Adaptive Wegstein method for a coefficient inverse problem for one model of HIV infection

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Abstract

We consider a coefficient inverse problems for one model of HIV infection. The problem is formulated as an minimization problem of a quadratic residual functional. The last one is turned to the fixed point problem. We study two approaches to obtaining approximations such as the adaptive Wegstein method to solutions of the fixed point problem. One way is the vector approach, this method uses the ratio of the norms of residuals for finding parameters of the method. The other way is the componentwise approach that shift tracking of approximations in each coordinate more subtle. Numerical results are presented.

1 Adaptive Wegstein method for fixed point problem

There are an impressive number of methods for the approximate solutions of nonlinear scalar equations and systems. The search for new methods of solving such equations and ways to improve the efficiency of the well-known and practically proven methods remains important. Newton's method and simple iterations method, being the simplest to build and structure and most capable of an exhaustive study, often serve as the starting point for this.

One way to improve the convergence and extend the scope of applicability of linearly convergent iterative processes is to build processes of the Fejer type [1] which are called Mann iterations (see [2, 3, etc.]). Suppose that the problem of a fixed point is defined by the equality

$$\mathbf{x} = \mathbf{\Phi}(\mathbf{x}). \tag{1}$$

Here $\mathbf{\Phi} : \mathbb{R}^n \to \mathbb{R}^n$ is a given continuous nonlinear mapping. These iterations are based on the formula

$$\mathbf{x}^{(k+1)} = \lambda \mathbf{\Phi}\left(\mathbf{x}^{(k)}\right) + (1-\lambda)\mathbf{x}^{(k)} \quad (k = 0, 1, 2, \dots). \tag{2}$$

Here λ is a scalar parameter or a sequence of parameters $\lambda = \lambda^{(k)}$. Different approaches to the method of fixing this parameter lead to different specific processes of the family (2). The Wegstein method [4] for solving one-dimensional equations (1) is one of sufficiently effective members of this family. In elaboration of this method, the authors of this paper proposed in [5] to fix the coefficients of the linear combination of the points $\mathbf{x}^{(k)}$ and

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$\mathbf{\Phi}\left(\mathbf{x}^{(k)}\right)$ to be inversely proportional to the values of taking residuals of these values. This method is defined by the following set of formulas:

$$\tilde{\mathbf{x}}^{(k+1)} = \frac{\lambda^{(k)}}{1+\lambda^{(k)}}\tilde{\mathbf{x}}^{(k)} + \frac{1}{1+\lambda^{(k)}}\mathbf{x}^{(k+1)}, \quad \mathbf{x}^{(k+1)} = \mathbf{\Phi}\left(\tilde{\mathbf{x}}^{(\mathbf{k})}\right), \tag{3}$$

$$\lambda^{(k)} = \frac{\mathbf{x}^{(k+1)} - \mathbf{\Phi}\left(x^{(k+1)}\right)}{\mathbf{x}^{(k+1)} - \tilde{\mathbf{x}}^{(k)}}, \quad k = 0, 1, 2, \dots \tag{4}$$

The resulting iterative method is identical to the Aitken Δ^2 method, in which the formula for acceleration is applied every other step of the method of simple iterations. The Aitken method in the form (3), (4) is convenient for studying the conditions of its quadratic convergence and gave rise to an adaptive algorithm in which the fulfillment of these conditions is checked and corrected in the process of its implementation [6].

When solving scalar equations, the parameters can be calculated using the formula

$$\lambda^{(k)} = \frac{\left|\mathbf{x}^{(k+1)} - \mathbf{\Phi}\left(\mathbf{x}^{(k+1)}\right)\right|}{\left|\mathbf{x}^{(k+1)} - \tilde{\mathbf{x}}^{(k)}\right|}, \tag{5}$$

which allows extending this method to the case of systems of nonlinear equations.

