Peak Estimation of Rational Systems using Convex Optimization

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Main Ideas

Rational dynamical systems have special structure

Deploy ‘trick’ from optimization towards dynamical systems

(Empirically) acquire tighter upper-bounds using the trick

Background

Peak Estimation Task

Find the maximum:

- Congestion in network
- Current across a power converter component
- Concentration of a chemical species
- Angular velocity of a motor

All instances of maximizing a state function p

Peak Estimation Problem

Find peak value P^* of $p(x)$ in state set X:

$$P^* = \sup_{t^*,\, x_0} \quad p(x(t \mid x_0))$$
$$\dot{x}(t) = f(t, x) \quad \forall t \in [0, t^*]$$
$$x_0 \in X_0 \text{ (initial set)}$$

Finite dimensional but (usually) nonconvex problem in (t^*, x_0)

This work: restrict to *rational* $f(t, x)$

Peak Estimation from Optimal Control

Peak estimation is an instance of Optimal Control (Stopping):

- Zero stage cost
- Terminal cost $p(x)$
- Free terminal time
- Choice of initial conditions (in X_0)

Rational Systems

Rational dynamical system (polynomials f_0, N_ℓ, D_ℓ):

$$\dot{x}(t) = f(t, x) = f_0(t, x) + \sum_{\ell=1}^{L} \frac{N_\ell(t, x)}{D_\ell(t, x)} \tag{1}$$

Commonly found in:

- Chemical reaction networks
- Telecommunications
- Population models
- Rigid-body kinematics

How do we solve peak estimation?

Lower bounds: sample, adjoint/trajectory optimization

Upper bounds: occupation measures/auxiliary functions

Sometimes (if lucky): explicit solutions

Auxiliary Function Methods

Auxiliary Function

A function $v(t, x)$ that behaves nicely along trajectories

Examples:

- Value function
- Lyapunov function
- Barrier function

Peak Function Program

Infinite-dimensional LP[1] with auxiliary function $v(t, x)$

$$d^* = \inf_{\gamma \in \mathbb{R}} \quad \gamma \tag{2a}$$

$$v(t, x) \geq p(x) \qquad \forall (t, x) \in [0, T] \times X \tag{2b}$$

$$(\partial_t + f \cdot \nabla_x) v(t, x) \leq 0 \qquad \forall (t, x) \in [0, T] \times X \tag{2c}$$

$$\gamma \geq v(0, x) \qquad \forall x \in X_0 \tag{2d}$$

$$v \in C^1([0, T] \times X) \tag{2e}$$

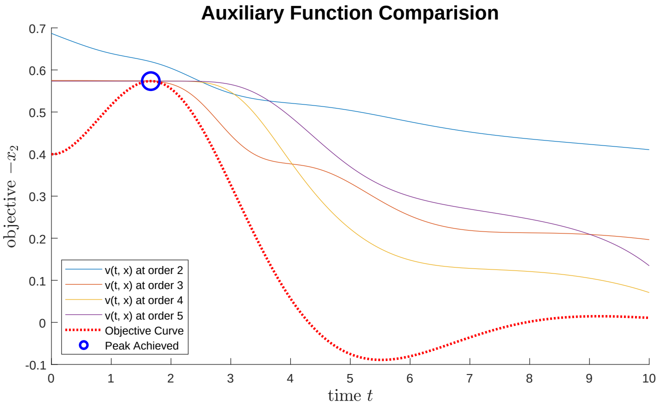
$P^* = d^*$ if $[0, T] \times X$ compact, p l.s.c., f **Lipschitz**

[1] Cho, Moon Jung, and Richard H. Stockbridge. "Linear programming formulation for optimal stopping problems." SIAM Journal on Control and Optimization 40.6 (2002): 1965-1982.

