

ADAPTIVE STEP SIZE INTEGRATION:
IT SEEMED LIKE SUCH A GOOD IDEA

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Abstract

Adaptive Step-Size Integration (ASSI) refers to a process of numerical integration in which the (n+1)-st integration step size h(n+1) is determined at the end of the n-th step without a trial solution and without computing the local truncation error. By analogy with discrete-data control systems which feature adaptive sampling intervals, the computation of the interval h(n+1) is based on the magnitude of the system sensitivity functions. For example, the influence of the interval size on the i-th state variable is given by the sensitivity function $\partial x/\partial h$. While adaptive step size control systems have been investigated in the past, ASSI has received very little attention.

This paper reviews the theory of ASSI in the light of recent results on the selection of the optimum criterion functions for the determination of the integration interval at each step. Since previous attempts to evaluate ASSI have been tested on very simple systems, a fourth order differential equation is used as a benchmark problem in the paper. The resulting fourth order system is solved by ASSI using three different step size "control laws" (adjustment algorithms) with Euler integration. For comparison the system is also integrated using a Runge-Kutta fixed step formula. The results show a slight advantage in total execution time for one of the ASSI algorithms. However, the results are difficult to generalize. Various limitations of the results are discussed. The paper concludes by indicating that the results are inconclusive, and that it still remains to be seen whether ASSI is a "good idea."

Introduction

Variable step size algorithms for the numerical solution of ordinary differential equations generally require either trial solutions or estimates of the local truncation error. Multiple step algorithms such as predictor-corrector methods utilize a sequence of trial values which can be used to adjust the step size until an appropriate error criterion is met. Other variable step size algorithms estimate the truncation error at each step in the integration process. Based on this estimate, the integration step size can then be doubled or cut in half. A review and analysis of many of these methods can be found in the references [1-3]. All the above mentioned algorithms share one common feature: they calculate a trial vector on the basis of which step sizes can be determined to fit predetermined accuracy requirements. By contrast, adaptive step size integration (ASSI) is defined here as a process of numerical integration in which the (n+1)-st integration step size h(n+1) is determined at the end of the n-th step without a trial solution and without computing the local truncation error. Rather, the determination of the step size is made on the basis of the sensitivity of the solution to changes in the step size. Hence, ASSI requires the evaluation of "sensitivity functions" [4], and the incorporation of these functions into appropriate step size adjustment subroutines.

Adaptive step size integration is analogous to the process of adaptive sampling in sampled data control systems. In a series of papers beginning in 1962 [5-13] various authors have investigated the performance of sampled data control systems with a

sampling interval dependent on some function of the state variables. While most of the above mentioned references are somewhat heuristic, other papers have investigated optimal control systems with state dependent sampling [14, 15]. In general, in a system of the type illustrated in Figure 1

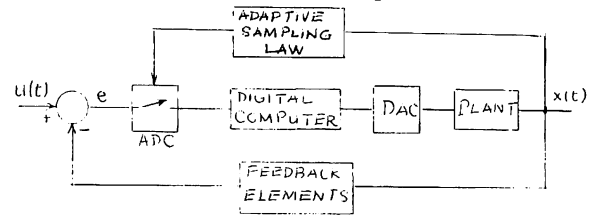


Fig. 1

it can be demonstrated that the use of state-dependent sampling can result in a requirement for fewer samples for a given accuracy criterion than that obtainable with a fixed sampling interval. Hsia [13] has examined a variety of control laws which have been used in adaptive sampling, and indicated how these could be derived from a general formulation. Among the control laws of interest are the following:

$$T_i = \frac{T_{max}}{G e^{\mu_i} + 1} \quad (1)$$

$$T_i = \frac{A}{G |\dot{e}_i|} \quad (2)$$

$$T_i = \frac{T_{max}}{G |\mu_i| + 1} \quad (3)$$

where T_i is the duration of the i-th sampling interval, T_{max} is the maximum allowable sampling interval, G is a gain constant, and μ_i is the sensitivity of a particular state variable to variations in the sampling interval. It is the control law of Equation (3) which appears to be suited to the problem of adaptive integration.