The method (3), (5) has more limited conditions for applicability, but the method (3) with the parameters

$$\lambda^{(k)} = \frac{\|\mathbf{x}^{(k+1)} - \mathbf{\Phi}\left(x^{(k+1)}\right)\|}{\|\mathbf{x}^{(k+1)} - \tilde{\mathbf{x}}^{(k)}\|} \tag{6}$$

is formally suitable for solving systems of nonlinear equations in the form (1). A careful study of the one-dimensional case [6] shows that, to ensure fast convergence of the method (3), when fixing the parameter $\lambda^{(k)}$ at each iterative step, it is important to consider the nature of convergence/divergence of simple iterations delivering the next intermediate value $\mathbf{x}^{(k+1)}$. In particular, it is important to know whether the points $\mathbf{x}^{(k+1)}$ and $\tilde{\mathbf{x}}^{(k)}$ are on the same side or on the opposite sides with respect to the fixed point $\mathbf{x}^*$. In an n-dimensional case, the behavior of the starting and intermediate points during each approximation can be similarly taken into account for each coordinate separately. The scalar parameter $\lambda^{(k)}$ becomes a vector $\lambda^k = \left(\lambda_i^{(k)}\right)$ for this purpose. The Mann process is implemented by coordinates as follows.

Let the given nonlinear system (1) in an expanded form be

$$\begin{cases} x_1 = \varphi_1(x_1, x_2, \dots, x_n), \\ x_2 = \varphi_2(x_1, x_2, \dots, x_n), \\ \qquad \dots \\ x_n = \varphi_n(x_1, x_2, \dots, x_n). \end{cases} \tag{7}$$

The transition from the value $\tilde{\mathbf{x}}^{(k)} = \left(\tilde{x}_i^{(k)}\right)$ to the value $\tilde{\mathbf{x}}^{(k+1)} = \left(\tilde{x}_i^{(k+1)}\right)$ is carried out based on formulas

$$x_i^{(k+1)} = \varphi_i\left(\tilde{x}_1^{(k)}, \tilde{x}_2^{(k)}, \dots, \tilde{x}_n^{(k)}\right), \tag{8}$$

$$\tilde{x}_i^{(k+1)} = \frac{\lambda^{(k)}}{1+\lambda^{(k)}}\tilde{x}_i^{(k)} + \frac{1}{1+\lambda^{(k)}}x_i^{(k+1)} \quad (k = 0,\ 1,\ 2,\ \dots), \tag{9}$$

The matrix-vector form of the method (8), (9) is

$$\begin{aligned} \tilde{\mathbf{x}}^{(k+1)} &= \Lambda^{(k)}\bar{\Lambda}^{(k)}\tilde{\mathbf{x}}^{(k)} + \bar{\Lambda}^{(k)}\mathbf{x}^{(\mathbf{k+1})}, \\ \mathbf{x}^{(k+1)} &= \mathbf{\Phi}\left(\tilde{\mathbf{x}}^{k}\right) \quad (k = 0,\ 1,\ 2,\ \dots), \end{aligned} \tag{10}$$

where $\Lambda^{(k)} = diag\left\{\lambda_1^{(k)}, \lambda_2^{(k)}, \dots, \lambda_n^{(k)}\right\}, \bar{\Lambda}^{(k)} = diag\left\{\frac{1}{1+\lambda_1^{(k)}}, \frac{1}{1+\lambda_2^{(k)}}, \dots, \frac{1}{1+\lambda_n^{(k)}}\right\}$.

We use two options for calculating values $\lambda_i^{(k)}$ required in (10).

1. $\lambda_i^{(k)} = \begin{cases} \beta^{(k)}, \text{if} \quad \operatorname{sgn}\left(\tilde{x}_i^{(k)} - x_i^{(k+1)}\right) = \operatorname{sgn}\left(\varphi_i(\mathbf{x}^{(k+1)}) - x_i^{(k+1)}\right), \\ -\beta^{(k)}, \text{if} \quad \operatorname{sgn}\left(\tilde{x}_i^{(k)} - x_i^{(k+1)}\right) = \operatorname{sgn}\left(x_i^{(k+1)} - \varphi_i(\mathbf{x}^{(k+1)})\right), \end{cases}$ where $\beta^{(k)} = \dfrac{\left\|\mathbf{x}^{(k+1)} - \Phi(\mathbf{x}^{(k+1)})\right\|}{\left\|\mathbf{x}^{(k+1)} - \tilde{\mathbf{x}}^{(k)}\right\|}$.

