Convergence of Discrete Aproximations of Inverse Problems in ODE Models

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Abstract
In this paper we prove a basic convergent result related with the numerical solution of the inverse problem in ODE dynamical models. First we recall the general approach to solve it, proposed in a preceding paper, using Adams' schemes with variable step size. Sufficient conditions for the convergence of sequences of stationary solutions of the discrete problems to a stationary solution of the continuous problem are established.

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1 General Approach

1.1 The parameter estimation problem

In [18] we considered the following continuous optimization problem:

$$\begin{array}{l} \min\ J(u) = \sum\limits_{i=1}^{s} \varphi_i \left[z_i(\tau_i), \bar{z}_i \right], \\ \dot{x}(t) = f\left(x(t), u, t \right),\ t \in [0,T], \\ x_0 = l(u), \\ z(t) = g\left(x(t), u, t \right),\ t \in [0,T], \\ 0 \leq \tau_i < \tau_{i+1} \leq T,\ i = 1, ..., s-1, \end{array} \tag{1}$$

where: $x \in \Re^n,\ u \in \Re^m,\ z \in \Re^p,\ \varphi_i : \Re^p \times \Re^p \to \Re,\ f : \Re^n \times \Re^m \times [0,T] \to \Re^n,\ l : \Re^m \to \Re^n,\ g : \Re^n \times \Re^m \times [0,T] \to \Re^p$. This means that we are modelling a dynamical process by a $n-$dimensional system of nonlinear ordinary differential equations, which depends on an unknown $m-$vector of parameters u. To this end, a set of data (measurements) $\{\bar{z}_1, \bar{z}_2, ..., \bar{z}_s\}$ of the observed $p-$vector variable $z(.)$, at s different instants of time $\{\tau_1, \tau_2, ..., \tau_s\}$, is given and we should minimize J, a sum of functions depending on model and observed vectors (most frequently it is a quadratic function of the residuals $(z_i(\tau_i) - \bar{z}_i)$).

Parameter estimation problems for ODE systems (or ODE inverse problems) is a classical matter and have been considered by many authors. Several methods and points of view were proposed and special structures or statistical concepts were exploited (see for example [1], [3], [13] [20]). New schemes of numerical integration were also designed in order to deal with stiff ODE (see [6], [9] and [4]), appearing frequently in chemical reaction models (see also [21], [22]) and other important fields of applications.

This paper is the second part of [18] where we were mainly interested in the numerical computation of the solution. It is clear that the problem (1) only can be approximately solved since, most time, the exact solution of the nonlinear differential equation can not be exactly calculated and the optimization algorithms are iterative process in character. Therefore, we proposed not to try to solve the continuous problem (1), but to transform it in such a way that we obtain a simpler problem which gives us a satisfactory approximated solution.

1.2 Problem transformation

The general idea introduced in [18] is to use numerical integration schemes as constraints, instead of the differential equation, transforming the continuous problem into a discrete one, which can be solved in an easier way. This transformation depends directly on the numerical scheme of integration that is used. As a general example, in [18] we considered the following discrete problem in which the system of ordinary differential equations is substituted by a multi-step scheme of variable order Q_i and variable step size h_i :

$$\begin{array}{l}
\min\ J_k(u) = \sum_{i=0}^{k} \tilde{\varphi}_i \left[z_i, \tilde{z}_i\right], \\
x_{i+1} = x_i + h_i F_i \left(x_i, x_{i-1}, ..., x_{i-Q_i+1}; u\right),\ i = 0, 1, 2, ..., k-1, \\
x_0 = l(u), \\
z_i = g_i \left(x_i, u\right),\ i = 0, 1, 2, ..., k.
\end{array} \tag{2}$$

The partition of integration:

$$\begin{aligned}
t_0 &= 0,\ t_k = T \\
t_{i+1} &= t_i + h_i,\ i = 0, 1, ..., k-1,
\end{aligned}$$

contains the set of measurement times $\{\tau_1, \tau_2, ..., \tau_s\}$ and hence, to each measurement index $j \in \{1, 2, ..., s\}$ corresponds an integration index $i \in \{0, 1, 2, ..., k\}$. We defined the index correspondence:

$$\mathcal{I}(i) = \begin{cases} j & \text{if } i \text{ corresponds to } j, \\ 0 & \text{otherwise,} \end{cases} \quad , \; i = 0, 1, ..., k \tag{3}$$

and denoted by M the set of integration indexes corresponding to measurements:

$$M = \{i \in \{0, 1, 2, ..., k\} \mid \mathcal{I}(i) \neq 0\},$$

then, the functions $\tilde{\varphi}_i$ in $J_k(u)$ are defined by:

$$\begin{aligned} \tilde{\varphi}_i[z_i, \tilde{z}_i] &= \varphi_{\mathcal{I}(i)}[z_i, \tilde{z}_i]\, \mathbf{1}_M[i], \\ \tilde{z}_i &= \bar{z}_{\mathcal{I}(i)}, \end{aligned}$$

where $\mathbf{1}_M$ is the characteristic function of the set M and $\varphi_0, \bar{z}_0$ can be given arbitrarily.

We also introduced $\mathcal{J} : \{1, ..., s\} \to \{0, 1, ..., k\}$ as a left inverse of $\mathcal{I}$ over $\{1, ..., s\}$, i.e. $\mathcal{J}(j)$ is equal to the unique $i \in \{0, ..., k\}$ such that $\mathcal{I}(i) = j$. Then,

$$\tilde{\varphi}_{\mathcal{J}(j)}[z_{\mathcal{J}(j)}, \bar{z}_j] = \varphi_j[z_j, \bar{z}_j]\, , \; j = 1, ..., s.$$

