A boundary value approach to dynamical systems estimation

Stephen Broadfoot *
and
M.R. Osborne †

Abstract

[1] Methods for the solution of the parameter estimation problem in ordinary differential equations fall into two categories (a) the simultaneous method in which the objective function (for example the sum of squares of residuals) is minimised subject to the differential system as imposed constraints, and (b) the embedding method in which auxiliary conditions are adjoined to take up the extra degrees of freedom in the differential system. If this is chaotic then the imposition of initial conditions in the embedding method becomes suspect. However,in [1] it is shown that provided system structure and data format can be married appropriately, a non-trivial condition, then a technique known as synchronization can be used successfully to overcome the disconnect between the initial conditions and the chaotic trajectory. This technique has a close similarity to the more familiar continuation methods. However, typically the form of data resembles multi point boundary conditions suggesting that a boundary value context would be more appropriate. Here we illustrate the inherent instability of the IVP formulation in chaotic dynamical systems, then show how to choose appropriate boundary conditions, and finally demonstrate the greater power and flexibility of the boundary value formulation in the estimation problem in this context.

*Australian Bureau of Statistics, Belconnen, ACT 2616, Australia
†MSI, Australian National University, ACT 0200, Australia, mailto:Mike.Osborne@anu.edu.au

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1 Introduction

The basic problem considered is given the system of differential equations of order p

$$\frac{d\mathbf{x}}{dt} = \mathbf{f}\left(t, \mathbf{x}, \boldsymbol{\beta}\right), \tag{1.1}$$

where $\boldsymbol{\beta} \in R^q$ is an unknown vector of parameters, estimate $\boldsymbol{\beta}$ given observational data

$$\mathbf{y}_i = \mathcal{O}\left(\mathbf{x}^*\left(t_i, \boldsymbol{\beta}^*\right)\right) + \boldsymbol{\varepsilon}_i, i = 1, 2, \cdots, n \tag{1.2}$$

where $\mathbf{y}_i \in R^s$ is vector of observations made on the system at t_i, $\mathcal{O}$ is the vector of linear functionals of the solution measured at t_i, and $\boldsymbol{\varepsilon}_i$ can be considered the corresponding measurement error, $i = 1, 2, \cdots, n$. Here $\mathbf{x}^*\left(t, \boldsymbol{\beta}^*\right)$ is the (unknown) exact solution.

The family of methods considered are the embedding methods. The idea is to impose auxilliary conditions

$$B\left(\mathbf{x}\right) = \mathbf{b}, \mathbf{b} \in R^p, \tag{1.3}$$

to take up the intrinsic degrees of freedom in the differential equation solution. Here $\mathbf{b}$ is a vector of additional parameters which are to be determined as part of the estimation process. The particular form assumed for the estimation problem is

$$\min_{\boldsymbol{\beta}, \mathbf{b}} F\left(\mathbf{x}, \boldsymbol{\beta}, \mathbf{b}\right), \tag{1.4}$$

$$F\left(\mathbf{x}, \boldsymbol{\beta}, \mathbf{b}\right) = \frac{1}{2}\Sigma_{i=1}^n r_i^2, \tag{1.5}$$

$$r_i = \mathbf{y}_i - \mathcal{O}\left(\mathbf{x}\left(t_i, \boldsymbol{\beta}, \mathbf{b}\right)\right). \tag{1.6}$$

The purpose of this investigation is to consider the implication of the choice of $B\left(\mathbf{x}\right)$ for the estimation process when the initial value problem $B\left(\mathbf{x}\right) = \mathbf{x}\left(0\right)$ for (1.1) is chaotic. Equation (1.1) supports chaotic trajectories if there exist trajectories $\mathbf{x}\left(t\right)$ such that the associated fundamental matrix $X\left(t\right)$ for the linearized equation

$$\frac{dX}{dt} = \nabla_x \mathbf{f}\left(t, \mathbf{x}, \boldsymbol{\beta}\right) X, X\left(0\right) = I, \tag{1.7}$$

has the property that

$$\Lambda = \lim_{t \to \infty} \left(X^T X\right)^{1/2t}$$

has eigenvalues $\exp(\lambda_i), i = 1, 2, \cdots, p$, where the λ_i are called Lyapunov exponents, and $\lambda_1 = \max_i \lambda_i > 0$. The implications are that the variational equation (1.7) has unbounded solutions to the initial value problem while (1.1) has bounded unstable solutions with the property of essentially forgetting their initial conditions corresponding to a form of capture by an attractor. This suggests that the initial value choice $B(\mathbf{x}) = \mathbf{x}(0)$ would be unsuitable for the estimation problem when the data is derived from observations made on chaotic system trajectories. This is confirmed in the next section, in particular by figure 2, where an example is given of the extreme instability of the response surface for the optimization problem (1.5) in this case.

