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Multiple Shooting-Local Linearization method for the identification of dynamical systems

F. Carbonell[a,*], Y. Iturria-Medina[b], J.C. Jimenez[c]

[a] *Biospective Inc., Montreal, Canada*
[b] *Montreal Neurological Institute, Montreal, Canada*
[c] *Institute for Cybernetics, Mathematics and Physics, Havana, Cuba*

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ABSTRACT

The combination of the multiple shooting strategy with the generalized Gauss–Newton algorithm turns out in a recognized method for estimating parameters in ordinary differential equations (ODEs) from noisy discrete observations. A key issue for an efficient implementation of this method is the accurate integration of the ODE and the evaluation of the derivatives involved in the optimization algorithm. In this paper, we study the feasibility of the Local Linearization (LL) approach for the simultaneous numerical integration of the ODE and the evaluation of such derivatives. This integration approach results in a stable method for the accurate approximation of the derivatives with no more computational cost than that involved in the integration of the ODE. The numerical simulations show that the proposed Multiple Shooting-Local Linearization method recovers the true parameters value under different scenarios of noisy data.

1. Introduction

Ordinary differential equations (ODEs) are extensively used for modeling the temporal evolution of complex dynamical systems in dissimilar fields such as physics, economy, ecology, biology, chemistry and social sciences [1]. Typically, these ODEs contain parameters that are associated to phenomenological factors that control the basic variables interplay of the models. However, the values of such parameters are usually unknown and must be determined in such a way that the models reproduce the observed experimental data at best. Despite a time series analysis of observed experimental data can determine useful quantities that characterize the system dynamics (e.g., Lyapunov exponents, attractor dimension), identifying the system structure and estimating the corresponding parameters would be a matter of greater practical value. Thus, an accurate estimation of the non observed states and models's parameters is not only critical to reproduce and describe a given dynamic behavior but also to understand the underlying causes of the analyzed processes. This is of particular importance for ODEs describing chaotic dynamics, where the trajectories of interest are very sensitive to small perturbations of the parameters and initial values [2–5]. In this circumstance, a major challenge is to find a proper numerical integrator able to preserve the stability of the solutions in situations of parameter-dependent instabilities in such a way that allows an accurate estimation of these parameters from noisy chaotic observations.

* Corresponding author. Tel.: +1 5142832667.
E-mail address: felix@biospective.com, felixmiguelc@yahoo.com (F. Carbonell).

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Several methods have been proposed for the parameter identification in ODEs given a set of (noisy) observations. A large class of methods, relying on synchronization phenomena of dynamical systems and control theory [5–8], has been successfully applied to a number of problems with either smooth or chaotic dynamics. The basic idea behind this class of methods is to couple a control term to the dynamics in order to synchronize the measured signal from the system and the controlled model. Then, parameter estimation is usually carried out by means of minimization of the synchronization errors. As pointed out by [7], these parameter estimation techniques can be broadly classified into two categories: on-line and off-line. The on-line techniques deal with the class of methods that involve the solution of additional differential equations governing a time evolution of the parameters, whereas the off-line techniques perform the direct minimization of a distance (cost function) between the observations and the model output. As explained in [5], this optimization procedure is equivalent to stabilize the synchronization manifold of the combined observed system plus the model state space. Typically, the on-line strategies are effective when the observations are collected on a sufficient large period of time in such a way that the transient in the parameter dynamics disappear and when the observed states of the model are sampled with a suitable high rate to resembling the truly continuous signal. Clearly, these requirements for the observations become in a serious drawback in many practical situations where it is difficult, costly or simply impossible to measure high frequency data during a large period of time. In these circumstances, the off-line techniques for the parameters estimation are more effective.