The functions F_i were defined by the Adams integration formulae, as a linear predictor-corrector scheme:

$$F_i\left(x_i, x_{i-1}, ..., x_{i-Q_i+1}, u\right) = K_0^{Q_i+1} f\left(y_{i+1}, u, t_{i+1}\right) + \sum_{j=1}^{Q_i} K_j^{Q_i+1} f\left(x_{i-j+1}, u, t_{i-j+1}\right), \tag{4}$$

$$y_{i+1} = x_i + h_i \sum_{j=1}^{Q_i} \Pi_j^{Q_i} f\left(x_{i-j+1}, u, t_{i-j+1}\right), \; i = 0, 1, ..., k-1. \tag{5}$$

where Π_j^Q, K_j^Q are the coefficients of the $Q-$order Adams-Bashford and Adams-Moulton schemes, respectively (see, for example, [23]). The order policy of the scheme was taken as:

$$Q_i = \min\left\{i + 1, Q_{\max} - 1\right\}, \; i = 0, 1, ...k - 1.$$

In addition, we considered a family of implicit multistep-multiderivative nonlinear $Q-$ order schemes with uniform steplength, proposed by Enright and Henrici in 1976, with several theoretical and practical advantages [4]. They are specially adapted for stiff problems and, for our purposes, we used the simpler and better known second order formula to construct various schemes:

$$\begin{aligned} x_{i+1} = x_i + h \sum_{j=1}^{Q} \rho_j^{Q+2} f(x_{i-j+1}, u) + h\rho_0^{Q+2} f\left(x_{i+1}, u\right) + \\ + h^2 \rho_0^{Q+2} D_x f\left(x_{i+1}, u\right).f\left(x_{i+1}, u\right). \end{aligned} \tag{6}$$

In order to decrease the complexity of the calculation of the resulting nonlinear equation and of the gradient computation, we used some explicit variants of such scheme. The idea was to improve the corrector evaluation, using the Enright's second order formula as a recorrector. For some details of the variants, gradient formulas, etc..., see [18].

The substitution we made is some kind of "direct method" approach for the solution of the inverse problem. At the end, we have an approximated problem and, as a consequence, we need some theoretical convergence theorem and we should solve this approximated problem in the most exact possible way.

2 Theoretical results

2.1 Gradient formulae

In the first part [18], the following "sensitivity form" of the continuous gradient was proved:

$$\nabla J(\bar{u}) = \sum_{i=1}^{s} \left[D_x \Phi_i(\bar{x}(\tau_i), \bar{u}) M(\tau_i) + D_u \Phi_i(\bar{x}(\tau_i), \bar{u}) \right],$$

or

$$\nabla J(\bar{u}) = \sum_{i=1}^{s} D_z \varphi_i[g(\bar{x}(\tau_i), \bar{u}, \tau_i), \overline{z}_i] \left[g_x(\bar{x}(\tau_i), \bar{u}, \tau_i) M(\tau_i) + g_u(\bar{x}(\tau_i), \bar{u}, \tau_i) \right], \quad (7)$$

where $M(t)$ is the solution of the "sensitivity " matrix differential system:

$$\begin{array}{l} \frac{dM(t)}{dt} = f_x(\bar{x}(t), \bar{u}, t) M(t) + f_u(\bar{x}(t), \bar{u}, t), \ t \in [0, T], \\ M(0) = D_u l(\bar{u}). \end{array} \quad (8)$$

and

$$\Phi_i(x, u) = \varphi_i[g(x, u, \tau_i), \overline{z}_i], \ i = 1, ..., s.$$

In addition, in [18] was also proved the "sensitivity form" of the discrete gradient:

$$\nabla J_k(\bar{u}) = \sum_{i=0}^{k} \left[D_x \Phi_i(\bar{x}_i, \bar{u}) M_i + D_u \Phi_i(\bar{x}_i, \bar{u}) \right], \quad (9)$$

where $\{M_i, \ i = 0, 1, ..., k\}$ is the solution of the discrete matrix system:

$$\begin{array}{l} M_0 = D_u l(\bar{u}), \\ M_{i+1} = M_i + h_i \left[\sum\limits_{j=1}^{Q_i} D_{x_{i-j+1}} F_i(\mathbf{\bar{x}}_i, \bar{u}) M_{i-j+1} + D_u F_i(\mathbf{\bar{x}}_i, \bar{u}) \right], \ i = \overline{0, k-1}, \end{array} \quad (10)$$

We shall use these results in the next section.

2.2 Convergence of discrete solutions sequences

The following theorem shows a limit relation between the discrete and continuous solutions, when we use the linear predictor-corrector scheme:

Theorem 1: Let be the continuous problem (1) and their associated discrete problems (2), using predictor-corrector scheme (5)-(4), and decreasing uniform step lengths $h_k = \frac{T}{k}$, $k = 1, 2, ...$ Assume that φ, f, l, g are continuous and continuously differentiable functions with respect to (x, u), such that f_x, f_u are bounded functions on $(x, u, t)-$bounded sets.

Let $\{u_k\}$ be any sequence of stationary points of the discrete problems, corresponding to the steps $\{h_k\}$, and orders $Q_i^k = \min\{i+1, Q_{\max} - 1\}$, $i = 0, 1, ..., k$, $k = 1, 2, ...$ Then, every accumulation point of the sequence $\{u_k\}$ is a stationary point of the continuous problem.

Proof. It is sufficient to show that if $\{u_k\}$ is a sequence convergent to u, then the sequence of discrete gradients $\{\nabla J_k(u_k)\}$ converges to the continuous gradient $\nabla J(u)$. In that case, if $\{u_k\}$ is any sequence of stationary points of (2), we have $\nabla J_k(u_k) = 0$ for all k. Then, at a limit point u of any convergent subsequence of $\{u_k\}$, we must have $\nabla J(u) = 0$. The proof of this property shall be done in several steps.