An ingenious method for working around this form of initial value instability is given in [1]. This approach requires that (1.1) be decomposable into drive and response subsystems, that the drive equations which determine the positive Lyapunov exponents be capable of being made stable by adding appropriate penalty terms, and that the estimation problem formulation include information that permits the system trajectory to be steered by the observed data. This steering process is called synchronisation. The estimation problem is then solved by relaxing the penalty terms to zero in a controlled fashion corresponding to a form of continuation. The method has a further disadvantage beyond the requirement that the system be drive decomposable because it requires the form of the observed data be compatible with this structure. In contrast, one advantage of our approach is there are no formal, a priori constraints imposed by the algorithm on the structure of the observed data.

Our approach has been to consider a boundary value form for the adjoined conditions.

$$B(\mathbf{x}) = B_0\mathbf{x}(t_1) + B_1\mathbf{x}(t_n). \tag{1.8}$$

This would seem to make sense for many applications as the form of the observed data does have some similarity to conditions appropriate for a multipoint form of boundary problem. Practical application requires the construction of appropriate boundary matrices B_0, B_1, and an approach which has proved successful [8] is discussed. It is of interest that, in the case of the Mattheij equation, our natural conditions are close numerically to conditions formulated by de Hoog and Mattheij [5] in order to demonstrate the possibility of relatively well conditioned problems in the class of possible solutions to strongly dichotomic system.

In the final section numerical examples are presented which permit direct comparison with problems considered in [1]. The results confirm the advantages claimed for the boundary form of the embedding method.

2 Initial value instability of response surfaces in chaotic systems

It proves convenient to start with a classic example of a chaotic system in order to demonstrate the instability problem.

Example 1 *The standard Lorenz system [2] is*

$$\frac{dx_1}{dt} = \beta_1 (x_2 - x_1), \tag{2.1}$$

$$\frac{dx_2}{dt} = x_1 (\beta_2 - x_3) - x_2, \tag{2.2}$$

$$\frac{dx_3}{dt} = x_1 x_2 - \beta_3 x_3. \tag{2.3}$$

The canonical parameters are $\beta_1 = 10, \beta_2 = 28, \beta_3 = 8/3$.

This system is chaotic with Lyapunov exponents $\lambda_1 = .905, \lambda_2 = 0., \lambda_3 = -14.57$. The instability of the system is illustrated in Figure 1 where plots of trajectories for two sets of initial values $\mathbf{x}^*(0)^T = [1, 1, 30]$, and $\widehat{\mathbf{x}}(0)^T = [-0.1, 2, 31]$ are displayed. Reasonably close initially, the trajectories begin to diverge seriously about $t = 1$, the divergence being more in phase rather than amplitude. The response surface plots are very revealing. Here $\mathbf{x}^*(0)$ is taken as the true vector of unknowns corresponding to the boundary value parameters in the embedding method. The response surfaces are plotted as functions of $x_1(0), x_2(0)$ and correspond to terminal integration values $t_n = 1, 3, 5, 10$. The plots correspond to the choice $n = 1000$. The instability of the response surfaces with respect to the initial value parameters as t_n increases is clearly evident, and the initial value problem solution becomes increasingly chaotic. These conclusions are valid despite the instability of the forward integration. The system actually possesses a backward stability property [4] which means that the visual impression is correct even if the fine numerical detail cannot be accurate.

The response surface diagram provides further evidence in support of [1] by showing that the initial value formulation of the embedding method in the case of chaotic system dynamics is a recipe for serious disappointment. It follows that the adjoining of auxiliary conditions in the embedding method must be done appropriately, and the a priori choice of initial values, if made at all, should be done with caution . To our cost we found this advice applies also to boundary value software that uses the quasi initial value device of compactification or condensation [6] when applied in the context of the boundary problems encountered here. The problem with this form of the solution algorithm should be well known. It is clearly described in [3], section 4.3.4.

