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Stepwise Solutions for Optimal Control Problems

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Abstract: A new stepwise method for solving optimal control problems is introduced. The main motivation for developing this new approach is the limitation of the continuous-time Pontryagin Maximum Principle (PMP) where all control functions must be continuous. However, in many real-world applications such as drug injection or resource allocation problems, it is not practical to continuously change the control. In dealing with these problems it is strictly preferred to change the control only at certain moments of time and keep it constant otherwise. Clearly, in this case the resulting stepwise solution cannot be calculated optimally using PMP since it is not continuous anymore. The other advantage of stepwise solutions is that they can be obtained much easier compared to the PMP approach when the system has complex dynamics or the cost function is more complicated. Some numerical examples are solved by using both the classical PMP and the proposed stepwise method and the results are compared, which prove the high performance of the proposed method.

Keywords: Optimal control theory, Heuristic and meta-heuristic optimization, Nonlinear dynamics.

1. Introduction

Optimal control theory is an effective tool to be applied to physical, biological, economical and other real-world models. Various examples of such applications are studied in [1] and [2]. As another example, the application of optimal control theory in chemotherapy of cancer and epidemiology can be found in [3] and [4], respectively. Currently, the most important classical method in optimal control theory is the remarkable Pontryagin Maximum Principle (PMP) which can be used in various forms in applied problems. Nonetheless, the application of PMP is somehow limited in practice since it finds the optimal control assuming it is continuous and has a continuous first derivative. Other less important limiting conditions are also posed on the state equations and the corresponding cost function. It should be noted that discontinuous optimal controls, which cannot be obtained by the standard PMP, are also desired in many practical problems, e.g. when a relay is involved or a medicine has to be injected in an stepwise manner.

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Here, we are interested in developing a new optimal control method which is capable of finding discontinuous optimal controls even for complicated dynamical systems. More precisely, in the proposed method the control functions are selected among the stepwise candidate solutions using heuristic and meta-heuristic optimization algorithms. In the forthcoming sections, the classical numerical forward-backward sweep method and the proposed stepwise method are applied to some problems and the results are compared to provide the reader with a clear vision of the potential applications and power of the new method.

2. Introductory Example and Definitions of the Stepwise Method with Fixed Step-size

In this section, we describe the proposed stepwise method by a simple example ([1], page 42). For this purpose, consider the constrained maximization problem:

$$max\ J = \int_0^2 (2x - 3u - u^2)dt, \tag{1}$$

subject to $x' = x + u$, $x(0) = 5$, and the control constraint $u \in \Omega = [0,2]$. The optimal solution $u(t)$ of this problem can be obtained using PMP as follows. First, we form the Hamiltonian as below

$$H = (2x - 3u - u^2) + \lambda(x + u) = (2 + \lambda)x - (u^2 + 3u - \lambda u).$$

Now, the optimal control can be calculated by differentiating H with respect to u and equating the result to zero as

$$\frac{\partial H}{\partial u} = -2u - 3 + \lambda = 0,$$

which yields $u(t) = (\lambda(t) - 3)/2$, where $u(t)$ must lie in the interval $\Omega = [0,2]$. In order to obtain λ we derive the adjoint equation as

$$\lambda' = -\frac{\partial H}{\partial x} = -2 - \lambda, \quad \lambda(2) = 0,$$

or equivalently,

$$\lambda' + \lambda = -2, \quad \lambda(2) = 0.$$

The solution of the above equation is $\lambda(t) = 2(e^{2-t} - 1)$. Considering the fact that the control must always lie in the interval $\Omega = [0,2]$, this leads to the following optimal control:

$$u = \begin{cases} 2 & \text{if} \quad e^{2-t} - 2.5 > 2, \\ e^{2-t} - 2.5 & \text{if} \quad 0 \le e^{2-t} - 2.5 \le 2, \\ 0 & \text{if} \quad e^{2-t} - 2.5 < 0. \end{cases} \tag{2}$$

As it is expected, the resultant optimal control is a continuous function in t. It can be easily verified that the total cost J using this control is equal to 68.93.

