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Peak Estimation of Time Delay Systems using Occupation Measures

Jared Miller[1,2], Milan Korda [3,4], Victor Magron [3,5], Mario Sznaier[2]

Abstract— **This work proposes a method to compute the maximum value obtained by a state function along trajectories of a Delay Differential Equation (DDE). An example of this task is finding the maximum number of infected people in an epidemic model with a nonzero incubation period. The variables of this peak estimation problem include the stopping time and the original history (restricted to a class of admissible histories). The original nonconvex DDE peak estimation problem is approximated by an infinite-dimensional Linear Program (LP) in occupation measures, inspired by existing measure-based methods in peak estimation and optimal control. This LP is approximated from above by a sequence of Semidefinite Programs (SDPs) through the moment-Sum of Squares (SOS) hierarchy. Effectiveness of this scheme in providing peak estimates for DDEs is demonstrated with provided examples.**

I. Introduction

This paper presents an algorithm to upper bound extreme values of a state function attained along trajectories of a Delay Differential Equation (DDE). The dynamics of a DDE depend on a history of the state, in contrast to an Ordinary Differential Equation (ODE) in which the dynamics are a function only of the present values of state [1], [2], [3], [4]. This paper will involve analysis of DDEs in a state space $X \subset \mathbb{R}^n$ over a time horizon $T < \infty$ with a single fixed discrete bounded delay $\tau \in (0, T)$.

Trajectory evolution of a DDE depends on an initial history $x_h : [-\tau, 0] \to X$ rather than simply an initial condition $x_0 \in X$ for a corresponding ODE. The evaluation at time t for a trajectory starting with a history x_h will be denoted as $x(t \mid x_h)$. A function class $\mathcal{H}$ of histories may be defined, allowing for the definition of differential inclusions of DDEs. A peak estimation problem may be defined on a time-delay system to find the maximum value of a state function p along system trajectories given a class of initial histories $\mathcal{H}$ as

$$
\begin{aligned}
P^* = & \sup_{t^* \in [0,T],\ x_h(\cdot)} p(x(t^* \mid x_h)) && \text{(1a)}\\
& \dot{x} = f(t, x(t), x(t-\tau)) \qquad \forall t \in [0, T] && \text{(1b)}\\
& x(t) = x_h(t) \qquad \forall t \in [-\tau, 0] && \text{(1c)}\\
& x_h(\cdot) \in \mathcal{H}. && \text{(1d)}
\end{aligned}
$$

The variables in Problem (1) are the stopping time t^* and the initial history x_h. Problem (1) is a DDE version of the (generically nonconvex) ODE peak estimation program studied in [5], [6]. The peak estimation task in (1) is an instance of a DDE Optimal Control Problem (OCP) with a free terminal time and a zero running (integrated) cost.

This work uses measure-theoretic methods in order to provide certifiable upper bounds on the peak value P^* from (1). The first application of measure-theoretic methods towards DDEs was in [7], in which the control input was relaxed into a Young Measure [8] (probability distribution at each point in time) [9]. This Young-Measure-based relaxed control yields the OCP optimal value in the case of a single discrete time delay under convexity, regularity, and compactness assumptions. However, the Young Measure control programs may result in a lower bound when there are two or more delays in the system dynamics (there exist Young-Measure solutions that do not correspond to OCP solutions) [10], [11]. Adding new measures and constraints allows for the construction of tight Young Measure OCP approximations at the cost of significantly more complicated programs [12].

Occupation measures are nonnegative Borel measures that contain all possible information about trajectory behavior, and are a step beyond Young Measures in terms of abstraction and relaxation. The work of [13] proves that a convex infinite-dimensional Linear Program (LP) in occupation measures for an ODE OCP has the same optimal value as the original OCP under compactness, convexity, and regularity conditions. The problem of estimation of the peak of the expected value of a given state function for stochastic processes may be solved using occupation measures under these same conditions [5]. The Moment-Sum of Squares (SOS) hierarchy offers a sequence of outer approximations (lower bounds on OCP/upper bounds on peak estimates) as found through solving Semidefinite Programs (SDPs) of increasing size [14]. The moment-SOS hierarchy has been applied to dynamical problems including barrier functions [15], OCPs [16], [17], peak estimation [6], [18], region of

[1]Automatic Control Laboratory (IfA), ETH Zürich, Physikstrasse 3, 8092, Zürich, Switzerland

[2]Robust Systems Lab, ECE Department, Northeastern University, Boston, MA 02115.

[3]Polynomial OPtimization Team, LAAS-CNRS, Toulouse, 31400, France

[4]Faculty of Electrical Engineering, Czech Technical University in Prague, Technická 2, CZ-16626 Prague, Czech Republic

[5]Institut de Mathématiques de Toulouse, 31062, France

emails: jarmiller@control.ee.ethz.ch, korda@laas.fr, vmagron@laas.fr, msznaier@coe.neu.edu

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attraction estimation [19], reachable set estimation [20] and distance estimation [21].

Use of the moment-SOS hierarchy towards analysis of DDEs includes finding stability and safety certificates [22], [23], [17]. Prior work on using occupation measures for problems in time delays includes ODE-PDE models in [24], [25], a Riesz-frame system in [26], and a gridded LP framework for optimal control given a single history x_h in [27]. Peak estimation has been conducted on specific time-delay systems such as the forced Liénard model [28] and compartmental epidemic models [29].

The contributions of this paper are:

- A theory of Measure-Valued (MV)-solutions to DDEs with multiple histories (in $\mathcal{H}$) and free terminal time
- A measure LP that upper-bounds problem (1)
- A convergent sequence of Linear Matrix Inequalities (LMIs) (and resultant SDPs) to the measure upper-bound

To the best of our knowledge, this is the first work that treats peak estimation of time-delay systems.

This paper is organized as follows: Section II formalizes notation and summarizes concepts in measure theory, time-delay, occupation measures, and ODE peak estimation. Section III defines an MV-solution for free-terminal-time DDE solutions to create a measure-LP that upper-bounds (1). Section IV reviews the Moment-SOS hierarchy and applies it to finding SDPs to upper-bound the peak-estimation measure LP. Section V provides two examples of DDE peak estimation. Section VI concludes the paper.

