Quadratizations of differential equations

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Computer Algebra for Functional Equations in Combinatorics and Physics
Institute Henri Poincaré, Paris, December 5

In this talk

Plan

1. Quadratization: what, why, and how?
2. Quadratizing systems of varying (sic!) dimension
3. Open problems

Part I
Quadratization: what, why, and how?

Quadratization: what?

Toy example

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$$x' = x^4$$

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DONE!

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Formal definition. Consider a system in $\bar{x} = (x_1, \ldots, x_n)$:

$$\begin{cases} x_1' = f_1(\bar{x}), \\ \ldots \\ x_n' = f_n(\bar{x}), \end{cases} \quad \text{where } f_1, \ldots, f_n \in \mathbb{C}[\bar{x}]. \tag{1}$$

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$n = 1$ & $f_1(x) = x^4$

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$$n = 1 \;\&\; f_1(x) = x^4 \implies m = 1 \;\&\; g_1(x) = x^3 \implies \begin{cases} x' = xy = h_1(x, y), \\ y' = 3y^2 = h_2(x, y) \end{cases}$$

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- Synthesis of chemical reaction networks:

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

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- Reachability analysis: explicit error bounds for Carleman linearization in the quadratic case
(Forets, Schilling ' 2021)
- Solving differential equations numerically
(Cochelin& Vergez'2009, Guillot, Cochelin, Vergez'2019)

Quadratization: why? Part 2

Main target application in this talk: Model Order Reduction.

Given:

- Learning quadratic reductions is well-understood
- Quadratic reductions are especially natural for quadratic systems
  (in particular projection of a quadratic model is quadratic)

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Main target application in this talk: Model Order Reduction.

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  (in particular projection of a quadratic model is quadratic)

Ergo: Quadratize and then Reduce

- Projection-based MOR
  (Gu'2011, Brenner & Breiten'2015, Kramer & Willcox' 2019)
- Lift & Learn *(Qian, Kramer, Peherstorfer, Willcox'2020)*

What do we know about quadratizations?

Theorem (e.g., Appelroth'1902, Lagutinskii'1911)

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BUT:

Theorem (Hemery, Fages, Soliman' 2020)

Computing optimal quadratization is an NP-hard problem.

Can we find quadratizations?

Existing software (monomial quadratizations)

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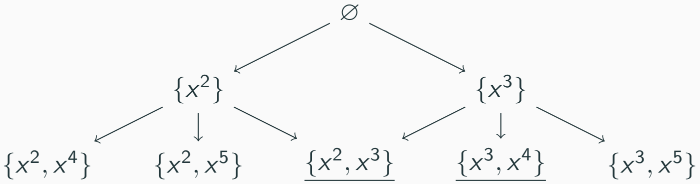
Example for QBEE: equation $x' = x^4 + x^3$



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30 sec.

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100 sec.

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4 vars $\implies \infty$

Part II
Quadratizing systems of varying dimension

Where can I get a high-dimensional ODE system?

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Recipy

Running example

Take one small PDE system and one large integer N

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Running example

$$\frac{\partial v}{\partial t} = v + v^2 \frac{\partial v}{\partial \xi}, \quad \text{where } v = v(t, \xi)$$

$$v(t, 0) = \frac{\partial v}{\partial \xi}(t, 1) = 0, \quad N = 100$$

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$$x_i(t) = v(t, i/N),$$

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$$\Downarrow$$

$$\underbrace{x_i' = x_i + N x_i^2 (x_i - x_{i-1}) \quad i = 1, \ldots, N}_{N\text{-dimensional system}}$$

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Goal: Quadratize efficiently systems appearing as discretizations

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Challenges

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Idea: equations are abundant but not so different!