For solving this problem using the proposed method, we first change the maximization problem under consideration to an equivalent minimization problem. This task can be performed e.g. by defining the cost function equal to $1/(1+J)$, where J is defined in (1) (assuming $J = 68.93$ the value of cost function is obtained as $1/(1+68.93) = 0.0143$). In the next step, we assume that the control cannot vary continuously with time; instead, it can be subjected only to stepwise changes. In other words, it is assumed that the control remains constant for some period of time and then its value is repeatedly changed to another constant value. Clearly, using this assumption, one must look for the optimal solution among stepwise functions. More precisely, in this problem assuming that the optimal solution has to be calculated in the time interval $[0,T]$, we divide this interval into three subintervals of length $T/3$ each, and assume that the control function $u(t)$ has a certain but unknown constant value in each subinterval. Note that the length of the subintervals can also be considered variable, which leads to the variable step-size method.

According to the above discussion, in order to find the optimal control for the dynamical system $x' = f(x,u,t)$, $x(0) = x_0$, in the time interval $[0,T]$ using the fixed step-size method we can assume that the control takes constant values α, β, and γ, in the time intervals $t \in [0, \frac{T}{3}]$, $t \in [\frac{T}{3}, \frac{2T}{3}]$, and $t \in [\frac{2T}{3}, T]$, respectively (obviously, the number of time intervals is arbitrary). Clearly, in order to calculate the cost function assuming that the control levels α, β, and γ are known, we can first solve the ordinary differential equation (ODE) $x' = f(x,\alpha,t)$, $x(0) = x_0$ in the time interval $t \in [0, \frac{T}{3}]$. Then, for $t \in [\frac{T}{3}, \frac{2T}{3}]$, we solve the ODE $x' = f(x,\beta,t)$ with the initial condition $x(0) = x(\frac{T}{3})$ where $x(\frac{T}{3})$ is the terminal point of the solution obtained in the past interval (i.e., the solution obtained in $t \in [0, \frac{T}{3}]$). Finally, we solve $x' = f(x,\gamma,t)$ using the initial condition $x(0) = x(\frac{2T}{3})$ to obtain x in the time interval $t \in [\frac{2T}{3}, T]$, where $x(\frac{2T}{3})$ refers to the terminal point of the solution obtained in $t \in [\frac{T}{3}, \frac{2T}{3}]$. Using this technique, x is known in all of the subintervals, and consequently, the cost function can be calculated as well. It is important to note that in this manner we actually convert the optimal control problem to an optimization problem where the optimal values of (α,β,γ) can be calculated using, e.g., any meta-heuristic optimization algorithm (the genetic algorithm (GA), simulated annealing (SA), and pattern search (PS) are used for this purpose in this paper, where only the first two are meta-heuristics).

A question may arise here about the possible difference between the final cost of PMP and the proposed stepwise method. We have the following simple lemma about the relation between stepwise and continuous functions.

Lemma 1. For every continuous function $u(t)$, there is a sequence $\{u_n(t)\}$ of stepwise functions such that $\lim_{n\to\infty} u_n(t) = u(t)$.

Using this lemma, we can be confident that the proposed stepwise method can generate useful solutions, which can mimic the results obtained by PMP. Moreover, it is also possible to find better optimal solutions compared to PMP since the limitation on the continuity of the solution and its derivative is removed using the stepwise method. Figure 1 shows the optimal control (2) obtained using PMP and the stepwise optimal control obtained using GA (For this purpose the GA of optimization toolbox of Matlab R2009a with default values for parameters is applied. The algorithm is run 20 times and the best result is reported here.). The final cost of the stepwise method is equal to 0.01430542.

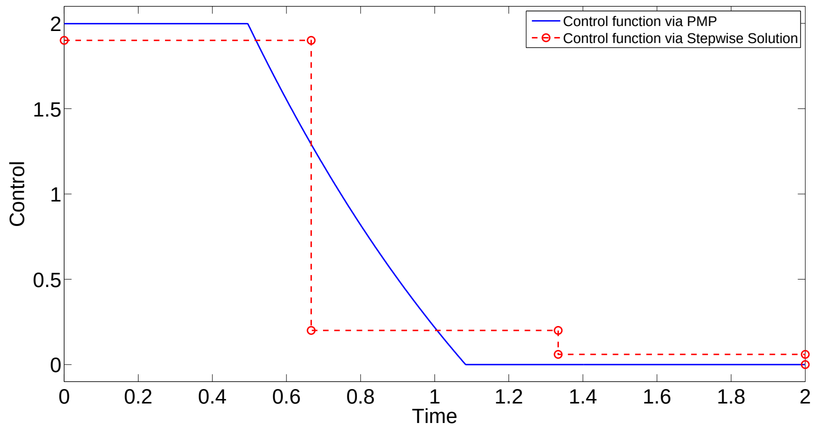

FIGURE 1. Optimal control obtained by using PMP (solid) and the stepwise method (dashed).

