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:

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

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 erf(x) evaulated at $x = 2$. The values, number of function evaluations, 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	168	126

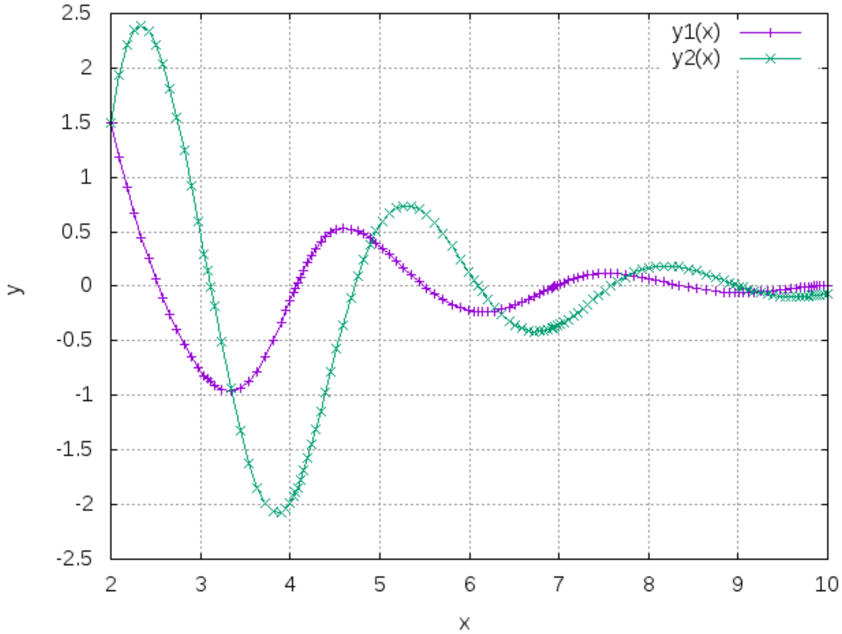

Figure 1: (x, y_1) and (x, y_2) for $0 \leq x \leq 10$.

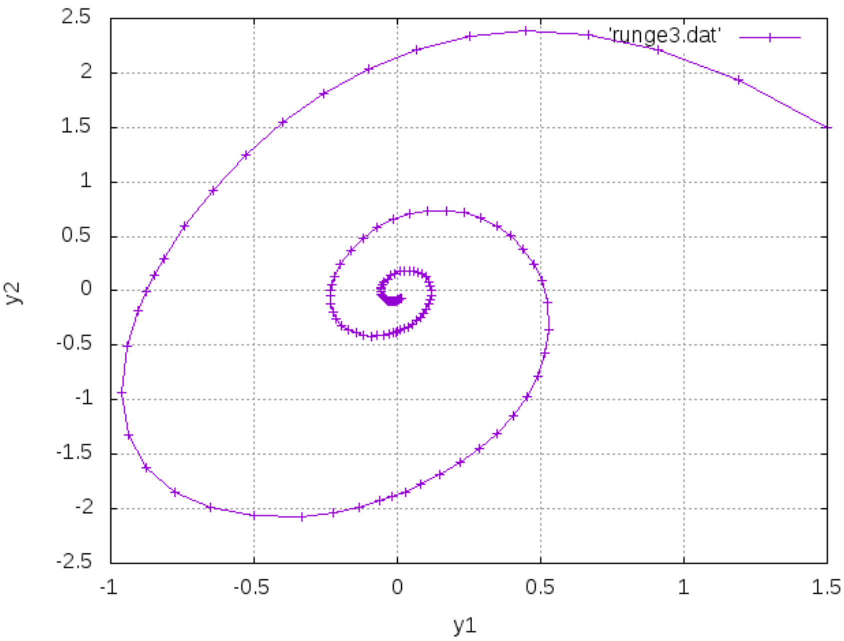

Figure 2: (y_1, y_2) for $0 \leq x \leq 10$.

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 $\vec{y}(x)$.

The number of function evaluation *does* differ between the two methods, with the adaptive Simpson's method requiring exactly three quarters of the function evaluations required for the original RK45, as expected from the fact we use 3 function evaluations per Runge-Kutta evaluation of the dependent variable vector at the $x + h$ from x.

In comparison to the fixed step Simpson's rule, which in the previous assignment obtained the same