2.2.1 Some properties of predictor-corrector schemes

Let u be an arbitrary vector in $\Re^m$. We denote by $\bar{x}^k = \left\{x_i^k,\ i = 0, 1, ..., k\right\}$ and $\bar{y}^k = \left\{y_i^k,\ i = 0, 1, ..., k\right\}$, the two vector sequence solutions of the difference system (4)-(5), corresponding to step h_k and vector u. Then, we have:

$$\begin{aligned} x_{i+1}^k &= x_i^k + h_k C_i(\mathbf{x}_i^k, y_{i+1}^k, u),\ i = 0, 1, ..., k-1, \\ x_0^k &= l(u), \end{aligned}$$

$$\begin{aligned} y_{i+1}^k &= x_i^k + h_k P_i(\mathbf{x}_i^k, u),\ i = 0, 1, ..., k-1, \\ y_0^k &= l(u), \end{aligned}$$

where $\mathbf{x}_i^k = (x_i^k, x_{i-1}^k, ..., x_{i-Q_i}^k)$ and

$$C_i(\mathbf{x}_i^k, y_{i+1}^k, u_k) = K_0^{Q_i+1} f\left(y_{i+1}^k, u, \tau_{i+1}^k\right) + \sum_{j=1}^{Q_i} K_j^{Q_i+1} f\left(x_{i-j+1}^k, u, \tau_{i-j+1}^k\right),$$

$$P_i(\mathbf{x}_i^k, u_k) = \sum_{j=1}^{Q_i} \Pi_j^{Q_i} f\left(x_{i-j+1}^k, u, \tau_{i-j+1}^k\right).$$

Observe that, for all i and k:

$$F_i(\mathbf{x}_i^k, u) = C_i(\mathbf{x}_i^k, y_{i+1}^k, u).$$

For the Adams' linear predictor-corrector schemes it is well known (see [23]) that piecewise polynomial approximations can be associated with $\bar{x}^k$ and $\bar{y}_k$. For example, to them correspond, respectively, the continuous functions $\bar{x}^k[t], \bar{y}^k[t]$ defined, at interval $[\tau_i^k, \tau_{i+1}^k]$, as the Q_i+1-degree interpolating polynomial (with vector coefficients), satisfying:

$$\begin{array}{l} \bar{x}^k[\tau_i^k] = x_i^k, \\ \frac{d}{dt}\bar{x}^k[\tau_j^k] = f(x_j^k, u, \tau_j^k), \quad j = i, i-1, ..., i-Q_i+1, \\ \frac{d}{dt}\bar{x}^k[\tau_{i+1}^k] = f(y_{i+1}^k, u, \tau_{i+1}^k), \end{array} \tag{11}$$

and the Q_i-degree interpolating polynomial, satisfying:

$$\begin{array}{l} \bar{y}^k[\tau_i^k] = x_i^k, \\ \frac{d}{dt}\bar{y}^k[\tau_j^k] = f(x_j^k, u, \tau_j^k), \quad j = i, i-1, ..., i-Q_i+1, \end{array} \tag{12}$$

for $i = 0, 1, ..., k-1$ and $k = 1, 2, ...$,where:

$$\tau_j^k = \frac{jT}{k} = jh_k, \;\; j = 0, ..., k,$$

are the points of $[0, T]$ defining the partition of integration.

If we denote by $x(t)$ the unique continuously differentiable solution of the Cauchy initial problem:

$$\begin{array}{rcl} \dot{x}(t) & = & f(x(t), u, t), \; t \in [0, T], \\ x(0) & = & x_0, \end{array}$$

corresponding to the vector u, and if (4)-(5) defines a $p-$order scheme (i.e. $Q_{\max} = p$) then, it is also known that the global errors tend to zero:

$$\begin{array}{l} e_x^k(t) = \left\| x(t) - \bar{x}^k[t] \right\|_\infty \to 0, \\ e_y^k(t) = \left\| x(t) - \bar{y}^k[t] \right\|_\infty \to 0, \end{array}$$

uniformly with respect to $t \in [0, T]$, if $k \to +\infty$. Furthermore, this limit is uniformly with respect to u in any bounded set of $\Re^m$ in the case that f_x and f_u are bounded, as we assumed here.

In particular, this property and the continuity of $x(t)$ show that the sequences $\{\|x_i^k\|\}_{i=0,k}$ and $\{\|y_i^k\|\}_{i=0,k}$ are uniformly bounded for all $k = 0, 1, ...$ and all u in any bounded set of $\Re^m$. We even have the estimations (see [23]):

$$e_x^k(t) \le \text{constant } \times h^{p+1},$$
$$e_y^k(t) \le \text{constant } \times h^{p},$$

for $t \in [\tau_{p-1}^k, T]$.

In addition, consider the following obvious inequality for $t \in [\tau_i^k, \tau_i^k + h_k]$:

$$\|\bar{x}^k[t] - x(t)\| \le \|\bar{x}^k[\tau_i^k] - x(\tau_i^k)\| + \int_{\tau_i^k}^t \left\| \frac{d\bar{x}^k[\tau]}{d\tau} - f(x(\tau), u, \tau) \right\| d\tau, \tag{13}$$

since f is Lipschitz continuous with respect to x (f_x is bounded), there exists a constant L_x, the same for all u in any bounded set, such that the following estimation hold:

$$\begin{array}{l} \left\| \frac{d\bar{x}^k[\tau]}{d\tau} - f(x(\tau), u, \tau) \right\| \le \|f(\bar{x}^k[\tau], u, \tau) - f(x(\tau), u, \tau)\| + \\ + \|f(\bar{x}^k[\tau_i^k], u, \tau_i^k) - f(\bar{x}^k[\tau], u, \tau)\| + \mathcal{O}_1(|\tau - \tau_i^k|) \le \\ \le L_x \|\bar{x}^k[\tau] - x(\tau)\| + L_x \|\bar{x}^k[\tau_i^k] - \bar{x}^k[t]\| + \mathcal{O}_2(|t - \tau_i^k|) \\ \le L_x \|\bar{x}^k[\tau] - x(t)\| + \mathcal{O}_3(|t - \tau_i^k|), \end{array}$$

where

$$\mathcal{O}_r(h) \to 0, \text{ if } h \to 0, \; r = 1, 2, 3,$$

and for all u in any bounded set of $\Re^m$.

Hence, substituting in (13) and applying Gronwall's inequality we obtain the estimation:

$$\|\bar{x}^k[t] - x(t)\| \le \left(\|\bar{x}^k[\tau_i^k] - x(\tau_i^k)\| + h_k \mathcal{O}_3(h_k)\right) \exp(L_x h_k),$$

for all $t \in [\tau_i^k, \tau_i^k + h_k]$. The same inequality holds for $\bar{y}^k[t]$:

$$\|\bar{y}^k[t] - x(t)\| \le \left(\|\bar{y}^k[\tau_i^k] - x(\tau_i^k)\| + h_k \mathcal{O}_3(h_k)\right) \exp(L_x h_k).$$

and this shows that the convergence at any point t depends on the convergence at the node points τ_i^k.

