Computational Methods Assignment 5 - ODE Integration

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1 Question 1

1(a) The program written for this assignment works by taking an arbitrary vector function of N variables corresponding to N coupled ordinary differential equations and initial state of the system, and implements the Runge-Kutta 45 method to determine the solution at a desired point. To obtain a 5th order accurate result optimally using a 4th order accurate method, an adaptive step size was used by implementing step-doubling. This worked by first calculating two estimates of the value of the dependent variable vector $\vec{y}(x)$ at the next step $x+h_1$, one with a single step h_1 and another with two half steps of size $h_1/2$. The difference in these two results gave an estimate Δ_1 for the error. To obtain an accuracy below Δ_0, the optimal step size h_0 was found by multiplying h_1 by $S(\Delta_0/\Delta_1)^{0.2}$, where S is a safety factor (chosen as 0.98).

If this optimal step size was smaller than the step already taken, then the step is redone with the optimal step size h_0, and step-doubling is implemented again so that a new error Δ can be calculated. This error is then used to obtain a 5th order accurate result of the evaluation at the end of the step by adding $\Delta/15$ to the value of $y(x+h_0)$ calculated using two half steps of size $h_0/2$. This means that the step is corrected so that it is within the required accuracy and does not miss important parts of a highly varying function.

If the step size taken is smaller than the calculated optimal step, then the step is not redone and the 5th order accurate results usedfor $y(x+h_1)$ is $y_2+\Delta_1/15$, where y_2 is the value of the dependent variable vector after two half steps of the original step size h_1. The optimal step size is then used for the next step. This means that unecessary detail and calculation is not given to determining the function over regions of the independent variable for which is does not vary much. This also means that the step size does not always decrease and allows flexibility. If the step size (optimal or current) used for that step took the independent variable over the range, then the step size was adjusted to that the desired end value was reached.

This was implemented in this program using a class which takes a vector function of a vector $\mathbf{f}(\vec{y},x)$ and upon iteration, will update its current values of the step size, independent variable, and dependent variable vector.

1(b) The plots for the coupled equations:

$$\frac{\mathrm{d}y_1}{\mathrm{d}x} = -y_1^2(x) - y_2(x)$$
$$\frac{\mathrm{d}y_2}{\mathrm{d}x} = 5y_1(x) - y_2(x)$$

for $y_1(0) = y_2(0) = 0$ are shown in Fig 1 (x vs y_1 and x vs y_2) and in Fig 2 (y_1 vs y_2).

2 Question 2

The N first order ODE solver was applied to determining the error function $\mathrm{erf}(x)$ evaulated at $x=2$. The values, number of function evaluations, number of repeated steps and number of steps taken are shown in table 1. This was done to achieve a relative accuracy of $\epsilon = 10^{-6}$.

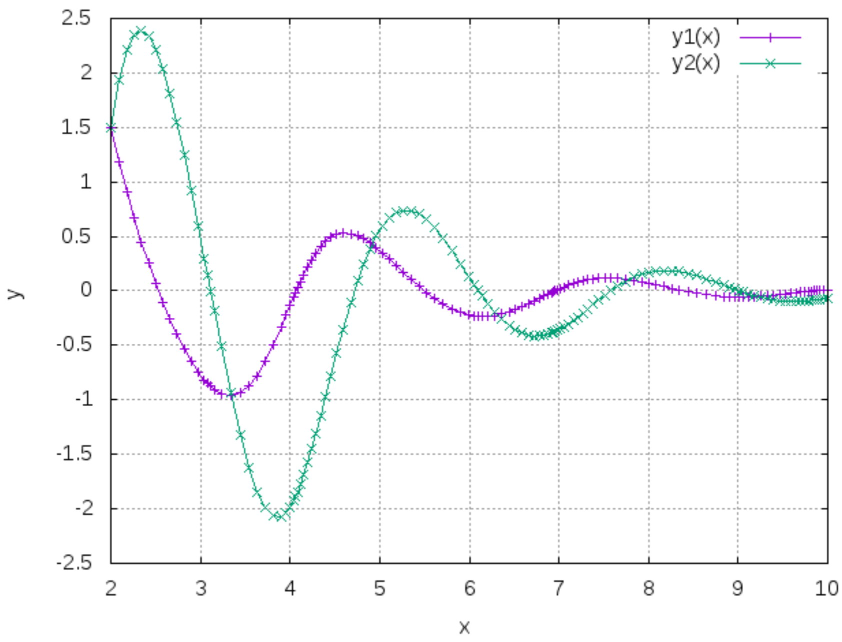

Figure 1: (x, y_1) and (x, y_2) for $0 \leq x \leq 10$.