Figure 2 shows the optimal stepwise controls obtained by using GA, SA, and PS. Table 1 and Figure 2 summarize the results in this case. Note that, in this table, the GA and SA are run for 20 times and the best result is reported, while PS is run only once since it is not a meta-heuristic.

Method	Final cost
Pattern search	0.01430542
Simulated annealing	0.01430682
Genetic algorithm	0.01435889

TABLE 1

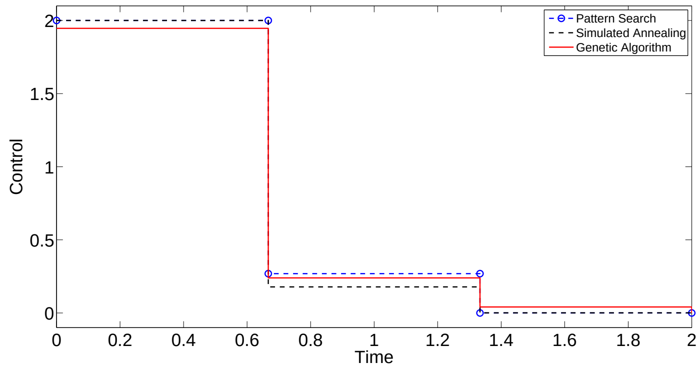

FIGURE 2. Optimal controls obtained by using GA, SA, and PS.

It is expected that increasing the number of the steps used in stepwise method leads to more optimal controls. The results obtained by applying 5-step function are summarized in Table 2 and Figure 3. Comparing Tables 1 and 2 shows that increasing the number of steps from 3 to 5 leads to decreasing the cost function in all cases which coincides with our expectations.

Method	Final cost
Pattern search	0.01428399
Simulated annealing	0.01430531
Genetic algorithm	0.01431998

TABLE 2

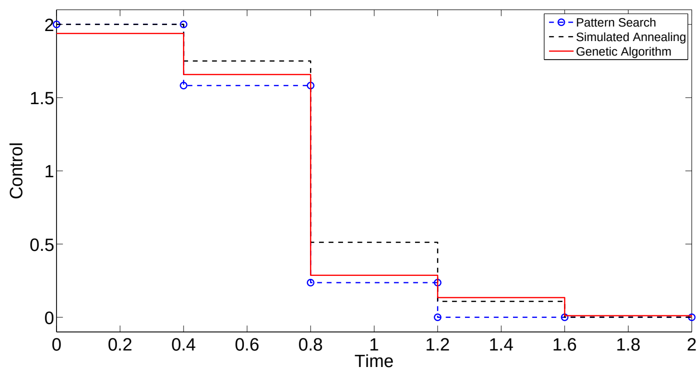

FIGURE 3. 5-step optimal controls (with fixed step size) obtained by using GA, SA, and PS.

3. Stepwise Method with Variable Step-size

In the previous section, we divided the interval into equal parts. Here, in order to arrive at better optimal controls, we let the optimization method decide about the width of subintervals. We reconsider the introductory example presented in the previous section. In dealing with this problem, instead of dividing the interval $[0,2]$ into equal subintervals $[0,2/3]$, $[2/3,4/3]$ and $[4/3,2]$, we divide it into $[0,a]$, $[a,b]$ and $[b,2]$, and let the optimization method find the optimal values of a and b such that $b > a$. Table 3 shows the value of the cost function for each optimization algorithm (in this table GA and SA are run 20 times and the best result is reported, while PS is run only once since it is not a meta-heuristic). The corresponding optimal intervals and optimal controls are presented in Table 4 and Figure 4, respectively. Note that the values obtained for the cost function in Table 3 are considerably smaller than the value obtained by PMP, which shows the advantage of the proposed stepwise method.

