \end{bmatrix}, \begin{bmatrix} -x_1 - 2x_2 \\ 2.5x_1 - x_2 \end{bmatrix} \right\} dt + \begin{bmatrix} 0 \\ 0.25x_2 \end{bmatrix} dw$$



Maximize $-x_2$ with d = 6 (dashed=50%, solid=85%)

Two-State Distance

Half-circle unsafe set X_u

Based on distance estimation program



Minimize L_2 distance to X_u with d = 6 (dashed=50%, solid=85%)

Time-Delay Peak Estimation

with M. Korda, V. Magron, M. Sznaier

Time-Delay Examples

Delay between state change and its effect on system

$$\dot{x}(t) = f(t, x(t), x(t - \tau)) \qquad \forall t \in [0, T]$$

 $x(s) = x_h(s) \qquad \forall s \in [-\tau, 0]$

System	Delay
Epidemic	Incubation Period
Population	Gestation Time
Traffic	Reaction Time
Congestion	Queue Time
Fluid Flow	Moving in Pipe

Dependence on History



$$x'(t) = -2x(t) - 2x(t-1)$$

All trajectories pass through (t, x) = (0, 1)Initial history determines behavior, not just initial point

Delay Bifurcation Example



Peak Value vs. Delay



(a) $I_h = 0.1$, peak decreases



$$\begin{bmatrix} S'(t) \\ I'(t) \end{bmatrix} = \begin{bmatrix} -0.4S(t)I(t) \\ 0.4S(t-\tau)I(t-\tau) - 0.1I(t) \end{bmatrix}$$

History $x_h(t)$ resides in a class of functions \mathcal{H}

Graph-constrained \mathcal{H} : $(t, x_h(t))$ contained in $H_0 \subset [-\tau, 0] \times X$

$$P^* = \sup_{\substack{t^*, x_h}} p(x(t^*))$$

$$\dot{x} = f(t, x(t), x(t - \tau)) \qquad t \in [0, t^*]$$

$$x(t) = x_h(t) \qquad t \in [-\tau, 0]$$

$$x_h(\cdot) \in \mathcal{H}$$

Represent $x(t \mid x_h) : t \in [-\tau, t^*]$ as occupation measure

Time-Varying Preview

Order 5 bound: 0.71826



Existing Methods (very brief)

Certificates of Stability

- Lyapunov-Krasovskii
- Razumikhin
- LMI, Wirtinger
- ODE-Transport PDE

Relaxed control (Warga 1974, Vinter and Rosenblueth 1991-2) Fixed-terminal-time OCP with gridding (Barati 2012) SOS Barrier (Papachristodoulou and Peet, 2010) Riesz Operators (Magron and Prieur, 2020)

Time-Delay Measure Program

Time-Delay Visualization



Time-Delay Embedding

Delay Embedding



Black curve: $(t, x(t), x(t - \tau))$

Tuple of measures for the delayed case

Peak Initial History Occupation Start Occupation End Time-Slack $\mu_{p} \in \mathcal{M}_{+}([0, T] \times X)$ $\mu_{0} \in \mathcal{M}_{+}(X_{0})$ $\mu_{h} \in \mathcal{M}_{+}(H_{0})$ $\bar{\mu}_{0} \in \mathcal{M}_{+}([0, T - \tau] \times X^{2})$ $\bar{\mu}_{1} \in \mathcal{M}_{+}([T - \tau, T] \times X^{2})$ $\nu \in \mathcal{M}_{+}([0, T] \times X)$

Initial Conditions

Liouville: Dynamics

Consistency: Time-delay overlaps

Point evaluation $\langle 1, \mu_0
angle = 1$ at time $t = 0^+$

History $(t, x_h(t))$ defines a curve $[-\tau, 0]$, point at $x_h(0)$ t-marginal of μ_h should be the Lebesgue measure in $[-\tau, 0]$ Treat $x(t - \tau) = x_1$ as an external input $\dot{x}_0 = f(t, x_0, x_1)$ Sum $\bar{\mu} = \bar{\mu}_0 + \bar{\mu}_1$ in times $[0, T - \tau] \cap [T - \tau, T] = [0, T]$ Based on the delay embedding $(t, x(t), x(t - \tau))$ For all test functions $v \in C^1([0, T] \times X)$:

$$\langle \mathbf{v}, \mu_{\mathbf{p}} \rangle = \langle \mathbf{v}(0, \mathbf{x}), \mu_{0}(\mathbf{x}) \rangle + \langle \mathcal{L}_{f(t, x_{0}, x_{1})} \mathbf{v}(t, x_{0}), \overline{\mu}(t, x_{0}, x_{1}) \rangle$$