II. Preliminaries

A. Notation

The n-dimensional real Euclidean vector space is $\mathbb{R}^n$. The set of natural numbers is $\mathbb{N}$, and the set of n-dimensional multi-indices is $\mathbb{N}^n$. The degree of a multi-index $\alpha \in \mathbb{N}^n$ is $|\alpha| = \sum_{i=1}^n \alpha_i$. The set of polynomials with real coefficients in an indeterminate x is $\mathbb{R}[x]$. Each polynomial $p(x) \in \mathbb{R}[x]$ has a unique representation in terms of a finite index set $\mathcal{J} \subset \mathbb{N}^n$ and coefficients $\{p_\alpha\}_{\alpha \in \mathcal{J}}$ with $p_\alpha \neq 0$ as $p(x) = \sum_{\alpha \in \mathcal{J}} p_\alpha \left(\prod_{i=1}^n x_i^{\alpha_i}\right) = \sum_{\alpha \in \mathcal{J}} p_\alpha x^\alpha$. The degree of a polynomial $\deg p(x)$ is equal to $\max_{\alpha \in \mathcal{J}} |\alpha_j|$. The subset of polynomials with degree at most d is $\mathbb{R}[x]_{\leq d} \subset \mathbb{R}[x]$.

B. Analysis and Measure Theory

Let X be a topological space. The set of continuous functions over a space X is $C(X)$, and its subcone of nonnegative functions over X is $C_+(X)$. The subset of once-differentiable functions over X is $C^1(X) \subset C(X)$. A single-variable function $g(t)$ is Piecewise Continuous (PC) over the domain $[a, b]$ if there exist $B \in \mathbb{N}\backslash\{0\}$ and a finite number of time-breaks $t_0 = a < t_1 < t_2 < \cdots < t_B < b = t_{B+1}$ such that the function $g(t)$ is continuous in each interval $[t_k, t_{k+1})$ for $k = 0..B$. The class of PC functions from the time interval $[-\tau, 0]$ to X is $PC([-\tau, 0], X)$.

The set of nonnegative Borel measures over X is $\mathcal{M}_+(X)$. A pairing exists between functions $p \in C(X)$ and measures $\mu \in \mathcal{M}_+(X)$ by Lebesgue integration with $\langle p, \mu \rangle = \int_X p(x) d\mu(x)$. This pairing is a duality pairing and defines an inner product between $C_+(X)$ and $\mathcal{M}_+(X)$ when X is compact. The μ-measure of a set $A \subseteq X$ may be defined in terms of A's indicator function ($I_A(x) = 1$ if $x \in A$ and $I_A(x) = 0$ otherwise) as $\mu(A) = \langle I_A(x), \mu(x) \rangle$. The quantity $\mu(X)$ is called the mass of μ, and μ is a probability distribution if $\mu(X) = 1$. The support of μ is the set of all points x such that all open neighborhoods $N_x \ni x$ satisfy $\mu(N_x) > 0$. Two special measures are the Dirac delta and the Lebesgue measure. The Dirac delta δ_x with respect to a point $x \in X$ obeys the point-evaluation pairing $\langle p, \delta_x \rangle = p(x)$ for all $p \in C(X)$. The Lebesgue (volume) distribution has the definition $\langle p, \lambda_X \rangle = \int_X p(x) dx$. Further details about measure theory are available in [30].

Given spaces X and Y, the projection $\pi^x : X \times Y \to X$ is the map $(x, y) \mapsto x$. For measures $\mu \in \mathcal{M}_+(X)$ and $\nu \in \mathcal{M}_+(Y)$, the product measure $\mu \otimes \nu \in \mathcal{M}_+(X \times Y)$ is the unique measure satisfying $(\mu \otimes \nu)(A \times B) = \mu(A)\nu(B)$ for all subsets $A \subseteq X,\ B \subseteq Y$. For two measures $\mu, \xi \in \mathcal{M}_+(X)$, the measure μ dominates ξ ($\xi \leq \mu$) if $\xi(A) \leq \mu(A),\ \forall A \subseteq X$. To every dominated measure $\xi \leq \mu$ there exists a slack measure $\hat{\xi} \in \mathcal{M}_+(X)$ such that $\xi + \hat{\xi} = \mu$.

The pushforward of a map $Q : X \to Y$ along a measure μ is $Q_\# \mu$, with the relation $\langle z, Q_\# \mu \rangle = \langle z \circ Q, \mu \rangle$ holding for all $z \in C(Y)$. Given $\eta \in \mathcal{M}_+(X \times Y)$, the projection-pushforward $\pi^x_\# \eta$ is the x-marginalization of η. The pairing of $p \in C(X)$ with $\pi^x_\# \eta$ may be equivalently expressed as $\langle p, \pi^x_\# \eta \rangle = \langle p, \eta \rangle$. The adjoint of a linear map $\mathcal{L} : C(X) \to C(Y)$ is a mapping $\mathcal{L}^\dagger : M(Y) \to M(X)$ satisfying $\langle \mathcal{L}p, \nu \rangle = \langle p, \mathcal{L}^\dagger \nu \rangle$ for all $p \in C(X)$ and $\nu \in M(Y)$.

C. Time Delay Systems

Given a PC state history $t \mapsto x_h(t),\ t \in [-\tau, 0]$, a unique forward trajectory $x(t \mid x_h)$ of (1b) exists on $t \in [0, T]$ if the function $(t, x_0, x_1) \mapsto f(t, x_0, x_1)$ is locally Lipschitz in all variables. Such locally Lipschitz dynamics satisfy a smoothing property: the order of trajectory time-derivatives that are continuous will increase by 1 every τ time steps [4].

The behavior of time-delay systems may change and bifurcate as the time delays change. A well-studied example of $\dot{x} = -x(t - \tau)$ in which the system is stable (to $x = 0$) for all bounded PC histories with $\tau \in [0, \pi/2)$, has bounded oscillations for some initial histories at $\tau = \pi/2$ (e.g. constant x_h in time), and is unstable (divergent oscillations to $\pm\infty$) for all similar histories with $\tau > \pi/2$ [4].