Method	Final cost
Pattern search	0.01256629
Simulated annealing	0.01334206
Genetic algorithm	0.01291203

TABLE 3

Method	Subintervals	control value
Pattern search	[0,0],[0,1],[1,2]	(0,2,0)
Simulated annealing	[0,0.0036],[0.0036,0.9738],[0.9738, 2]	(1.6336,1.8345,0.5623)
Genetic algorithm	[0,0.0034],[0.0034,0.9027],[0.9027,2]	(0.7718,1.9087,0.1524)

TABLE 4

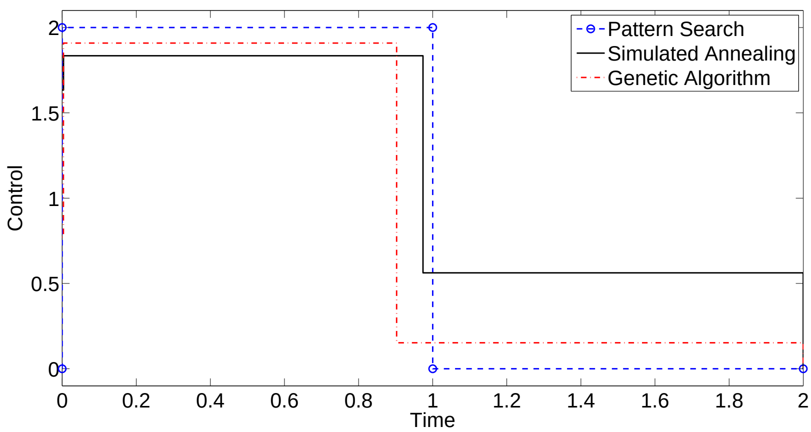

FIGURE 4. 3-step optimal controls (with variable step size) obtained by using GA, SA, and PS. Note that the fist step is very small in all cases.

4. Application of the Stepwise Method to Real-world Models

As mentioned before, there are some limitations such as continuity with respect to time for admissible controls in PMP. Such limitations are really restricting in practice, since we are often not able to change the value of the control function at every moment of time. Instead, one prefers to change the value of control only at several distinct moments of time. For example, when we want to make a decision about resource allocation in epidemiological models, we cannot alter our strategy in short periods of time. The reason is that changing the vaccination rate or prevention strategy often imposes heavy costs. An analogous problem occurs in optimal control of the treatment of diseases through the use of drugs. Thus, it seems that the stepwise method is a reasonable way to deal with certain real-world applications without facing the limitations of PMP. In the following examples, we apply the stepwise method to some real-world problems and compare the results with those obtained by using the classical PMP method.

4.1. Example: Chemotherapy

Optimal control methods are useful for optimal control of chemotherapy. For example, Renee Fister et al. [3, 2] studied different cell-kill models of chemotherapy. They characterized an optimal control strategy which minimizes the cancer mass and the cost of the total amount of drug applied. We apply the stepwise method to one of their models. The problem is

$$\min_{u} \int_0^T a(N(t) - N_d)^2 + bu^2(t)dt$$

subject to,

$$N'(t) = rN\ln\left(\frac{1}{N}\right) - u(t)\delta N(t)$$

$$N(0) = N_0, \quad u(t) \geq 0.$$

The parameters in this model are:

- $N(t)$: the normalized density of the tumor at time t,
- r: the growth rate of the tumor,
- δ: the magnitude of the dose,
- $u(t)$: the time dependent pharmacokinetics of the drug,
- N_d: the desired tumor density.

Without loss of generality, we perform our optimization assuming $r = 0.1$, $a = 3$, $b = 1$, $\delta = 0.45$, $N_d = 0$, $N_0 = 0.975$, and $T = 20$. Figure 5 shows the tumor density and the corresponding optimal control strategy obtained by using the PMP method. The optimal control obtained by using our stepwise method (with 5 fixed steps) is shown in Fig. 6. The final cost of PMP and the 5-step stepwise method is equal to 10.7758 and 10.8666, respectively. As it is observed, the final cost of the proposed method is fairly close to PMP, while it has the advantage of being constant at each step and can be applied much easier in practice.