Adaptive Integration

Consider the block diagram of Figure 2

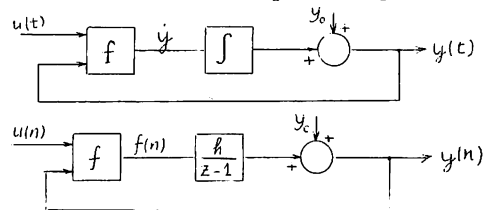


Fig. 2

Figure 2a represents an analog computer solution of the differential equation

$$\dot{y} = f(y, u) \quad (4)$$

while Figure 2b represents the numerical solution of the same equation by means of Euler or rectangular integration formula

$$y(n+1) = y(n) + hf(n) \quad (5)$$

The numerical integration formula is represented by its discrete transfer function [16]. By analogy with Figure 1 it seems reasonable to construct a feedback control law for adjustment of the step size h by means of a control law similar to that in Equation (3). Further, it is intuitively appealing to suggest that when the solution to Equation (4) is highly sensitive to changes

in the step size, h should be small; on the other hand, when the solution is relatively insensitive to changes in the step size, then large steps may be taken with small error penalties. Such a philosophy is embodied in Equation (3), where the sensitivity μ_i is defined by

$$\mu(t_n) \triangleq \lim_{\Delta h \rightarrow 0} \frac{y(t_n, h_n + \Delta h) - y(t_n, h_n)}{\Delta h} \quad (6)$$

or

$$\mu(t_n) = \mu(n) = \frac{\partial y(t_n)}{\partial h} \quad (7)$$

If one applies the definition of the sensitivity coefficient or sensitivity function in Equation (7) to the rectangular integration formula of Equation (5), we can differentiate this expression term by term and obtain

$$\frac{\partial y(n+1)}{\partial h} = \frac{\partial y(n)}{\partial h} + h \frac{\partial f(n)}{\partial h} + f(n) \quad (8)$$

or

$$\mu(n+1) = \mu(n) + h \dot{\mu}(n) + \dot{y}(n) \quad (9)$$

Equation (9) is a sensitivity difference equation [9] which can be solved to obtain the desired sensitivity coefficient for substitution into a control law such as that given by Equation (3). Once μ_{n+1} is found, we can proceed to the calculation of the step size h_{n+1} for the next interval. Note that trial solutions of the difference Equation (5) are not required. In general, for an n -th order system there will also be an n -th order system of sensitivity equations with respect to the parameter h .

A large number of control laws were investigated. The best results were obtained from the following:

$$h(n) = \frac{1}{G|\mu_{\max}(n)|} \quad (10)$$

$$h(n) = \frac{A}{\sqrt{|\dot{\mu}_1(n)|}} \quad (11)$$

$$h(n) = \frac{h_{\max}}{G\mu_1(n) + 1} \quad (12)$$

$$h(n) = \frac{h_{\max}}{G\mu_1^2(n) + 1} \quad (13)$$

A Test Problem

The combination of the system equations and sensitivity equations represents a nonlinear system of difference equations. Hence, the application of ASSI is highly specific to any particular example problem, and generalization is very difficult. Consider for example the two curves of Figure 3

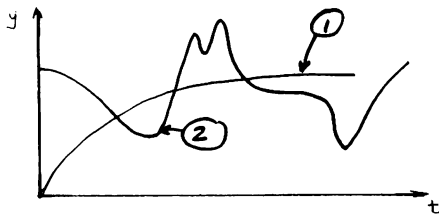


Fig. 3

Curve # 1 is typical of the response of a first order system to a step input. It is intuitively evident that if the solution is discretized, that the variable y will become less and less sensitive to changes in integration step size as the solution proceeds. On the other hand the curve indicated by the number 2 has periods of greater and lesser sensitivity which appear to be related to its slope. The solution of any equation which follows curve 1 can be made to favor adaptive step size integration by simply taking a long enough solution time since as time progresses one can take larger and larger steps without incurring significant errors. For this reason a fourth order differential equation with a known solution was taken as a benchmark problem. The specific equation selected for solution is given by

$$\frac{d^4 y}{dt^4} + a \frac{d^3 y}{dt^3} + b \frac{d^2 y}{dt^2} + c \frac{dy}{dt} + dy = 0 \quad (14)$$

where $a=2.9$, $b=2.7$, $c=0.7$, $d=-0.1$ and the initial conditions are

$$\begin{aligned} y(0) &= .01 & \dot{y}(0) &= 1.001 \\ \ddot{y}(0) &= -1.9999 & \ddot{y}(0) &= 3.00001 \end{aligned}$$

The solution to this equation is given by

$$y(t) = \frac{e^{-t/10}}{100} + te^{-t} \quad (15)$$

For computer solution, Equation (14) is transformed into a system of first order differential equations:

$$\begin{aligned} \dot{y}_1 &= y_2 \\ \dot{y}_2 &= y_3 \\ \dot{y}_3 &= y_4 \end{aligned} \quad (16)$$

$$\dot{y}_4 = -2.9y_4 - 2.7y_3 - 0.7y_2 + 0.1y_1$$

$$y_1(0) = .01 \quad y_2(0) = 1.001$$

$$y_3(0) = -1.9999 \quad y_4(0) = 3.00001$$

where the variables y_1, y_2, y_3 and y_4 represent the variable y and its first, second and third derivatives respectively.