Approach: Motivating example

Running example restated

$$\frac{\partial v}{\partial t} = v + v^2 \frac{\partial v}{\partial \xi} \implies x_i' = x_i + N x_i^2 (x_i - x_{i-1}),\; i = 1, \ldots, N$$

Approach: Motivating example

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$$\frac{\partial v}{\partial t} = v + v^2 \frac{\partial v}{\partial \xi} \implies \mathbf{x}' = \mathbf{x} + \mathbf{x}^2 \odot (\mathbf{D}\mathbf{x})$$

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Where:

- $\mathbf{x} = [x_1, \dots, x_N]^T$; $[a_1, a_2, \dots]^T \odot [b_1, b_2, \dots]^T = [a1 b_1, a_2 b_2, \dots]$;
- $\mathbf{D} \in \mathbb{R}^{N \times N}$ is a matrix with $\mathbf{D}_{i,j} = \begin{cases} N, \text{ if } i = j, \\ -N, \text{ if } i = j + 1, \\ 0, \text{ otherwise.} \end{cases}$

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Quadratization

The following works for every N:

$$\mathbf{w}_1 = \mathbf{x}^2 \quad \text{and} \quad \mathbf{w}_2 = \mathbf{x} \odot \mathbf{S}\mathbf{x}$$

where $\mathbf{S}$ is a shift operator: $\mathbf{S}\mathbf{x} = [0, x_1, \ldots, x_{N-1}]^T$.

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Quadratization

The following works for every N:

$$\mathbf{w}_1 = \underbrace{\mathbf{x}^2}_{\text{uncoupled}} \quad \text{and} \quad \mathbf{w}_2 = \underbrace{\mathbf{x} \odot \mathbf{S}\mathbf{x}}_{\textit{coupled}}$$

where $\mathbf{S}$ is a shift operator: $\mathbf{S}\mathbf{x} = [0, x_1, \ldots, x_{N-1}]^T$.

Approach: Formal statement

Consider scalar case only to keep notation simple

Input family of ODE systems indexed by number N and matrix $\mathbf{D} \in \mathbb{C}^{N \times N}$:

$$\mathbf{x}' = p_0(\mathbf{x}) + p_1(\mathbf{x}) \odot (\mathbf{D}\mathbf{x})$$

where $\mathbf{x} = [x_1, \ldots, x_N]^T$ and $p_0, p_1 \in \mathbb{C}[x]$ are polynomials.

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Output family of quadratizations valid of **all** N and $\mathbf{D}$ consisting of

- *uncoupled*: blocks of new variables of the form $\{q(x_1), \ldots, q(x_N)\}$ (like $\mathbf{x}^2$)

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We will call this dimension-agnostic quadratization.

Approach: Underlying theory

One quadratization to rule them all . . . too much to ask?

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Theorem (Bychkov, Issan, P., Kramer, 2023)

No, it's okay

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Every family of the form $\mathbf{x}' = p_0(\mathbf{x}) + p_1(\mathbf{x}) \odot (\mathbf{D}\mathbf{x})$
has a (monomial) dimension-agnostic quadratization.

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Idea

Fix N and $\mathbf{D}$ and use QBee to search for
a quadratization of such *uncoupled+coupled* form.

Approach: Underlying theory

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Theorem (Bychkov, Issan, P., Kramer, 2023)

Every family of the form $\mathbf{x}' = p_0(\mathbf{x}) + p_1(\mathbf{x}) \odot (\mathbf{D}\mathbf{x})$
has a (monomial) dimension-agnostic quadratization.

Idea

Fix N and $\mathbf{D}$ and use QBEE to search for
a quadratization of such *uncoupled+coupled* form.

Wanted: N_0 and $\mathbf{D}_0$ such that

$$\text{quadratization for } N_0, \mathbf{D}_0 \implies \text{quadratization for } \textbf{any } N, \mathbf{D}$$

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$$N_0 = 4, \qquad \mathbf{D}_0 = \begin{pmatrix} 1 & 1 & 0 & 1 \\ 0 & 1 & 1 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}$$

Algorithm

Summary

Input Family of the form $\mathbf{x}' = p_0(\mathbf{x}) + p_1(\mathbf{x}) \odot (\mathbf{D}\mathbf{x})$ (not necessarily a single x!)