2.2.2 Applications to the sensitivity matrix cases

Analogous results can be obtained if we apply the linear predictor-corrector scheme to the matrix ODE system (8). Introducing the notations:

$$\mathbf{x}()_i^k = \left(x(\tau_i^k), x(\tau_{i-1}^k), ..., x(\tau_{i-Q_i}^k)\right), \tag{14}$$

$$\mathfrak{M}_i^k = \left(\mathcal{M}_i^k, \mathcal{M}_{i-1}^k, ..., \mathcal{M}_{i-Q_i}^k\right), \tag{15}$$

$$D_x\mathcal{C}_i\left(\mathbf{x}()_i^k, \mathfrak{M}_i^k, \mathcal{N}_{i+1}^k, u\right) = K_0^{Q_i+1} f_x\left(x(\tau_{i+1}^k), u, \tau_{i+1}^k\right)\mathcal{N}_{i+1}^k + \sum_{j=1}^{Q_i} K_j^{Q_i+1} f_x\left(x(\tau_{i-j+1}^k), u, \tau_{i-j+1}^k\right)\mathcal{M}_{i-j+1}^k \quad (16)$$

$$D_x\mathcal{P}_i\left(\mathbf{x}()_i^k, \mathfrak{M}_i^k, u\right) = \sum_{j=1}^{Q_i} \Pi_j^{Q_i} f_x\left(x(\tau_{i-j+1}^k), u, \tau_{i-j+1}^k\right)\mathcal{M}_{i-j+1}, \quad (17)$$

and the corresponding meaning for $D_u\mathcal{C}_i(\mathbf{x}_i^k, y_{i+1}^k, \mathcal{N}_{i+1}^k, u)$ and $D_u\mathcal{P}_i(\mathbf{x}_i^k, \mathfrak{M}_i^k, u)$, it is easy to see that we have the following equations:

$$\mathcal{M}_0^k = D_u l(u),$$
$$\mathcal{M}_{i+1}^k = \mathcal{M}_i^k + h_k\left[D_x\mathcal{C}_i\left(\mathbf{x}()_i^k, \mathfrak{M}_i^k, \mathcal{N}_{i+1}^k, u\right) + D_u\mathcal{C}_i\left(\mathbf{x}()_i^k, \mathfrak{M}_i^k, \mathcal{N}_{i+1}^k, u\right)\right],\ i = \overline{0, k-1}, \quad (18)$$
$$\mathcal{N}_{i+1}^k = \mathcal{M}_i^k + h_k\left[D_x\mathcal{P}_i\left(\mathbf{x}()_i^k, \mathfrak{M}_i^k, u\right) + D_u\mathcal{P}_i\left(\mathbf{x}()_i^k, \mathfrak{M}_i^k, u\right)\right],\ i = \overline{0, k-1}, \quad (19)$$

for the scheme (4)-(5) in the case when it is applied to (8).

To the solution sequence $\overline{\mathfrak{M}}^k = \left\{\mathcal{M}_i^k,\ i = 0, 1, ..., k\right\}$ of (18)-(19) corresponds the piecewise polynomial approximation $\overline{\mathfrak{M}}^k[t]$, defined at interval $[\tau_j^k, \tau_{j+1}^k]$ as the $Q_i + 1$−degree interpolating polynomial (with matrix coefficients), satisfying:

$$\overline{\mathfrak{M}}^k[\tau_i^k] = \mathcal{M}_i^k,$$
$$\tfrac{d}{dt}\overline{\mathfrak{M}}^k[\tau_j^k] = f_x(x(\tau_j^k), u, \tau_j^k)\mathcal{M}_j^k + f_u(x(\tau_j^k), u, \tau_j^k),\quad j = i, ..., i - Q_i + 1, \quad (20)$$
$$\tfrac{d}{dt}\overline{\mathfrak{M}}^k[\tau_{i+1}^k] = f_x(x(\tau_{j+1}^k), u, \tau_{j+1}^k)\mathcal{N}_{j+1}^k + f_u(x(\tau_{j+1}^k), u, \tau_{j+1}^k),$$

for $i = 0, 1, ..., k-1$; $k = 1, 2, ...$, and the error convergence to zero:

$$\mathcal{E}^k(t) = \left\|\overline{\mathfrak{M}}^k[t] - M(t)\right\| \to 0, \text{ for } h_k \to 0,$$

uniformly with respect to u in any bounded set. Here $M(t)$ denotes the unique matrix solution of the sensitivity ODE system (8). We have similar results for the solution sequence $\overline{\mathfrak{N}}^k = \left\{\mathcal{N}_i^k,\ i = 0, 1, ..., k\right\}$ and, in addition, the estimates:

$$\left\|\overline{\mathfrak{M}}^k[t] - M(t)\right\| \le \left(\left\|\overline{\mathfrak{M}}^k[\tau_i^k] - M(\tau_i^k)\right\| + h_k\mathcal{O}(h_k)\right)\exp(L_x h_k),$$
$$\left\|\overline{\mathfrak{N}}^k[t] - M(t)\right\| \le \left(\left\|\overline{\mathfrak{N}}^k[\tau_i^k] - M(\tau_i^k)\right\| + h_k\mathcal{O}(h_k)\right)\exp(L_x h_k),$$

for all $t \in [\tau_i^k, \tau_i^k + h_k],\ i = 0, 1, ..., k,\ k \in \aleph$ and the uniform boundedness properties:

$$\|\mathcal{N}_i^k\| \le K_1,\ \|\mathcal{M}_i^k\| \le K_2,$$
$$\text{for } i = 0, 1, ..., k,\ k \in \aleph,\ u \text{ bounded}.$$

