International Journal of Applied Mathematics

Volume 33 No. 5 2020, 919-928
ISSN: 1311-1728 (printed version); ISSN: 1314-8060 (on-line version)
doi: http://dx.doi.org/10.12732/ijam.v33i5.12

PICARD-LINDELÖF ITERATIONS AND MULTIPLE SHOOTING METHOD FOR PARAMETER ESTIMATION

Stanislav Slavov[1], Tsvetelin Tsvetkov[2 §]

[1]Department of Physics
University of Chemical Technology and Metallurgy
8, Kliment Ohridski, Blvd., Sofia, 1756, BULGARIA

[2]Department of Mathematics
University of Chemical Technology and Metallurgy
8, Kliment Ohridski, Blvd., Sofia, 1756, BULGARIA

Abstract: In this article, we modify the Picard-Lindelöf iteration scheme in order to show an iteration algorithm for parameter estimation of ordinary differential equations. The proposed algorithm inherited the advantages exhibited in the classical algorithms and, moreover, the parameters can be transformed to a form that are convenient and suitable for computation. In the end, a numerical example has also been discused to highlight the results.

AMS Subject Classification: 62F12, 34A55, 62F99
Key Words: parameter identification for ODE, parameter estimation, Picard-Lindelöf iterations, multiple shooting method

1. Introduction: Multiple Shooting Method

Let

$$\Theta = \{(t_i, \boldsymbol{X}_i) : i = 1, \dots, m\}$$

be a set of given data. In general, we may interpret t_i as measurement moments

Received: July 23, 2020

[§]Correspondence author

of some, for example, experimental d-dimensional progress test or data $\boldsymbol{X}_i \in \mathbb{R}^d$. Of course, we suppose: $0 < t_1 < t_2 < \cdots < t_m$ and $\boldsymbol{X}_i = (X_{i1} \ \cdots \ X_{id})^T$, $i = 1, \ldots, m$.

Also, let

$$\dot{\boldsymbol{x}} = f(t, \boldsymbol{x}, \boldsymbol{p}) \tag{1}$$

be a d-dimensional differential equation. We suppose that any trajectory of equation (1) is defined and unique in the time-interval $[0, T]$, $T > t_m$, for all initial conditions and all parameters $\boldsymbol{p} \in \mathbb{R}^p$.

Let the data Θ satisfy the following observation law

$$X_{ij} = g_j(\boldsymbol{x}(t_i), \boldsymbol{p}) + a_{ij}\varepsilon_{ij}, \quad i = 1, \ldots, m, \ j = 1, \ldots, d, \tag{2}$$

where:

1. the function $g = (g_1 \ \cdots \ g_d) : \mathbb{R}^{d+p} \to \mathbb{R}^d$ is continuous;
2. a_{ij} are positive constants.
3. ε_{ij} are independent and standard Gaussian distributed random variables.

On the basis of data Θ and law (2), the goal is to estimate the initial condition $\boldsymbol{x}_0 \in \mathbb{R}^d$ and the parameter vector $\boldsymbol{p}_0 \in \mathbb{R}^p$ for differential equation (1) such that

$$\mathcal{L}(\boldsymbol{x}_0, \boldsymbol{p}_0) = \min \left\{ \mathcal{L}(\boldsymbol{y}, \boldsymbol{p}) : \boldsymbol{y} \in \mathbb{R}^d, \ \boldsymbol{p} \in \mathbb{R}^p \right\}, \tag{3}$$

where

$$\mathcal{L}(\boldsymbol{y}, \boldsymbol{p}) = \sum_{i=1}^{m} \sum_{j=1}^{d} \frac{(X_{ij} - g_j(\boldsymbol{x}(t_i; \boldsymbol{y}, \boldsymbol{p}), \boldsymbol{p}))^2}{2a_{ij}}$$

and $\boldsymbol{x}(t; \boldsymbol{y}, \boldsymbol{p})$ is the solution of (1) with initial condition $\boldsymbol{x}(0; \boldsymbol{y}, \boldsymbol{p}) = \boldsymbol{y}$.