2. $\lambda_i^{(k)} = \dfrac{x_i^{(k+1)} - x_i^{(k)}}{\tilde{x_i}^{(k-1)} - \tilde{x_i}^{(k)}}; \quad i = 1, \ldots, n.$

Theorem 1. *Let a vector-valued function* $\mathbf{\Phi}$ *be continuously differentiable in some domain* $M \subseteq \mathbb{R}^n$, *that contains its fixed point* ξ. *Let there exist nonnegative constants* a_k, b_k, $k = 0, 1, \ldots,$ *such that*

$$\max_i \left| \frac{1}{1 + \lambda_i^{(k)}} \right| \leqslant a_k, \quad \max_i \left| \lambda_i^{(k)} + \sum_{j=1}^{n} \frac{\partial \varphi(\mathbf{x})}{\partial x_j} \right| \leqslant b_k.$$

If there exist q, *that the following inequality holds*

$$a_k b_k \leqslant q < 1 \tag{11}$$

and all members of the sequence $\left(\tilde{\mathbf{x}}^{(k)}\right)$ *and* $\left(\mathbf{x}^{(k)}\right)$, *defined by* (10), *do not leave the* M, *then the sequence* $\left(\tilde{\mathbf{x}}^{(k)}\right)$ *converges to* ξ *provided that the initial point* $\tilde{\mathbf{x}}^{(0)} \in M$.

P r o o f. Regardless of the way in which parameters $\lambda_i^{(k)}$, $i = 1, \ldots, n$ is chosen, we deduce from equality (10) that

$$\xi - \tilde{\mathbf{x}}^{(k+1)} = \xi - \Lambda^{(k)} \bar{\Lambda}^{(k)} \tilde{\mathbf{x}}^{(k)} - \bar{\Lambda}^{(k)} \mathbf{x}^{(k+1)} = \bar{\Lambda}^{(k)} \left[\xi - \mathbf{x}^{(k+1)} + \Lambda^{(k)} \left(\xi - \tilde{\mathbf{x}}^{(k)} \right) \right],$$

because

$$\bar{\Lambda}^{(k)} + \bar{\Lambda}^{(k)} \Lambda^{(k)} = diag \left(\frac{1}{1 + \lambda_i^{(k)}} \right) + diag \left(\frac{1}{1 + \lambda_i^{(k)}} \right) \cdot diag \left(\lambda_i^{(k)} \right) = diag \left(\frac{1}{1 + \lambda_i^{(k)}} + \frac{\lambda_i^{(k)}}{1 + \lambda_i^{(k)}} \right) =$$
$$= diag \left(\frac{1 + \lambda_i^{(k)}}{1 + \lambda_i^{(k)}} \right) = E,$$

where E is the identity matrix.

Using the equality $\xi = \mathbf{\Phi}(\xi)$ and the mean-value theorem for each row vector function $\xi - \mathbf{x}^{(k+1)}$, we obtain

$$\xi - \tilde{\mathbf{x}}^{(k+1)} = \bar{\Lambda}^{(k)} \left[\mathbf{\Phi}(\xi) - \mathbf{\Phi}\left(\tilde{\mathbf{x}}^{(k)} \right) + \Lambda^{(k)} \left(\xi - \tilde{\mathbf{x}}^{(k)} \right) \right] = \bar{\Lambda}^{(k)} \left(\Gamma_k + \Lambda^{(k)} \right) \left(\xi - \tilde{\mathbf{x}}^{(k)} \right), \tag{12}$$

where $\Gamma_k = \Gamma\left(\theta_1^{(k)}, \ldots, \theta_n^{(k)}\right) = \begin{pmatrix} \frac{\partial \varphi_1}{\partial x_1} & \frac{\partial \varphi_1}{\partial x_2} & \cdots & \frac{\partial \varphi_1}{\partial x_n} \\ \frac{\partial \varphi_2}{\partial x_1} & \frac{\partial \varphi_2}{\partial x_2} & \cdots & \frac{\partial \varphi_2}{\partial x_n} \\ \cdots & \cdots & \cdots & \cdots \\ \frac{\partial \varphi_n}{\partial x_1} & \frac{\partial \varphi_n}{\partial x_2} & \cdots & \frac{\partial \varphi_n}{\partial x_n} \end{pmatrix}$ is the matrix, in which the partial derivatives are calculated with $\mathbf{x} = \theta_i^{(k)}$, $i = 1, \ldots, n$. If the following inequality holds $\left\|\xi - \theta_i^{(k)}\right\| \leqslant \left\|\xi - \tilde{\mathbf{x}}^{(k)}\right\|$, equality (12) implies the inequality