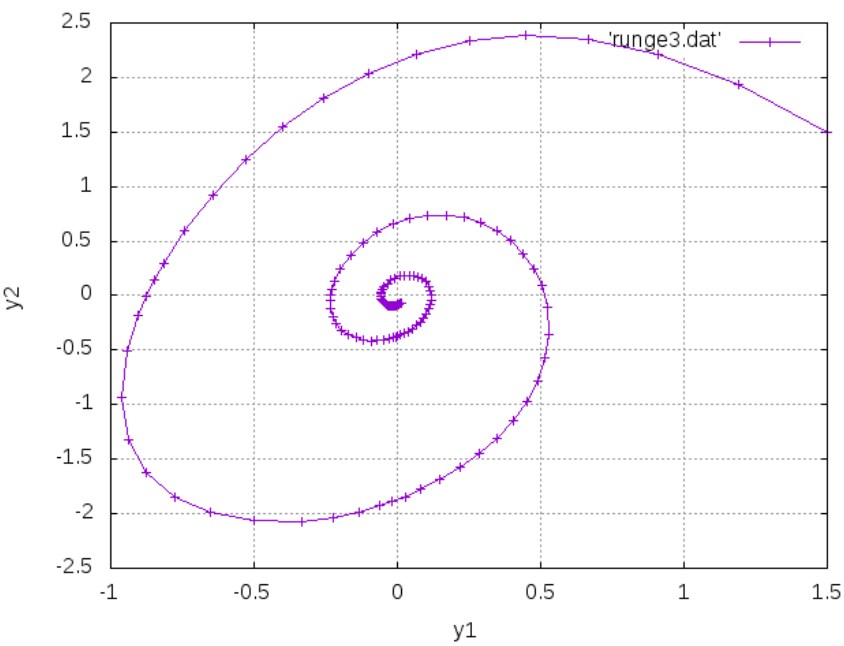

Figure 2: (y_1, y_2) for $0 \leq x \leq 10$.

	RK45	Adaptive Simpson's
erf$(x = 2)$	0.995322265	0.995322265
No. Steps	12	12
Fnc. Evaluations	140	98
Repeats	2	2

It can be seen by comparison that the RK45 with adaptive step size and the adaptive Simpson's rule produce the same result. This is the same because the algorithm has not changed, as the function being evaluated in this problem does not depend on the vector of dependent variables $\vec{y}(x)$, meaning that the function is not evaluated unecessarily in the Runge-Kutta steps. Similarly, the number of steps taken, also matches for this reason, with the step size not being determined by removal of a function evaluation which is a repeated step of the k_2 quantity in the Runge-Kutta method, for a function that does not depend of $\vec{y}(x)$. Also, it can be seen that the number of repeated steps, for both methods is identical, and significantly lower that the number of steps taken, representing a small fractional increase in function evaulations of 1.167.

The number of function evaluation *does* differ between the two methods, with the adaptive Simpson's method requiring $98/140 = 0.7$ the amount of function evaluations that the original RK45 uses. This is because, primarily, for each individual step of the RK45 method, being either 1 full step or 1 half step, 3 out of 4 of the function evaluations are needed for that particular step if the vector function is independent of $\vec{y}(x)$ (which the error function is). The reason it is less than 0.75, is that the full step and the first step of the two half steps use the same value of $\vec{f}(\vec{y}, x)$ in their k_1 vector in the Runge-Kutta 4 method. So by having an updatable value which can be used for k_1 in the full step and in the first half step, one-less function evaluation is performed per step-doubling implementation. Also, if the step is recalculated because the original step is too large, then this function evaulation $\vec{f}(\vec{y}, x)$ can be used for the full step and the first half step of the repeated step-doubling procedure, which further reduces the number of step evaluations needed to obtain the 5th order accurate estimation of the integral. Overall, for a single step, assuming it does not have to be repeated, the adaptive Simpson's rule brings the number of function evaluations in this step-doubling procedure down from 11 to 8. If the step must be re-calculated, then the number of function evaluations is brought down from 21 to 15.

In comparison to the fixed step Simpson's rule which required 65 function evaluations for the same relative accuarcy $\epsilon = 10^{-6}$, the adaptive Simpson's rule obtained the same value for erf(2) but the number of function evaluations approximately 1.5 times that of the fixed-step Simpson's rule.