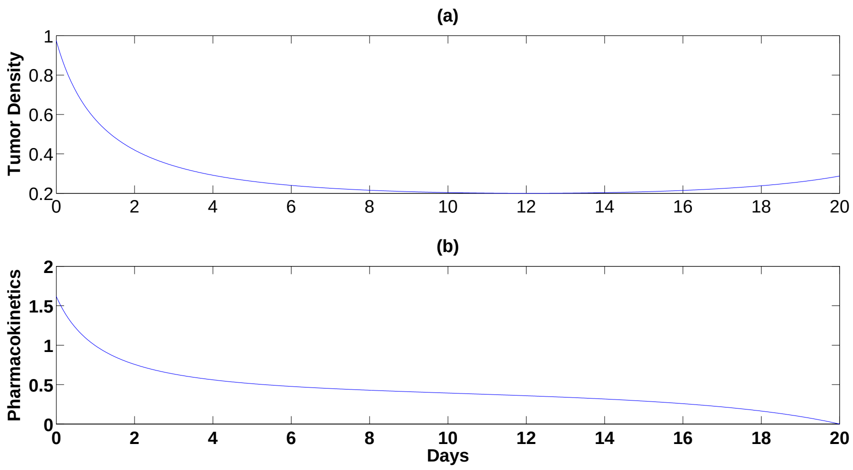

FIGURE 5. (a) Tumor density, (b) the optimal control obtained using PMP method.

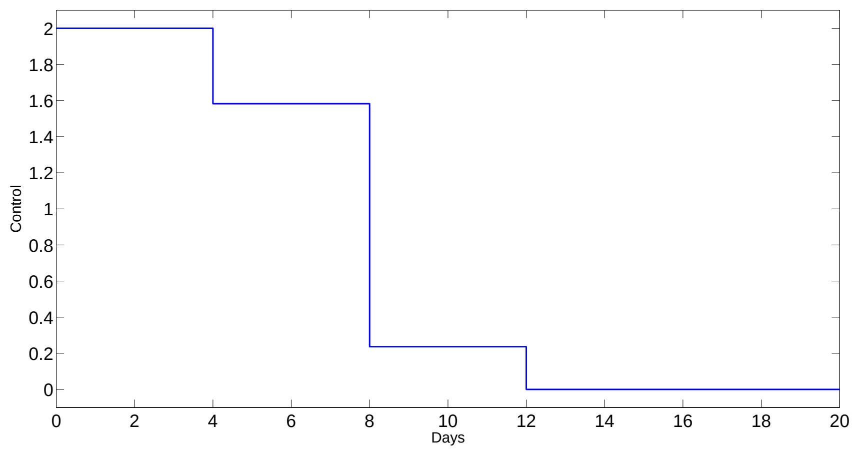

FIGURE 6. The 5-step optimal control (with fixed step size) obtained using the proposed stepwise method.

4.2. Example: Differential Susceptibility and Differential Infectivity (DSDI) model

Based on [4], we develop an optimal control formulation of the DSDI model with two groups of susceptible and two groups of infected individuals [5]. The reason for proposing the idea of dividing the susceptible and infected population into two subgroups is that, in many diseases, the pattern of spreading the disease is different for male and female, children and adults, addicted and nonaddicted, and so on. Define the groups S_1 and S_2 and suppose that the individuals in different groups have different susceptibility, whereas the susceptibility is homogeneous in each group based on its inherent susceptibility. The infected community is subdivided into two subgroups, I_1 and I_2. The following parameters appear in our proposed model:

- μ: natural death rate,
- ν_i: the rate at which infectives in I_i are removed or become immune,
- δ: disease-induced mortality rates for the infectives,
- λ_i: The rate of infection for susceptibles in group S_i $(i = 1,2)$.

The infectivity rate λ_i is given by $\lambda_i = r\alpha_i \sum_{j=1}^{2} \beta_j I_j$, where β_i is the transmission probability per contact and r is the number of contacts of an individual per unit of time. The following system of ODEs, which also includes the controls, is proposed in this paper for modelling the system.

$$\begin{cases} S_1{}' &= \mu(p_1 S^0 - S_1) - \lambda_1 S_1(1-u_1) \\ S_2{}' &= \mu(p_2 S^0 - S_2) - \lambda_2 S_2(1-u_2) \\ I_1{}' &= q_{11}\lambda_1 S_1(1-u_1) + q_{21}\lambda_2 S_2(1-u_2) - (\mu+\nu_1+u_3)I_1 \\ I_2{}' &= q_{12}\lambda_1 S_1(1-u_1) + q_{22}\lambda_2 S_2(1-u_2) - (\mu+\nu_2+u_4)I_2 \\ R' &= (\nu_1+u_3)I_1 + (\nu_2+u_4)I_2 - (\mu+\delta)R \end{cases} \tag{3}$$

