Dissipative quadratizations of polynomial ODE systems

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April 10 - TACAS 2024 - Luxembourg

Quadratization: what is it?

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DONE!

Quadratization: formal definition

Consider a **polynomial** system of differential equations

$$\mathbf{x}' = \mathbf{p}(\mathbf{x}), \tag{1}$$

where $\mathbf{x} = \mathbf{x}(t) = (x_1(t), \ldots, x_n(t))$ is a vector of unknown functions and $\mathbf{p} = (p_1, \ldots, p_n)$ s.t. $p_1, \ldots, p_n \in \mathbb{R}[\mathbf{x}]$.

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New variables $y_1 = g_1(\mathbf{x}), \cdots, y_m = g_m(\mathbf{x})$ are called **quadratization** if there exist

$$\mathbf{q}_1(\mathbf{x}, \mathbf{y}) = (q_{1,1}(\mathbf{x}), \dots, q_{1,n}(\mathbf{y})) \quad \text{and} \quad \mathbf{q}_2(\mathbf{x}, \mathbf{y}) = (q_{2,1}(\mathbf{x}, \mathbf{y}), \dots, q_{2,m}(\mathbf{x}, \mathbf{y}))$$

such that $\deg(\mathbf{q}_1), \deg(\mathbf{q}_2) \leqslant 2$, we have

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Previous example: for $x' = x^4$ we have $n = 1, m = 1$

$$x' = p_1(x) = x^4 \Rightarrow y = g_1(x) = x^3 \Rightarrow \begin{cases} x' = xy = q_{1,1}(x, y) \\ y' = 3y^2 = q_{2,1}(x, y) \end{cases}$$

Quadratization: why important?

- Synthesis of chemical reaction networks:

$$\deg \leqslant 2 \Leftrightarrow \text{bimolecular network}$$

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A chemical reaction network (CRN) comprises a set of reactants, a set of products, and a set of reactions:

$$C + O_2 \longrightarrow CO_2$$

We express the concentration of chemicals as $[\cdot]$ and k as the reaction rate constant, we can write the chemical kinetics functions:

$$\frac{d[C]}{dt} = -k \cdot [C] \cdot [O_2]$$
$$\frac{d[O_2]}{dt} = -k \cdot [C] \cdot [O_2]$$
$$\frac{d[CO_2]}{dt} = k \cdot [C] \cdot [O_2]$$

Quadratization: why important?

But, how quadratization helps?

From **Collision theory**, the reactions involving 3+ reactants are **rare** $\Rightarrow$ Restriction of at most two reactant molecules in reactions is practically important $\Rightarrow$ Elementary CRN (ECRN)

Advantages of Elementary CRN (ECRN):

- Turing-complete model of analog computation
- Get accurate results in arbitrary precision

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  - Quadratize
  - Use a dedicated algorithm for reducing a quadratic system

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- **Reachability analysis:** explicit error bounds for Carleman linearization in the quadratic case
  (Marcelo Forets & Christian Schilling 2021, more in later)

Quadratization: what do we know about it?

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1. Every ODE system has a quadratization.
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Consider an ODE $x' = -x + x^3$, add a new variable $y = g_1(x) = x^2$:

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We can add/subtract $y - x^2$ with any coefficients from the RHS:

$$x' = -x + xy \quad \text{and} \quad y' = -2y + 2y^2 + 12(y - x^2) = 10y - 12x^2 + 2y^2. \tag{3}$$

Our problem?

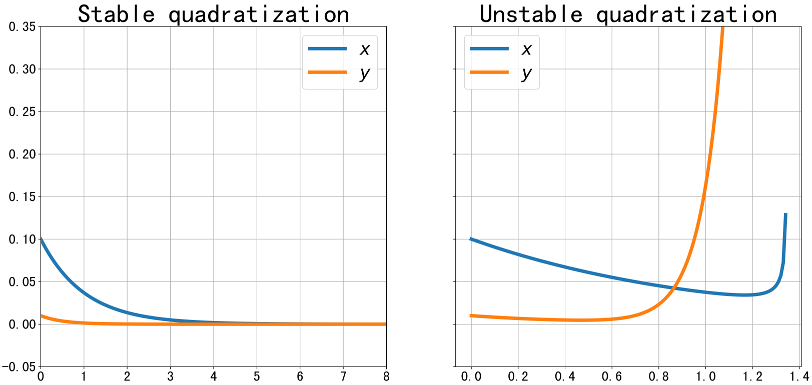

Figure: Plot of the equation (2) and (3) after quadratizaiton with initial condition $\mathcal{X}_0 = [x_0, y_0 = x_0^2] = [0.1, 0.01]$.