The above mentioned off-line identification techniques are actually more in correspondence with the so-called Initial Value approach, which is perhaps the most known class of methods for parameter estimation of ODEs. In this approach, the estimated parameters are those that minimize the least square errors resulting from fitting the numerical solution of the corresponding Initial Value problem to the given observation data. However, according to [9–11], the estimators resulting from this approach are very sensitive to the initial guess of the parameters and usually turn out only local optimum solutions. Moreover, for certain initial parameter values, the solution of the ODEs might not even exist over the whole integration interval, producing overflow in the numerical integration, and so, the failure of the optimization algorithm. A class of estimation methods that overcome these drawbacks was originally introduced in [9] and it is currently known as the Boundary Value approach (see, e.g., [3,10,12,13]). This approach has two distinctive components: 1) the introduction of several multiple shooting nodes for solving the ODE as multiple Initial Value Problems (IVPs) in smaller subintervals, and 2) the solution of a constrained least squares problem in an augmented set of parameters. The main advantage of this multiple shooting method is that the whole observed data can be easily used to bring information about the true solution of the ODE on the whole integration interval [10]. In such a way, the numerical solution of the multiple IVP remains close to the true solution since the first iteration of the optimization algorithm. This limits the propagation of the integration error, reduces the sensitivity of the estimators respecting to possible bad initial guess of the unknown parameters, reduces the number of iterations of the optimization algorithm, and allows the estimation of parameters even in the case of chaotic systems ([2], [3]). Besides, the splitting of a single IVP into multiple IVPs with independent initial conditions allows an efficient evaluation of the cost function by means of parallel algorithms, which significantly reduces the computational burden of the multiple shooting methods as compared with the single shooting ones. Despite the introduction of additional variables seems to yield a more complicated estimation procedure, it is actually increasing computational efficiency and numerical stability of the estimation method [10], [3]. A third type of off-line technique, called nonparametric, employs nonparametric functions to represent the unknown solutions of the ODEs (see, e.g., [14], [15], [16], [11], [17]). Typically, this class of estimators require two levels of optimization. The lower level approximates non parametric functions to the ODE trajectories conditional on the ODE parameters, while the upper optimization level does the estimation of the parameters of interest. Clearly, as compared to the previous two approaches, this procedure increases the computational burden of the parameters estimation process.

As remarked in [11], a common difficulty of these off-line estimation strategies is the numerical computation of the derivatives of the trajectories with respect to the parameters of the ODE. With this respect, three main approximations have been commonly employed. The simplest one, finite differences, also called external differentiation [9], [10] is not usually recommended due to the high computational cost required for achieving numerically stable derivatives (see further discussion in [13]). The second one, called internal differentiation, consists on differentiating the numerical integrator corresponding to the original differential equation [9], [10], [18]. In general, internal differentiation is a mechanism less computationally intensive than the external differentiation but, it might introduce also high computational cost in the case of implicit integrators or integrators defined trough some numerical derivatives. The third approach ([9], [10], [13]) consists on approximating the variational equations that describe the temporal evolution of the required derivatives, which must be integrated simultaneously to original equation. As in the second kind of approximation, this can be also computationally intensive for certain types of numerical schemes.

In this paper, we study the feasibility of the Local Linearization (LL) approach (see, e.g., [19], [20]) for the simultaneous numerical integration of the IVPs and the evaluation of the numerical derivatives that appear in the multiple shooting method. In previous works [21], [22], [23] this LL technique has been successfully applied for the parameter estimation of ODEs in the context of the Initial-Value approach. This has been possible thanks to the convenient trade-off between the numerical accuracy, stability and computational cost of the LL integrators and their capability of preserve a number of dynamical behaviors of the ODEs, which became relevant for the parameter estimation. In addition to this and following the ideas used in [24] for the computation of the Lyapunov Exponents, the LL technique can be used for the numerical integration of the variational equations associated to the derivative with respect to the parameters and initial conditions with no more computational cost than that involved in the integration of the ODE. Therefore, the application of the LL technique for identification of ODEs in the framework of Boundary Value approach is also attractive. The inference method