Complementary Slackness Interpretation

Consider tuple (x_0^*, t_p^*) with $d^* = p(x(t_p^* \mid x_0^*))$

Comp. slackness: $v^*(t_p^*, x(t_p^* \mid x_0^*)) = d^*$, can fall after



Ways to Discretize

Infinite-dimensional LP must be discretized for computation

More complexity: more accurate solutions

Method	Increasing Complexity
Gridding (MDP)	# Grid Points
Basis Functions (ADP)	# Functions
Random Sampling	# Samples
Sum-of-Squares	Polynomial Degree
Neural Nets (FOSSIL)	Width and Depth
Your Favorite Method	Some Accuracy Parameter

Runtime usually exponential in dimension, complexity

Rational Peak Estimation

Rational Structure

Liouville equation involves term

$$\langle(\partial_t + f \cdot \nabla_x)v(t,x), \mu(t,x)\rangle \tag{3}$$

Use rational structure of dynamics

$$\dot{x}(t) = f(t,x) = f_0(t,x) + \sum_{\ell=1}^{L} \frac{N_\ell(t,x)}{D_\ell(t,x)} \tag{4}$$

Removal of Lipschitz Assumption

Trajectories with rational f may be non-Lipschitz

Use arguments from non-smooth analysis[2]

Lipschitz f not needed assuming $[0, T] \times X$ compact

(theory contribution)

[2] L. Ambrosio and G. Crippa, "Continuity equations and ODE flows with non-smooth velocity," Proceedings of the Royal Society of Edinburgh Section A: Mathematics, vol. 144, no. 6, pp. 1191–1244, 2014.

Lie Derivative Constraint

Expand Lie derivative constraint ($\forall (t, x) \in [0, T] \times X$):

$$(\partial_t + f \cdot \nabla_x) v(t, x) \leq 0 \qquad (5)$$

$$(\partial_t + f_0 \cdot \nabla_x) v(t, x) + \sum_{\ell=1}^{L} \frac{N_\ell(t, x)}{D_\ell(t, x)} \cdot \nabla_x v(t, x) \leq 0 \qquad (6)$$

Key: affine in rational terms N_ℓ / D_ℓ

Prior Methods

Prior Methods (in SOS)

Two dominant approaches:

- Add new states (lifting) [3]
- Clear to common denominators[4]

Ours is a third approach (Sum-of-Rational Lie Constraint)

[3] V. Magron, M. Forets, and D. Henrion, "Semidefinite approximations of invariant measures for polynomial systems," Discrete & Continuous Dynamical Systems - B, vol. 22, no. 11, p. 1–26, 2017

[4] J. P. Parker, D. Goluskin, and G. M. Vasil, "A study of the double pendulum using polynomial optimization," Chaos: An Interdisciplinary Journal of Nonlinear Science, vol. 31, no. 10, 2021

Add new states

Define new variable y_ℓ for each rational term

Augmented space Ω :

$$\Omega = \{(t, x, y) \in [0, T] \times X \times \mathbb{R}^L \mid \ \forall \ell : \ y_\ell D_\ell(t, x) = 1\}$$

Lie derivative constraint reformulation $\forall (t, x, y) \in \Omega$:

$$\mathcal{L}_{f_0} v(t, x) + \sum_{\ell=1}^{L} y_\ell (N_\ell \cdot \nabla_x v(t, x)) \leq 0 \qquad (7)$$

Large number of states (t, x, y): curse of dimensionality

Clear to Common Denominators

Product of denominators $\Phi(t, x) = \prod_{\ell=1}^{L} D_\ell(t, x)$

Assuming that $\forall \ell : \; D_\ell > 0$, it holds that $\Phi > 0$

Multiply Lie constraint by $\Phi(t, x)$ to get polynomial

$$\Phi \left((\partial_t + f_0 \cdot \nabla_x) v + \sum_{\ell=1}^{L} \frac{N_\ell}{D_\ell} \cdot \nabla_x v \right) \leq 0 \qquad (8)$$

High-degree verification needed when L large

Our Approach

Employ trick from optimization

Add new function $q_\ell \in C([0, T] \times X)$ for each rational term[5]:

$$D_\ell(t,x)q_\ell(t,x) \leq N_\ell(t,x) \cdot \nabla_x v(t,x) \tag{9}$$

Sandwiched Lie derivative constraint, same solution:

$$(\partial_t + f_0 \cdot \nabla_x)v(t,x) + \sum_{\ell=1}^{L} q_\ell(t,x) \leq 0 \tag{10}$$