Consistency Issue



Consistency Fix



Early stopping in delayed time

Consistency Constraint

Inspired by changing limits of integrals $t' \leftarrow t - \tau$

$$\begin{pmatrix} \int_0^{t^*} + \int_{t^*}^{\min(\tau, t^* + \tau)} \end{pmatrix} \phi(t, x(t - \tau)) dt \\ = \left(\int_{-\tau}^0 + \int_0^{\min(t^*, \tau - \tau)} \right) \phi(t' + \tau, x(t')) dt'.$$

Shift-push $S^{\tau}_{\#}$ with $\langle \phi, S^{\tau}_{\#} \mu \rangle = \langle S^{\tau} \phi, \mu \rangle = \langle \phi(t + \tau, x), \mu \rangle$

Consistency constraint with time-slack ν

$$\pi_{\#}^{tx_1}(\bar{\mu}_0 + \bar{\mu}_1) + \nu = S_{\#}^{\tau}(\mu_h + \pi_{\#}^{tx_0}\bar{\mu}_0).$$

Linear program for time-delay peak estimation

$$p^{*} = \sup \langle p, \mu_{p} \rangle$$
(8a)
History-Validity(μ_{0}, μ_{h}) (8b)
Liouville($\mu_{0}, \mu_{p}, \bar{\mu}_{0}, \bar{\mu}_{1}$) (8c)
Consistency($\mu_{h}, \bar{\mu}_{0}, \bar{\mu}_{1}, \nu$) (8d)
Measure Definitions for ($\mu_{h}, \mu_{0}, \mu_{p}, \bar{\mu}_{0}, \bar{\mu}_{1}, \nu$) (8e)

Largest measures $\bar{\mu}_0, \bar{\mu}_1$ have 2n + 1 variables

Time-Delay Examples

Delay Comparision



Delayed Flow System



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Time-Varying System (Reprise)

Order 5 bound: 0.71826





Noted importance of safety quantification

Extended occupation measure methods for peak estimation

Performed data-driven analysis using robust counterparts

Adapted to non-ODE systems (Hybrid, SDE, Time-Delay)
- No-relaxation-gap for chance-peak and time-delay system
- High-order concentration inequalities
- Other time-delay models
- Lévy processes, Poisson jumps
- Distance-maximizing control
- Increased scalability, robotic systems
- Real-time computation

Safety is Important



Quantify using Peak Estimation

Published:

 J. Miller, D. Henrion, and M. Sznaier, "Peak Estimation Recovery and Safety Analysis," *IEEE Control Systems Letters*, vol. 5, no. 6, pp. 1982–1987, 2021 [link]

Conditionally Accepted:

 J. Miller and M. Sznaier, "Bounding the Distance to Unsafe Sets with Convex Optimization," (Conditionally accepted by IEEE Transactions on Automatic Control in 2022) [link]

Conference Proceedings

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- J. Miller and M. Sznaier, "Facial Input Decompositions for Robust Peak Estimation under Polyhedral Uncertainty," *IFACPapersOnLine*, vol. 55, no. 25, pp. 55–60, 2022. [link]. IFAC Young Author Award (ROCOND)
- J. Miller, D. Henrion, M. Sznaier, and M. Korda, "Peak Estimation for Uncertain and Switched Systems," in 2021 60th IEEE Conference on Decision and Control (CDC), pp. 3222–3228, 2021. [link]. Outstanding Student Paper Award (CDC 2021)

Preprints

- J. Miller, M. Korda, V. Magron, and M. Sznaier "Peak Estimation of Time Delay Systems using Occupation Measures, " 2023. [link]
- J. Miller, M. Tacchi, M. Sznaier, and A. Jasour, "Peak Value-at-Risk Estimation for Stochastic Differential Equations using Occupation Measures," 2023. [link]
- 3. J. Miller and M. Sznaier, "Peak Estimation of Hybrid Systems with Convex Optimization, " 2023. [link]
- J. Miller and M. Sznaier "Quantifying the Safety of Trajectories using Peak-Minimizing Control," 2023. [link]
- J. Miller and M. Sznaier, "Analysis and Control of Input-Affine Dynamical Systems using Infinite-Dimensional Robust Counterparts," 2023. [link]