On the other hand, using definitions in (4)-(5), it is not difficult to see that:

$$D_{x_s}F_i(\mathbf{x}_i^k,u)=K_0^{Q_i+1}f_x(y_{i+1}^k,u,\tau_{i+1}^k)\frac{\partial y_{i+1}}{\partial x_s}+K_{i-s+1}^{Q_i+1}f_x(x_s^k,u,\tau_s^k),\ s=i,...,i-Q_i+1,$$

$$D_uF_i(\mathbf{x}_i^k,u)=K_0^{Q_i+1}f_u\left(y_{i+1},u,t_{i+1}\right)+\sum_{j=1}^{Q_i}K_j^{Q_i+1}f_u\left(x_{i-j+1},u,t_{i-j+1}\right),$$

$$\begin{aligned}\frac{\partial y_{i+1}}{\partial x_i}&=I+h_k\Pi_1^{Q_i}f_x(x_i^k,u,\tau_i^k),\\ \frac{\partial y_{i+1}}{\partial x_s}&=h_k\Pi_{i-s+1}^{Q_i}f_x(x_s^k,u,\tau_s^k),\ s=i-1,...,i-Q_i+1.\end{aligned}$$

Hence, if we denote by $\bar{\mathbf{M}}^k=\left\{M_i^k,\ i=0,1,...,k\right\}$ the matrix sequence, solution of the "sensitivity" discrete system (10) corresponding to step h_k, then:

$$\begin{aligned}&\sum_{j=1}^{Q_i}D_{x_{i-j+1}}F_i(\mathbf{x}_i^k,u)M_{i-j+1}^k=\\ &=\sum_{j=1}^{Q_i}\left[K_0^{Q_i+1}f_x(y_{i+1}^k,u,\tau_{i+1}^k)\tfrac{\partial y_{i+1}}{\partial x_{i-j+1}}+K_j^{Q_i+1}f_x(x_{i-j+1}^k,u,\tau_{i-j+1}^k)\right]M_{i-j+1}^k=\\ &=K_0^{Q_i+1}f_x(y_{i+1}^k,u,\tau_{i+1}^k)\left[M_i^k+h_k\sum_{j=1}^{Q_i}\Pi_j^{Q_i}f_x(x_{i-j+1}^k,u,\tau_{i-j+1}^k)M_{i-j+1}^k\right]+\\ &\quad+\sum_{j=1}^{Q_i}K_j^{Q_i+1}f_x(x_{i-j+1}^k,u,\tau_{i-j+1}^k)M_{i-j+1}^k.\end{aligned}$$

Defining the matrix sequence $\left\{N_i^k,\ i=1,...,k\right\}$ as:

$$N_{i+1}^k=M_i^k+h_k\sum_{j=1}^{Q_i}\Pi_j^{Q_i}\left[f_x(x_{i-j+1}^k,u,\tau_{i-j+1}^k)M_{i-j+1}^k+f_u(x_{i-j+1}^k,u,\tau_{i-j+1}^k)\right],\ i=\overline{0,k-1},$$

we obtained that the "sensitivity" system (10) can also be written in the following form:

$$\begin{aligned}&M_0^k=D_ul(u),\\ &M_{i+1}^k=M_i^k+h_kK_0^{Q_i+1}\left[f_x(y_{i+1}^k,u,\tau_{i+1}^k)N_{i+1}^k+f_u(y_{i+1}^k,u,\tau_{i+1}^k)\right]+\\ &\qquad+h_k\sum_{j=1}^{Q_i}K_j^{Q_i+1}\left[f_x(x_{i-j+1}^k,u,\tau_{i-j+1}^k)M_{i-j+1}^k+f_u(x_{i-j+1}^k,u,\tau_{i-j+1}^k)\right],\end{aligned}$$

or equivalently:

$$\begin{aligned}&M_0^k=D_ul(u),\\ &M_{i+1}^k=M_i^k+h_k\left[D_x\mathcal{C}_i\left(\mathbf{x}_i^k,\mathbf{M}_i^k,N_{i+1}^k,u\right)+D_u\mathcal{C}_i\left(\mathbf{x}_i^k,\mathbf{M}_i^k,N_{i+1}^k,u\right)\right],\ i=\overline{0,k-1},\end{aligned}\tag{21}$$

$$N_{i+1}^k = M_i^k + h_k \left[D_x\mathcal{P}_i\left(\mathbf{x}_i^k, \mathbf{M}_i^k, u\right) + D_u\mathcal{P}_i\left(\mathbf{x}_i^k, \mathbf{M}_i^k, u\right)\right],\ i = \overline{0, k-1}, \qquad (22)$$

with the same meanings as in (14)-(17) for the notation $\mathbf{x}_i^k$, $\mathbf{M}_i^k, D_x\mathcal{C}_i, D_x\mathcal{P}_i$ and $D_u\mathcal{C}_i, D_u\mathcal{P}_i$, changing $x(\tau_i^k), \mathcal{M}_i^k$ and $\mathcal{N}_i^k$ by x_i^k, M_i^k and N_i^k respectively.

Now it is clear that the only difference between the matrix schemes (18)-(19) and (21)-(22) is the evaluation of the matrix coefficients at $x(\tau_i^k)$ instead of x_i^k. Therefore, if $\bar{\mathbf{M}}^k[t]$ denotes the piecewise polynomial approximation, analogous to (20) and corresponding to $\bar{\mathbf{M}}^k$, it satisfies the equalities:

$$\begin{array}{l} \bar{\mathbf{M}}^k[\tau_i^k] = M_i^k, \\ \frac{d}{dt}\bar{\mathbf{M}}^k[\tau_j^k] = f_x(x_j^k, u, \tau_j^k) M_j^k + f_u(x_j^k, u, \tau_j^k),\quad j = i, i-1, ..., i-Q_i+1, \\ \frac{d}{dt}\bar{\mathbf{M}}^k[\tau_{i+1}^k] = f_x(x_{j+1}^k, u, \tau_{j+1}^k) N_{j+1}^k + f_u(x_{j+1}^k, u, \tau_{j+1}^k), \end{array} \qquad (23)$$

for all $i = 0, 1, ..., k$ and $k \in \aleph$.

