Stepsize Control in Numerical Integration of ODE's

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Abstract

This is the final report of the STU project 88-1611. It describes a project aiming at solving a problem of stepsize control in numerical integration of ordinary differential equations. The problem is analyzed and a new improved stepsize control algorithm is derived. The algorithm is tested through an implementation in the simulation program Simnon.

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1. Introduction

A common way to simulate reality is to use models based on differential equations in combination with a program package for numerical simulation. The program package implements a numerical integration method, and is normally constructed such that the user only supplies the differential equations while the program takes care of everything regarding the integration. This normally works quite well, but there are exceptions. An example from a simulation of a simple control system is show in Figure 1. The oscillating component in the signal to the left is not a part of a true solution of the equations. The accuracy requirements were set to 0.1%, and even though the deviations in the incorrect signal are much larger the simulation program does not succeed in detecting it.

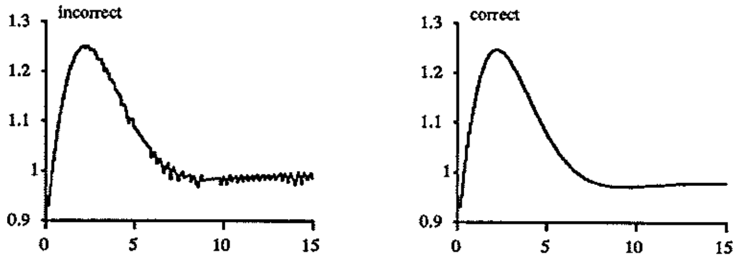

Figure 1. A signal drawn from a simple control system simulation. The oscillatory component, in the signal to the left, is caused by an irregular stepsize sequence. The correct signal, to the right, is obtained by improving the stepsize control algorithm.

The artifact in Figure 1 is caused by the algorithm for stepsize control in the integration method. An integration method calculates the solution to the differential equations at a number of discrete (time)points. The distance between the points is called the stepsize and control the accuracy of the produced solution. Small steps makes the solution accurate but requires a lot of computations. Therefore, the stepsize is normally chosen as large as possible within the accuracy requirements, since that gives an acceptable solution with the least computations. The appropriate stepsize varies along the solution of the differential equations. It is hard for the user to relate a given stepsize to a specific accuracy and therefore one would like a simulation program where the user only prescribes the accuracy and the program chooses a corresponding stepsize.

There are algorithms for stepsize selection but for some differential equations they behave poorly. The symptom is an highly irregular stepsize sequence. The irregularities make the estimation of the error in the produced solution hard, and may result (see Figure 1) in an incorrect solution. In the example above it is not hard to see that something is wrong, but often the discrepancies are more subtle and it is hard for the user to judge the quality of the user.

It is important to solve the stepsize control problem. By improving the stepsize control algorithm, the robustness of the simulation programs is improved.

2. Feedback Control View of Stepsize Selection

A numerical integration method can be viewed as a complicated dynamic system, where the stepsize is the input and the error estimate the output. In the stepsize control algorithm the estimated error is compared with a user-specified tolerance, and the result is used to decide upon the next stepsize. The method can be viewed as a control loop with feedback from the estimated error to the stepsize (see Figure 2). The mission of the controller is to keep the the output (the solution error) under control by choosing the input (the stepsize) appropriately.

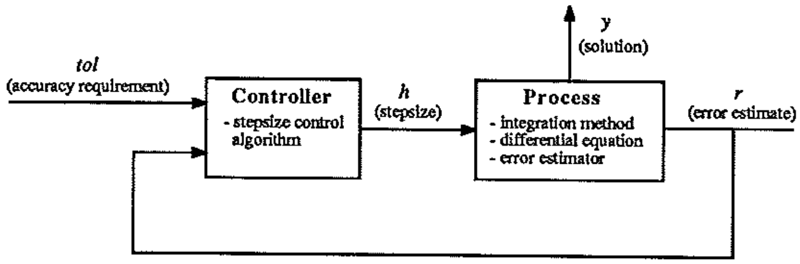

Figure 2. Feedback control view of stepsize control.

Earlier treatments of the stepsize control problem have focused mainly on explaining the observed irregularities in the stepsize sequence [Shampine 1975, Hall 1985, Hall 1986, Hall and Higham 1987]. The studies have in common that they describe and characterize the problem but do not present a solution. An exception is [Higham and Hall 1987], where the integration method is changed while the stepsize control algorithm is kept as is, in an attempt to solve the problem. They manage to improve the stepsize control, but the accuracy of the integration method as well as its stability region is sacrificed in order to achieve this end.