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Last but not least



The Warden

Thank you again for your attention



Thank you again for your attention



Cookies in Dana 429 (RSL)

Bonus: Data-Driven Program

Auxiliary Evaluation along Optimal Trajectory



Optimal v(t, x) should be constant until peak is achieved

Polytopic region for L_{∞} -bounded noise

2 linear constraints for each coordinate i, sample j

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

Intersection of ellipsoids for L_2 -bounded noise

$$\|f_0(t_j, x_j) + \sum_{\ell=1}^L w_\ell f_\ell(t_j, x_j) - (\dot{x}_j)\|_2 \le \epsilon$$

Robust Counterpart Theory

Semidefinite-representable uncertainty set

$$W = \bigcap_{s} \{ \exists \lambda_{s} \in \mathbb{R}^{q_{s}} : A_{s}w + G_{s}\lambda_{s} + e_{s} \in K_{s} \}$$

Lie constraint (based on Ben-Tal, Nemirovskii, 2009)

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

Nonconservative robust counterpart with multipliers ζ

$$\begin{split} \mathcal{L}_{f_0} v(t,x) + \sum_{s=1}^{N_s} e_s^T \zeta_s(t,x) &\leq 0 & \forall [0,T] \times X \\ G_s^T \zeta_s(t,x) &= 0 & \forall s = 1..N_s \\ \sum_{s=1}^{N_s} (A_s^T \zeta_s(t,x))_\ell + f_\ell(t,x) \cdot \nabla_x v(t,x) &= 0 & \forall \ell = 1..L \\ \zeta_s(t,x) \in K_s^* & \forall s = 1..N_s \end{split}$$

Peak Decomposed Program

Example: Polytopic uncertainty $W = \{w \mid Aw \le b\}$ Only the Lie Derivative constraint changes

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

$$\gamma \ge v(0, x) \qquad \forall x \in X_0$$

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

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

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

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

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

Peak Estimation Example (Flow)



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Peak Estimation Example (Flow)



Consistency sets

$$Z = [0, J_{\max}] \qquad \Omega = \{(w, z) \in W \times Z : J(w) \le z\}.$$

Optimal Control Problem with auxiliary $v(t, x, z) \in C^1$

$$d^* = \sup_{\gamma \in \mathbb{R}, v} \gamma$$

$$v(0, x, z) \ge \gamma \qquad \forall (x, z) \in X_0 \times Z$$

$$v(t, x, z) \le z \qquad \forall (t, x, z) \in [0, T] \times X_u \times Z$$

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

Exploit affine structure of $J(w) = \|\Gamma w - h\|_{\infty}$

Nonconservatively robustified Lie constraint

$$\begin{aligned} d^* &= \sup_{\gamma \in \mathbb{R}, \ v} \ \gamma \\ & v(0, x, z) \geq \gamma & \forall (x, z) \in X_0 \times Z \\ & v(t, x, z) \leq z & \forall (t, x, z) \in [0, T] \times X_u \times Z \\ & \mathcal{L}_{f_0} v - (z\mathbf{1} + h)^T \zeta \geq 0 & \forall (t, x, z) \in [0, T] \times X \times [0, J_{\max}] \\ & (\Gamma^T)_{\ell} \zeta + f_{\ell} \cdot \nabla_x v = 0 & \forall \ell = 1..L \\ & \zeta_j \in C_+([0, T] \times X \times Z) & \forall j = 1..2nT. \end{aligned}$$

Every $c \in \mathbb{R}$ satisfies $c^2 \ge 0$ Sufficient: $q(x) \in \mathbb{R}[x]$ nonnegative if $q(x) = \sum_i q_i^2(x)$ Exists $v(x) \in \mathbb{R}[x]^s$, *Gram* matrix $Z \in \mathbb{S}^s_+$ with $q = v^T Z v$ Sum-of-Squares (SOS) cone $\Sigma[x]$

$$x^{2}y^{4} - 6x^{2}y^{2} + 10x^{2} + 2xy^{2} + 4xy - 6x + 4y^{2} + 1$$

=(x + 2y)² + (3x - 1 - xy²)²

Motzkin Counterexample (nonnegative but not SOS)