Differentiation of Equation (16) with respect to the step size h , followed by a certain amount of algebraic substitution results in the system of sensitivity equations

$$\mu_1(n+1) = \mu_1(n) + h\mu_2(n) + y_2(n)$$

$$\mu_2(n+1) = \mu_2(n) + h\mu_3(n) + y_3(n) \quad (17)$$

$$\mu_3(n+1) = \mu_3(n) + h\mu_4(n) + y_4(n)$$

$$\mu_4(n+1) = \mu_4(n) + h[-2.9\mu_4(n) - 2.7\mu_3(n) - 0.7\mu_2(n) + 0.1\mu_1(n)] + \dot{y}_4(n)$$

A simplified flow chart for the solution of Equation (16) and (17) is shown in Figure 4

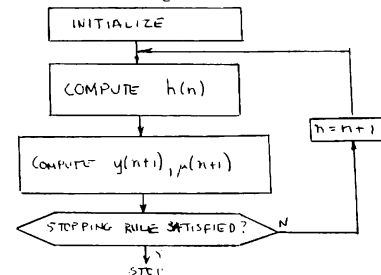


Fig. 4

Note that the following sequence of operations is followed: a) calculation of the sensitivity vector $\mu(n+1)$; b) calculation of the step size $h(n+1)$. (the inequality $h \geq h_{min}$ is included to insure that the program does not result in infinitesimal steps under any circumstances); c) calculation of $y(n+1)$ by any single step algorithm. While Euler integration was used in this study, any single step algorithm can be used. However, multiple step algorithms such as predictive-corrective formulas can not be used because of the nonuniform size of h . A second order Runge-Kutta algorithm was chosen for this test case as a reference digital solution. In order to have a meaningful comparison, all cases were adjusted to have the same mean square per step error when compared to the known analytical solutions. A comparison of execution times and the number of integration steps taken in the same solution interval for several control laws and the Runge-Kutta fixed step-size formula are given in Table 1. The three control laws for which results are included are representative of a number of other control formulas which were investigated. It can be concluded from an investigation of this table and other similar results that those control laws which were based on the sensitivity function μ_1 (i.e. a partial derivative of y_1 with respect to h) did not yield any significant improvement over the fixed step size R-K formula. An attempt to search among the four sensitivity coefficients for the largest numerical value at each step in general produced considerably worse results in the sense that more steps were required and a longer solution time was required to obtain the same first step error. Interestingly enough, the best results were obtained from control laws which were based on the rate of change of a sensitivity function as shown in the second column of Table 1 which indicates a saving of approximately 20%.

Discussion of Results and Conclusions

Unfortunately, the results of Table 1 are specific to the test problem being investigated. On the basis of this problem alone, it can not be stated whether any of the control laws investigated here will in fact result in reductions of computer time in integration of any other differential equations. Furthermore, the results of Table 1 were obtained by trial and error. In view of the nonlinearity of the system, it is entirely possible that other combinations of the parameters G , β , and h_{min} will yield the same first step mean square error with a problem time $t_{max} = 40$ seconds. The use of an optimization algorithm for the determination of the optimum parameters of the control laws which would yield the best possible match to the known analytical solution was not justified in view of the fact that the results would still not be general, but only specific to this particular problem. A previous paper by Nilsen [17] also raised some reservations about the generality and usefulness of ASSI.

A further difficulty arises from the very fact that the step size is adaptive. This variability means that error analysis is difficult if not impossible. While in the benchmark problem investigated above the accuracy of ASSI can be investigated, in general of course the exact solution of the system being studied is not known and hence the only input a user would have would be that of adjusting the parameters of the control law to see whether a solution with smaller steps would in fact be different from one with larger steps, after making allowances for accumulation of roundoff error.

Furthermore, note that the overhead associated with the calculation of sensitivity functions at least doubles the execution time required for the solution of the differential equation itself. If one uses a better integration formula than the simple rectangular

integration routine used here, this increase in time can be formidable, to say nothing of the additional analysis and precalculation required for the preparation of the system of sensitivity equations.

In summary, adaptive step size integration has been and continues to be an intuitively appealing concept. However, the selection of the optimum control law for ASSI, and general results for its application to realistic problems remain lacking. It is the authors' hope to stimulate further research so that ASSI can be either validated or laid to rest once and for all.

Table 1

Control Law	$\frac{1}{G \mu_{max} }$	$\frac{1}{G\sqrt{\mu_1}}$	$\frac{1}{G\mu_1^2 + \beta}$	R-K 2nd order
Execution time	.81 sec.	.43 sec.	.54 sec.	.55 sec.
Number of steps	127	78	99	101
Largest step taken	1.63	1.81	0.5	.3984
h_{min}	0.2	0.2	0.3	.3984

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