Proceedings of the 14th KACC, Octorber 1999

Two Phase Algorithm in Optimal Control

° Chungsik Park*, and Tai-yong Lee**

Dept. of Chemical Engineering, KAIST, 373, Kusung-dong, Yusong-gu, Taejon, 305-701 Korea
*(Tel : 82-42-869-3966; Fax : 82-42-869-3910 ; E-mail: cspark@nectar.kaist.ac.kr)
**(Tel : 82-42-869-3926; Fax : 82-42-869-3910 ; E-mail: tylee@nectar.kaist.ac.kr)

Abstract

Feed rate in the fed-batch reactor is the most important control variable in optimizing the reactor performance. Exact solution can be obtained only for limited cases of simple reactor. The complexity of the model equations makes it extremely difficult to solve for the general class of system models. Evolutionary programming method is proposed to get the information of the profile types, and the final profile is calculated by that information. The modified evolutionary programming method is used to get the more optimal profiles and it is demonstrated that proposed method can solve a wide range of optimal control problems.

1. Introduction

In fed-batch reactors, optimal control of the feed rate is crucial to maximize the yield of the valuable product. In order to maximize the desired product quantity or minimize the process time, there have been suggested various ways to find the profiles of the time-dependent feeding rate. These optimal control problems are notoriously difficult to solve especially when the system dynamics are nonlinear and the control and/or state variables are constrained. Therefore, most existing methods can only solve restricted ranges of problems. Many authors have used the Pontryagin's maximum principle to solve these optimal control problems, but this approach is restricted to a problem with simple system dynamics.

One approach to modify maximum principle is the method of sequential strategies. Cuthrell and Biegler [1] presented a simultaneous optimization and solution method based on orthogonal collocation and sequential quadratic programming. Chen and Hwang [2] proposed a method based on piecewise constant control parameterization to convert the original problem into a sequence of finite dimensional nonlinear programming problems that were solved by a sequential quadratic programming algorithm. Luus [3] has improved the previous methods by the use of penalty function approach together with iterative dynamic programming methods to solve the constrained optimal control problems. Dadebo and McAuley modified this method that may be useful in obtaining feasible control profiles [4]. An alternative approach, which does not use maximum principle, is termed direct optimization methods. These methods are based on the parameterization of the control variables via variable length piecewise linear polynomials and the solution of the resulting nonlinear programming problem. But, it is not easy to find and update appropriate polynomials during iterations. So, Banga [5] suggested the stochastic algorithm combined with random search method. But because of the random search, when the number of parameters to be determined increases, it makes the solving time explosively increase.

Recently genetic algorithm (GA) and evolutionary programming (EP) have been widely accepted as a new optimization technique, which is robuster than the above-mentioned algorithms [6,7]. Muhlenbein [8] and Scott [9] use GA to find the function optimum. They combined parallel GA with the deterministic methods, and could get better performance than those of the deterministic only methods. In the present study, EP is used combined with spline method (EPS) which is similar to parameterization method in Banga. In this study, smooth curve forms are added as a feasible solution by spline method and compete with others to find more accurate and fast search. It will be demonstrated that proposed method, EPS plays a good alternative role in optimal control of fed-batch reactors.

2. Optimization Problems

The following general form expresses the model equations considered

$$\frac{d\underline{x}}{dt} = \underline{a}(\underline{x}) + \underline{b}(\underline{x})u, \qquad 0 \le t \le t_f \tag{1}$$

Here, $\underline{x}$ is the n-dimensional state variable vector and u is a scalar control variable. The objective function is given by J and J should be maximized with respect to $u(t)$.

$$J[u(t)] = G[\underline{x(t_f)}] \tag{2}$$

The control variable $u(t)$ is constrained as following.

$$u_* \le u(t) \le u^* \tag{3}$$

3. Maximum Principle Method

In order to solve the problem by maximum principle methods, Hamiltonian is defined as.

$$H = \underline{\lambda}^T \{\underline{a}(\underline{x}) + \underline{b}(\underline{x})u\} \tag{4}$$

Here, $\underline{\lambda}$ is the Lagrange multiplier vector of time-dependent function defined by

$$\frac{d\underline{\lambda}}{dt} = -\frac{\partial H}{\partial \underline{x}} = -\underline{\lambda}^T(\underline{a}_x + \underline{b}_x u) \qquad \lambda_i(t_f) = \frac{\partial G}{\partial x_i} \qquad (5)$$

The control $u(t)$ maximizes the objective J only if the following equation is true for unconstrained portion of the path, where the Hamiltonian H is maximized along the constrained portion of the path.

$$\frac{\partial H}{\partial u} = 0 = \underline{\lambda}^T \underline{b}(\underline{x}) \qquad (6)$$

The optimal profile $u(t)$ is obtained to satisfy the following constraints.