2.2.3 Two essential estimations

Moreover, we have the estimations:

$$\bar{v}_{i+1}^k \leq (1 + h_k V_1)\bar{w}_i^k + h_k V_2, \qquad (24)$$

$$\bar{w}_{i+1}^k \leq (1 + h_k W_1)\bar{w}_i^k + h_k W_2, \qquad (25)$$

for $i = 0, 1, ..., k$ and $k \in \aleph$, and all u in any bounded set, where:

$$\begin{array}{rcl} v_i^k &=& \left\| N_i^k - \mathcal{N}_i^k \right\|,\ w_i^k = \left\| M_i^k - \mathcal{M}_i^k \right\|, \\ \bar{v}_i^k &=& \max\left\{ v_j^k,\ i - Q_i + 1 \leq j \leq i \right\}, \\ \bar{w}_i^k &=& \max\left\{ w_j^k,\ i - Q_i + 1 \leq j \leq i \right\}, \end{array}$$

and V_1, W_1, V_2, W_2 are constants, independent on i and k.

In fact, for any k and reasoning by induction, for $i = 0$ we can write:

$$\begin{array}{l} \left\| N_1^k - \mathcal{N}_1^k \right\| \leq h_k \left\| D_x\mathcal{P}_0\left(\mathbf{x}_0^k, \mathbf{M}_0^k, u\right) - D_x\mathcal{P}_0\left(\mathbf{x}()_0^k, \mathcal{M}_0^k, u\right)\right\| + \\ + h_k \left\| D_u\mathcal{P}_0\left(\mathbf{x}_0^k, \mathbf{M}_0^k, u\right) - D_u\mathcal{P}_0\left(\mathbf{x}()_0^k, \mathcal{M}_0^k, u\right)\right\| \leq \\ \leq \left\| M_0^k - \mathcal{M}_0^k \right\| + h_k \left\| f_x(x_0^k, u, \tau_0^k) - f_x(x(\tau_0^k), u, \tau_0^k) \right\| \left\| M_0^k \right\| + \\ + h_k \left\| f_x(x_0^k, u, \tau_0^k) \right\| \left\| M_0^k - \mathcal{M}_0^k \right\| + h_k \left\| f_u(x_0^k, u, \tau_0^k) - f_u(x(\tau_0^k), u, \tau_0^k) \right\|, \end{array}$$

and by the continuity of $x(t), f_x, f_u$, the uniform convergence of $x^k[\tau]$ to $x(\tau)$ and the uniform boundedness of the sequences $\{x_0^k\}, \{\tau_0^k\}, \{\left\| M_0^k \right\|\}$ and of the function f_x, we have:

$$\begin{array}{rcl} \left\| N_1^k - \mathcal{N}_1^k \right\| &\leq& (1 + h_k V_1)\left\| M_0^k - \mathcal{M}_0^k \right\| + o(h_k) V_2, \\ \dfrac{o(h_k)}{h_k} &\to& 0,\ k \to +\infty, \end{array} \qquad (26)$$

for some constants V_1, V_2, independent on u and k. In addition,

$$\begin{array}{l}\left\|M_1^k - \mathcal{M}_1^k\right\| \leq \left\|M_0^k - \mathcal{M}_0^k\right\| + \\ +h_k \left\| D_x\mathcal{C}_i\left(\mathbf{x}_i^k, \mathbf{M}_i^k, N_{i+1}^k, u\right) - D_x\mathcal{C}_i\left(\mathbf{x}()_i^k, \mathfrak{M}_i^k, \mathcal{N}_{i+1}^k, u\right)\right\| + \\ +h_k \left\| D_u\mathcal{C}_i\left(\mathbf{x}_i^k, \mathbf{M}_i^k, N_{i+1}^k, u\right) - D_u\mathcal{C}_i\left(\mathbf{x}()_i^k, \mathfrak{M}_i^k, \mathcal{N}_{i+1}^k, u\right)\right\| \leq \\ \leq \left\|M_0^k - \mathcal{M}_0^k\right\| + h_k K_0^{Q_0+1}\left\|f_x(y_1^k, u, \tau_1^k) - f_x(x(\tau_1^k), u, \tau_1^k)\right\| \left\|N_1^k\right\| + \\ +h_k K_0^{Q_0+1}\left\|f_x(x(\tau_1^k), u, \tau_1^k)\right\| \left\|N_1^k - \mathcal{N}_1^k\right\| + \\ +h_k K_0^{Q_0+1}\left\|f_u(y_1^k, u, \tau_1^k) - f_u(x(\tau_1^k), u, \tau_1^k)\right\| + \\ +h_k K_1^{Q_0+1}\left\|f_x(x_0^k, u, \tau_0^k) - f_x(x(\tau_0^k), u, \tau_0^k)\right\| \left\|M_0^k\right\| + \\ +h_k K_1^{Q_0+1}\left\|f_x(x(\tau_0^k), u, \tau_0^k)\right\| \left\|M_0^k - \mathcal{M}_0^k\right\| + \\ +h_k K_1^{Q_0+1}\left\|f_u(x_0^k, u, \tau_0^k) - f_u(x(\tau_0^k), u, \tau_0^k)\right\|.\end{array}$$

Once more, continuity of $x(t), f_x, f_u$, uniform convergence of $x^k[t]$ to $x(t)$ and boundedness of sequences and functions involved, jointly with (26), give the inequality:

$$\left\|M_1^k - \mathcal{M}_1^k\right\| \leq (1 + h_k W_1)\left\|M_0^k - \mathcal{M}_0^k\right\| + o(h_k)W_2,$$

for some constants W_1, W_2 independent on k and u.