The direct mimimization of $\mathcal{L}$ with respect to vectors $\boldsymbol{y}$ and $\boldsymbol{p}$ is exactly *initial value approach.*

It is well-known that the direct optimization metods used for problem (3) are highly nonlinear and in the general case computational complexity (and therefore the computational cost) is also high.

The *multiple shooting method* is an efficient and robust method minimising these two effects. Following Bock, see [2], [3], [4] (also see [1], [10] and references therein), we divide the interval $[0, T]$ into subintervals $[\tau_{i-1}, \tau_i]$ such that

$$t_0 = \tau_0 = 0; \ \tau_i \in (t_i, t_{i+1}), \ i = 1, \ldots, m-1; \ t_{m+1} = \tau_m = T.$$

For every $i = 0, \dots, m-1$, we consider a different initial value problem

$$\dot{\boldsymbol{x}} = f(t, \boldsymbol{x}, \boldsymbol{p}), \quad t \in [\tau_i, \tau_{i+1}], \tag{4}$$

$$\boldsymbol{x}(\tau_i) = \boldsymbol{x}_0^{(i)}, \tag{5}$$

with corresponding solution $\boldsymbol{x}\left(t; \boldsymbol{x}_0^{(i)}, \boldsymbol{p}\right)$.

Consider the cost function

$$\mathcal{L}_{\boldsymbol{x}}\left(\boldsymbol{x}_0^{(0)}, \dots, \boldsymbol{x}_0^{(m-1)}, \boldsymbol{p}\right) = \sum_{i=1}^{m} \sum_{j=1}^{d} \frac{\left(X_{ij} - g_j\left(\boldsymbol{x}\left(t_i; \boldsymbol{x}_0^{(i)}, \boldsymbol{p}\right), \boldsymbol{p}\right)\right)^2}{2a_{ij}} \tag{6}$$

and the minimization problem

$$\min\left\{\mathcal{L}_{\boldsymbol{x}}\left(\boldsymbol{x}_0^{(0)}, \dots, \boldsymbol{x}_0^{(m-1)}, \boldsymbol{p}\right) : \boldsymbol{x}_0^{(i)} \in \mathbb{R}^d,\ \boldsymbol{p} \in \mathbb{R}^p\right\} \tag{7}$$

subject to

$$\lim_{t \to \tau_i - 0} \boldsymbol{x}\left(t; \boldsymbol{x}_0^{(i-1)}, \boldsymbol{p}\right) = \lim_{t \to \tau_i + 0} \boldsymbol{x}\left(t; \boldsymbol{x}_0^{(i)}, \boldsymbol{p}\right),\ i = 1, \dots, m-1. \tag{8}$$

Obviously (8) is equivalent to the following equality

$$\boldsymbol{x}\left(\tau_i; \boldsymbol{x}_0^{(i-1)}, \boldsymbol{p}\right) = \boldsymbol{x}_0^{(i)},\ i = 1, \dots, m-1. \tag{9}$$

2. Picard-Lindelöf Iterations

Let us set

$$\phi_0(t) = \begin{cases} \boldsymbol{X}_1, & \text{if } t \in [\tau_0, \tau_1), \\ \boldsymbol{X}_2, & \text{if } t \in [\tau_1, \tau_2), \\ \vdots & \\ \boldsymbol{X}_m, & \text{if } t \in [\tau_{m-1}, \tau_m] \end{cases} \tag{10}$$

and

$$\phi_{k+1}(t)=\begin{cases} \boldsymbol{C}_{k+1}^{(0)}+\int\limits_{\tau_0}^{t} f(s,\boldsymbol{\phi}_k(s),\boldsymbol{p})\,ds, & \text{if } t\in[\tau_0,\tau_1),\\ \boldsymbol{C}_{k+1}^{(1)}+\int\limits_{\tau_1}^{t} f(s,\boldsymbol{\phi}_k(s),\boldsymbol{p})\,ds, & \text{if } t\in[\tau_1,\tau_2),\\ \vdots & \\ \boldsymbol{C}_{k+1}^{(m-1)}+\int\limits_{\tau_{m-1}}^{t} f(s,\boldsymbol{\phi}_k(s),\boldsymbol{p})\,ds, & \text{if } t\in[\tau_{m-1},\tau_m], \end{cases} \tag{11}$$