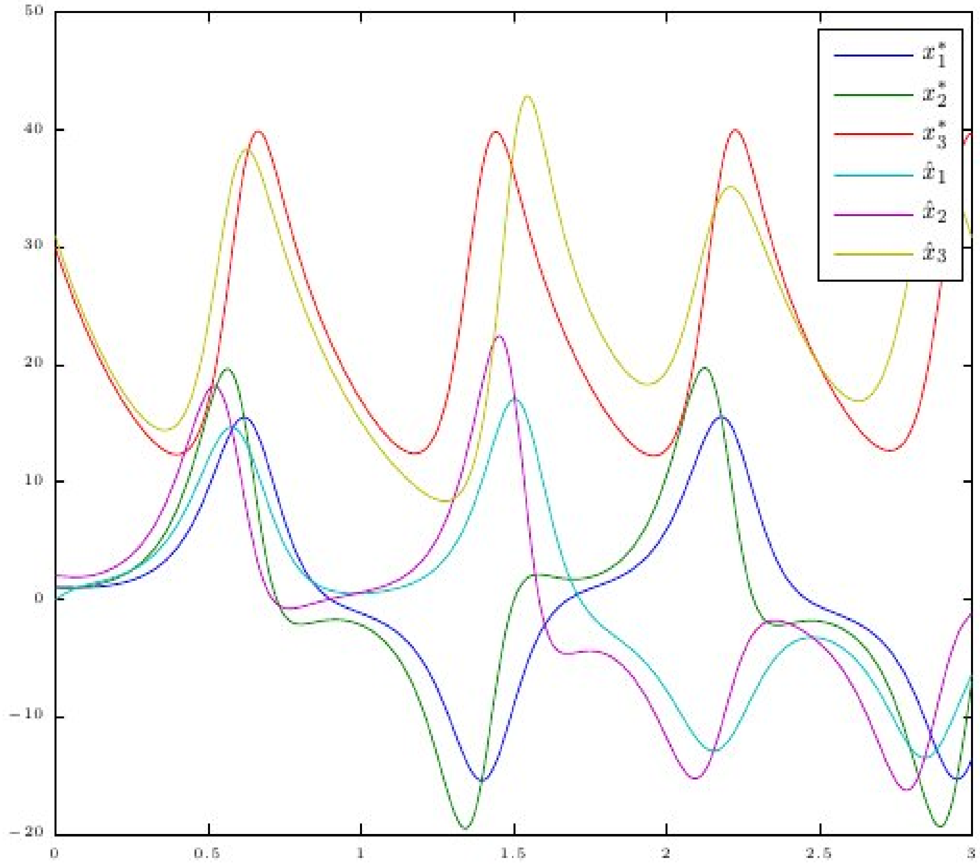

Figure 1: Diverging trajectory plots for the Lorenz system

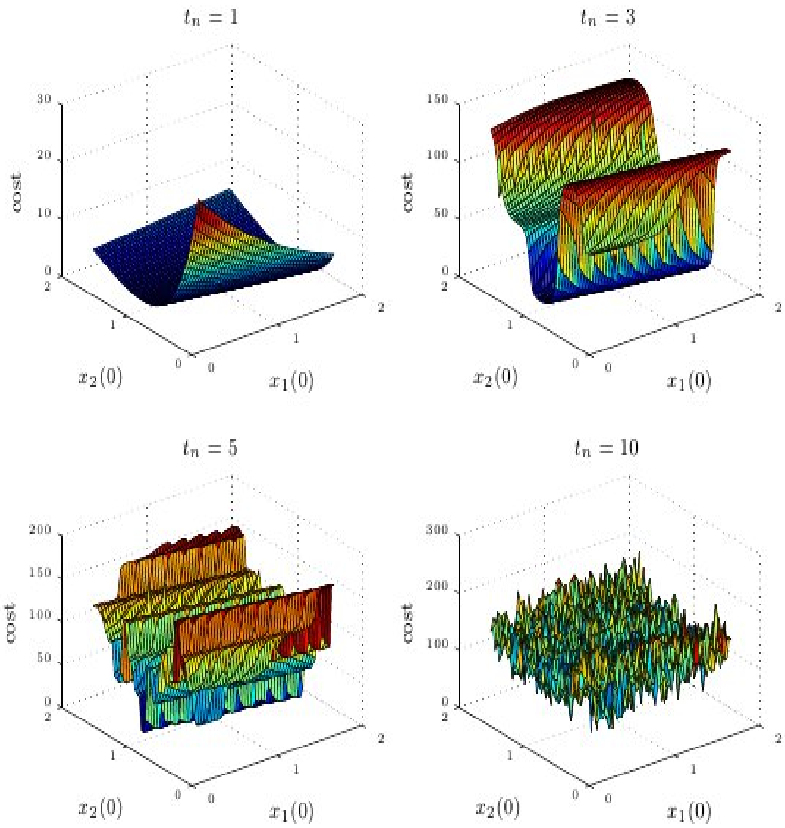

Figure 2: IVP response surface plots for Lorenz equations

3 How to choose the boundary conditions

The embedding approach has the advantage that it leads to algorithms that are relatively simple to formulate. It follows from (1.1) that the gradient of the objective function (1.5) is

$$\nabla_{(\boldsymbol{\beta},\mathbf{b})} F = -\frac{1}{n}\sum_{i=1}^{n} \mathbf{r}_i^T O_i^T \nabla_{(\boldsymbol{\beta},\mathbf{b})} \mathbf{x}\left(t_i\right), \tag{3.1}$$

where the gradient term components can be evaluated by solving the linear boundary value problems

$$B_1 \frac{\partial \mathbf{x}}{\partial \boldsymbol{\beta}}(0) + B_2 \frac{\partial \mathbf{x}}{\partial \boldsymbol{\beta}}(1) = 0, \tag{3.2}$$

$$\frac{d}{dt}\frac{\partial \mathbf{x}}{\partial \boldsymbol{\beta}} = \nabla_{\mathbf{x}} \mathbf{f} \frac{\partial \mathbf{x}}{\partial \boldsymbol{\beta}} + \nabla_{\boldsymbol{\beta}} \mathbf{f}, \tag{3.3}$$

and

$$B_1 \frac{\partial \mathbf{x}}{\partial \mathbf{b}}(0) + B_2 \frac{\partial \mathbf{x}}{\partial \mathbf{b}}(1) = I, \tag{3.4}$$

$$\frac{d}{dt}\frac{\partial \mathbf{x}}{\partial \mathbf{b}} = \nabla_{\mathbf{x}} \mathbf{f} \frac{\partial \mathbf{x}}{\partial \mathbf{b}}. \tag{3.5}$$

Given this information then the scoring (Gauss-Newton) algorithm [7] is applied readily.