Output dimension-agnostic quadratization

1. Consider a specific ODE system in the family using $N_0, \mathbf{D}_0$
2. Find a quadratization matching the *uncoupled+coupled* pattern (using QBee)
3. Return the corresponding dimension-agnostic quadratization

Example: Tubular reactor

Model

$$\boldsymbol{\psi}' = \mathbf{b}_\psi - \mathcal{D}\boldsymbol{\psi} \odot (\mathbf{c}_0 + \mathbf{c}_1 \odot \boldsymbol{\theta} + \mathbf{c}_2 \odot \boldsymbol{\theta}^2 + \mathbf{c}_3 \odot \boldsymbol{\theta}^3) + \mathbf{A}_\psi \boldsymbol{\psi},$$
$$\boldsymbol{\theta}' = \mathbf{b}_\theta + \mathbf{b}u + \mathcal{B}\mathcal{D}\boldsymbol{\psi} \odot (\mathbf{c}_0 + \mathbf{c}_1 \odot \boldsymbol{\theta} + \mathbf{c}_2 \odot \boldsymbol{\theta}^2 + \mathbf{c}_3 \odot \boldsymbol{\theta}^3) + \mathbf{A}_\theta \boldsymbol{\theta}$$

where

- $\boldsymbol{\theta}$, $\boldsymbol{\psi}$ — N-dimensional vectors of variables;
- $\mathbf{A}_\psi, \mathbf{A}_\theta$ — $N \times N$ matrices;
- u — external input;
- the rest are constant parameters.

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We find $6N$-dimensional automatically.

New variables: $\boldsymbol{\theta}^2$, $\boldsymbol{\theta}^3$, $\boldsymbol{\psi} \odot \boldsymbol{\theta}$, $\boldsymbol{\psi} \odot \boldsymbol{\theta}$.

Case study: Solar wind model (quadratization)

Model

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Result

- Uncoupled: $\frac{1}{\mathbf{v}}, \ \frac{\mathbf{w}}{\mathbf{v}}$;
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Using extra observation + specific form of $\mathbf{D}$

$\implies$ $3N$-dimensional quadratization

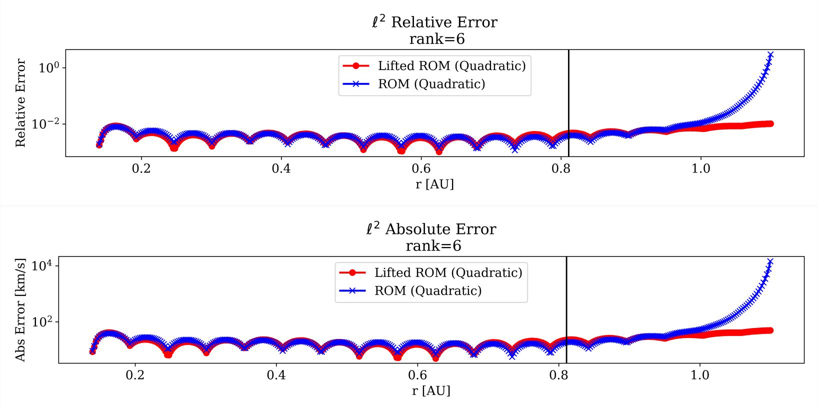
Case study: Solar wind model (order reduction)

Reduction

- $N = 129$;
- reduced to $\ell = 6$.

Learned models

- Blue: learn from original data;
- Red: learn from quadratized data.



Part III
Quadratizing systems of varying dimension

Size of the output

Theorem (Hemery, Fages, Soliman' 2020)

Computing optimal quadratization is an NP-hard problem.

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(particular proposed system $x_i' = x_{i+1}^2 + \prod_{j=1}^{n} x_j^2$*; values:* $3, 10, \leqslant 25$*)*

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Problem

Find algorithm for finding optimal Laurent monomial quadratizations.

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Work in progress to find quadratizations on the level of PDEs (good news — always exists!).

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Inspired open problem

Input differential polynomials $p(x, x', x'', \ldots), q_1(x, x', \ldots), q_n(x, x', \ldots)$ and integer d;

Ouptut TRUE if p can be written as a differential polynomial in $q_1, \ldots, q_n$ of degree at most d, otherwise FALSE.

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Remarks

- I think I can solve $d = 1$;
- For quadratization, $d = 2$ is needed.

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- Was relatively understood in the simplest finite-dimensional case.
- And now settled for coupled families of systems.
- Many things left: PDEs, Laurent monomials, arbitrary polynomials, etc.

Thank you!

Partially supported by the PANTOMIME project (AAP INS2I CNRS) and Paris Ile-de-France region.