SOS: Restrict $v, \{q_\ell\}$ to polynomials

[5]Bugarin, Florian, Didier Henrion, and Jean Bernard Lasserre. "Minimizing the sum of many rational functions." Mathematical Programming Computation 8.1 (2016): 83-111. (used in optimization, not dynamical systems)

Other applications

Can be used many in continuous-time analysis/control tasks

- Peak estimation (this work)
- Reachable set estimation
- Optimal control
- Stochastic analysis/control (SDE with rational drift)
- Global attractor estimation

Does not work for discrete-time systems

Examples

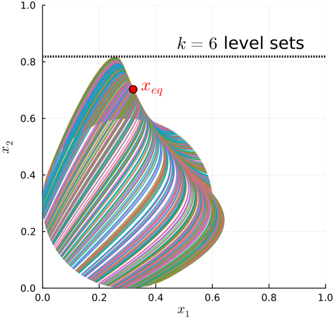
Michaelis-Menten Kinetics

Rational-inhibited chemical reaction network

Structurally stable [6] with equilibrium $x_{eq} = [0.3203, 0.7027]$

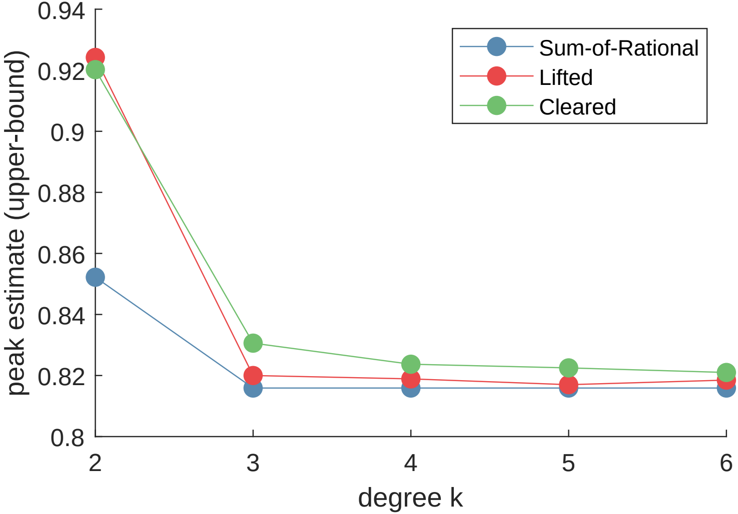
$$\dot{x}_1 = -\frac{3}{4}x_1 + \frac{1}{1 + 4.5x_2}$$

$$\dot{x}_2 = -\frac{9}{16}x_2 + \frac{1.25}{1 + 6.75x_1}$$



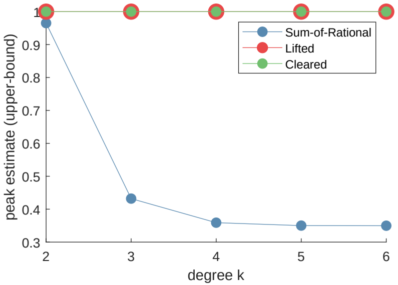
[6] Blanchini, Franco, et al. "Michaelis–Menten networks are structurally stable." Automatica 147 (2023): 110683.

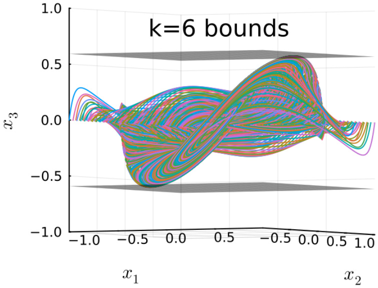
Michaelis-Menten Comparison



Rational Twist Example

System structure: linear plus (sum of cubic-over-quadratics)





Take-aways

Conclusion

Formulated sandwiched-Liouville sum-of-rational program

Gets better upper-bounds in experiments

Applicable to rational continuous-time dynamics (e.g. SDE)

Still vulnerable to the curse of dimensionality

Use Rational Structure!

Also, I’ll be on the job market soon