The suggestion is that the boundary matrices B_0, B_1 be chosen to ensure the satisfactory integration of the linear differential equation corresponding to variation of (1.1) with respect to $\mathbf{x}$. Here this corresponds to equation (3.5). There is an assumption here that variation of $\boldsymbol{\beta}$ is not going to affect stability unduly, and this assumption would be expected to hold quite generally. In exceptional cases it would be possible to augment the state vector by $\boldsymbol{\beta}$, (1.1) by $\frac{d\boldsymbol{\beta}}{dt} = 0$, and treat $\mathbf{b}$ as the parameter vector to be estimated.

If a two point discretization (for example, the trapezoidal rule) is employed to link adjacent points of the linearised equation on the data grid then the resulting difference equation matrix X has the block bi-diagonal form:

$$X = \begin{bmatrix} X_{11} & X_{12} & & & & \\ & X_{22} & X_{23} & & & \\ & & X_{33} & X_{34} & & \\ & & & \cdots & \cdots & \\ & & & & X_{(n-1)(n-1)} & X_{(n-1)n} \end{bmatrix}$$

The next step involves interchanging the first column of X to the last position using the permutation matrix P followed followed by orthogonal reduction of the modified matrix to upper triangular form using the orthogonal matrix Q computed, for example, using Householder transformations, to give

$$XP \to Q \left[\begin{array}{cccccccc} R_{11} & R_{12} & & & & & 0 & R_{1n} \\ & R_{22} & R_{23} & & & & 0 & R_{2n} \\ & & \cdots & \cdots & \cdots & & & \\ & & & & & R_{(n-2)(n-2)} & R_{(n-2)(n-1)} & R_{(n-2)n} \\ & & & & & & H & G \end{array} \right].$$