where for any $k=0,1,\dots,$ the parameter $\boldsymbol{p}$ and constant vectors $C_{k+1}^{(i)}$ are obtained as the solution of following constrained problem

$$\min\left\{\mathcal{L}_{\boldsymbol{\phi}_{k+1}}\left(\boldsymbol{C}_{k+1}^{(0)},\dots,\boldsymbol{C}_{k+1}^{(m-1)},\boldsymbol{p}\right):\boldsymbol{C}_{k+1}^{(i)}\in\mathbb{R}^d,\ \boldsymbol{p}\in\mathbb{R}^p\right\} \tag{12}$$

subject to

$$\boldsymbol{\phi}_{k+1}\left(\tau_i;\boldsymbol{C}_{k+1}^{(i-1)},\boldsymbol{p}\right)=\boldsymbol{C}_{k+1}^{(i)},\ i=1,\dots,m-1. \tag{13}$$

Let us mark that (12), (13) is a classical constrained optimization problem. Hence, we may use any well-known solution metod such as any non-linear programming method.

Theorem 1. *Let there exist a vector $\boldsymbol{X}_0$ and two numbers $a>0$, $b>0$ such that:*

1. *The function f is continuous in cylinder $C_{a,b}(\boldsymbol{X}_0)=\{(t,\boldsymbol{x}):t\in[0,T],\ \|\boldsymbol{x}-\boldsymbol{X}_0\|\le b\}$ and uniformly Lipschitz continuous with respect to $\boldsymbol{x}$.*
2. *$\|\boldsymbol{X}_i-\boldsymbol{X}_0\|\le b/2$, $i=1,\dots,m$ and $\|\boldsymbol{C}_k^{(j)}-\boldsymbol{X}_0\|\le b/2$, $k=0,1,\dots$.*
3. *$T\le\min\left\{a,\frac{b}{M}\right\}$.*

Then the limit

$$x(t)=\lim_{k\to\infty}\phi_k(t),\quad t\in[0,T]$$

exists and the function $x(t)$ is a solution of minimization problem (7), (9).

Proof. We will follow the classical approach and techniques proving the convergence of Picard-Lindelöf iterations.

In the space $C^0([0,T], B_b(\boldsymbol{X}_0))$ of all continuous functions from $[0,T]$ to $B_b(\boldsymbol{X}_0) = \{\boldsymbol{x} : \|\boldsymbol{x} - \boldsymbol{X}_0\| \le b\}$ we consider the metric induced by sup-norm $\|\psi\|_\infty = \sup\{\|\psi(t)\| : t \in (0,T)\}$.

We define the Picard operator as follows

$$\Gamma : ([0,T], B_b(\boldsymbol{X}_0)) \to ([0,T], B_b(\boldsymbol{X}_0)),$$

$$\Gamma\psi(t) = \begin{cases} \boldsymbol{C}^{(0)} + \int\limits_{\tau_0}^{t} f(s, \boldsymbol{\psi}(s), \boldsymbol{p})\, ds, & \text{if } t \in [\tau_0, \tau_1), \\ \boldsymbol{C}^{(1)} + \int\limits_{\tau_1}^{t} f(s, \boldsymbol{\psi}(s), \boldsymbol{p})\, ds, & \text{if } t \in [\tau_1, \tau_2), \\ \vdots & \\ \boldsymbol{C}^{(m-1)} + \int\limits_{\tau_{m-1}}^{t} f(s, \boldsymbol{\psi}(s), \boldsymbol{p})\, ds, & \text{if } t \in [\tau_{m-1}, \tau_m], \end{cases}$$

where the parameter $\boldsymbol{p}$ and constant vectors $\boldsymbol{C}^{(i)}$ are obtained as the solution of the following constrained problem

$$\min\left\{\mathcal{L}_{\boldsymbol{\psi}}\left(\boldsymbol{C}^{(0)}, \dots, \boldsymbol{C}^{(m-1)}, \boldsymbol{p}\right) : \boldsymbol{C}^{(i)} \in \mathbb{R}^d,\ \boldsymbol{p} \in \mathbb{R}^p\right\}$$

subject to

$$\lim_{t \to \tau_i - 0} \boldsymbol{\psi}(t) = \boldsymbol{C}^{(i)},\ i = 1, \dots, m-1.$$

