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 potentially rapidly-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 it does not vary greatly. 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 so that the desired end value iss reached.

This was implemented 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. To minimize the number of function evaluations required, the value of k_1 was stored prior to the three steps needed for the step-doubling, since the full step and the first hald step share the same starting values which means k_1 can be reused. This same k_1 value can also be used if the step is repeated since, again, the starting point is the same, which reduces the computational cost if the step needs re-doing.

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 $y_1(0) = y_2(0) = 1.5$ are shown in Fig 1 (x vs y_1 and x vs y_2) and in Fig 2 (y_1 vs y_2) over $0 \leq x \leq 10$.

2 Question 2

For ODE problems where the function that represents the set of N coupled ODE's does not depend on any of the dependent variables, the RK45 method 'collapses' to an adaptive Simpson's rule. The amount of function evaluations and hence the computational overhead can be reduced by reusing k_2 as k_3 for all

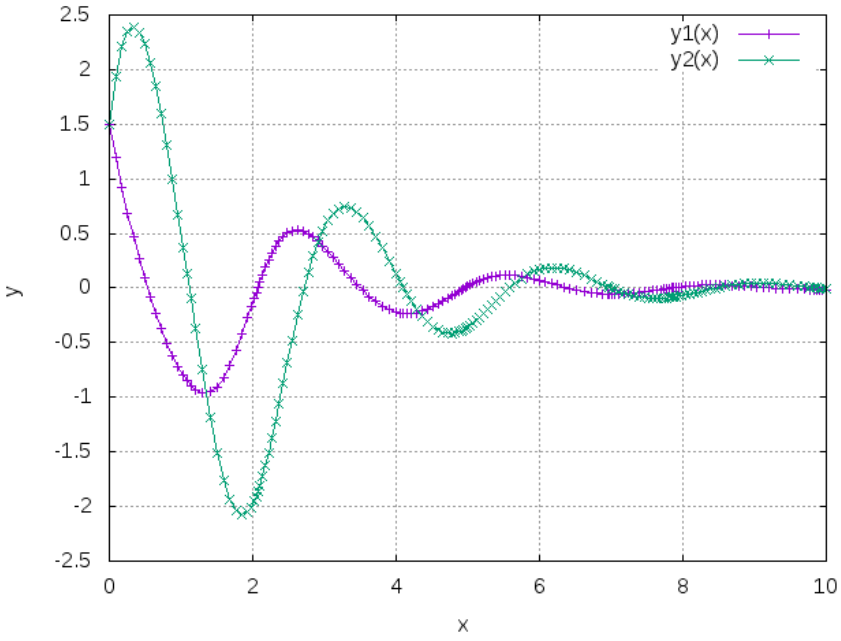

Figure 1: (x, y_1) and (x, y_2) for $0 \leq x \leq 10$.

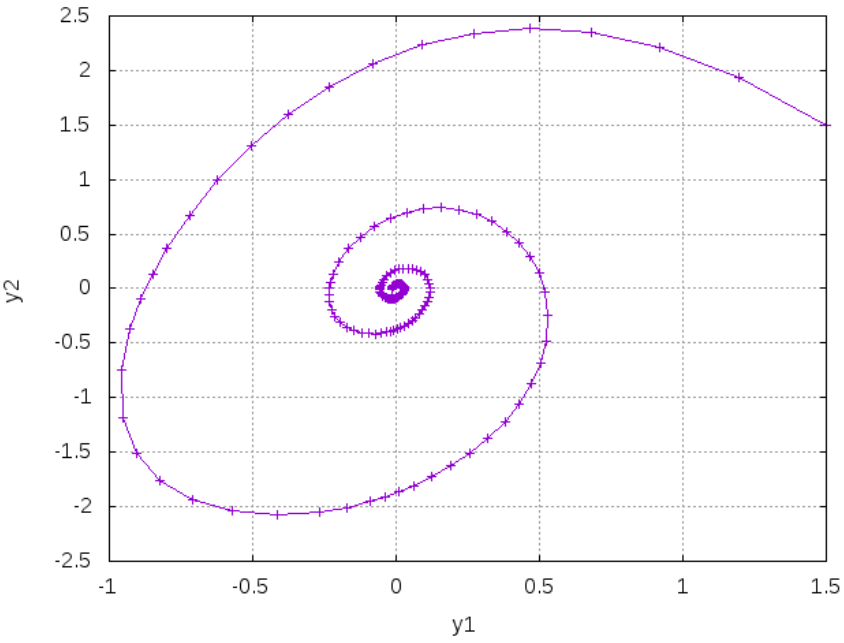

Figure 2: (y_1, y_2) for $0 \leq x \leq 10$.

iterations of Runge-Kutta. Also, for this method, it is noted that the last function evaluation used in the nth step, $k_4^{(n)}/h^{(n)}$, can be used as the first function evaluation for the $(n+1)$th step, $k_1^{(n+1)}/h^{(n+1)}$. This, along with $k_2 = k_3$, was added to the Runge-Kutta iterating class as an optional feature for $\vec{y}$-independent functions. The N first order ODE solver was applied to determining the error function $\text{erf}(x)$ 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 $\epsilon = 10^{-6}$.

	RK45	Adaptive Simpson's
erf($x = 2$)	0.995322265	0.995322265
No. Steps	12	12
Fnc. Evaluations	152	85
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 $85/152 \approx 0.56$ the amount of function evaluations (nearly half) 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, at most 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). This further reduces as $k_4^{(n)}/h^{(n)} = k_1^{(n+1)}/h^{(n+1)}$, so the edge values of each block of adaptive Simpson's rule need only be calculated once. Overall, it can be seen that when the Runge-Kutta 45 is collapsed into the 3-point adaptive Simpson's rule, the efficiency is almost doubled due to the lack of $\vec{y}$ dependence of the function that represents the ODE, whilst the accuracy for both methods is the same.

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 with the number of function evaluations approximately 1.3 times that of the fixed-step Simpson's rule. While Simpson's fixed point rule has an error of order h^5, the adaptive step size is order h^6 accurate, which comes as a trade-off for the slight increase in function evaluations. However, the order of the error is h^5 for the entire calcuation of the fixed point Simpson's rule, whilst the error in the adaptive step size Simpson's rule used here has a local error of the order h^6. Thus the cummulative error in this calculation can be expected to be of the order $N \times h^6$ where N is the number of steps. This means that for larger numbers of steps, error in the adaptive Simpson's rule may scale as order $h^{(n<5)}$, so that the error scaling of these methods is comparable. Using the RK45 method implemented in this task, the order h^6 error cannot be determined, so neither can the cummulative error.