Problem (1) involves a class of histories $\mathcal{H}$. In this paper, we will impose that $\mathcal{H}$ is graph-constrained,

Definition 2.1: The history class $\mathcal{H}$ is **graph-constrained** if $\mathcal{H}$ is the set of histories whose graph lies within a given set $H_0 \subseteq [-\tau, 0] \times X$,

$$\mathcal{H} = \{x_h \in PC([-\tau, 0], X) \mid (t, x_h(t)) \in H_0\ \forall t \in [-\tau, 0]\},$$

and there are no other continuity restrictions on histories.

D. Occupation Measures

The **occupation measure** associated with an interval $[a, b] \subset \mathbb{R}$ and a curve $t \mapsto x(t) \in PC([a, b], X)$ is the pushforward of the Lebesgue distribution (in time) $\lambda_{[a,b]}$ along the curve evaluation. Such an occupation measure $\mu_{x(\cdot)} \in \mathcal{M}_+([a,b] \times X)$ satisfies a relation for all $v \in C([a,b] \times X)$:

$$\langle v, \mu_{x(\cdot)} \rangle = \textstyle\int_a^b v(t, x(t)) dt. \tag{2}$$

Occupation measures can be extended to controlled dynamics. Let $U \subset \mathbb{R}^m$ be a set of input-values and define the following controlled dynamics (with $\forall t \in [0,T]: \ u(t) \in U$)

$$\dot{x}(t) = f(t, x(t), u(t)). \tag{3}$$

The occupation measure of a trajectory of (3) given a stopping time t^*, a distribution of initial conditions $\mu_0 \in \mathcal{M}_+(X_0)$ with $X_0 \subset X$ and a measurable control $u(\cdot)$ (such that $u(t)$ is a probability distribution over U for each $t \in [0, t^*]$) for sets $A \subseteq [0,T], \ B \subseteq X, \ C \subseteq U$ is

$$\mu(A \times B \times C \mid t^*) = \tag{4}$$
$$\int_{X_0} \int_{[0,t^*]} I_{A\times B\times C}\left((t, x(t \mid x_0, u(\cdot)), u(t)\right) dt d\mu_0(x_0).$$

A linear operator $\mathcal{L}_f$ may be defined for every $v \in C^1([-\tau, T] \times \mathbb{R}^n)$ by

$$\mathcal{L}_f v(t,x) = \partial_t v(t,x) + f(t,x,u) \cdot \nabla_x v(t,x). \tag{5}$$

A distribution of initial conditions $\mu_0 \in \mathcal{M}_+(X_0)$, free-terminal-time values $\mu_p \in \mathcal{M}_+([0,T] \times X)$, and occupation measures $\mu \in \mathcal{M}_+([0,T] \times X \times U)$ from (4) are connected together by Liouville's equation for all $v \in C^1([0,T] \times X)$

$$\langle v, \mu_p \rangle = \langle v(0,x), \mu_0(x) \rangle + \langle \mathcal{L}_f v, \mu \rangle \tag{6a}$$
$$\mu_p = \delta_0 \otimes \mu_0 + \pi^{tx}_\# \mathcal{L}_f^\dagger \mu. \tag{6b}$$

Equation (6b) is a shorthand notation for (6a) when applied to all C^1 functions v. Note that the $\pi^{tx}_\#$ marginalizes out the input u in the occupation measure μ. Any μ as part of a tuple of measures (μ_0, μ_p, μ) satisfying (6) is referred to as a **relaxed occupation measure**.

III. Peak Measure Program

This section will formulate a measure-valued LP which upper-bounds Problem (1) in objective.

A. Assumptions

The following assumptions will be imposed on the peak estimation Problem (1):

- A1 The set $[-\tau, T] \times X$ is compact with $\tau < T$;
- A2 The function f is Lipschitz inside $[0,T] \times X^2$;
- A3 Any trajectory $x(\cdot \mid x_h)$ with $x_h \in \mathcal{H}$ such that $x(t \mid x_h) \notin X$ for some $t \in [0,T]$ also satisfies $x(t' \mid x_h) \notin X$ for all $t' \geq t$;
- A4 The objective p is continuous;
- A5 The history class $\mathcal{H}$ is graph-constrained by $H_0 \subset [-\tau, 0] \times X$.

In the case where $\tau > T$, the delayed state $t \mapsto x(t-\tau)$ is fully specified in time $[0,T]$ without requiring dynamical information, and (1) reduces to a peak estimation problem over ODEs. All tracked histories in $\mathcal{H}$ are bounded due to assumption A1 (since the range X is compact). The nonreturn assumption A3 ensures that a trajectory cannot leave and then return to X to produce a lower value of p, given that the occupation-measure-based techniques used in this paper can only track trajectories while they are in X (Remark 1 of [21]).

B. Measure-Valued Solution

The initial set X_0 is the $t = 0^+$ slice of H_0. Equation (7) describes the measures $(\mu_h, \mu_0, \mu_p, \bar{\mu}_0, \bar{\mu}_1, \nu)$ that will be used to form a free-terminal-time MV-solution to the DDE (1b) with multiple histories (in $\mathcal{H}$):

History	$\mu_h \in \mathcal{M}_+(H_0)$	(7a)
Initial	$\mu_0 \in \mathcal{M}_+(X_0)$	(7b)
Peak	$\mu_p \in \mathcal{M}_+([0,T] \times X)$	(7c)
Occupation Start	$\bar{\mu}_0 \in \mathcal{M}_+([0, T-\tau] \times X^2)$	(7d)
Occupation End	$\bar{\mu}_1 \in \mathcal{M}_+([T-\tau, T] \times X^2)$	(7e)
Time-Slack	$\nu \in \mathcal{M}_+([0,T] \times X)$	(7f)

The joint (relaxed) occupation measure $\bar{\mu} \in \mathcal{M}_+([0,T] \times X^2)$ is constructed from the sum $\bar{\mu} = \bar{\mu}_0 + \bar{\mu}_1$. An MV solution to the DDE in (1b) is a set of measures from (7) that satisfies three types of constraints: History-Validity, Liouville, Consistency.