$$x^2y^4 + x^4y^2 - x^2y^2 + 1$$

Putinar Positivestellensatz (Psatz) nonnegativity certificate over set $\mathbb{K} = \{x \mid g_i(x) \ge 0, h_j(x) = 0\}$:

$$q(x) = \sigma_0(x) + \sum_i \sigma_i(x)g_i(x) + \sum_j \phi_j(x)h_j(x)$$
(9a)
$$\exists \sigma_0(x) \in \Sigma[x], \quad \sigma_i(x) \in \Sigma[x], \quad \phi_j \in \mathbb{R}[x].$$
(9b)

Psatz at degree 2*d* is an SDP, monomial basis: $s = \binom{n+d}{d}$ Archimedean: $\exists R \ge 0$ where $R - ||x||_2^2$ has Psatz over \mathbb{K}

Optimal Trajectories (Distance)



Optimal trajectories described by $(x_p^*, y^*, x_0^*, t_p^*)$:

- x_p^* location on trajectory of closest approach
- y^* location on unsafe set of closest approach
- x_0^* initial condition to produce x_p^*
- t_p^* time to reach x_p^* from x_0^*

Measures from Optimal Trajectories

Form measures from each $(x_p^*, x_0^*, t_p^*, y^*)$

Atomic Measures (rank-1)

$$\mu_0^*: \qquad \delta_{x=x_0^*} \\ \mu_p^*: \qquad \delta_{t=t_p^*} \otimes \delta_{x=x_p^*} \\ \eta^*: \qquad \delta_{x=x_p^*} \otimes \delta_{y=y^*}$$

Occupation Measure $\forall v(t, x) \in C([0, T] \times X)$

$$\mu^*$$
: $\langle v(t,x), \mu \rangle = \int_0^{t_\rho^*} v(t,x^*(t \mid x_0^*)) dt$

Hybrid Systems

State guards and transitions



 L_2 bound 0.0891: uncontrolled to boundary, controlled to sphere

Bonus: Chance-Peak

Reformulate as infinite-dimensional second-order cone program SOC set $Q^3 = \{(s, \kappa) \in \mathbb{R}^3 \times \mathbb{R}_{\geq 0} \mid \|s\|_2 \leq \kappa\}$

$$p_r^* = \sup_{z \in \mathbb{R}} rz + \langle p, \mu_\tau \rangle$$
 (10a)

$$\mu_{\tau} = \delta_0 \otimes \mu_0 + \mathcal{L}^{\dagger} \mu \tag{10b}$$

$$s = [1 - \langle p^2, \mu_\tau \rangle, \ 2z, \ 2\langle p, \mu_\tau \rangle]$$
(10c)

$$(s, 1 + \langle p^2, \mu_\tau \rangle) \in Q^3$$
 (10d)

$$\mu, \ \mu_{\tau} \in \mathcal{M}_{+}([0, T] \times X).$$
(10e)

Moment-SOS: $p_d^* \ge p_{d+1}^* \ge \ldots \ge p_r^* = P_r^* \ge P^*$

Bonus: Time Delay

Use moment-SOS hierarchy (Archimedean assumption) Degree *d*, dynamics degree $\tilde{d} = d + \max(\lfloor \deg f/2 \rfloor, \deg g - 1)$ Bounds: $p_d^* \ge p_{d+1}^* \ge \ldots \ge p_r^* = P_r^* \ge P^*$

Measure
$$\mu_p(t, x) \quad \mu(t, x)$$

PSD Size $\binom{1+n+d}{d} \quad \binom{1+n+\tilde{d}}{\tilde{d}}$

Timing scales approximately as $(1+n)^{6\widetilde{d}}$ or $\widetilde{d}^{4(n+1)}$

Propagation of Continuity



$$x'(t) = -2x(t) - 2x(t-1)$$

Continuity increases every τ_r time steps

Computational Complexity

Use moment-SOS hierarchy (Archimedean assumption) Degree d, dynamics degree $\widetilde{d} = d + \lfloor \deg f/2 \rfloor$