$$\left\|\xi - \tilde{\mathbf{x}}^{(k+1)}\right\| \leqslant \left\|\bar{\Lambda}^{(k)}\right\| \cdot \left\|\Gamma_k + \Lambda^{(k)}\right\| \cdot \left\|\xi - \tilde{\mathbf{x}}^{(k)}\right\| \leqslant$$
$$\leqslant a_k b_k \left\|\xi - \tilde{\mathbf{x}}^{(k)}\right\| \leqslant q \left\|\xi - \tilde{\mathbf{x}}^{(k)}\right\|.$$

Successive iterations of this inequality yield

$$\left\|\xi - \tilde{\mathbf{x}}^{(k+1)}\right\| \leqslant q^2 \left\|\xi - \tilde{\mathbf{x}}^{(k-1)}\right\| \leqslant \cdots \leqslant q^k \left\|\xi - \tilde{\mathbf{x}}^{(0)}\right\|.$$

We have (11). It is now obvious that the above estimate for the error of the approximation $\left(\tilde{\mathbf{x}}^{(k+1)}\right)$ implies the convergence of the sequence $\left(\tilde{\mathbf{x}}^{(k)}\right)$ to ξ for each $\tilde{\mathbf{x}}^{(0)} \in M$. □

Theorem 2. *Let a vector-valued function* $\mathbf{\Phi}$ *be continuously differentiable in some domain* $M \subseteq \mathbb{R}^n$, *that contains its fixed point* ξ. *Let there exist nonnegative constants* a, b c, *such that*

$$\max_i \left| \frac{1}{1+\lambda_i^{(k)}} \right| \leqslant a, \quad \max_i \left| \lambda_i^{(k)} \right| \leqslant b, \quad \max_i \sum_{j=1}^{n} \left| \frac{\partial \varphi(\mathbf{x})}{\partial x_j} \right| \leqslant c.$$

If the following inequality holds

$$a(b+c) < 1$$

and all members of the sequence $\left(\tilde{\mathbf{x}}^{(k)}\right)$ *and* $\left(\mathbf{x}^{(k)}\right)$, *defined by* (10), *do not leave the* M, *then the sequence* $\left(\tilde{\mathbf{x}}^{(k)}\right)$ *converges to* ξ *provided that the initial point* $\tilde{\mathbf{x}}^{(0)} \in M$.

To illustrate good properties of the elaborated method we apply it for solving one inverse coefficient problem for a model of HIV dynamics. An observer measures the concentration of viral particles in blood as well as a serum level of immunocompetent cells. These data are used to estimate coefficients of the model. This is a typical inverse dynamic problem and to deal with it a quadratic residual functional is introduced and the identification problem is formulated as a minimization problem. As a necessary condition for extremum dictates the last problem is reduced to a nonlinear system to be solved numerically. To accelerate a convergence of iterative process we use method (10). The implementation of these ideas in a formal and precise way is given in a paragraph 3 while a concise description of the HIV model is given in a paragraph 2.

2 Description of the model

Mathematical models provide a means to understand the human immunodeficiency virus (HIV)-infected immune system as a dynamic process. Models formulated as differential equations for the dynamic interactions of CD4+ lymphocytes and virus populations are useful in identifying essential characteristics of HIV pathogenesis and chemotherapy [7, 8]. The equations for the model with treatment are as follows:

