

# Optimal monomial quadratization for ODE systems

## Extended Abstract

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### ABSTRACT

Transformation of a polynomial ODE system to a special quadratic form has been successfully used recently as a preprocessing step for model order reduction methods. However, to the best of our knowledge, there has been no practical algorithm for performing this step automatically with any optimality guarantees.

We present an algorithm that, given a system of polynomial ODEs, finds a transformation into a quadratic ODE system by introducing new variables which are monomials of the original variables. The algorithm is guaranteed to produce an optimal transformation of this form. The algorithm is implemented, and we demonstrate it on examples from the literature.

### CCS CONCEPTS

• **Computing methodologies** → *Hybrid symbolic-numeric methods*.

### KEYWORDS

nonlinear ODE systems, model order reduction, quadratic-linear representation, graph traversals, variable transformation

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## 1 INTRODUCTION

The *quadratization* problem considered in this paper is, given a system of ODEs with polynomial right-hand side, reduce the system to a system with quadratic right-hand side by introducing as few new variables as possible (see formal definition in Definition 2.1). We illustrate the problem on a simple example of a scalar ODE:

$$\dot{x} = x^5. \quad (1)$$

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The right-hand side has degree larger than two but if we introduce a new variable  $y := x^4$ , then we can write:

$$\begin{cases} \dot{x} = xy, \\ \dot{y} = 4x^3\dot{x} = 4x^4y = 4y^2. \end{cases} \quad (2)$$

The right-hand sides of (2) are of degree at most two, and every solution of (1) is a component of a solution of (2).

The motivation for this problem comes from recent developments in the area of model order reduction [3, 7] that are based on the following observation. For ODE systems with at most quadratic right-hand side, there are dedicated model order reduction methods that can produce a better reduction than the general ones. Therefore, it can be beneficial first to bring a general polynomial system to such quadratic form, and then use the dedicated methods. For more details about this approach and examples of applications, we refer to [3, 6, 7, 9].

To the best of our knowledge, so far the quadratization step has been always carried out by hand following a procedure outlined in [3, Section G.] thus limiting the applicability of the approach. Also, since one would like to perform a model reduction on the quadratized system, it is desirable to add as few new variables as possible. We design and implement an algorithm that finds a quadratization for a given system with new variables being monomials in the original variables such that the number of new variables is the smallest possible.

## 2 FORMAL SETUP

*Definition 2.1.* Consider a system of ODEs

$$\begin{cases} \dot{x}_1 = f_1(\bar{x}), \\ \dots \\ \dot{x}_n = f_n(\bar{x}), \end{cases} \quad (3)$$

where  $\bar{x} = (x_1, \dots, x_n)$  and  $f_1, \dots, f_n \in \mathbb{C}[x]$ . Then a list of new variables

$$y_1 = g_1(\bar{x}), \dots, y_m = g_m(\bar{x}), \quad (4)$$

is said to be a *quadratization* of (3) if there exist polynomials  $h_1, \dots, h_{m+n} \in \mathbb{C}[\bar{x}, \bar{y}]$  of degree at most two such that

- $\dot{x}_i = h_i(\bar{x}, \bar{y})$  for every  $1 \leq i \leq n$ ;
- $\dot{y}_j = h_{j+n}(\bar{x}, \bar{y})$  for every  $1 \leq j \leq m$ .

The number  $m$  will be called the *order of quadratization*. A quadratization of the smallest possible order will be called an *optimal quadratization*.

**Definition 2.2.** If all the polynomials  $g_1, \dots, g_m$  are monomials, the quadratization is called a *monomial quadratization*. If a monomial quadratization of a system has the smallest possible order among all the monomial quadratizations of the system, it is called an *optimal monomial quadratization*.

Now we are ready to precisely state the main problem we tackle.

**Input** A system of ODEs of the form (3).

**Output** An optimal monomial quadratization of the system.

**Example 2.3.** Consider a single scalar ODE  $\dot{x} = x^5$  from (1), that is  $f_1(x) = x^5$ . As has been show in (2),  $y = x^4$  is a quadratization of the ODE with  $g(x) = x^4$ ,  $h_1(x, y) = xy$ , and  $h_2(x, y) = 4y^2$ . Moreover, this is a monomial quadratization.

Since the original ODE is not quadratic, the quadratization is optimal, so it is also an optimal monomial quadratization.

### 3 OUTLINE OF THE ALGORITHM

From a high-level point of view, the algorithm is organized as a search of a shortest path in an implicitly defined directed graph, in which vertices are sets of new variables of the form (4) and, for each such set of size  $m$ , a directed edge goes to every set of size  $m + 1$  having the same  $g_1, \dots, g_m$ . In this graph, we would like to find a shortest path from the original system (that is, the empty set of new variables with  $m = 0$ ) to the set of vertices representing quadratizations.

