Globally Optimal Parameter Estimation for Autonomous Nonlinear Dynamical Models is an Eigenvalue Problem

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1 Introduction

Complex real-world phenomena, ranging from chemical reaction networks to meteorological systems, are often described using nonlinear models. A crucial aspect of understanding these phenomena is accurately estimating the parameters of the physical models from empirical data. Despite the availability of numerous estimation techniques, most depend on numerical optimization methods, which do not always guarantee finding the global optimum. Building upon our prior work on Autonomous Linear Time-Invariant (LTI) [2] models, this study extends the methodology to Nonlinear Autonomous Time-Invariant models. We demonstrate that globally optimal least squares parameters for these models can be effectively determined through a multiparameter eigenvalue problem.

2 Problem statement

We will consider Nonlinear Autonomous Time-Invariant models of the form

$$\Sigma : \begin{cases} \hat{\mathbf{x}}_{k+1} = \mathbf{f}(\hat{\mathbf{x}}_k, \theta) \\ \hat{y}_k = g(\hat{\mathbf{x}}_k, \theta) \end{cases} \tag{1}$$

where $\hat{\mathbf{x}} \in \mathbb{R}^n$ are the state variables, $\hat{y} \in \mathbb{R}$ is the output, $\theta \in \mathbb{R}^l$ are the model parameters, $\mathbf{f} : \mathbb{R}^n \to \mathbb{R}^n$, $g : \mathbb{R}^n \to \mathbb{R}$ are rational functions describing the model. Given a sequence of output data $\mathbf{y} \in \mathbb{R}^{\mathrm{N}}$ our objective is to estimate the model parameters θ in a manner that minimizes the 2-norm of the misfit. Here, the misfit $\tilde{\mathbf{y}} \in \mathbb{R}^{\mathrm{N}}$ refers to the necessary adjustments applied to the observed data $\mathbf{y}$ so that the modified sequence $\hat{\mathbf{y}} = \mathbf{y} - \tilde{\mathbf{y}} \in \mathbb{R}^{\mathrm{N}}$ perfectly aligns with the model equations of the identified model.

3 Research Methodology

When Σ is a LTI model, we can easily derive a difference equation which is a linear combination of the consecutive samples $\hat{y}_k$ where the coefficients are polynomial functions of the model parameters θ. This difference equation can be recursively shifted to generate a banded Toeplitz matrix $\mathbf{T}$ of appropriate dimensions in whose null space lies vectors whose components are the optimal data sequence $\hat{\mathbf{y}}$. The misfit problem can then be written as

$$\begin{aligned} &\min_{\theta} \|\tilde{\mathbf{y}}\|_2^2 \\ &\text{s.t. } \mathbf{T}\hat{\mathbf{y}} = \mathbf{0}. \end{aligned} \tag{2}$$

However, when Σ is nonlinear as in (1), a relation between the consecutive samples $\hat{y}_k$ and the model parameters θ can be expressed using a multivariate polynomial equation , $h(\hat{y}_{k+n}, \ldots, \hat{y}_k, \theta) = 0$ found via elimination in a parametric polynomial ring [1]. This difference equation can be recursively shifted to generate a block banded Toeplitz matrix $\mathbf{T}_b$ of appropriate dimensions in whose null space lies vectors $\mathbf{y}_b$ whose components are the optimal data sequence (and/or) monomials evaluated in this sequence. After incorporating this nonlinear structure in the misfit problem in (2), the cost function can be re-written such that the first order optimality conditions result in a multiparameter eigenvalue problem whose eigentuples correspond to the stationary points of the optimization problem from which we can recover globally optimal least-squares parameters.

4 Presentation outline

In our presentation we will show how we can compute this nonlinear difference equation corresponding to a state space model (1) and set up the block banded Toeplitz matrix. We will then show how to derive the multiparameter eigenvalue problem and to solve it using the block Macaulay algorithm [2] to find the optimal parameters. Finally, we will corroborate our theoretical findings through several numerical examples.

References

[1] D. Cox, J. Little, and D. OShea. *Ideals, Varieties, and Algorithms: an Introduction to Computational Algebraic Geometry and Commutative Algebra*. Springer Science & Business Media, 2013.

[2] B. De Moor. Least squares optimal realisation of autonomous LTI systems is an eigenvalue problem. *Communications in Information and Systems*, 20(2):163–207, 2020.

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