The control functions $u_1(t)$, $u_2(t)$, $u_3(t)$ and $u_4(t)$ have to be bounded on $[0,1]$ and Lebesgue integrable. $u_1(t)$ and $u_2(t)$ denote the time dependent efforts (i.e., the prevention strategy) on the susceptible individuals in S_1 and S_2, respectively, to reduce the number of individuals that may be infectious. Similarly, the control functions $u_3(t)$ and $u_4(t)$ denote the time dependent efforts for treatment of infected individuals in I_1 and I_2, respectively. The objective functional to be minimized is considered as

$$J(u_1,u_2,u_3,u_4) = \int_0^T (AI_1^2 + BI_2^2 + Cu_1^2 + Du_2^2 + Eu_3^2 + Fu_4^2)dt, \tag{4}$$

where A, B, C, D, and E are adjustment weights. The optimization goal is to find the optimal control set $(u_1^*,u_2^*,u_3^*,u_4^*)$ such that

$$J(u_1^*,u_2^*,u_3^*,u_4^*) = \min\{J(u_1,u_2,u_3,u_4) | (u_1,u_2,u_3,u_4) \in U\}$$

where $U = \{(u_1,u_2,u_3,u_4)|\ u_i \text{ measerable}, 0 \leq u_i \leq 1, t \in [0,T], i = 1,2,3,4\}$ is the control set. The values of the parameters used in model are $S^0 = 1$, $\delta = 0$, $\mu = .012$, $r = 25$, $p_1 = 0.5$, $p_2 = 0.5$, $S_1(0) = 0.47$, $S_2(0) = 0.47$, $I_1(0) = 0.02$, $I_2(0) = 0.04$, $R(0) = 0$, $\alpha_1 = 0.05$, $\alpha_2 = 0.2$, $\beta_1 = 0.2$, $\beta_2 = 0.06$, $\nu_1 = 0.15$, $\nu_2 = 0.6$, $q_{11} = 0.9$, $q_{12} = 0.1$, $q_{21} = 0.1$, $q_{22} = 0.9$,$A = 3$, $B = 3$, $C = 0.002$, $D = 0.002$, $E = 0.002$, $F = 0.002$, $T = 1000$. Figure 7 shows the optimal controls calculated using the PMP method, which lead to the cost function value 0.1059. Figure 8 shows the optimal controls calculated using the 3-step stepwise method, which lead to the cost function value 0.11107136.

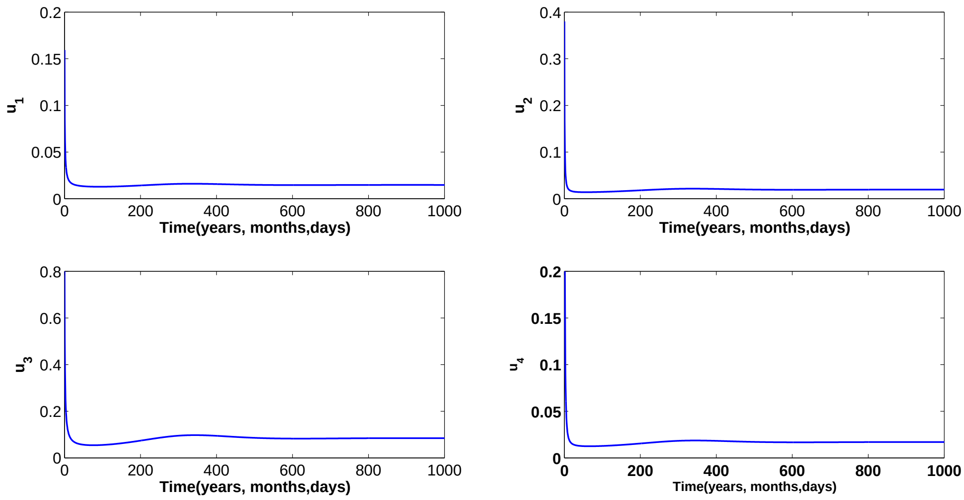

FIGURE 7. Optimal controls calculated for the DSDI model via PMP.