Note the move of X_{11} to the last column introduces fill in this column. If the boundary matrices are introduced at this stage then the first step in a backsubstitution would require the solution of the linear system with matrix

$$\left[\begin{array}{cc} H & G \\ B_1 & B_0 \end{array} \right].$$

The basic idea is that B_0, B_1 be chosen so that the resulting system is relatively well conditioned. This can be achieved by starting with an orthogonal factorization:

$$\left[\begin{array}{cc} H & G \end{array} \right] = \left[\begin{array}{cc} U^T & 0 \end{array} \right] \left[\begin{array}{c} Q_1^T \\ Q_2^T \end{array} \right],$$

and setting

$$\left[\begin{array}{cc} B_1 & B_0 \end{array} \right] = Q_2^T. \tag{3.6}$$

Here U provides an indication of the sensitivity of the differential system to two point boundary conditions.

4 Computational experience

The first example compares the performance of initial value and boundary value methods on the Lorenz equations (2.1), (2.2), (2.3). The reference data is obtained by solving the initial value problem with $\mathbf{x}^*(0)^T = [1, 1, 30]$ on $0 \le t \le 3$. It will be seen from Figure 2 that the effects of chaos are by no means as severe as they become for larger values of t_n. However, it still proved necessary to adjust the form of the estimation data on the initial value form of this problem to obtain any results at all. The final form used was

$$\mathbf{y}_i = \left[\begin{array}{ccc} 1 & 0 & 0 \\ 0 & 0 & 1 \end{array} \right] \mathbf{x}^*(t_i) + \mathbf{e}_i, i = 1, 2, \cdots, n,$$

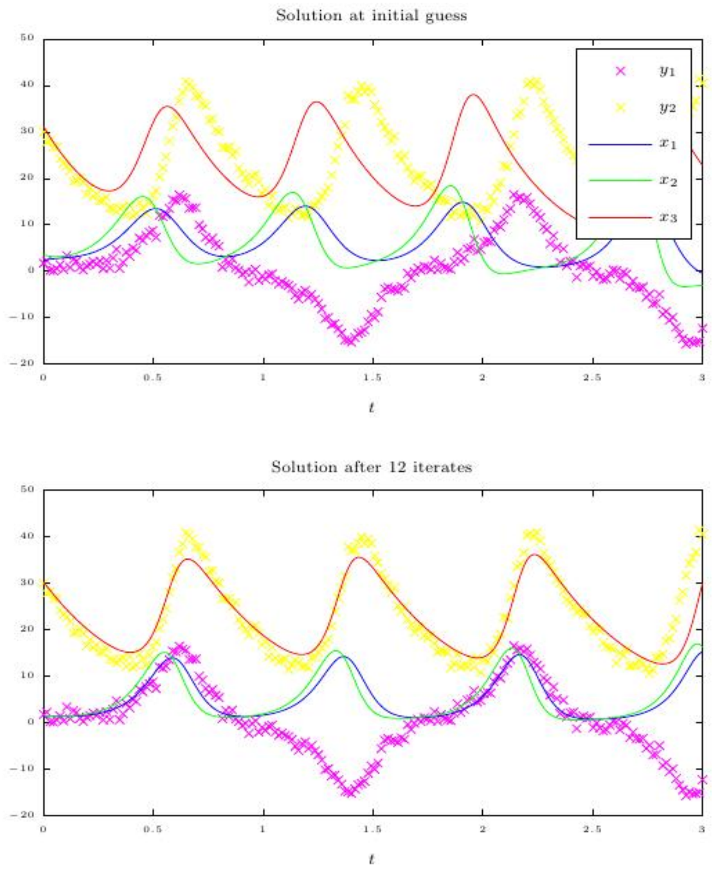

Figure 3: Initial and converged solutions for the initial value formulation

where $\mathbf{e}_i \sim N(\mathbf{0}, I)$, and $n = 200$. Starting estimates for $\mathbf{b}$ and $\boldsymbol{\beta}$ are generated by adding random noise to the exact values