Suppose (24)-(25) are true for all $j \leq i$, from (18)-(19) and (21)-(22), we can write the inequalities:

$$\begin{array}{l}\left\|N_{i+1}^k - \mathcal{N}_{i+1}^k\right\| \leq \left\|M_i^k - \mathcal{M}_i^k\right\| + \\ +h_k \left\| D_x\mathcal{P}_i\left(\mathbf{x}_i^k, \mathbf{M}_i^k, u\right) - D_x\mathcal{P}_i\left(\mathbf{x}()_i^k, \mathcal{M}_i^k, u\right)\right\| + \\ +h_k \left\| D_u\mathcal{P}_i\left(\mathbf{x}_i^k, \mathbf{M}_i^k, u\right) - D_u\mathcal{P}_i\left(\mathbf{x}()_i^k, \mathcal{M}_i^k, u\right)\right\|,\end{array}$$

$$\begin{array}{l}\left\|M_{i+1}^k - \mathcal{M}_{i+1}^k\right\| \leq \left\|M_i^k - \mathcal{M}_i^k\right\| + \\ +h_k \left\| D_x\mathcal{C}_i\left(\mathbf{x}_i^k, \mathbf{M}_i^k, N_{i+1}^k, u\right) - D_x\mathcal{C}_i\left(\mathbf{x}()_i^k, \mathfrak{M}_i^k, \mathcal{N}_{i+1}^k, u\right)\right\| + \\ +h_k \left\| D_u\mathcal{C}_i\left(\mathbf{x}_i^k, \mathbf{M}_i^k, N_{i+1}^k, u\right) - D_u\mathcal{C}_i\left(\mathbf{x}()_i^k, \mathfrak{M}_i^k, \mathcal{N}_{i+1}^k, u\right)\right\|.\end{array}$$

Then, using again the continuity of $x(t), f_x, f_u$, the uniform convergence of $x^k[t]$ to $x(t)$, the uniform boundedness of the sequences $\{x_i^k\}, \{y_i^k\}, \{\tau_i^k\}, \{M_i^k\}, \{N_i^k\}$ and of the function f_x, and induction, we obtain the estimations:

$$\begin{array}{l}\left\|N_{i+1}^k - \mathcal{N}_{i+1}^k\right\| \leq (1 + h_k V_1)\bar{w}_i^k + o(h_k)V_2, \\ \left\|M_{i+1}^k - \mathcal{M}_{i+1}^k\right\| \leq (1 + h_k W_1)\bar{w}_i^k + o(h_k)W_2.\end{array}$$

From induction hypothesis, we also have for all $j \leq i-1$:

$$\begin{array}{l}\left\|N_{j+1}^k - \mathcal{N}_{j+1}^k\right\| \leq (1 + h_k V_1)\bar{w}_j^k + o(h_k)V_2 \leq (1 + h_k V_1)\bar{w}_i^k + o(h_k)V_2, \\ \left\|M_{j+1}^k - \mathcal{M}_{j+1}^k\right\| \leq (1 + h_k W_1)\bar{w}_j^k + o(h_k)W_2 \leq (1 + h_k W_1)\bar{w}_i^k + o(h_k)W_2,\end{array}$$

and then:

$$\max_{i-Q_i+2\le j\le i+1}\left\|N_j^k-\mathcal{N}_j^k\right\|=\bar{v}_{i+1}^k\le(1+h_kV_1)\bar{w}_i^k+o(h_k)V_2,$$
$$\max_{i-Q_i+2\le j\le i+1}\left\|M_{i+1}^k-\mathcal{M}_{i+1}^k\right\|=\bar{w}_{i+1}^k\le(1+h_kW_1)\bar{w}_i^k+o(h_k)W_2.$$

2.2.4 Convergence of sensitivity matrices

Now we can apply the following well known Lemma (for a proof see [24]):

Lemma 2: Suppose the real numbers $\{\xi_i\}_{i=0,1,...}$satisfy a recurrence estimate of the form:

$$\left|\xi_{i+1}\right|\le(1+\delta)\left|\xi_i\right|+B,\ i=0,1,...$$

for some fixed $\delta>0$ and $B\ge 0$. Then, we have the global estimate:

$$\left|\xi_i\right|\le e^{i\delta}\left|\xi_0\right|+\frac{e^{i\delta}-1}{\delta}B,\ n=1,2,...$$

Applying Lemma 2 to the sequences $\xi_i^k=\bar{w}_i^k$, and recalling that $\bar{w}_0^k=0$, we have the global estimate:

$$\bar{w}_i^k\le\frac{e^{ih_kW_2}-1}{h_kW_1}o(h_k)W_2,$$

for all $i=0,1,...,k$, and all $k\in\aleph$, and this implies:

$$\left\|M_i^k-\mathcal{M}_i^k\right\|\le\left(\frac{\left(e^{TW_2}-1\right)W_2}{W_1}\right)\frac{o(h_k)}{h_k}\to 0\text{ if }k\to+\infty. \tag{27}$$

From this last estimation we obtain:

$$\left\|\bar{\mathbf{M}}^k[t]-\overline{\mathfrak{M}}^k[t]\right\|\to 0,\text{ if }k\to\infty,$$

since from (20), (23) and (27) the values of the interpolating polynomials converge uniformly to zero:

$$\left\|\bar{\mathbf{M}}^k[\tau_i^k]-\overline{\mathfrak{M}}^k[\tau_i^k]\right\|\underset{k}{\to}0,$$
$$\left\|\tfrac{d}{dt}\bar{\mathbf{M}}^k[\tau_j^k]-\tfrac{d}{dt}\overline{\mathfrak{M}}^k[\tau_j^k]\right\|\underset{k}{\to}0,\ j=i-Q_i+1,....,i+1,$$

and the finite and fixed number of coefficients of those interpolating polynomials depend continuosly on this values.

Then, we have the convergence of the sequence $\bar{\mathbf{M}}^k[t]$ to $M(t)$ for each $t\in[0,T]$, because:

$$\left\|\bar{\mathbf{M}}^k[t]-M(t)\right\|\le\left\|\bar{\mathbf{M}}^k[t]-\overline{\mathfrak{M}}^k[t]\right\|+\left\|\overline{\mathfrak{M}}^k[t]-M(t)\right\|\underset{k}{\to}0.$$

2.2.5 Convergence of gradients

Now we are ready to prove the convergence of the sequence of discrete gradients $\{\nabla J_k(u)\}_{k\in\aleph}$ to the continuous gradient $\nabla J(u)$. We recall the expressions of the continuous and discrete gradient for this case:

$$\nabla J(u) = \sum_{j=1}^{s} \left[D_x \tilde{\Phi}_j(x(\tau_j), u) M(\tau_j) + D_u \tilde{\Phi}_j(x(\tau_j), u) \right], \tag{28}$$

$$\nabla J_k(u) = \sum_{i=0}^{k} \left[D_x \Phi_i(x_i^k, u) M_i^k + D_u \Phi_i(x_i^k, u) \right],$$

where:

$$\tilde{\Phi}_j(x(\tau_j), u) = \varphi_j[g(x(\tau_j), u, \tau_j), \bar{z}_j], \; j = 1, 2, ..., s,$$

$$\Phi_i(x_i^k, u) = \tilde{\varphi}_i[g(x_i^k, u, \tau_i^k), \bar{z}_{\mathcal{I}(i)}], \; i = 0, 1, ..., k,$$

$$\tilde{\varphi}_i[z_i, \tilde{z}_i] = \varphi_{\mathcal{I}(i)}[z_i, \bar{z}_{\mathcal{I}(i)}]\, \mathbf{1}_M[i], \; i = 0, 1, ..., k,$$

$$M = \{i \in \{0, 1, 2, ..., k\} \mid \mathcal{I}(i) \neq 0\},$$

and the numbers $\{\tau_j, \; j = 1, 2, ..., s\}$ are the measure points in $[0, T]$.