First we have to show that Γ maps $C^0([0,T], B_b(\boldsymbol{X}_0))$ into itsef. Indeed, let $\|\psi\|_\infty < b$. Then for any $t \in [0,T]$, we have $t \in [\tau_i, \tau_{i+1})$ for some $i = 0, \dots, m-1$, i.e.

$$\begin{aligned} \|\Gamma\psi(t) - \boldsymbol{C}^{(i)}\| &\le \left\|\Gamma\psi(t) - \boldsymbol{X}_0 + \boldsymbol{X}_0 - \boldsymbol{C}^{(i)}\right\| \\ &\le \|\Gamma\psi(t) - \boldsymbol{X}_0\| + \left\|\boldsymbol{X}_0 - \boldsymbol{C}^{(i)}\right\| \\ &= \left\|\int\limits_{\tau_i}^{t} f(s, \psi(s), \boldsymbol{p})\, ds\right\| + \left\|\boldsymbol{X}_0 - \boldsymbol{C}^{(i)}\right\| \\ &\le M|t - \tau_i| + \left\|\boldsymbol{X}_0 - \boldsymbol{C}^{(i)}\right\| \\ &\le MT + \frac{b}{2} \le \frac{b}{2} + \frac{b}{2} = b. \end{aligned}$$

Next we have to prove that Γ is a contraction, i.e. for any two functions $\psi_1, \psi_2 \in C^0([0,T], B_b(\boldsymbol{X}_0))$, we have (for some $q < 1$)

$$\|\Gamma\psi_1 - \Gamma\psi_2\|_\infty \le q\|\psi_1 - \psi_2\|_\infty.$$

Let us fix $t^* \in [0,T]$ such that

$$\|\Gamma\psi_1 - \Gamma\psi_2\|_\infty = \|(\Gamma\psi_1 - \Gamma\psi_2)(t^*)\|.$$

Let the index i be chosen such that $t^* \in [\tau_i, \tau_{i+1})$. Using the definition of Γ (as in classical case) we have

$$\begin{aligned}\|(\Gamma\psi_1 - \Gamma\psi_2)(t^*)\| &= \left\| \int_{\tau_i}^{t^*} (f(s,\psi_1(s),\boldsymbol{p}) - f(s,\psi_2(s),\boldsymbol{p}))(t^*)\, ds \right\| \\ &\le \int_{\tau_i}^{t^*} \|(f(s,\psi_1(s),\boldsymbol{p}) - f(s,\psi_2(s),\boldsymbol{p}))(t^*)\|\, ds \\ &\le L \int_{\tau_i}^{t^*} \|\psi_1(s) - \psi_2(s)\|\, ds \\ &\le LT\,\|\psi_1 - \psi_2\|_\infty < q\,\|\psi_1 - \psi_2\|_\infty.\end{aligned}$$

Therefore, using the Banach fixed point theorem, there exists a unique fixed point of Γ, i.e. there exists a unique function ϕ such that $\Gamma\phi = \phi$. □

3. A Two-Dimensional Example

As an example, let us consider the two-dimensional data

$$\Theta = \{(0.1, 1), (0.3, 0.34), (0.5, 0.2), (0.7, 0.15), (0.9, 0.1)\},$$

and linear model

$$\dot{\boldsymbol{x}} = p_1 x + p_2. \tag{14}$$

In this example we seek the parameters p_1, p_2, and x_0 such that the solution of equation (14) with initial condition $x(0) = x_0$ best fits the given data Θ.

It is suitable to choose $\tau_i = \frac{i}{5}$, $i = 0, 1, 2, 3, 4, 5$.

