# Learning Exact and Optimal Quadratic Forms for Nonlinear Non-autonomous Ordinary Differential Equations

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**Motivation** Evolutionary processes in engineering and science are often modeled with nonlinear non-autonomous ordinary differential equations that describe the time evolution of the states of the system, i.e., the physically necessary and relevant variables. However, these models are not unique: the same evolutionary process can be modeled with different variables, which can have tremendous impact on computational modeling and analysis. This idea of variable transformations—referred to as *lifting* when extra variables are added—to promote model structure and discover new model forms is found across different communities and spanning half a century. For instance, lifting transformations can make model learning and model reduction much more feasible, see [3, 4]. This is the key motivation for our work.

**What original discovery problem did you want to solve?** We are interested in the scientific discovery problem of finding quadratic forms for non-polynomial and higher-order polynomial dynamical systems of the form

$$\dot{\mathbf{x}} = \mathbf{p}_0(\mathbf{x}) + \sum_{i=1}^{r} \mathbf{p}_i(\mathbf{x}) u_i, \tag{1}$$

where $\mathbf{p}_0(\mathbf{x})$ and $\mathbf{p}_0(\mathbf{x})$ are vectors of polynomials. The models are allowed to be non-autonomous with external inputs $u_i(t)$ and the $n$-dimensional state vector is denoted as $\mathbf{x}(t)$. We also consider non-polynomial functions $\mathbf{p}_0$ and $\mathbf{p}_i$.

**How did you formulate the problem in computational terms?** We formulated the problem as a symbolic computing problem and solved it using the techniques from combinatorial optimization by combining general branch-and-bound paradigm with problem-specific selection strategy and pruning rules to achieve efficiency.

**What data and knowledge did you provide as system inputs?** As inputs to our quadratization system, we provide the symbolic model form of the (non-polynomial or non-quadratic) dynamical system (1) along with information about the regularity of the inputs $\mathbf{u}(t)$. This makes the formulation and problem data free in that sense as it works in symbolic expressions and not with simulated data.

**What types of models did your system produce as outputs?** The models produced by our QBee algorithm[1] (building on [2]) are quadratic-bilinear dynamical systems of the form

$$\dot{\mathbf{x}} = \mathbf{A}\mathbf{x} + \mathbf{H}(\mathbf{x} \otimes \mathbf{x}) + \sum_{i=1}^{r} \mathbf{N}_i \mathbf{x} u_i + \mathbf{B}\mathbf{u}, \tag{2}$$

where $\mathbf{A} \in \mathbb{R}^{n \times n}, \mathbf{H} \in \mathbb{R}^{n \times n^2}$, $\mathbf{N}_i \in \mathbb{R}^{n \times n}$ for $1 \leqslant i \leqslant r$, and $\mathbf{B} \in \mathbb{R}^{n \times r}$.

[1] `https://github.com/AndreyBychkov/QBee`

**What criteria did you use to evaluate candidate models?** At the moment, success of the method is determined when a quadratization is found. We can prove that that is the case for almost all model forms. Other criteria, such as: numerical advantages (reduced stiffness, better stability) of quadratizations are not quantified yet.

**How did you interpret results that the system generated?** Quadratized systems have many advantages. We performed model learning on the original system and on the quadratized system, and evaluated the results with respect to the better predictive capabilities of the learned reduced models when the correct model form is used. A physical interpretation of the new state variables of the quadratized system remains a challenge.

**Highlights of method:** There are several novelties of the presented work [1]. First, the presented algorithms have a functionality to quadratize systems with time-dependent inputs and with non-polynomial terms. Moreover, we provide new theorems (with constructive proofs) of existence of such quadratizations for different classes of dynamical systems models. Second, we demonstrate how this new scientific discovery method performs on models from chemical engineering, space weather modeling and combustion. The method finds quadratizations with fewer additional variables than previously reported in the literature. In some cases, we can prove that those are optimal—i.e., the quadratized models were achieved with the minimal possible number of extra variables. Third, we show some numerical results where we demonstrate how these lifting transformations can create coordinate systems that improve the predictive capabilities of reduced-order models learned from data, which is a key use case of quadratization.

## References


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