$$\begin{cases} \dfrac{dT(t)}{dt} = S_1 - \dfrac{S_2 V_S(t)}{B_S + V_S(t)} - \mu_T T(t) + \dfrac{\lambda_1}{C + V_S(t)} T(t) V(t) - \left(k_S V_S(t) + k_r V_r(t)\right) T(t), \\ \dfrac{dT_S(t)}{dt} = k_S V_S(t) T(t) - \mu_{T_i} T_S(t) - \dfrac{\lambda_2}{C_i + V_S(t)} T_S(t) V(t), \\ \dfrac{dT_r(t)}{dt} = k_r V_r(t) T(t) - \mu_{T_i} T_r(t) - \dfrac{\lambda_2}{C_i + V_S(t)} T_r(t) V(t), \\ \dfrac{dV_S(t)}{dt} = (1-q) \dfrac{\lambda_3}{C_i + V_S(t)} T_S(t) V(t) - k_V T(t) V_S(t) + \dfrac{G_S V_S}{B + V(t)}, \\ \dfrac{dV_r(t)}{dt} = \dfrac{\lambda_3 T_r(t)}{C_i + V_S(t)} V(t) + q \dfrac{\lambda_3 T_S(t)}{C_i + V_S(t)} V(t) - k_V T(t) V_r(t) + G_r\left(V(t)\right) \dfrac{V_r(t)}{B + V(t)}, \end{cases} \tag{13}$$

where $V(t) = V_S(t) + V_r(t)$, $G_r = (G_S e^{(V-V_0)p})/(1 + e^{(V-V_0)p})$, the initial conditions are $T(0) = T_0$, $T_S(0) = 0$, $T_r(0) = 0$, $V(0) = V_0$, the dependent variables are T is uninfected CD4+ T-cell population, T_s is CD4+ T-cell population infected by virus sensitive to the treatment, T_r is CD4+ T-cell population infected by virus restrictive to the treatment, V_s is infectious HIV population sensitive to the treatment, V_r is infectious HIV population restrictive to the treatment.

In equation 1 the term $S_1 - S_2 V_S(t)/(B_S + V_S(t))$ represents the external input of uninfected CD4+ T-cells from the thymus, bone marrow, or other sources. It is assumed that there is a deterioration of this source as the viral level increases during the course of HIV infection, μ_T is the death rate of uninfected CD4+ T-cells whose average lifespan is $1/\mu_T$. The term $\lambda_1 T(t) V(t)/(C + V_S(t))$ represents CD4+ T-cell proliferation in the plasma due to an immune response that incorporates both direct and indirect effects of antigen stimulation, where C is a saturation constant. The form assumed here idealizes the growth mechanisms of CD4+ T-cells, since subpopulations of antigen specific CD4+ T-cells are not modeled. In equation 1 k_S is the infection rate of CD4+ T cells by virus (it is assumed that the rate of infection is governed by the mass action term $k_S V_S(t) T(t)$). In the absence of virus the CD4+ T-cell population converges to a steady state of S_1/μ_T.

In equation 2 there is a gain term $k_S V_S(t) T(t)$ of CD4+ T-cells infected by drug-sensitive virus, a loss term $\mu_{T_i} T_S(t)$ due to the death of these cells independent of the virus population, and a loss term $\lambda_2 T_S(t) V_S(t)/(C_i + V_S(t))$ dependent on the virus population due to bursting or other causes. The dependence of the loss term

$\lambda_2 T_S(t)V_S(t)/(C_i+V_S(t))$ allows for an increased rate of bursting of infected cells as the immune system collapses and fewer of these cells are removed by CD8+ T-cells. The structure of equation 3 is the same.

In equation 4 the virus population is increased by the term $\lambda_3 T_S(t)V(t)/(C_i+V_S(t))$. This term corresponds to the internal production of virus in the blood. The dependence of this term on $T_S(t)$ allows for a decreased rate of viral production in the plasma when the infected CD4+ T-cell population in the plasma collapses. Since most of the plasma virus is contributed by the external lymph source, the plasma virus population still increases steeply at the end stage of the disease. In equation 4 the virus population is decreased by the loss term $k_V T(t)V_S(t)$, which represents viral clearance. In equation 4 there is a source of virus from the external lymphoid compartment, which is represented by the term $G_S V_S/(B+V(t))$ (B is a saturation constant). This term accounts for most of the virus present in the blood. the structure of equation 5 is the same.

A complete list of parameters and their estimated values for model (13) is given in [8]. Figure 1 shows a schematic diagram of the entire immune response process.