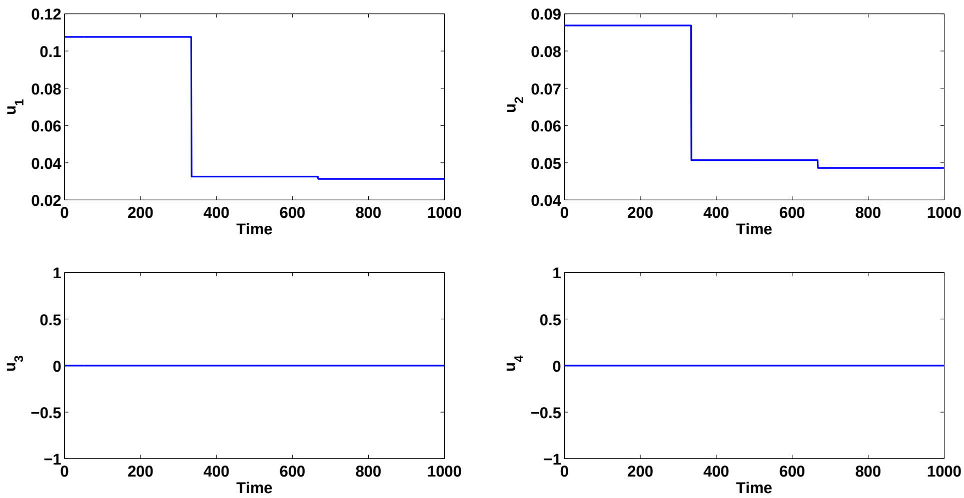

FIGURE 8. Optimal controls calculated for the DSDI model via 3-step stepwise method (using PS algorithm).

5. Convergence

One important point in numerical methods is the convergence of an algorithm and its rate. In this paper, the stepwise method is proposed in contrast to a forward-backward sweep method (used in PMP) for the numerical solution of optimal control problems. The convergence of the forward-backward sweep method and its rate has already been discussed in [9]. In heuristic and meta-heuristic algorithms, the convergence rate is often measured by counting the number of function evaluations, i.e., the number of recalls of the main (cost) function. Hence, in this case the structure of the cost function J is not really important when evaluating the computational cost of the algorithm. In contrary, in the forward-backward sweep method, the cost function has an important role in the structure of the algorithm. In fact, the forward-backward sweep method does not work based on function calls, and consequently, it is not meaningful to compare the performance of forward-backward sweep method and the stepwise method. Hence, in the following we only present the rate of convergence of the stepwise method for the introductory example (with 3-step fixed and 3-step variable step sizes) based on the number of function evaluations when different algorithms are applied. The results are presented in Figures 9 and 10. Note that similar to previous simulations, in these figures the GA and SA are run 20 times and the average results are presented.

The convergence rate of this method depends on the convergence rate of the heuristic or meta-heuristic method being used. From our experience, the differential evolution (DE) method appears to yield satisfying convergence rates in various examples.

