# Safety Quantification for Nonlinear and Time-Delay Systems using Occupation Measures (Bonus Content)

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# **Bonus: Data-Driven Program**

#### Auxiliary Evaluation along Optimal Trajectory



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

Polytopic region for  $L_{\infty}$ -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  $\zeta$ 

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

#### 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)



#### Peak Estimation Example (Flow)



#### **Crash-Bound Program**

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)<sup>2</sup> + (3x - 1 - xy<sup>2</sup>)<sup>2</sup>

Motzkin Counterexample (nonnegative but not SOS)

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

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

$$q(x) = \sigma_0(x) + \sum_i \sigma_i(x)g_i(x) + \sum_j \phi_j(x)h_j(x)$$
(1a)  
$$\exists \sigma_0(x) \in \Sigma[x], \quad \sigma_i(x) \in \Sigma[x], \quad \phi_j \in \mathbb{R}[x].$$
(1b)

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  $Q^3 = \{(s, \kappa) \in \mathbb{R}^3 \times \mathbb{R}_{\geq 0} \mid \|s\|_2 \leq \kappa\}$ 

$$p_r^* = \sup_{z \in \mathbb{R}} rz + \langle p, \mu_\tau \rangle$$
 (2a)

$$\mu_{\tau} = \delta_0 \otimes \mu_0 + \mathcal{L}^{\dagger} \mu \tag{2b}$$

$$\mathbf{s} = [1 - \langle \boldsymbol{p}^2, \boldsymbol{\mu}_{\tau} \rangle, \ 2z, \ 2\langle \boldsymbol{p}, \boldsymbol{\mu}_{\tau} \rangle]$$
(2c)

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

$$\mu, \ \mu_{\tau} \in \mathcal{M}_{+}([0, T] \times X).$$
(2e)

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  $\begin{pmatrix} 1+n+d \\ d \end{pmatrix} \begin{pmatrix} 1+n+\tilde{d} \\ \tilde{d} \end{pmatrix}$ 

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  $\tau_r$  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  $ar{\mu}$ 

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

$$egin{aligned} &\langle \phi_1(t,x_1),ar{\mu}
angle &= \int_0^T \phi_1(t,x(t- au\mid x_h))dt \ &= \int_{- au}^{T- au} \phi_1(t+ au,x(t\mid x_h))dt \ &= \int_{- au}^0 \phi_1(t+ au,x_h(t))dt + \langle \phi_1(t+ au,x),oldsymbol{
u}_0
angle \end{aligned}$$

#### 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  $\mu$ 

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

$$\mu = c_1 \delta_{x_1'} + c_2 \delta_{x_2'} \qquad c > 0, \ x_1' \neq x_2'$$

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  $\mu = \delta_{x^*}$ 

#### **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  $|\alpha| = \sum_{i} \alpha_{i}$  $\alpha$ -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  $\mu$ ?

#### 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  $2 \times 2 = 4$ 

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

 $\mu$  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 :

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

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  $\lim_{d \to \infty} p_d^* \to p^* = P^*$