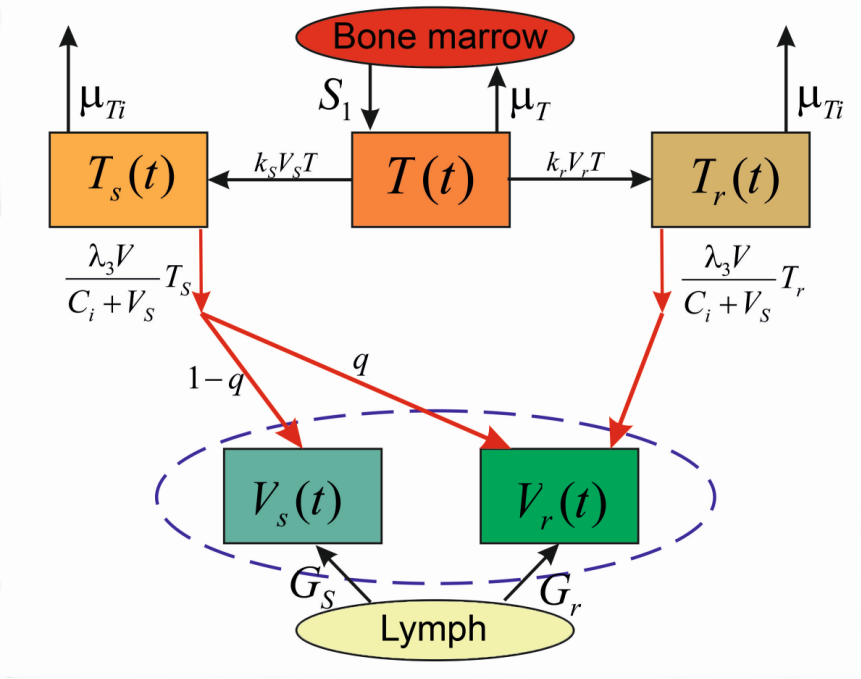

Figure 1: Schematic diagram of the working immune system

Figure 2 represents the progression to AIDS, the total number of viruses increased rapidly after 3000 days, while the population of CD4+ T-cells decline to zero.

3 A coefficient inverse problem and numerical experiments

Let t_k, $k = 1, \ldots, m$, $t_1 < t_2 < \cdots < t_m$ are fixed time moments of measurements. We also defined state vector $\mathbf{x} = \mathbf{x}(t) = (T(t), T_S(t), T_r(t), V_S(t), V_r(t))$ and the vector of the parameters $\mathbf{a}^* = (a_1, \ldots, a_p)$ to be estimated, $1 \leqslant p \leqslant 16$. We denote by $\mathbf{x}(\mathbf{a}) = \mathbf{x}(t; \mathbf{a})$ the solution obtained with the given parameters $\mathbf{a}$, $\mathbf{x}_k(\mathbf{a}) = \mathbf{x}(t_k; \mathbf{a})$.

Let us denote by $\mathbf{y}_k$ the results of measurements at moment t_k, and the accuracy of measurements satisfies $|y_{i,k} - x_{i,k}| \leqslant \xi_i$, $i = 1, \ldots, 5$, where ξ_i are given.

Let the initial approximation $\mathbf{a}^0 = (a_1^0, \ldots, a_p^0)$ is known, it is required to estimate the parameters $\mathbf{a}^*$. We consider a quadratic residual functional

$$\Phi(\mathbf{a}) = \sum_{i=1}^{5} \sum_{k=1}^{m} \frac{1}{\xi_i} \left(x_{i,k}(\mathbf{a}) - y_{i,k}\right)^2. \tag{14}$$

A minimization problem for a functional (14) is turned to solving of nonlinear equation