1) History-Validity: The first History-Validity constraint is that μ_0 should be a probability distribution over the initial state condition (at $t = 0$). The second is that the history measure μ_h should represent an averaged occupation measure of histories that are defined between $[-\tau, 0]$, which implies that the t-marginal of μ_h should be Lebesgue-distributed. The two History-Validity constraints are,

$$\langle 1, \mu_0 \rangle = 1, \qquad\qquad \pi^t_\# \mu_h = \lambda_{[-\tau, 0]}. \tag{8}$$

2) Liouville: The true occupation measure $(t, x_0, x_1) \mapsto \bar{\mu}(t, x_0, x_1)$ has a time t, a current state $x_0 = x(t \mid x_h)$, and an external input $x_1 \in X$ with $x_1(t) = x(t - \tau \mid x_h)$. Use of the Liouville equation in (6) applied to the joint occupation measure $\bar{\mu} = \bar{\mu}_0 + \bar{\mu}_1$ leads to

$$\mu_p = \delta_0 \otimes \mu_0 + \pi^{tx_0}_\# \mathcal{L}_f^\dagger (\bar{\mu}_0 + \bar{\mu}_1). \tag{9}$$

3) Consistency: The x_1 input of f from the Liouville equation (9) is not arbitrary; it should be equal to a time-delayed $x_1(t) = x_0(t - \tau)$. This requirement will be imposed by a Consistency constraint.

Lemma 3.1: Let $x(\cdot)$ be a solution to (1b) for some history x_h with an initial time of 0 and a stopping time of $t^* \in [0,T]$. Then the following two integrals are equal for all $\phi \in C([0,T] \times X)$:

$$\left(\int_0^{t^*} + \int_{t^*}^{\min(T, t^*+\tau)}\right) \phi(t, x(t-\tau)) dt$$
$$= \left(\int_{-\tau}^{0} + \int_0^{\min(t^*, T-\tau)}\right) \phi(t' + \tau, x(t)) dt'. \tag{10}$$

Proof: This follows from $t' \leftarrow t - \tau$. ■

Equation (10) inspires a consistency constraint for the free-terminal-time MV-solution in (7). The left-hand-side of (10) may be generalized to

$$\langle \phi(t, x_1), \bar{\mu}_0(t, x_0, x_1) + \bar{\mu}_1(t, x_0, x_1)\rangle + \langle \phi(t, x), \nu(t, x)\rangle, \tag{11}$$

in which $\bar{\mu}_0$ is supported in times $[0, \min(t^*, T-\tau)]$, $\bar{\mu}_1$ is supported in times $[T-\tau, t^*]$ if $t^* > T-\tau$, and the slack measure ν implements the $[t^*, \min(T, t^*+\tau)]$ limits. The right-hand-side of (10) may be interpreted as

$$\langle \phi(t+\tau, x), \mu_h(t, x)\rangle + \langle \phi(t+\tau, x_0), \bar{\mu}_0(t, x_0, x_1)\rangle. \tag{12}$$

Define S^τ as the shift operator $S^\tau \phi(t, x) = \phi(t+\tau, x)$. With an abuse of notation, the pushforward operation $S^\tau_\#$ applied to a measure (such as μ_h) will have the expression

$$\langle \phi, S^\tau_\# \mu_h\rangle = \langle S^\tau \phi, \mu_h\rangle = \langle \phi(t+\tau, x), \mu_h(t, x)\rangle. \tag{13}$$

The Consistency constraint inspired by Lemma 3.1 is

$$\pi^{tx_1}_\#(\bar{\mu}_0 + \bar{\mu}_1) + \nu = S^\tau_\#(\mu_h + \pi^{tx_0}_\# \bar{\mu}_0). \tag{14}$$

Remark 1: Equation (14) may also be written as $\pi^{tx_1}_\#(\bar{\mu}_0 + \bar{\mu}_1) \leq S^\tau_\#(\mu_h + \pi^{tx_0}_\# \bar{\mu}_0)$ with slack ν.

C. Measure Program

An infinite-dimensional LP in terms of the measures from (7) to upper-bound Problem (1) is,

$$p^* = \sup \quad \langle p, \mu_p\rangle \tag{15a}$$
$$\langle 1, \mu_0\rangle = 1 \tag{15b}$$
$$\pi^t_\# \mu_h = \lambda_{[-\tau, 0]} \tag{15c}$$
$$\mu_p = \delta_0 \otimes \mu_0 + \pi^{tx_0}_\# \mathcal{L}^\dagger_f(\bar{\mu}_0 + \bar{\mu}_1) \tag{15d}$$
$$\pi^{tx_1}_\#(\bar{\mu}_0 + \bar{\mu}_1) + \nu = S^\tau_\#(\mu_h + \pi^{tx_0}_\# \bar{\mu}_0) \tag{15e}$$
$$\text{Measure Definitions from (7).} \tag{15f}$$

Remark 2: Membership in the history class $\mathcal{H}$ is imposed by the History-Validity constraint (15c) and through support of μ_h in (7a).

Definition 3.1: An MV-solution to the DDE (1b) with free-terminal-time and histories in $\mathcal{H}$ is a tuple of measures that satisfy (15b)-(15f) and (7a)-(7f).

Theorem 3.2: Under assumptions A1-A5, (15) will upper bound (1) with $p^* \geq P^*$ when $\mathcal{H}$ is graph-constrained.