1. $u = u^*$ if $\frac{\partial H}{\partial u} > 0$,
2. $u = u_*$ if $\frac{\partial H}{\partial u} < 0$, or
3. $u = u_s(t)$ if $\frac{\partial H}{\partial u} = 0$

The gradient of Hamiltonian is calculated by eq. (1), (5) and (6). In addition to that, the type of profile is different only with initial condition of the system. Lim [10] showed that various profile types could exist in the same system equation. These mean that physical insights are needed to solve these kinds of problems.

Since the Hamiltonian functional is linear with respect to the control variable, $u(t)$, the optimal problem of this fed-batch fermentation process is a singular control problem. Generally it involves bang-bang control and state feedback control of singular arcs [11]. The maximum principle of Pontryagin is used to solve this problem, but fails to provide a solution for singular arcs. Because no useful sufficient conditions for optimality of singular arcs are available, and in some cases a singular solution may not be unique. It is not surprising that most existing methods may fail to solve many of these problems. Therefore, several alternative methods have been proposed which are based on the parameterization of the control variables via variable length piecewise linear polynomials.

4. Evolutionary Programming with Spline Method (EPS)

For the singular control problem, optimal control profile is expected to be a smooth curve. To represent the smooth curve, spline method is added to EP method. The new smooth feasible solutions are made from the best solution in the iteration procedure using spline fitting, and compete with the others to survive. This evolutionary programming with spline method (EPS) enables faster convergence and gets smoother curves. Fig. 1 shows the procedure. Spline fitting is made from (a) to solution like (b), and new solution is added to the iteration procedure as (c). One iteration procedure of EPS is shown in the Fig. 2. When the new generation is made from the evolutionary programming method, spline method is applied to the populations of the new generation, and prepares the next generation.

This EPS method often shows slow convergence near the optimum, so two phase algorithm is suggested. IF EPS reached near optimum, then the second algorithm is triggered. The content of the two phase algorithm is the following:

Phase I: Apply EPS methods to find optimal profile.

Phase II: Check the profile. If profile reached lower or upper bound of the $u(t)$, the value is fixed as that constraint in that interval. For the singular interval, new search region is reset as within 20% of the result of Phase I.

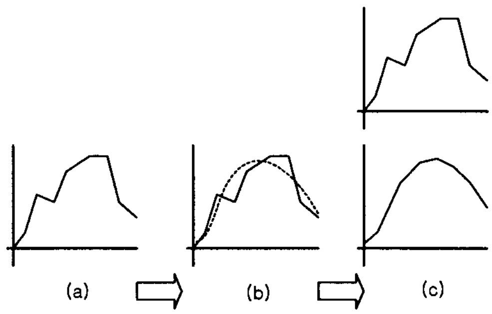

Fig. 1: The procedure of EP with spline fitting

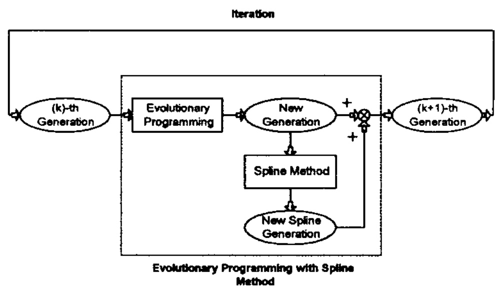

Fig. 2: The block diagram of EPS

5. Results and Discussion

In this section, two types of optimal control problems are introduced. The first case study has simple model equation and analytic solution is available. For this problem the results of EP and EPS methods are compared to that of exact solution by analytic method. The other case study is fed-batch reactor for ethanol production and many researchers used various methods to solve optimal control problems. EPS method is applied to these case studies as a more general solver and the results are compared to those of others.

Case Study 1

Consider the following reactor model equations:

$$\frac{dx_1}{dt} = -(u + 0.5u^2)x_1, \qquad x_1(0) = 1$$

$$\frac{dx_2}{dt} = ux_1, \qquad x_2(0) = 0$$

$$u_* \le u(t) \le u^*$$

where $u_* = 0$ and $u^* = 4$. The objective is to find $u(t)$ maximizing $x_2(t_f)$ when $t_f = 1$, and the objective function is expressed by $J[u(t)] = x_2(t_f)$. In this problem, the exact solution can be obtained based on the maximum principle as

$$u(t) = \begin{cases} u_s(t), & 0 \le t \le t^* \\ u^*, & t^* \le t \le 1 \end{cases}$$