$$\boldsymbol{\beta} = \boldsymbol{\beta}^* + \delta\boldsymbol{\beta},$$
$$\mathbf{b} = \mathbf{b}^* + \delta\mathbf{b},$$

with $\delta\mathbf{b} \sim N(0, 3I)$, $\delta\boldsymbol{\beta} \sim N(0, 0.15I)$. Although a convergent iteration was obtained,the result did not correspond to the expected solution. Results are summarised in Figure 3: The natural boundary matrices corresponding to the true solution $\mathbf{x}^*(t)$ are

$$B_1 = \begin{bmatrix} -0.0155 & 0.0084 & -0.2942 \\ 0.0483 & 0.0061 & 0.8043 \\ -0.9790 & 0.1958 & 0.0574 \end{bmatrix},$$

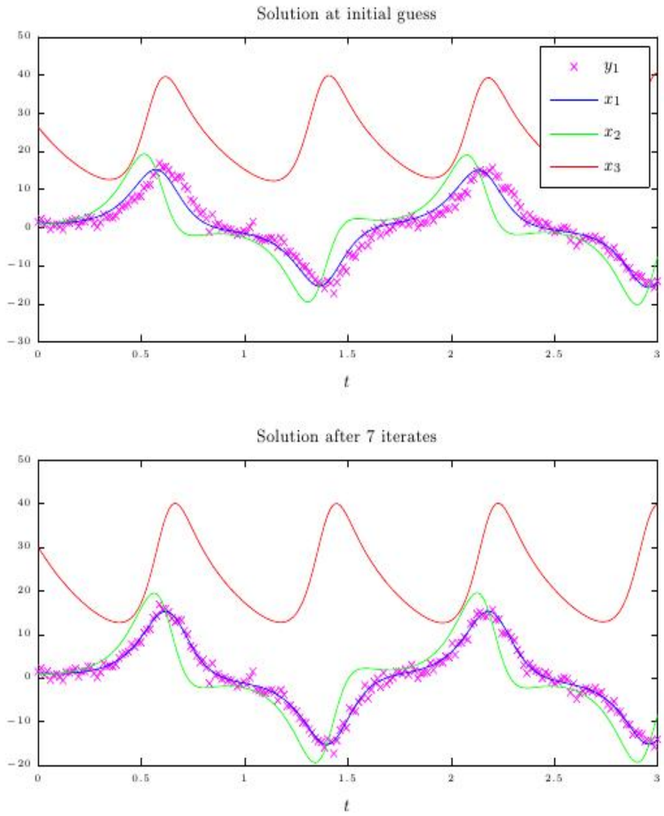

Figure 4: Initial and converged solutions for the boundary value formulation

and

$$B_2 = \begin{bmatrix} -0.4504 & -0.7696 & 0.3434 \\ 0 & -0.4694 & -0.3611 \\ 0 & 0 & 0 \end{bmatrix}.$$

These are used here to define the particular form of the embedding method. This time a satisfactory computation is achieved. Results are summarised in Figure 4:

An example of a system with two positive Lyapunov exponents is given by the Lorenz (1996) equations

$$\begin{aligned}
\frac{dx_1}{dt} &= x_5\left(x_2 - x_3\right) - x_1 + f \\
\frac{dx_2}{dt} &= x_1\left(x_3 - x_4\right) - x_2 + f, \\
\frac{dx_3}{dt} &= x_2\left(x_4 - x_5\right) - x_3 + f, \\
\frac{dx_4}{dt} &= x_3\left(x_5 - x_1\right) - x_4 + f, \\
\frac{dx_5}{dt} &= x_4\left(x_1 - x_2\right) - x_5 + f,
\end{aligned}$$

with f=8.17. The estimation problem based on this system is discussed in some detail in [1] where it is noted that the presence of two positive Lyapunov exponents requires modification of their basic synchronized initial value method and a consequent need to collect a minimum of two suitably chosen data items at each observation point . This formal constraint on the provision of estimation problem data is not so obvious in the boundary value approach. This point is illustrated here using a single data sequence in the embedding algorithm. This sequence is chosen as