Proof: This proof will proceed by demonstrating that every (t^*, x_h) candidate from (1) may be expressed by a unique MV-solution from Defn. 3.1. The history measure μ_h is the $[-\tau, 0]$ occupation measure of $x(t)$, and the initial measure μ_0 is the Dirac-delta $\delta_{x_h(0^+)}$. The peak measure μ_p is the Dirac-delta $\delta_{t=t^*} \otimes \delta_{x=x(t^* | x_h)}$. The relaxed occupation measures $(\bar{\mu}_0, \bar{\mu}_1, \nu)$ will now be considered. For convenience, define $z(t) = (t, x(t \mid x_h), x(t-\tau \mid x_h))$ as the delay embedding of the trajectory $x(t \mid x_h)$. In the case where $t^* \in [0, T-\tau]$, then $\bar{\mu}_0$ is the $[0, t^*]$ occupation measure of $z(t)$, $\bar{\mu}_1$ is the zero measure, and ν is the $[t^*, t^*+\tau]$ occupation measure of $(t, x(t-\tau \mid x_h))$. Alternatively when $t^* \in (T-\tau, T]$, $\bar{\mu}_0$ is the $[0, T-\tau]$ occupation measure of $z(t)$, $\bar{\mu}_1$ is the $[T-\tau, t^*]$ occupation measure of $z(t)$, and ν is the $[t^*, T]$ occupation measure of $(t, x(t-\tau \mid x_h))$. All of the measures in (7) have been defined for each input (t^*, x_h), which proves that $p^* \geq P^*$. ■

IV. Peak Moment Program

This section will briefly review the moment-SOS hierarchy [14] in order to approximate-from-above Program (15) by a sequence of finite-dimensional SDPs.

A. Review of Moment-SOS Hierarchy

Let $\mu \in \mathcal{M}_+(X)$ be a measure, and let $\alpha \in \mathbb{N}^n$ be a multi-index. The α-moment of μ is the pairing $\mathbf{m}_\alpha = \langle x^\alpha, \mu\rangle$. The moment sequence $\mathbf{m} = \{\mathbf{m}_\alpha\}_{\alpha \in \mathbb{N}^n}$ is the infinite collection of moments of μ. A unique (Riesz) linear functional $L_\mathbf{m}$ exists operating on each polynomials $p = \sum_{\alpha \in \mathcal{J}} p_\alpha x^\alpha \in \mathbb{R}[x]$ as $L_\mathbf{m}(p) = \sum_{\alpha \in \mathcal{J}} p_\alpha \mathbf{m}_\alpha$ for a finite index set $\mathcal{J} \subset \mathbb{N}^n$.

A set is Basic Semialgebraic (BSA) if it is defined by a finite number of polynomial inequality constraints, such as by $\mathbb{K} = \{x \in \mathbb{R}^n \mid g_k(x) \geq 0 : \ k = 1 \ldots N_c\} \subseteq \mathbb{R}^n$. The measure μ is supported on $\mathbb{K}$ if $\mu \in \mathcal{M}_+(\mathbb{K})$. Given a polynomial $g = \sum_{\gamma \in \mathcal{J}} g_\gamma x^\gamma$, the localizing matrix $\mathbb{M}[g\mathbf{m}]$ induced by the constraint $g(x) \geq 0$ with respect to the moment sequence $\mathbf{m}$ is the infinite-dimensional matrix indexed by $\alpha, \beta \in \mathbb{N}^n$ as $\mathbb{M}[g\mathbf{m}]_{\alpha,\beta} = L_\mathbf{m}(x^{\alpha+\beta} g) = \sum_{\gamma \in \mathbb{R}^n} g_\gamma \mathbf{m}_{\alpha+\beta+\gamma}$. The moment matrix $\mathbb{M}[\mathbf{m}]$ is the localizing matrix associated with $g = 1$. The matrix $\mathbb{M}[\mathbb{K}\mathbf{m}]$ is the block-diagonal matrix comprised of $\mathbb{M}[\mathbf{m}]$ and $\mathbb{M}[g_k \mathbf{m}]$ for $k = 1 \ldots N_c$.

Let $\{\tilde{\mathbf{m}}_\alpha\}_{\alpha \in \mathbb{N}^n}$ be a sequence of real numbers. If there exists some measure $\tilde{\mu} \in \mathcal{M}_+(\mathbb{K})$ such that $\forall \alpha \in \mathbb{N}^n$: $\langle x^\alpha, \mu\rangle = \tilde{\mathbf{m}}_\alpha$ then $\tilde{\mu}$ is a representing measure for $\tilde{\mathbf{m}}$, and $\tilde{\mathbf{m}}$ is a moment-sequence for $\tilde{\mu}$. Such a representing measure (if it exists) could be nonunique. The stronger condition that there is a unique representing measure for $\tilde{\mathbf{m}}$ is called moment determinacy. A necessary condition for $\tilde{\mathbf{m}}$ to have a representing measure is that the block-diagonal matrix $\mathbb{M}[\tilde{\mathbf{m}}]$ is Positive Semidefinite (PSD). This necessary condition is also sufficient if $\mathbb{K}$ satisfies an *Archimedean* condition (stronger than compactness, equivalent after a ball constraint $R - \|x\|_2^2 \geq 0$ is added to $\mathbb{K}$ for sufficiently large $R > 0$ if $\mathbb{K}$ is compact). In general we will call $\tilde{\mathbf{m}}$ a *pseudo-moment* sequence.

The order-d truncation of $\mathbb{M}[\mathbb{K}\mathbf{m}]$ (for $d \in \mathbb{N}$ and expressed as $\mathbb{M}_d[\mathbb{K}\mathbf{m}]$) keeps entries of degree $\leq 2d$, and preserves the top-corner of each matrix in the block-diagonal. The moment matrix $\mathbb{M}_d[\mathbf{m}]$ is a PSD matrix of size $\binom{n+d}{d}$ assuming a monomial basis for x is employed. The size of each truncated localizing matrix $\mathbb{M}_d[g_k\mathbf{m}]$ is $\binom{n+d-\lceil d_k/2\rceil}{d-\lceil d_k/2\rceil}$, where $d_k = \deg g_k$. The moment-SOS hierarchy is the process of increasing the degree $d \to \infty$ when forming moment programs associated to measure LPs.

B. Moment Program

Additional assumptions are required in order to approximate (15) using the moment-SOS hierarchy:

A6 The sets H_0, X_0, and X are Archimedean BSA sets.
A7 Both p and f are polynomials.