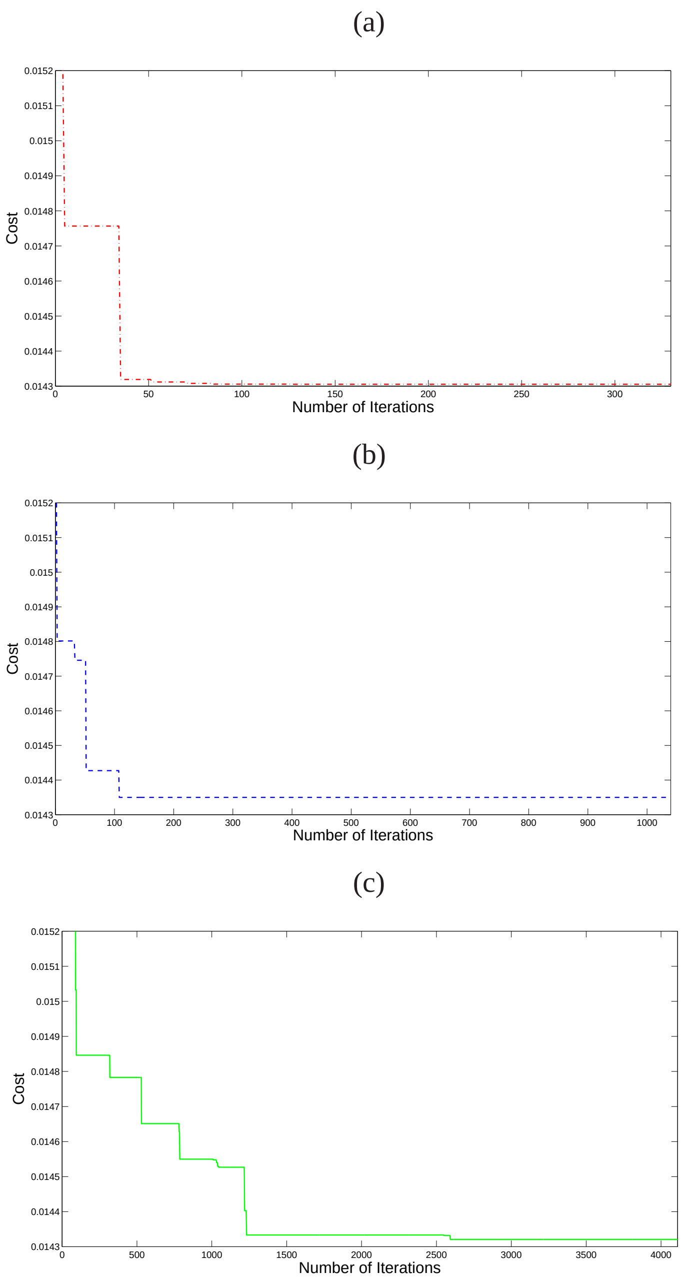

FIGURE 9. The rate of convergence of the fixed endpoint stepwise method versus iteration number, (a) GA, (b) SA, (c) PS.

6. Conclusion

We introduced the stepwise method for optimal control problems. This method can replace the classical PMP method when dealing with certain real-world problems. The proposed method is applied to several problems and the results are satisfactory.

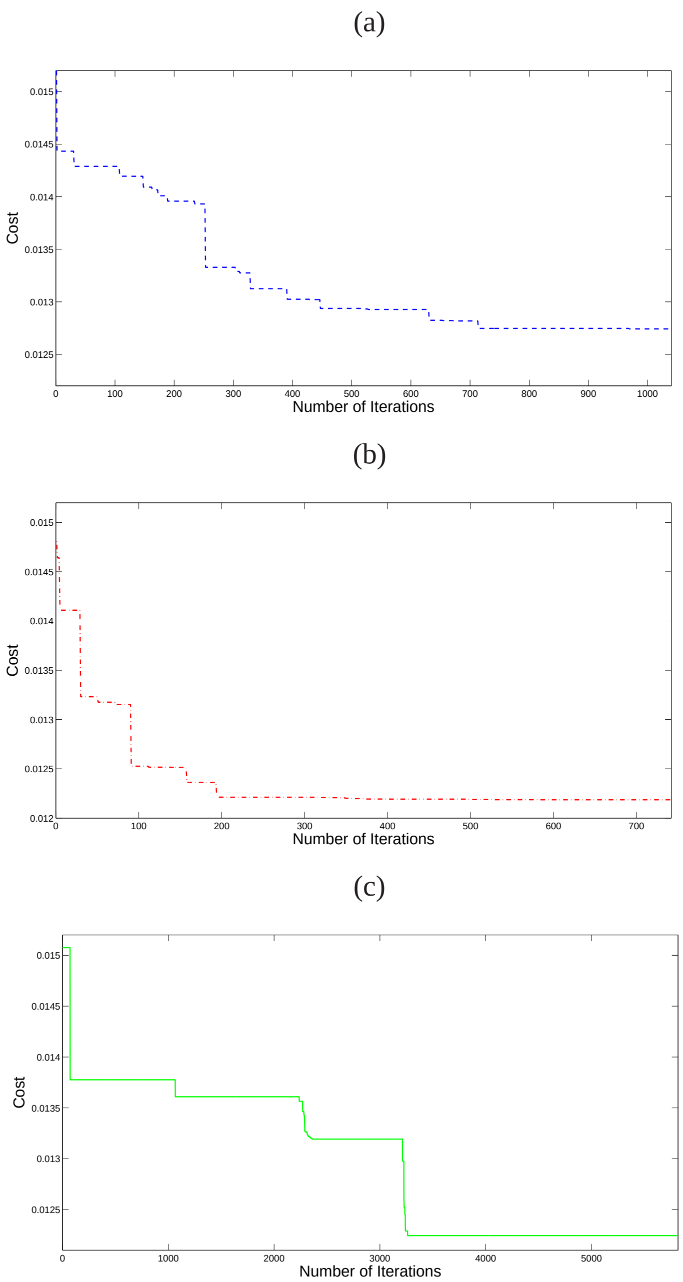

FIGURE 10. The rate of convergence of variable endpoint stepwise method versus iteration number, (a) GA, (b) SA, (c) PS.

7. Acknowledgement

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