We define an initial gues for the approximation as:

$$\phi_0(t) = \begin{cases} 1, & \text{if } t \in [\tau_0, \tau_1), \\ 0.34, & \text{if } t \in [\tau_1, \tau_2), \\ 0.2, & \text{if } t \in [\tau_2, \tau_3), \\ 0.15, & \text{if } t \in [\tau_3, \tau_4), \\ 0.1, & \text{if } t \in [\tau_4, \tau_5]. \end{cases}$$

The calculation algorithm listed below is based on CAS Maple.

```
restart;with(GlobalOptimization);with(plots);
data:=[[.1,1],[.3,.34],[.5,.2],[.7,.15],[.9,.1]];
grid_data:=[0,.2,.4,.6,.8,1];
f:=(A,B,y)->A*y+B;
x[0]:=t->piecewise(0<=t and t<.2,data[1][2],
        .2<=t and t<.4,data[2][2],
        .4<=t and t<.6,data[3][2],
        .6<=t and t<.8,data[4][2],
        .8<=t and t<=1,data[5][2]);
p1:=pointplot(data,color=red);
p3:=plot(x[0](t),t=0..1,color=blue);
display(p1,p3);

x[1]:=t->piecewise(
 0<=tandt<.2,C[1]+int(f(A[k],B[k],x[k-1](s)),s=.1..t),
 .2<=tandt<.4,C[2]+int(f(A[k],B[k],x[k-1](s)),s=.3..t),
 .4<=tandt<.6,C[3]+int(f(A[k],B[k],x[k-1](s)),s=.5..t),
 .6<=tandt<.8,C[4]+int(f(A[k],B[k],x[k-1](s)),s=.7..t),
 .8<=tandt<=1,C[5]+int(f(A[k],B[k],x[k-1](s)),s=.9..t));

sol:=GlobalSolve(sum((x[k](data[i][1])-data[i][2])^2,
        i=1..5),
        [seq(limit(x[k](t),t=grid_data[i],left)
          =x[k](grid_data[i]),i=2..5)],
        A[k]=-10..10,B[k]=-10..10,
        seq(C[j]=0..1,j=1..5));

assign(sol[2]);

p1:=pointplot(data,color=red);
p3:=plot(x[k](t),t=0..1,color=blue);
display(p1,p3)
```

The output of *GlobalSolve* is (the decimal place accuracy is 4)

```
sol:=[0.0016,[A[1]=-5.7411,B[1]=.6842,C[1]=.9948,
        C[2]=.3623,C[3]=.1892,C[4]=.1251,C[5]=.1184]]
```

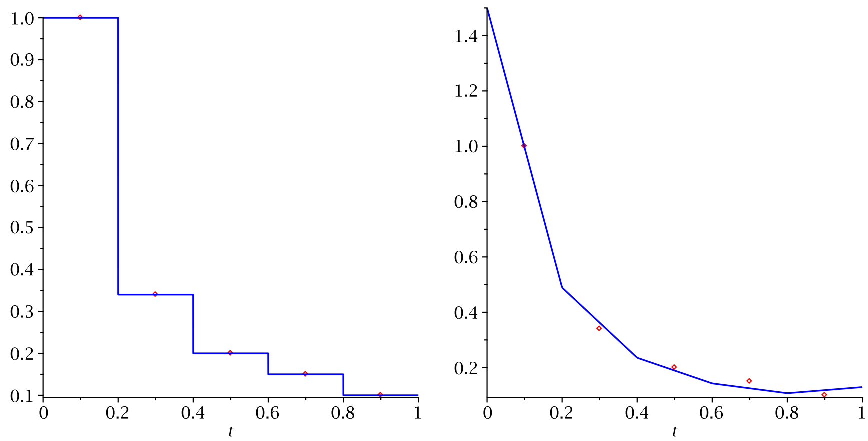

Figure 1: Initial gues and first iteration

and the output graphics are ploted of Figure 1.

Continuing algorithm, on the second step we receive

$$x_2(t) = \begin{cases} 0, & t < 0, \\ 1.7379 - 9.1097t + 16.5583t^2, & t \in [\tau_0, \tau_1), \\ 1.2416 - 4.1468t + 4.1509t^2, & t \in [\tau_1, \tau_2), \\ 0.8205 - 2.0413t + 1.5191t^2, & t \in [\tau_2, \tau_3), \\ 0.4822 - 0.9133t + 0.57918t^2, & t \in [\tau_3, \tau_4), \\ -0.1193 + 0.5905t - 0.3607t^2, & t \in [\tau_4, \tau_5), \\ 0, & t > 1. \end{cases} \quad (15)$$

It is not hard to calculate directly the solution of linear equation and to verify that the quadratic error is less than 0.00234.