Let the measures $(\mu_h, \mu_0, \mu_p, \bar{\mu}_0, \bar{\mu}_1, \nu)$ have associated pseudo-moment sequences $(\mathbf{m}^h, \mathbf{m}^0, \mathbf{m}^p, \bar{\mathbf{m}}^0, \bar{\mathbf{m}}^1, \mathbf{m}^\nu)$ respectively. Let $\alpha \in \mathbb{N}^n$ and $\beta \in \mathbb{N}$ be multi-indices that define monomial test functions $x_0^\alpha t^\beta$. For each multi-index tuple (α, β), the operator $\text{Liou}_{\alpha\beta}(\mathbf{m}^0, \mathbf{m}^p, \bar{\mathbf{m}}^0, \bar{\mathbf{m}}^1)$ may be derived from the linear relations induced by the Liouville equation (15d) (in which $\delta_{\beta 0} = 1$ is a Kronecker delta):

$$0 = \langle x^\alpha, \mu_0 \rangle \delta_{\beta 0} + \langle \mathcal{L}(x_0^\alpha t^\beta), \bar{\mu}^0 + \bar{\mu}^1 \rangle - \langle x^\alpha t^\beta, \mu_\tau \rangle. \quad (16)$$

Similarly, the operator $\text{Cons}_{\alpha\beta}(\mathbf{m}^h, \mathbf{m}^\nu, \bar{\mathbf{m}}^0, \bar{\mathbf{m}}^1)$ may be derived from the consistency constraint (15e) by

$$\begin{aligned} 0 =& \langle x_1^\alpha t^\beta, \bar{\mu}^0 + \bar{\mu}^1 \rangle + \langle x^\alpha t^\beta, \nu \rangle - \langle x^\alpha (t+\tau)^\beta, \mu_h \rangle \quad (17) \\ & - \langle x_0^\alpha (t+\tau)^\beta, \bar{\mu}^0 \rangle. \end{aligned}$$

Given a degree $d \in \mathbb{N}$, the dynamics degree $\tilde{d} \geq d$ may be defined as $\tilde{d} = d + \lfloor \deg f/2 \rfloor$.

Problem 4.1: Program (15) is upper-bounded by the following order-d LMI in pseudo-moments:

$$\begin{aligned}
p_d^* = \max \quad & L_{\mathbf{m}^p}(p) && (18a)\\
& \mathbf{m}_0^0 = 1 && (18b)\\
& \forall (\alpha, \beta) \in \mathbb{N}^{n+1}_{\leq 2d}: \\
& \quad \mathbf{m}^h_\beta = \textstyle\int_{-\tau}^0 t^\beta dt = -(-\tau)^{\beta+1}/(\beta+1) && (18c)\\
& \quad \text{Liou}_{\alpha\beta}(\mathbf{m}^0, \mathbf{m}^p, \bar{\mathbf{m}}^0, \bar{\mathbf{m}}^1) = 0 && (18d)\\
& \quad \text{Cons}_{\alpha\beta}(\mathbf{m}^h, \mathbf{m}^\nu, \bar{\mathbf{m}}^0, \bar{\mathbf{m}}^1) = 0 && (18e)\\
& \mathbb{M}_d((X_0)\mathbf{m}^0), \ \mathbb{M}_{\tilde{d}}((H_0)\mathbf{m}^h) \succeq 0 && (18f)\\
& \mathbb{M}_d(([0,T] \times X)\mathbf{m}^p) \succeq 0 && (18g)\\
& \mathbb{M}_{\tilde{d}}(([0, T-\tau] \times X^2)\bar{\mathbf{m}}^0) \succeq 0 && (18h)\\
& \mathbb{M}_{\tilde{d}}(([T-\tau, T] \times X^2)\bar{\mathbf{m}}^1) \succeq 0 && (18i)\\
& \mathbb{M}_{\tilde{d}}(([0,T] \times X)\mathbf{m}^\nu) \succeq 0. && (18j)
\end{aligned}$$

The objective (18a) is the pseudo-moment version of $\langle p, \mu_p \rangle$. Constraints (18c) and (18b) are History-Validity constraints from (8) when applied to the pseudo-moments $(\mathbf{m}^\nu, \mathbf{m}^0)$. Constraints (18d) and (18e) are the Liouville and Consistency constraints respectively. Constraints (18f)-(18j) are support constraints necessary for the pseudo-moments to have representing measures.

Boundedness of all moments of measures in (7) is required to obtain convergence of (18) to (15) as $d \to \infty$.

Lemma 4.2: All measures from (7) in an MV-solution (Defn. 3.1) are bounded under assumptions A1-A7.

Proof: Boundedness of a measure's mass and support is a sufficient condition that all of the measure's moments are bounded. Assumption A1 ensures compactness, with the requirement from Defn. 2.1 that $H_0 \subseteq [-\tau, X]$ and $X_0 \subseteq X$. The remainder of this proof will involve finding upper bounds on the masses of all measures in (7).

The initial measure μ_0 has a mass of 1, and the history measure μ_h has a mass of τ by the History-Validity constraints (15b) and (15c). Substitution of the test function $v(t,x) = 1$ in the Liouville (15d) leads to $\langle 1, \mu_p \rangle = \langle 1, \mu_0 \rangle = 1$. Since T is finite, the moment $\langle t, \mu_p \rangle \leq \langle 1, \mu_p \rangle \, (\sup_{t \in [0,T]} t) = T$ is also finite. Use of the test function $v(t,x) = t$ into the Liouville (15d) yields $\langle t, \mu_p \rangle = \langle 1, \bar{\mu}_0 + \bar{\mu}_1 \rangle \leq T$. Because $\bar{\mu}_0$ and $\bar{\mu}_1$ are both nonnegative Borel measures, it holds that $\langle 1, \bar{\mu}_0 \rangle \leq T$ and $\langle 1, \bar{\mu}_1 \rangle \leq T$. The final constraint involves substitution of $\phi(t,x) = 1$ into the Consistency (15e), resulting in

$$\begin{aligned} \langle 1, \bar{\mu}_0 + \bar{\mu}_1 \rangle + \langle 1, \nu \rangle &= \langle 1, \mu_h \rangle + \langle 1, \bar{\mu}_0 \rangle \quad (19) \\ \langle 1, \nu \rangle &= \langle 1, \mu_h \rangle - \langle 1, \bar{\mu}_1 \rangle = \tau - \langle 1, \bar{\mu}_1 \rangle. \end{aligned}$$

Given that $\bar{\mu}_1$ and ν are nonnegative Borel measures and cannot have negative masses, the mass $\langle 1, \nu \rangle$ is constrained within $[0, \tau]$. All masses are demonstrated to be finite, thus proving boundedness. ■

Remark 3: Neglecting the History-Validity constraint (15c) allows for μ_h in (19) to have infinite mass, violating the boundedness principle.