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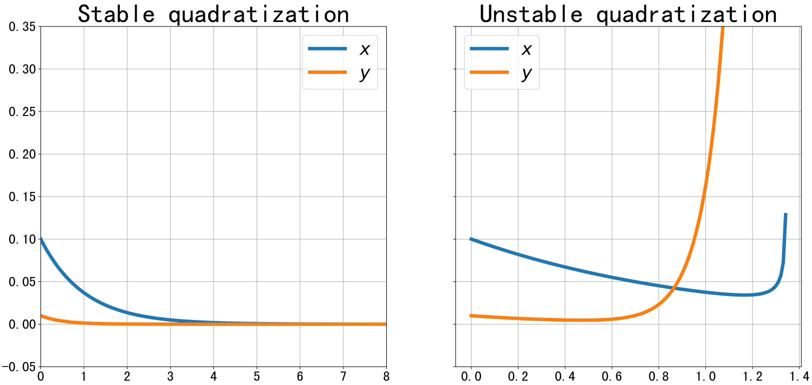


Figure: Plot of the equation (2) and (3) after quadratizaiton with initial condition $\mathcal{X}_0 = [x_0, y_0 = x_0^2] = [0.1, 0.01]$.

The two systems are mathematically equivalent; however, the results obtained through numerical integration differ!!!

Our solution: some definitions

What is equilibrium, dissipativity of an ODE system?

Definition (Equilibrium)

For a polynomial ODE system $\mathbf{x}' = \mathbf{p}(\mathbf{x})$, a point $\mathbf{x}^* \in \mathbb{R}^n$ is called an *equilibrium* if $\mathbf{p}\left(\mathbf{x}^*\right) = 0$.

Example: Consider

$$x' = -x(x-1)(x-2) \tag{4}$$

Set the RHS equal to 0 $\Rightarrow$ three equilibria: $0, 1, 2$.

Our solution: some definitions

Definition (Dissipativity)

An ODE system $\mathbf{x}' = \mathbf{p}(\mathbf{x})$ is called *dissipative* at an equilibrium point $\mathbf{x}^*$ if all the eigenvalues of the Jacobian $J(\mathbf{p})|_{\mathbf{x}=\mathbf{x}^*}$ of $\mathbf{p}$ and $\mathbf{x}^*$ have negative real part.

Important fact: Dissipativity at $\mathbf{x}^* \implies$ Asymptotic stability at $\mathbf{x}^*$
(i.e. exponential convergence to $\mathbf{x}^*$ in a small neighbourhood)

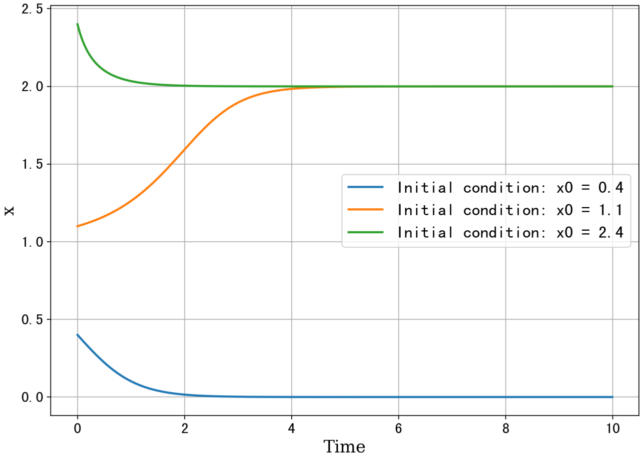
Example: Among the three equilibria $0, 1, 2$ of $x' = -x(x-1)(x-2)$, $x = 0$ and $x = 2$ are dissipative but $x = 1$ is not:

$$J(\mathbf{p})|_{x=1} = \left[-3x^2 + 6x - 2\right]\Big|_{x=1} = [1]$$

which has a positive real part in its eigenvalue.