References

[1] J.P.N. Bishwal, *Parameter Estimation in Stochastic Differential Equations*, Lecture Notes in Math., **1923**, Springer, Berlin, 2008.

[2] H.G. Bock, Numerical treatment of inverse problems in chemical reaction kinetics, In: *Modelling of Chemical Reaction Systems* (Ed-s: K. Ebert, P. Deuflhard, and W. Jäger), Springer, 1981, 102-125.

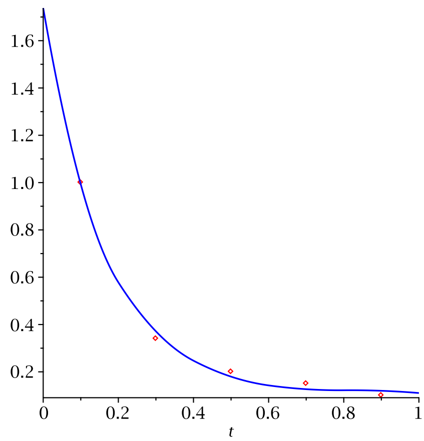

Figure 2: Second iteration

[3] H.G. Bock, Recent advances in parameter identification techniques for ordinary differential equations, In: *Numerical Treatment of Inverse Problems in Differential and Integral Equations* (Ed-s: P. Deuflhard and E. Hairer), Birkhaüser, 1983, 95-121.

[4] H.G. Bock, *Randwertproblemmethoden zur Parameteridenti Fizierung in Systemen Nichtlinearer Differentialgleichungen*, PhD Thesis, Universität Bonn, 1987.

[5] N. J-B. Brunel, Parameter estimation of ODE's via nonparametric estimators, *Electronic Journal of Statistics*, **2** (2008), 1242-1267, doi: 10.1214/07-EJS132.

[6] A. Dishliev, K. Dishlieva, S. Nenov, *Specific Asymptotic Properties of the Solutions of Impulsive Differential Equations. Methods and Applications*, Academic Publication, 2011.

[7] N. Kyurkchiev, On a sigmoidal growth function generated by reaction networks. some extensions and applications, *Communications in Applied Analysis*, **23**, No. 3 (2019), 383-400.

[8] N. Kyurkchiev, A. Iliev, and A. Rahnev, On a special choice of nutrient supply for cell growth in a continuous bioreactor. Some modeling and approximation aspects, *Dynamic Systems and Applications*, **28**, No. 3 (2019), 587-606.

[9] V. Kyurkchiev, A. Iliev, A. Rahnev and N. Kyurkchiev, *Some New Logistic Differential Models: Properties and Applications*, Lambert, 2019.

[10] H. Miao, X. Xia, A.S. Perelson, Hulin Wu, On identifiability of nonlinear ode models and applications in viral dynamics, *SIAM Review*, **53**, No. 1 (2011), 3-39, doi: 10.1137/090757009.

[11] S.I. Nenov, Impulsive controllability and optimization problems in population dynamics, *Nonlinear Analysis: Theory, Methods & Applications*, Pergamon, **36**, No. 7 (1999).

[12] A. Papavasiliou, Ch. Ladroue, Parameter estimation for rough differential equations, *The Annals of Statistics*, **39**, No. 4 (2011), 2047-2073, doi: 10.1214/11-AOS893.

[13] D. Rocha, S. Gouveia, C. Pinto, M. Scotto, J.N. Tavares, E. Valadas, and L.F. Caldeira, On the parameters estimation of HIV dynamic models, *REVSTAT – Statistical Journal*, **17**, No. 2 (2019), 209-222.

[14] D.S. Stratiev, R.K. Dinkov, I.K. Shishkova, A.D. Nedelchev, T. Tsaneva, E. Nikolaychuk, I.M. Sharafutdinov, N. Rudney, S. Nenov, M. Mitkova, M. Skunov, D. Yordanov, An investigation on the feasibility of simulating the distribution of the boiling point and molecular Weight of heavy oils, *Petroleum Science and Technology*, **33**, No. 5 (2015), 527-541.