Theorem 4.3: The optima in (18) will converge as $\lim_{d \to \infty} p_d^* = p^*$ to (15) under assumptions A1-A6.

Proof: This follows from Corollary 8 of [31] under the boundedness condition in Lemma 4.2. ■

Remark 4: Assumption $A6$ can be generalized to cases where the sets (H_0, X_0, X) are the unions of BSA sets. As an example, consider $H_0 = H_0^1 \cup H_0^2$ in which $\pi^t H_0^1 = [-\tau, -\tilde{\tau}]$ and $\pi^t H_0^2 = [-\tilde{\tau}, 0]$ for some $\tilde{\tau} \in (0, \tau)$. Then the pseudo-moments $\mathbf{m}^h = \mathbf{m}^h_1 + \mathbf{m}^h_2$ can be implicitly constructed from $\mathbb{M}_d((H_0^1)\mathbf{m}^h_1)$, $\mathbb{M}_d((H_0^2)\mathbf{m}^h_2) \succeq 0$.

C. Computational Complexity

Table I lists the size of the order-d PSD moment matrices associated with the pseudo-moment sequences $(\mathbf{m}^h, \mathbf{m}^0, \mathbf{m}^p, \bar{\mathbf{m}}^0, \bar{\mathbf{m}}^1, \mathbf{m}^\nu)$.

TABLE I: Size of Moment Matrices in LMI (18)

Matrix:	$\mathbb{M}_d(\mathbf{m}^0)$	$\mathbb{M}_{\tilde{d}}(\mathbf{m}^p)$	$\mathbb{M}_d(\mathbf{m}^h)$
Size:	$\binom{n+d}{d}$	$\binom{n+1+d}{d}$	$\binom{n+1+\tilde{d}}{\tilde{d}}$
Matrix:	$\mathbb{M}_d(\bar{\mathbf{m}}^0)$	$\mathbb{M}_{\tilde{d}}(\bar{\mathbf{m}}^1)$	$\mathbb{M}_d(\mathbf{m}^\nu)$
Size:	$\binom{2n+1+\tilde{d}}{\tilde{d}}$	$\binom{2n+1+\tilde{d}}{\tilde{d}}$	$\binom{n+1+\tilde{d}}{\tilde{d}}$

The largest size written in Table I is $\binom{2n+1+\tilde{d}}{\tilde{d}}$, which occurs with the pseudo-moment sequences $(\bar{\mathbf{m}}^0, \bar{\mathbf{m}}^1)$ associated to the two joint occupation measures $(\bar{\mu}_0, \bar{\mu}_1)$. Equality constraints between entries of the moment matrices must be added to convert the LMI into an SDP for use in symmetric-cone Interior Point Methods. The per-iteration complexity of solving an SDP derived from an order-d LMI involved in the moment-SOS hierarchy scales as $O(n^{6d})$ [14] with n. In the case of LMI (18), the complexity of solving (18) will scale approximately as $(2n+1)^{6\tilde{d}}$ (based on $\bar{\mathbf{m}}^0, \bar{\mathbf{m}}^1$).

V. Numerical Examples

All experiments were developed in MATLAB 2021a, and code is available at https://github.com/Jarmill/timedelay. Dependencies include Gloptipoly [32], YALMIP [33], and Mosek [34] in order to formulate and solve moment-SOS LMIs and SDPs.

In this section, a notational convention where (x_1, x_2) correspond to coordinates of $x \in X$ will be used. All sampled histories in visualizations are piecewise-constant inside H_0 with 10 randomly-spaced jumps between $[-\tau, 0]$.

A. Delayed Flow System

A time-delayed version of the Flow system from [15] is

$$\dot{x}(t) = \begin{bmatrix} x_2(t) \\ -x_1(t-\tau) - x_2(t) + x_1(t)^3/3 \end{bmatrix}. \quad (20)$$

Figure 1 plots the delayed Flow system (20) without lag ($\tau = 0$ in blue) and with a lag ($\tau = 0.75$ in orange) starting from the constant initial history $x_h(t) = (1.5, 0),\ \forall t \in [-\tau, 0]$ (black circle).

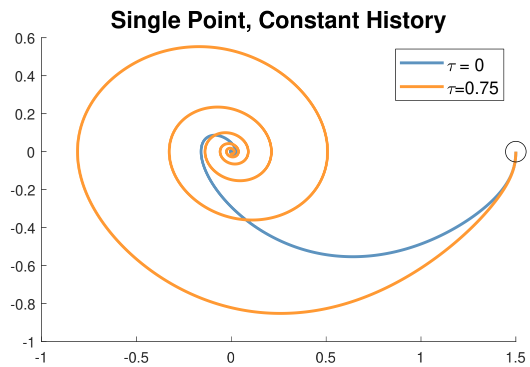

Fig. 1: Comparison of delayed Flow systems (20) with lags $\tau = 0$ and $\tau = 0.75$ in times $t \in [0, 20]$

The time-zero set of allowable histories is $X_0 = \{x \in \mathbb{R}^2 \mid (x_1 - 1.5)^2 + x_2^2 \leq 0.4^2\}$. The history class $\mathcal{H}$ will be the set of functions $x_h \in PC([-\tau, 0])$ whose graphs $(t, x(t))$ are contained within the cylinder $H_0 = [-0.75, 0] \times X_0$. No further requirements of continuity are posed on histories in $\mathcal{H}$. The considered peak estimation aims to find the minimum value of x_2 (maximize $p(x) = -x_2$) for trajectories following (20) starting from H_0, within the state set $X = [-1.25, 2.5] \times [-1.25, 1.5]$ and time horizon $T = 5$. The first five bounds on the maximum value of $-x_2$ by solving (18) are $p^*_{1:5} = [1.25, 1.2183, 1.1913, 1.1727, 1.1630]$.