Bounds: $p_d^* \ge p_{d+1}^* \ge ... = p^* \ge P^*$

Size of Moment Matrices Peak Estimation

Timing scales approximately as $(2n+1)^{6 ilde{d}}$ or $ilde{d}^{4(2n+1)}$

SIR Peak Estimation Example



Upper bound $I_{max} \ge 56.9\%$ with order 3 LMI

Recovery: $t_* = 15.6$ days, $(S^*, I^*) = (56.9\%, 5.61\%)$

Time-Varying System



Time-Varying Histories



History restrictions and trajectories of system

Joint+Component Consistency



 (t, x_0) marginal of $\bar{\mu}$

For all test functions $\phi_0 \in C([0, T] \times X)$

$$\begin{split} \langle \phi_0(t, x_0), \bar{\mu} \rangle &= \int_0^T \phi_0(t, x(t \mid x_h)) dt \\ &= \left(\int_0^{T-\tau} + \int_{T-\tau}^T \right) \phi_0(t, x(t \mid x_h)) dt \\ &= \langle \phi_0(t, x), \nu_0 + \nu_1 \rangle \end{split}$$

Joint+Component Consistency (cont.)



 (t, x_1) marginal of $\bar{\mu}$

For all test functions $\phi_1 \in C([0, T] \times X)$

$$egin{aligned} &\langle \phi_1(t,x_1),ar{\mu}
angle &= \int_0^T \phi_1(t,x(t- au\mid x_h))dt \ &= \int_{- au}^{T- au} \phi_1(t+ au,x(t\mid x_h))dt \ &= \int_{- au}^0 \phi_1(t+ au,x_h(t))dt + \langle \phi_1(t+ au,x),
u_0
angle \end{aligned}$$

Joint+Component Experiment

Table 1: Objective values for Flow experiment

degree <i>d</i>	1	2	3	4	5
Joint+Component	1.25	1.223	1.1937	1.1751	1.1636
Standard	1.25	1.2183	1.1913	1.1727	1.1630

Table 2: Time (seconds) to obtain SDP bounds in Table 1

degree <i>d</i>	1	2	3	4	5
Joint+Component	0.782	0.991	5.271	31.885	336.509
Standard	0.937	1.190	9.508	105.777	552.496

Bonus: Measure Background
Nonnegative Borel Measure μ

Assigns each set $A \subseteq X$ a 'size' $\mu(A) \ge 0$ (Measure)

Mass $\mu(X) = \langle 1, \mu \rangle = 1$: Probability distribution

 $\mu \in \mathcal{M}_+(X)$: space of measures on X $f \in C(X)$: continuous function on XPairing by Lebesgue integration $\langle f, \mu \rangle = \int_X f(x) d\mu(x)$

Dirac delta
$$\delta_{x'}(A) = egin{cases} 1 & x' \in A \ 0 & x'
ot \in A \end{cases}$$

Probability: $\delta_{x'}(X) = 1, \ \langle f(x), \delta_{x'} \rangle = f(x')$ $\mu(A) = 1$: Solid Box $\mu(A) = 0$: Dashed Box



Rank-1 atomic measure

$$\mu = c\delta_{x'} \qquad \qquad c > 0$$

Rank-2 atomic measure

$$\mu = c_1 \delta_{x'_1} + c_2 \delta_{x'_2}$$
 $c > 0, \ x'_1 \neq x'_2$

Rank-r atomic measure

$$\mu = \sum_{i=1}^{r} c_i \delta_{x'_i} \qquad c > 0, \ \{x'_i\}_{i=1}^{r} \text{distinct}$$

Example of Measure Optimization



Optimum $\mathbb{E}_{\mu}[f] = \langle f, \mu \rangle$ at $\mu = \delta_{\mathsf{x}^*}$

Measure Optimization

Nonconvex problems could be convex in measures

$$\min_{x\in K} p(x) o \min_{\mu\in \mathcal{M}_+(K)} \langle p,\mu
angle, \quad \langle 1,\mu
angle = 1$$



 $f(\frac{1}{2}(1+(-1))) = 1$, but $\frac{1}{2}(f(1)+f(-1)) = 0$

Bonus: Approximating Measure LPs

Measure LPs are infinite-dimensional

Linear Matrix Inequality: convex problem

$$\max_{y} b^{T} y \qquad C + \sum_{i=1}^{m} A_{i} y_{i} \geq 0$$

Solve LMIs through (interior point, ADMM, etc.) Approximate infinite LPs by finite-dimensional LMIs Monomial $x^{\alpha} = \prod_{i} x_{i}^{\alpha_{i}}$ for power $\alpha \in \mathbb{N}^{n}$ Degree $|\alpha| = \sum_{i} \alpha_{i}$ α -moment of measure $y_{\alpha} = \langle y_{\alpha}, \mu \rangle$

Measure uniquely described by infinite set $\{y_{\alpha}\}_{\alpha \in \mathbb{N}^n}$

When does a sequence $\{y_{\alpha}\}_{\alpha \in \mathcal{A}}$ correspond to a measure μ ?