$$y_i = x^*\left(t_i\right)_5 + \varepsilon_i, i = 1, 2, \cdots, 251$$

where $\varepsilon_i \sim N\left(0, \sigma^2\right)$, $\sigma = 0.3$, and the $*$ is used to denote exact quantities. This does not correspond to either of the observed data sets in the [1] application. The computed boundary matrices are

$$B_1 = \begin{bmatrix} -0.2466 & 0.3415 & -0.0282 & 0.4924 & 0.6841 \\ -0.1790 & -0.2863 & -0.1201 & 0.3459 & -0.1249 \\ 0.3798 & -0.3457 & -0.6443 & 0.2565 & 0.2039 \\ -0.7452 & 0.0797 & -0.5354 & -0.1267 & -0.2342 \\ -0.2778 & -0.5959 & 0.1805 & -0.4544 & 0.5535 \end{bmatrix},$$

and

$$B_2 = \begin{bmatrix} -0.2674 & -0.0961 & 0.1433 & -0.0095 & 0.0998 \\ 0 & 0.4998 & 0.2637 & 0.6186 & -0.1854 \\ 0 & 0 & -0.4222 & -0.1365 & -0.1302 \\ 0 & 0 & 0 & -0.2775 & -0.0612 \\ 0 & 0 & 0 & 0 & -0.1493 \end{bmatrix}.$$

Starting estimates for $\mathbf{b}$ and $\boldsymbol{\beta}$ are generated by adding random noise to the

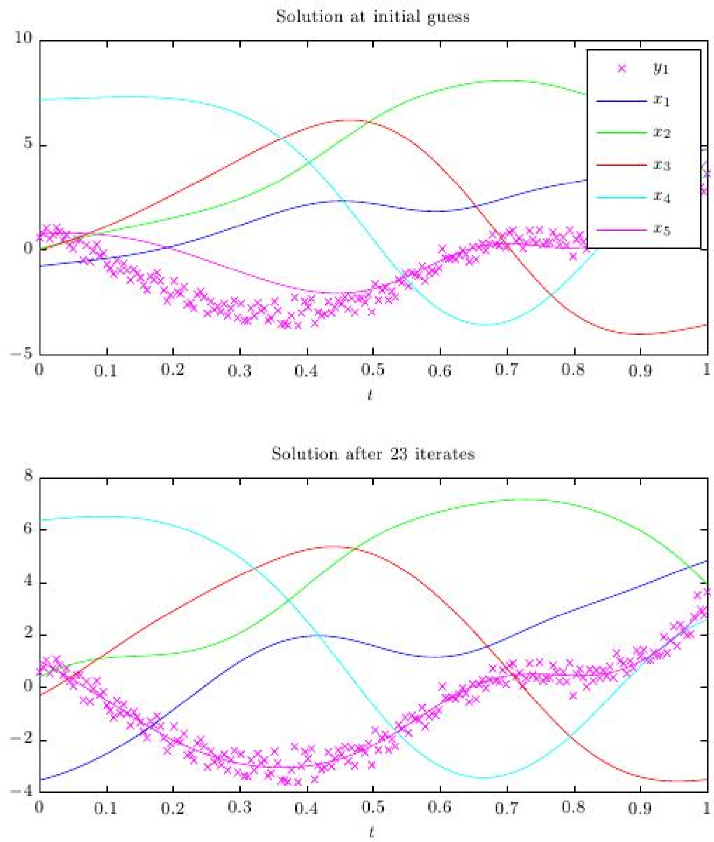

Figure 5: Initial and converged solutions for the Lorenz 1996 model

exact values

$$\boldsymbol{\beta} = \boldsymbol{\beta}^* + \delta\boldsymbol{\beta},$$
$$\mathbf{b} = \mathbf{b}^* + \delta\mathbf{b},$$

with $\delta\mathbf{b} \sim N(0,1), \delta\boldsymbol{\beta} \sim N(0, 0.15)$.

The results for the Gauss-Newton algorithm are displayed in figure 5. They show that rate of convergence measured by number of iterations in this application, while still reasonably satisfactory, proved distinctly slower than in the previous example with little evidence of the asymptotic second order convergence expected for large n. This may be a hint that a different choice of observed data could be more satisfactory. The drive component of the Lorenz system involves the first and third equations, and it is this property that influenced the choice of data selection made in [1]. The data choice made here is more directly associated with the response subsystem.

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