Our solution: some definition

Trajectories of the differential equation $x' = -x(x-1)(x-2)$



Trajectory from $x_0 = 1.1$ converge to equilibrium $x = 2$ instead of $x = 1$

Definition (Dissipative quadratization)

Assume that a system $\mathbf{x}' = \mathbf{p}(\mathbf{x})$ is dissipative at an equilibrium $\mathbf{x}^* \in \mathbb{R}^n$. Then a quadratization given by $\mathbf{y} = \mathbf{g}$ (new variables introduced), $\mathbf{q}_1$ and $\mathbf{q}_2$ is called *dissipative* at $\mathbf{x}^*$ if the system

$$\mathbf{x}' = \mathbf{q}_1(\mathbf{x}, \mathbf{y}), \quad \mathbf{y}' = \mathbf{q}_2(\mathbf{x}, \mathbf{y})$$

is dissipative at a point $(\mathbf{x}^*, \mathbf{g}(\mathbf{x}^*))$.

Dissipative quadratization: what?

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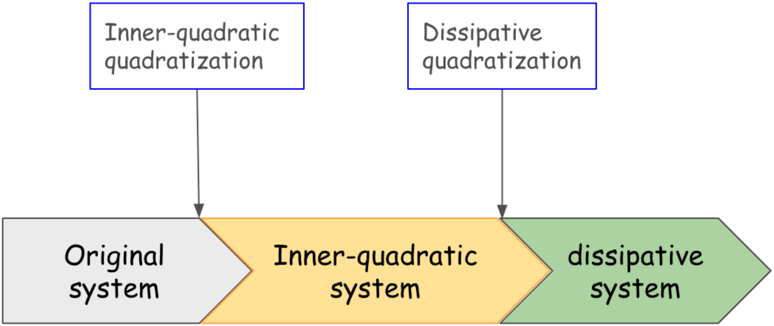
How we find such a quadratization?

Dissipative quadratization: How? (Overview)



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$\Rightarrow$

We can add $y - x^2$ (**stabilizer**) to RHS:

$$\begin{aligned} x' &= -xy + 3x^2 - 2x \\ y' &= -2y^2 + 6xy - 4x^2 - \lambda\left(y - x^2\right) \end{aligned}$$

$\uparrow$

still a quadratization

Dissipative quadratization: How? (Example, cntd.)

Jacobian of the previous system:

$$J = \underbrace{\begin{bmatrix} -y + 6x - 2 & -x \\ 6y - 8x & -4y + 6x \end{bmatrix}}_{\boxed{\text{inner-quadratic}}} - \lambda \underbrace{\begin{bmatrix} 0 & 0 \\ -2x & 1 \end{bmatrix}}_{\boxed{\text{stabilizer}}}$$

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For $\lambda = 1, 2, 4, 8, \cdots$ we check the eigenvalues on equilibria $(0, 0)$ and $(2, 4)$, results summarized in the following table:

λ	at $(0, 0)$	at $(2, 4)$
1	$-2, -1$	$-2, \mathbf{3}$
2	$-2, -2$	$-2, \mathbf{2}$
4	$-2, -4$	$-2, \mathbf{0}$
8	$-2, -8$	$\boxed{-2,-4}$

Dissipative quadratization: How? (Formalization)

What is the "good" combinatorial property: **Inner-quadratic**.

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How to find the inner-quadratic quadratization: Branch & Bound search.

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- Construct a quadratic system Σ_λ

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- Check if Σ_λ dissipative at $\left(\mathbf{x}_i^*, \mathbf{g}\left(\mathbf{x}_i^*\right)\right)$ for every $1 \leqslant i \leqslant \ell$, if yes, **return**, otherwise, set $\lambda = 2\lambda$.

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As λ is large enough, the system Σ_λ is dissipative at all equilibria: Proofs in **Proposition 2 and 3** in the paper.

Inner-quadratic: Why and How?

Retinal behind:

Quadratic relation between variables ⇒ Flexibility to "tune" the RHS ⇒ Adding the stabilizers to force the trajectory to be stable.