Phrasing the problem of stepsize selection as a feedback control problem separates the system into two parts: the process and the controller (see Figure 2). It is then natural to keep the process as is, and solve the problem by improving the stepsize controller using some of the analysis and synthesis tools provided by control theory. This view of the problem motivated the study [Gustafsson et al. 1988]. Here a simple standard control scheme was tried as stepsize controller, with very promising results. The tried control scheme could be motivated heuristically, but a thorough understanding of the positive results was lacking. Such an understanding is crucial if one wants to find out if even better control is possible, and if so, how to do it. Moreover, all controller parameters were determined experimentally using simulation. That is a straight forward method to determine parameters for one integration method, but since different methods need different parameters, a better way to tune the controller parameters is needed if the control algorithm is to be used generally.

The research project, of which this is the final report, was motivated by the positive preliminary results achieved by viewing stepsize selection as a feedback control problem. By continuing that path it seemed possible to derive a new stepsize control algorithm together with tuning rules for its parameters, that would solve the problem of irregular stepsize sequences and resulting incorrect solutions.

3. The Research Project

To be able to solve the stepsize control problem it is vital to have a good understanding of the relation between solution error and stepsize. The standard stepsize controller is derived assuming a static relation, but in reality the relation is a complicated nonlinear dynamic system. Fortunately, the dominating properties of the relation can be captured with a rather simple dynamic model. The derivation and verification of such a model for explicit Runge-Kutta methods was done and is presented in [Gustafsson 1988, Gustafsson 1989].

Using the derived model it is possible to evaluate different control schemes. The evaluation reveals that the standard controller fails to stabilize the dynamic model, which explains its poor behavior. On the other hand, the control scheme tried in [Gustafsson et al. 1988] does not have any problems stabilizing the model, and hence its performance is better.

In [Gustafsson 1988, Gustafsson 1989] the model is used to further improve the controller from [Gustafsson et al. 1988]. The result is a robust controller with very good properties. To be able to use the controller in different integration methods a systematic way to determine the controller methods is needed. In [Gustafsson 1989] such a method is derived for explicit Runge-Kutta methods.

To test the new stepsize controller an implementation of it was done in the simulation program Simnon [Elmqvist et al. 1986]. The algorithm has been used on a daily bases since November 1988 with very good results. During a student course (Adaptive Control, Jan 89 – March 89) with large simulation projects, the new controller was used and gave good results in every case where the standard controller failed.

4. Conclusions

Treating stepsize control in numerical integration as a feedback control problem has proven very successful. Control theory has provided tools for analyzing. The result has been a deep understanding of the mechanisms underlying the problem, making it possible to construct a new improved stepsize control algorithm. Such an algorithm has been presented, Moreover, a definite procedure for choosing the controller parameters has been given for the case of explicit Runge-Kutta methods.

The algorithm and the tuning procedure will shortly be published [Gustafsson 1989] in a forum for people that deal with implementation of simulation programs. It is presented in a form facilitating its incorporation in new and existing software.

Practical tests of the algorithm have been very successful. The availability of Simnon made it possible to make an implementation at an early stage. This implementation gave valuable feedback on the properties of the algorithm.

The reactions from the numerical analysis community regarding the algorithm have been very positive. It is worth noting that some parts of the algorithm are counterintuitive if regarded in the light of standard numerical analysis, whereas they are very natural in the feedback control point of view. Hence, the combination of the two research fields gave insight and constructive ideas. It is likely that there are other numerical problems that could be approached in a similar way.

5. References

ELMQVIST, H, ÅSTRÖM, K. J., and SCHÖNTHAL, T. (1986): *SIMNON, User's Guide for MS-DOS Computers*, Department of Automatic Control, Lund Institute of Technology, Lund, Sweden.

GUSTAFSSON, K., LUNDH, M., and SÖDERLIND, G. (1988): "A PI stepsize control for the numerical solution of ordinary Differential Equations," *BIT*, **28**, 2, 270–287.

GUSTAFSSON, K. (1988): *Stepsize Control in ODE-Solvers–Analysis and Synthesis*, Licentiate Thesis, CODEN:LUTFD2/(TFRT-3199), Department of Automatic Control, Lund Institute of Technology, Lund, Sweden.

GUSTAFSSON, K. (1989): "Control theoretic methods for stepsize selection in ODE's," *Submitted to ACM Transaction on Mathematical Software.*

HALL, G. (1985): "Equilibrium states of Runge-Kutta schemes: part I," *ACM Transactions on Mathematical Software*, **11**, 3, 289–301.

HALL, G. (1986): "Equilibrium states of Runge-Kutta schemes: part II," *ACM Transactions on Mathematical Software*, **12**, 3, 183–192.

HALL, G., and HIGHAM, D. J. (1987): "Analysis of stepsize selection for Runge-Kutta codes," NA report No. 137, University of Manchester.

HIGHAM, D. J., and HALL, G. (1987): "Embedded Runge-Kutta formulae with stable equilibrium states," NA report No. 140, University of Manchester.

SHAMPINE, L. F. (1975): "Stiffness and nonstiff differential equation solvers," in L. Collatz (Ed.): *Numerische Behandlung von Differentialgleichungen*, Information Series of Numerical Mathematics 27, Birkhauser Verlag, Basel, pp. 287–301.