The graph described above is infinite and each vertex has an infinite degree, so we start with observing that we can restrict ourselves to the case when  $g_{m+1}$  divides one of the monomials in  $\dot{x}_i$  or  $\dot{y}_j$  for  $1 \leq j \leq m$  (see also [3, Theorem 3]). Although the outdegrees of vertices become finite, they may still be pretty large, so finding a shortest path using BFS turns out to be very inefficient. Instead of BFS, we employ *limited iterative deepening depth-first search* (ID-DLS) — a modification of iterative deepening depth-first search (ID-DFS, [5]). At each step of the traversal, the next vertex to explore is determined using one of the domain specific heuristics we came up with. The implementation is available at <https://github.com/AndreyBychkov/QBee>.

**Example 3.1.** Figure 3.1 below shows a part of the graph for (1). The starting vertex is  $\emptyset$  which corresponds to the original system (that is, no new variables). There are three outgoing edges corresponding to proper divisors of  $x^5$  distinct from  $x$ . The underlined vertex corresponds to an optimal quadratization, so the algorithm will return it.

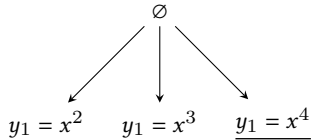


Figure 1: A part of the graph corresponding to (1)

## 4 EXAMPLES

In this section we will apply our algorithm to nonlinear dynamic systems from literature. For the sake of illustration, we have chosen systems with relatively high density of nonquadratic terms.

### 4.1 Rabinovich-Fabrikant system

*Rabinovich-Fabrikant system* [8, Eq. (2)] (see also [1, 4]) is defined as follows:

$$\begin{cases} \dot{x} = y(z - 1 + x^2) + ax, \\ \dot{y} = x(3z + 1 - x^2) + ay, \\ \dot{z} = -2z(b + xy). \end{cases} \quad (5)$$

Our algorithm finds an optimal monomial quadratization of order three:

$$y_1 = x^2, \quad y_2 = xy, \quad y_3 = y^2.$$

The resulting quadratic system is:

$$\begin{cases} \dot{x} = y(y_0 + z - 1) + ax, \\ \dot{y} = x(3z + 1 - y_0) + ay, \\ \dot{z} = -2z(b + y_1), \\ \dot{y}_1 = 2y_1(a + y_2) + 2y_2(z - 1), \\ \dot{y}_2 = 2ay_2 + y_1(3z + 1 - y_1 + y_3) + y_3(z - 1), \\ \dot{y}_3 = 2ay_3 + 2y_2(3z + 1 - y_1). \end{cases}$$

It took  $9 \pm 5$  steps for algorithm to achieve this quadratization. Dispersion occurs because, at some steps of the algorithms, different options may have the same value of the heuristic score function, so the algorithm will choose a random one.

**Example 4.1.** We will discuss in detail the choice of the new variable  $y_1$ .

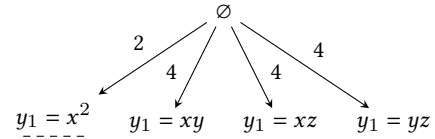


Figure 2: Possible first steps of the algorithm for (5). Edges labeled with the values of the heuristic score function used.

Each option affects two monomials in (5), reducing the degree of each by 1. However, the equations introduced by these new variables are qualitatively different. According to the chain rule,  $y_1 = x^2$  introduces  $\dot{y}_1 = 2x\dot{x}$ , which involves fewer non-quadratic monomials than, for example,  $\dot{y}_1 = \dot{x}y + x\dot{y}$ , generated by  $y_1 = xy$ . Therefore, the algorithm will choose  $y_1 = x^2$ .

### 4.2 Two-parameter model for the blue-sky catastrophe

Consider *Two-parameter model for the blue-sky catastrophe* [2, Eq. (1)] (see also [4, 10]):

$$\begin{cases} \dot{x} = x(2 + a - 10(x^2 + y^2)) + y^2 + 2y + z^2, \\ \dot{y} = -z^3 - (1 + y)(y^2 + 2y + z^2) - 4x + ay, \\ \dot{z} = (1 + y)z^2 + x^2 - b \end{cases} \quad (6)$$

Our algorithm finds an optimal monomial quadratization of order four:

$$y_1 = z^2, y_2 = x^2, y_3 = yz, y_4 = y^2$$

The resulting system is:

$$\begin{cases} \dot{x} &= x(a + 2 - 10(y_2 + y_4)) + 2y + y_1 + y_4 \\ \dot{y} &= y(a - 2 - y_1 - y_4) - y_1(z + 1) - 4x - 3y_4 \\ \dot{z} &= y_1(y + 1) + y_2 - b \\ \dot{y}_1 &= 2z(y_1 + y_2 - b) + 2y_1y_3 \\ \dot{y}_2 &= 2y_2(a + 2 + 2x - 10(y_2 + y_4)) + 2x(y_1 + y_4) \\ \dot{y}_3 &= y(y_1 + y_2 - 3y_3 - b) + y_1(y_4 - y_3 - y_1 - z) \\ &\quad + y_3(a - y_4 - 2) - xz \\ \dot{y}_4 &= 2y_4(a - 2 - y_1 - y_4) - 2y(4x + y_1 + 3y_4) - 2y_1y_3 \end{cases}$$

It took  $470 \pm 260$  steps for algorithm to achieve this quadratization.

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