Applications

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- Reachability analysis
  (more details later)

Application to reachability analysis

Given an ODE system $\mathbf{x}' = \mathbf{p}(\mathbf{x})$, a set $S \subseteq \mathbb{R}^n$ of possible initial conditions, and a time $t \in \mathbb{R}_{>0}$, compute a set containing the set

$$\big\{\mathbf{x}(t) \mid \mathbf{x}' = \mathbf{p}(\mathbf{x}) \;\&\; \mathbf{x}(0) \in S\big\} \subseteq \mathbb{R}^n$$

of all points reachable from S at time t.

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One recent approach: Using Carleman linearization to reduce the problem to the linear case. (Forets, Schilling ' 2021)

Application to reachability analysis

Given an ODE system $\mathbf{x}' = \mathbf{p}(\mathbf{x})$, a set $S \subseteq \mathbb{R}^n$ of possible initial conditions, and a time $t \in \mathbb{R}_{>0}$, compute a set containing the set

$$\{\mathbf{x}(t) \mid \mathbf{x}' = \mathbf{p}(\mathbf{x}) \;\&\; \mathbf{x}(0) \in S\} \subseteq \mathbb{R}^n$$

of all points reachable from S at time t.

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Restriction: quadratic system with dissipativity and weak nonlinearity.

Our algorithm relaxes the restriction!

Application to reachability analysis

Consider the Duffing equation:

$$x'' = x + \underline{x^3} - x'$$

rewrite as a first-order system by introducing $x_1 := x, x_2 := x'$:

$$x_1' = x_2, \quad x_2' = x_1 + x_1^3 - x_2.$$

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Dissipative equilibrium: Origin $(0,0)$.

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Inner-quadratic quadratization: via a new variable $y(\mathbf{x}) = x_1^2$:

$$x_1' = x_2, \quad x_2' = x_1 y - x_2 + x_1, \quad y' = 2x_1x_2.$$

Dissipative quadratization: take $\lambda = 1$ and add the stabilizer:

$$\begin{cases} x_1' = x_2 \\ x_2' = x_1 y + x_1 - x_2 \\ y' = -y + x_1^2 + 2x_1x_2 \end{cases}$$

For the initial conditions $x_1(0) = 0.1, x_2(0) = 0.1, y(0) = x_1(0)^2 = 0.01$, the system satisfies dissipativity and weak nonlinearity, we apply the reachability algorithm with truncation order $N = 5$:

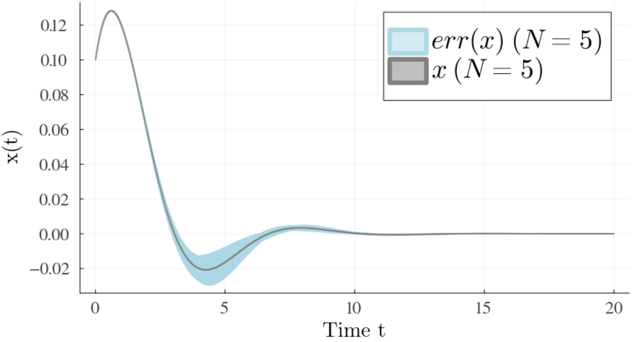

Figure: Reachability analysis results with the computed trajectory (gray) and overapproximation of the reachable set (light blue). The estimate reevaluation time $t = 4$.

Conclusion and future work

Summary:

- We proved that in any dissipative equilibria of the polynomial ODE system, the dissipative quadratization exists.
- We presented an algorithm capable of computing dissipative quadratization by first transforming the system into an inner-quadratic system.
- We showed applications in reachability analysis and numerical simulations.

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Summary:

- We proved that in any dissipative equilibria of the polynomial ODE system, the dissipative quadratization exists.
- We presented an algorithm capable of computing dissipative quadratization by first transforming the system into an inner-quadratic system.
- We showed applications in reachability analysis and numerical simulations.

Future work:

- Extend the results and algorithms beyond the polynomial system
- Exploring the preservation of other stability properties, such as limit cycles, attractors, and Lyapunov functions.

Thank you for your attention!

DQbee: https://github.com/yubocai-poly/DQbee

Figure: Paper

Figure: Code

I would like to express my gratitude to the ETAPS community and École Polytechnique for the financial support provided for this conference, as well as to my supervisor, Professor Gleb Pogudin, for his meticulous guidance.