For the index function $\mathcal{J}$ we have:

$$\tau_{\mathcal{J}(j)}^k = \tau_j, \; j = 1, ..., s,$$

since $\mathcal{J}(j)$ is precisely the index i, corresponding to the $j-$th measure, in the partition of integration $\left\{\tau_i^k, \; i = 0, 1, ..., k\right\}$. Then, we can write:

$$\begin{aligned}
&\nabla J_k(u) = \textstyle\sum_{i=0}^{k} \left[D_x \Phi_i(x_i^k, u) M_i^k + D_u \Phi_i(x_i^k, u) \right] = \\
&= \textstyle\sum_{i=0}^{k} \mathbf{1}_M[i] \left[D_x \varphi_{\mathcal{I}(i)}[g(x_i^k, u, \tau_i^k), \bar{z}_{\mathcal{I}(i)}] M_i^k + D_u \varphi_{\mathcal{I}(i)}[g(x_i^k, u, \tau_i^k), \bar{z}_{\mathcal{I}(i)}] \right] = \\
&= \textstyle\sum_{j=1}^{s} \left[D_x \varphi_j[g(x_{\mathcal{J}(i)}^k, u, \tau_{\mathcal{J}(i)}^k), \bar{z}_j] M_{\mathcal{J}(i)}^k + D_u \varphi_j[g(x_{\mathcal{J}(i)}^k, u, \tau_{\mathcal{J}(i)}^k), \bar{z}_j] \right] = \\
&= \textstyle\sum_{j=1}^{s} \left[D_x \varphi_j[g(\bar{\mathbf{x}}^k[\tau_{\mathcal{J}(i)}^k], u, \tau_{\mathcal{J}(i)}^k), \bar{z}_j] \bar{\mathbf{M}}^k[\tau_{\mathcal{J}(i)}^k] + D_u \varphi_j[g(\bar{\mathbf{x}}^k[\tau_{\mathcal{J}(i)}^k], u, \tau_{\mathcal{J}(i)}^k), \bar{z}_j] \right] = \\
&= \textstyle\sum_{j=1}^{s} \left[D_x \varphi_j[g(\bar{\mathbf{x}}^k[\tau_j], u, \tau_j), \bar{z}_j] \bar{\mathbf{M}}^k[\tau_j] + D_u \varphi_j[g(\bar{\mathbf{x}}^k[\tau_j], u, \tau_j), \bar{z}_j] \right],
\end{aligned}$$

and

$$\nabla J_k(u) = \sum_{j=1}^{s} \left[D_x \tilde{\Phi}_j(\mathbf{x}^k[\tau_j], u) \bar{\mathbf{M}}^k[\tau_j] + D_u \tilde{\Phi}_j(\mathbf{x}^k[\tau_j], u) \right]. \tag{29}$$

Comparing (28) with (29), it is clear that the convergence of $\nabla J_k(u)$ to $\nabla J(u)$, if $k \to +\infty$, is a consequence of the uniform convergence of $\mathbf{x}^k[\tau_j]$ to $x(\tau_j)$ and $\bar{\mathbf{M}}^k[\tau_j]$ to $M(\tau_j)$ for all $j = 1, 2, ..., s$, and all u in any bounded set, and using the continuity of φ and g.

Finally, from the continuity of ∇J at u, for every $\dot{\varepsilon} > 0$ there exists $r > 0$ such that if v belongs to the closed ball $\bar{B}_r$, with center at u and radius r, then

$$\|\nabla J(v) - \nabla J(u)\| < \varepsilon.$$

If $\{u_k\}$ is any sequence of vectors in $\Re^m$ converging to u, for k big enough ($\geq N_1$), the sequence $\{u_k\}$ belongs to the compact neighborhood $\bar{B}_r$ of u. Since the convergence of $\mathbf{x}^k[\tau_j]$ to $x(\tau_j)$ and $\bar{\mathbf{M}}^k[\tau_j]$ to $M(\tau_j)$ is also uniform for u in $\bar{B}_r$, we have for any $\varepsilon > 0$, the existence of $N_2 = N_2(\varepsilon)$, such that:

$$\|\nabla J_k(v) - \nabla J(v)\| < \varepsilon, \text{ if } k \geq N_2 \text{ and for any } v \in \bar{B}_r.$$

Then,

$$\begin{aligned} &\|\nabla J_k(u_k) - \nabla J(u)\| \leq \|\nabla J_k(u_k) - \nabla J(u_k)\| + \|\nabla J(u_k) - \nabla J(u)\| \\ &\|\nabla J_k(u_k) - \nabla J(u)\| \leq 2\varepsilon, \text{ for } k \geq N = \max(N_1, N_2). \blacksquare \end{aligned}$$

3 Conclusions

In the present paper we stated and proved fundamental results related with inverse problems in ODE modelling which we resume as follows:

1) We proposed some kind of "direct approach " for the solution of the inverse problem, substituting the ordinary differential equation by a difference scheme. This is a general approach and can be used also for other dynamical model (as PDE),

2) We strongly recommend to use the exact formulas for the gradients of the discrete approximation schemes instead of using a finite difference approach. In [18] we give a general algorithm to their calculation.

3) We proved the convergence of sequences of discrete gradients to the continuous gradient. This implies that limit points of sequences of stationary points for the discrete problems are stationary points of the continuos problem.

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