$$\frac{\partial \Phi(\mathbf{a})}{\partial a_l} = 0, \tag{15}$$

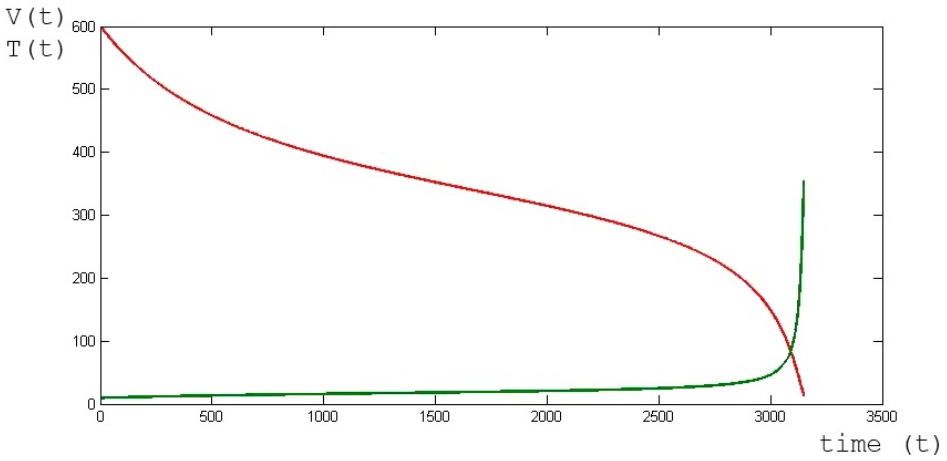

Figure 2: This is the numerical solution of model (13). Parameter values used to generate this figure can be found in [8]

it is easy to check that $\dfrac{\partial \Phi(\mathbf{a})}{\partial a_l} = 2 \sum\limits_{i=1}^{5} \sum\limits_{k=1}^{m} \dfrac{1}{\xi_i} \left(x_{i,\,k}(\mathbf{a}) - y_{i,\,k} \right) \dfrac{\partial x_{i,\,k}(\mathbf{a})}{\partial a_l}, \;\; l = 1, \ldots, p.$

Method (10) is applied for solving the problem (15). We use a priory information to set the initial approximation of the vector $\mathbf{a}^0$. Calculation of the function in (15) implies a numerical solving of the differential equations (13). Because of stiffness we use implicit fourth order Runge-Kutta method each step of which implies solving of an appropriate nonlinear system, and adaptive method (10) is used for this too.

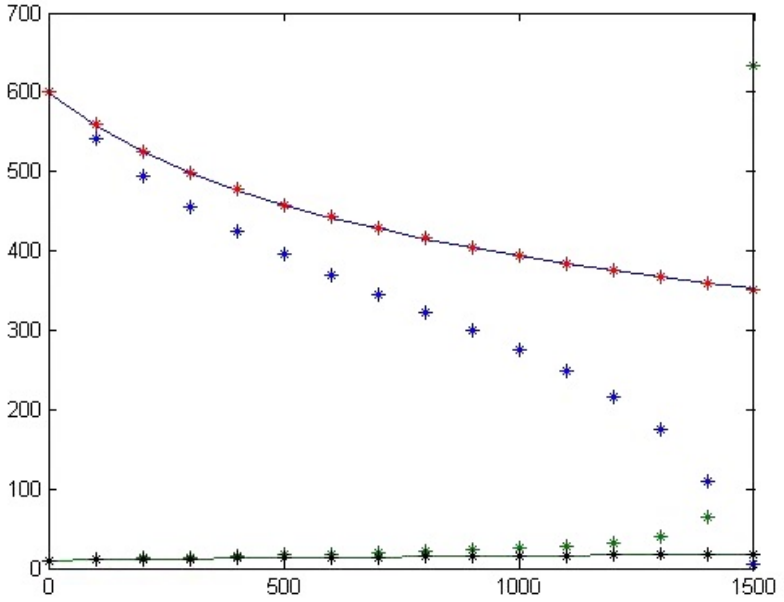

Figure 3: This is the results of parameters estimation for model (13)

To illustrate good properties of the proposed method (10) and efficiency of the approach described above we performed several numerical experiments. Let B and B_S are unknown parameters to be estimated, so $a = (B, B_S)$. To simulate the system dynamics and obtain the observations $\mathbf{a}^*$ was defined according to [8] as $\mathbf{a}^* = (2, 13.8)$. The initial approximation was taken as $\mathbf{a}^0 = (3, 18)$.

The system dynamics for true parameters value is depicted by solid lines, for initial value $\mathbf{a}^0$ by green and blue

stars, and as it clearly seen in the picture it is rather far. Numerical algorithm (10) found $\mathbf{a} = (2.1207, 13.4800)$, the corresponding dynamics is depicted by red and black stars and is extremely closed to the true one.

4 Conclusions

The advantage of the proposed method (10) for solving nonlinear systems is that only one function calculation is required on each iterative step, while the calculation of the derivatives and matrix inversion is not required at all. In one-dimensional case the proposed method has the quadratic convergence; in general case according to the results of numerical estimations method (10) converges not slower than Newton's method.

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