Linear Functional polynomial \rightarrow moments

$$f(x)
ightarrow \int_X f(x) d\mu = \int_X \sum_{lpha} f_{lpha} x^{lpha} d\mu = \sum_{lpha} f_{lpha} y_{lpha}$$

Bivariate Example

$$2 + x_1 x_2 - 3x_1^2 + x_1 x_2^3 \rightarrow 2 + y_{11} - 3y_{20} + y_{13}$$

Moment Matrices

Squares $f(x)^2$ are nonnegative (real) $f(x)^2 \ge 0$ implies that $\langle f(x)^2, \mu \rangle \ge 0 \quad \forall f \in \mathbb{R}[x]$:

$$\langle f(x)^2, \mu
angle = \int_X \sum_{lpha, eta} (f_lpha x^lpha) (f_eta x^eta) d\mu = \int_X \sum_{lpha, eta} (f_lpha f_eta x^{lpha+eta}) d\mu \ge 0$$

Moment matrix $\mathbb{M}[y] \succeq 0$ has $\mathbb{M}[y]_{\alpha,\beta} = y_{\alpha+\beta}$

$$\langle f(\mathbf{x})^2, \mu \rangle = \mathbf{f}^T \mathbb{M}[\mathbf{y}] \mathbf{f} \ge 0$$

Moments up to degree $2 \times 2 = 4$

$$\mathbb{M}_{2}[y] = \begin{cases} y_{00} & y_{10} & y_{01} & y_{20} & y_{11} & y_{02} \\ y_{10} & y_{20} & y_{11} & y_{30} & y_{21} & y_{12} \\ y_{01} & y_{11} & y_{02} & y_{21} & y_{12} & y_{03} \\ y_{20} & y_{30} & y_{21} & y_{40} & y_{31} & y_{11} \\ y_{11} & y_{21} & y_{12} & y_{31} & y_{22} & y_{13} \\ y_{02} & y_{12} & y_{03} & y_{22} & y_{13} & y_{04} \end{cases}$$

 μ supported on set $K = \{x \mid g_i(x) \ge 0, i = 1...N\}$ $g_i(x)f(x)^2 \ge 0$ implies that $\langle g_i(x)f(x)^2, \mu \rangle \ge 0$

$$\langle g_i(x)f(x)^2,\mu\rangle = \int_X \sum_{lpha,eta,\gamma} (f_lpha f_eta g_\gamma x^{lpha+eta+\gamma}) d\mu \ge 0$$

Localizing matrix $\mathbb{M}[g_i m] \succeq 0$ has $\mathbb{M}[g_i m]_{\alpha,\beta} = \sum_{\gamma} g_{\gamma} m_{\alpha+\beta+\gamma}$ $\langle g_i(x) f(x)^2, \mu \rangle = \mathbf{f}^T \mathbb{M}[g_i y] \mathbf{f} \ge 0$ Polynomial optimization problem example :

$$p^* = \max_{x \in K} p(x) = \max_{\mu \in \mathcal{M}_+(K)} \langle p(x), \mu
angle, \quad \mu(K) = 1$$

Keep moments up to degree *d*:

$$p_d^* = \max_{y} \sum_{|\alpha| \le 2d} p_{\alpha} m_{\alpha}$$
$$\mathbb{M}_d[y], \ \mathbb{M}_{d-\deg(g_i)}[g_i y] \succeq 0$$

Finite-dimensional SDP: $\mathbb{M}_d[y]$ has size $\binom{n+d}{d}$

Bounds $p_d^* \geq p_{d+1}^* \geq p_{d+2}^* \dots$ converge to p^* as $d o \infty$

- 1. Trajectory Program
- 2. Measure LP
- 3. Moment LMI

Increase degree d of LMI to get better bounds

Prove conditions under which $\lim_{d\to\infty} p_d^* o p^* = P^*$