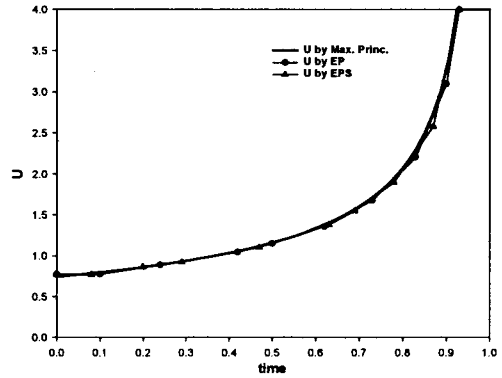

Fig. 3: Control variable $u(t)$ using the result of maximum principle, EP and EPS for case study 1

Fig. 3 shows the results by analytic method and those by EP and EPS. The solid line represents control variable $u(t)$ of the exact solution and the solid line with circular or triangular symbols represent the results of EP and EPS by discretizing $u(t)$ into 10 intervals. In this figure, result of maximum principle and those of EP and EPS are indistinguishable. The population size is 70 and GENOCOP starts from a random population. The performance indexes of EP and EPS are plotted in Fig. 4 as the iteration proceeds. EP combined with spline method shows the faster convergence feature than plain EP, and as a result of splining, we can get smooth curve. These EP and EPS solutions are obtained after 200 generations and it takes 30 seconds on HP 710, to reach the 99% of the analytic solution by EPS.

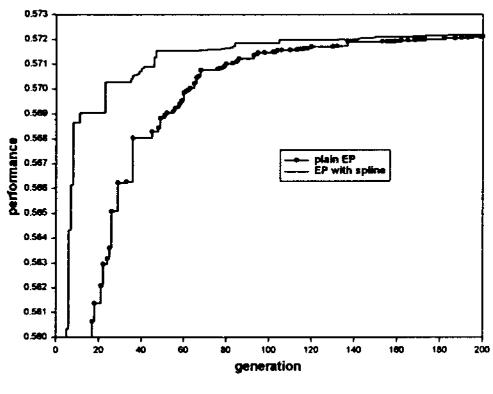

Fig. 4: The plot of generation vs. performance index for case study 1

In this section, EPS gives the control profile without the discrimination between the singular control interval and u^* control interval. Phase I is enough to this case. EPS, taking the control action each interval, gives the $u(t)$ profile identical to the results by maximum principle, even when the control action may exist on the constrained boundary. The time needed to get the profile by EPS method is reasonable to apply to the optimal control problems.

Case Study 2

Fed-batch reactor for ethanol production is described by the following equations.

$$\frac{dx_1}{dt} = g_1 x_1 - u\left(\frac{x_1}{x_4}\right)$$

$$\frac{dx_2}{dt} = -10 g_1 x_1 + u\left(\frac{150 - x_2}{x_4}\right)$$

$$\frac{dx_3}{dt} = g_2 x_1 - u\left(\frac{x_3}{x_4}\right)$$

$$\frac{dx_4}{dt} = u$$

where

$$g_1(\underline{x}) = \left(\frac{0.408}{1 + x_3/16}\right)\left(\frac{x_2}{0.22 + x_2}\right)$$

$$g_2(\underline{x}) = \left(\frac{1}{1 + x_3/71.5}\right)\left(\frac{x_2}{0.44 + x_2}\right)$$

Here, x_1, x_2, x_3 are the cell mass, substrate and ethanol concentrations (g/L), respectively, and x_4 is the volume (L). The optimal control problem is to maximize the yield of ethanol, $J(u) = x_2(t_f)x_4(t_f)$, using the feed rate $u(t)$ as the control variable. The initial conditions are $\underline{x}(t_0) = [1, 150, 0, 10]^T$.

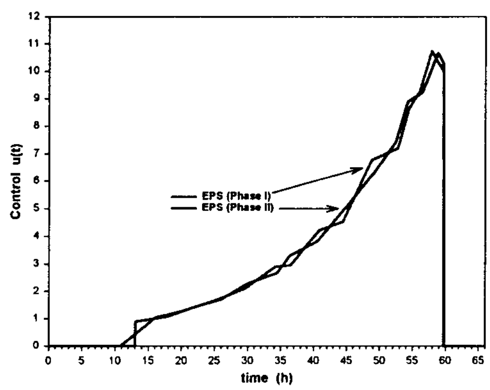

Fig. 5: Sate variable profile by the result of EPS for case study 2

Table 1: The results of other researchers for case study 2

Literature	Reformulation	Treatment of t_f	Initial guess	t_f	Performance
Chen and Hwang (1990)	Necessary	Sequential	User-supplied	54.0 h	20073
Luus (1993)	Necessary	Sequential	Chen and Hwang's Optimum	54.0 h 62.9 h	20430 20841
Banga (1997)	not necessary	Sequential	Random	54.0 h 62.9 h	20423 20715
Present study	not necessary	Simultaneous	Random	62.7 h	20842

To solve this problem, $u(t)$ is composed of 20 piecewise linear lines and final time t_f is not fixed. The result of proposed EPS method, Phase I and Phase II algorithms are shown in Fig. 5. At the end of Phase I, we can guess that this problem has the optimum profile as the minimum-singular-minimum or singular-minimum type. Initial part of the optimal profile is regarded as minimum type, and Phase II algorithm is started to find the smooth curve and switching time where the type change occurs.