Figure 2 plots trajectories and peak information associated with this example. The black circle is the initial set X_0. The initial histories inside X_0 are plotted in grey. These sampled histories are piecewise constant with 10 uniformly spaced jumps (moving to a new point uniformly sampled in X_0) within $[-0.75, 0]$. The cyan curves are the DDE trajectories of (20) starting from the grey histories. The red dotted line is the p^*_5 bound on the minimum vertical coordinate of a point on any trajectory starting from $\mathcal{H}$ up to $T = 5$.

B. Delayed Time-Varying System

This example involves peak estimation of a DDE version of the time-varying Example 2.1 of [6]

$$\dot{x}(t) = \begin{bmatrix} x_2(t)t - 0.1x_1(t) - x_1(t-\tau)x_2(t-\tau) \\ -x_1(t)t - x_2(t) + x_1(t)x_1(t-\tau) \end{bmatrix}. \quad (21)$$

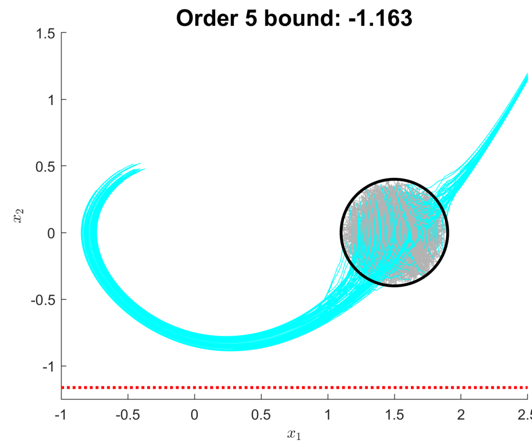

Fig. 2: Minimize x_2 on the delayed Flow system (20)

The considered support parameters are $\tau = 0.75,\ T = 5$, and $X = [-1.25, 1.25] \times [-0.75, 1.25]$. The time-zero set is the disk $X_0 = \{x \in \mathbb{R}^2 \mid (x_1 + 0.75)^2 + x_2^2 \leq 0.3^2\}$. The only restriction on allowable histories $\mathcal{H}$ is that their graphs are contained in the history set $H_0 = [-0.75, 0] \times X_0$.

Solving the SDP associated with the LMI (18) to maximize the peak function $p = x_1$ yields the sequence of five bounds $p^*_{1:5} = [1.25, 1.25, 1.1978, 0.8543, 0.718264618]$. Figure 3 plots system trajectories and the p^*_5 bound on x_1 using the same visual convention as Figure 2 (black circle X_0, grey histories $x_h(t)$, cyan trajectories $x(t \mid x_h)$, red dotted line $x_1 = p^*_5$).

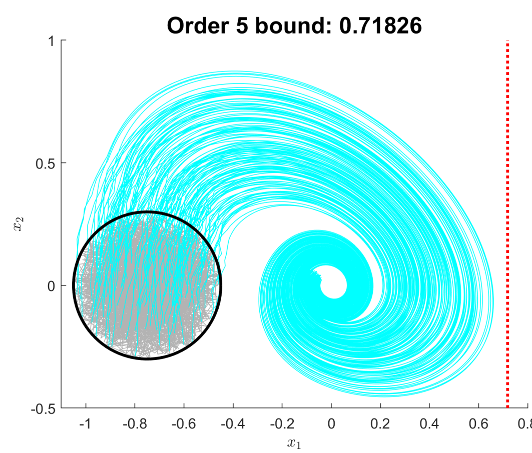

Fig. 3: Maximize x_1 on the delayed time-varying (21)

Figure 4 plots the corresponding trajectory and bound information in 3d (t, x_1, x_2). The black circles denote the boundary of H_0. The history structure inside H_0 between times $[-0.75, 1]$ is clearly visible in grey.

The peak estimation of $p = x_2$ under the same system parameters leads to the sequence of five bounds $p^*_{1:5} = [1.25, 1.25, 0.9557, 0.9138, 0.9112]$.

VI. Conclusion

This paper presented a formulation of MV-solutions for free-terminal-time DDEs with multiple histories (Definition

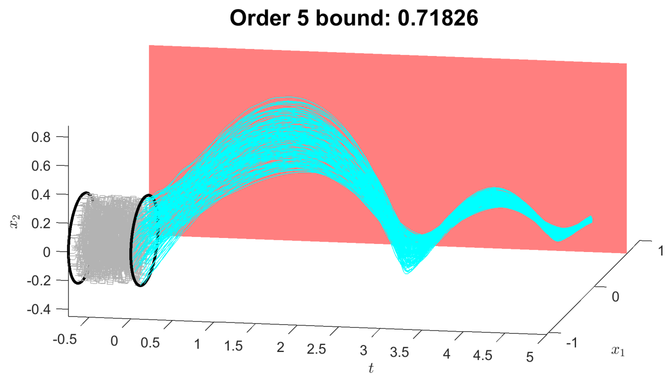

Fig. 4: A 3d plot of (21) and its x_1 bound

3.1). These MV-solutions are formed by the conjunction of Validity, Liouville and Consistency constraints. These MV-solutions may be used to provide upper bounds on peak estimation problems over DDEs by Program (15).

A vital area for future work is determining the conditions under which $P^* = p^*$ between (1) and (15). Other areas for future work include applying MV-solutions to other problems (such as optimal control and reachable set estimation), analyzing systems with multiple time-delays, improving approximation quality by spatio-temporal partitioning [35], developing MV-solutions for discrete-time systems with large time delays, handling graph-constrained history classes $\mathcal{H}$ that have additional requirements (e.g., constant x_h in time), and formulating MV-solutions for DDEs with other types of time delays (e.g., proportional, distributed, unknown-but-bounded, time-varying).

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