For the ethanol production model in this section, EPS found a simple and good profile to use in industry. The control profile $u(t)$ gives a performance index of $J = 20842$ with the final time $t_f = 62.7$. Table 1 shows the results of other researchers on this problem. The result of Luus [3] showed similar performance to that of present study. But, Luus started this problem with the initial control profiles close to the global optimum. Luus used Chen's [2] results as an initial guess and modified the performance index as penalty function, and thus his algorithm depends heavily on the initial guesses of the decision variables. On the contrary, proposed EPS method starts without any *a priori* knowledge, and exhibits good performance, and need not change the problem formulation.

6. Conclusion

Control law nonlinearity is increased by the interaction of many factors: the process system, the performance objective, and the constraints. Besides, the $u(t)$ profile is different only with different initial conditions. So, other deterministic algorithms often fail. Thus, control parameterization methods are widely used, and to modify the set of time and profile, EP method is proposed. To enhance the performance and to get smoother curves than plain EP, adding the spline method modifies EP. These techniques get better performances than other control parameterization methods.

This method has the advantages that no adjoint equations need to be solved, and thus it does not require the information of switching times and the shape of optimal control. In the absence of physical feelings for the shape of optimal control, piecewise linear polynomials are used to represent the optimal control profile, and the optimization performed with respect to the profile. Several starting points are always used to ensure that the algorithm has converged to the global optimum, because multiple optima are possible in the optimal control problems.

In the present study, EPS is used to find optimal control profile for biological fed-batch reactors. The approach is powerful and easy to implement since it is rarely affected by the characteristic of reactor model and initial conditions. EPS does not require to be tailored to suit each optimal control problem, and one algorithm tackles all. In particular, the only real input required of the user is the model equation and performance index function.

Acknowledgement

This work was supported by the Korea Science and Engineering Foundation (KOSEF) through the Automation Research Center at POSTECH.

References

[1] J. E. Cuthrell, and L. T. Biegler, "Simultaneous optimization and solution methods for batch reactor control profiles", *Comput. Chem. Eng.*, **13**, pp. 49-62, 1989

[2] C. T. Chen, and C. Hwang, "Optimal on-off control for fed-batch fermentation processes", *Ind. Eng. Chem. Res.*, **29**, pp. 1869-1875, 1990

[3] R. Luus, "Application of dynamic programming to differential algebraic process systems", *Comput. Chem. Eng.*, **17**, pp. 373-377, 1993

[4] S. A. Dadebo and K. B. McAuley, "Dynamic optimization of constrained chemical engineering problems using dynamic programming", *Comput. Chem. Eng.*, **19**, pp. 513-525, 1995

[5] J. R. Banga, A. A. Antonio, R. Paul Singh, "Stochastic dynamic optimization of batch and semicontinuous bioprocesses", *Biotechnol. Prog.*, **13**, pp. 326-335, 1997

[6] D. E. Goldberg, *Genetic Algorithms in Search, Optimization and Machine Learning*, Addison-Wesley, 1989

[7] Z. Michalewicz, *Genetic Algorithms + Data Structure = Evolution Programs*, 2nd ed., Springer-Verlag, 1994

[8] H. Muhlenbein, H. Schomisch, and J. Born, "The parallel genetic algorithm as function optimizer", *Parallel Comput.*, **17**, pp. 619-632, 1991

[9] G. V. Scott, and D. Whitley, "Serial and parallel genetic algorithms as function as function optimizer. In: Forrest, S. (Ed.)", *Proc. 5th Int. Conf. on Genetic Algorithms*, San Mateo, CA: Morgan Kaufmann, 1993

[10] H. C. Lim, Y. J. Tayeb, J. M. Modak, and P. Bonte, "Computational algorithms for optimal feed rates for a class of fed-batch fermentation: Numerical results for penicillin and cell mass production", *Biotech. and Bioeng.*, **28**, pp. 1408-1420, 1986

[11] A. E. Bryson, Jr., and Y. C. Ho, *Applied Optimal Control*, John Wiley & Sons, 1975