The Commuting Mathematician goes to a Wedding

For a short time I was a celebrity. Not only was I employed as a mathematician on Auckland buses, adding value to the ordinary traveller's commuting experience through my stimulating and arcane conversation, but I was also commissioned to expand this valued service through the recruitment of colleagues to assist me. And then the final accolade of a celebrity – my television appearance. What a dream!

Many years ago, after a visit to a North American University, I was sent to the airport in a chauffeured vehicle. The driver was trying to better himself by studying the type of introductory mathematics popular at that time, full of Venn diagrams and truth tables. He tried to explain what he was doing by working through notebooks with me as the car sped along icy highways. I had some concerns, but we got to the airport safely and I flew away. Perhaps it was this commuting tutorial that came back as the source of my dream last night.

Today I join in the celebration of the marriage of Nicolette Moir. Nicolette is one of the stars of my mathematical career; I have known her since her undergraduate days and have helped to guide her through her MSc and through her almost completed PhD. Her research is on numerical solutions of ordinary differential equations using what we call ARK ("Almost Runge-Kutta") methods. I would like to offer this brief introduction to her work on this happy day.

Numerical methods for solving differential equations are generally based on two types of operations: evaluating derivatives and forming linear combinations of already computed quantities. Suppose the differential equation is $y'(x) = f(x, y(x))$, and an approximation has already been found after $n-1$ steps: $y_{n-1} \approx y(x_{n-1})$. The aim is now to advance the solution one step further by computing $y_n \approx y(x_n)$, where $x_n = x_{n-1} + h$. In one particular family of Runge-Kutta methods, discovered by Kutta in 1901, a sequence of four derivative approximations, F_1, F_2, F_3, F_4 is computed corresponding to approximation solutions at x_{n-1}, $x_{n-1} + th$, $x_{n-1} + \frac{1}{2}h$ and $x_{n-1} + h$. These are given by

$$\begin{aligned}
Y_1 &= y_{n-1}, & F_1 &= f(x_{n-1}, Y_1) & &\approx y'(x_{n-1}),\\
Y_2 &= y_{n-1} + thF_1, & F_2 &= f(x_{n-1}+th, Y_2) & &\approx y'(x_{n-1}+th),\\
Y_3 &= y_{n-1} + \tfrac{4t-1}{8t}hF_1 + \tfrac{1}{8t}hF_2, & F_3 &= f(x_{n-1}+\tfrac{1}{2}h, Y_3) & &\approx y'(x_{n-1}+\tfrac{1}{2}h),\\
Y_4 &= y_{n-1} + \tfrac{1-2t}{2t}hF_1 - \tfrac{1}{2t}hF_2 + 2hF_3, & F_4 &= f(x_{n-1}+h, Y_4) & &\approx y'(x_{n-1}+h).
\end{aligned}$$

These computed results are sufficiently accurate to enable y_n to be computed using Simpson's rule, without detracting significantly from the quality of that famous integration rule. That is,

$$y_n = y_{n-1} + \tfrac{1}{6}hF_1 + \tfrac{2}{3}hF_3 + \tfrac{1}{6}hF_4.$$

If $t = -1$ or $t = -\frac{1}{2}$, it is possible to lower the cost of the algorithm, but with some impact on the computational properties, by replacing F_2 by either F_1 or F_3 as computed in the *previous* step. In ARK methods we take this idea a little further by using information from the previous step combined in a package which approximates not just $hy'(x_{n-1})$, available here as hF_1, which could equally well have been computed as part of the previous step, but also $h^2y''(x_{n-1})$. Things can be contrived so that the modified methods have the same stability properties as for a standard Runge-Kutta method and, furthermore, the derivative approximations on which the method is built are more accurate than for a Runge-Kutta method. This last feature has several advantages including the ability to obtain realistic error estimates and the ability to obtain reasonably accurate and, at the same time inexpensive, interpolations.

One of Nicolette's special contributions has been the extension of ARK methods to the solution of so-called stiff problems. The crucial difference between stiff and non-stiff problems is that stiff problems need to be solved using implicit methods. Implicit methods cost a great deal more per step but there is a hope that there will be many fewer steps required to obtain comparable accuracy, because of better stability. A second significant contribution has been in the design of a new fourth order ARK method which can be implemented in such a way that it acts as though it were fifth order, even when h changes from step to step.

This new explicit method passes approximations to y, hy' and h^2y'' from step to step. Denote these approximations, as computed in step number n, by y_n, hy'_n and $h^2y''_n$. The formula for these quantities, and for the stage values which lead to them are

$$\begin{aligned}
Y_1 &= y_{n-1} + \tfrac{1}{4}hy'_{n-1} + \tfrac{1}{32}h^2y''_{n-1}, & F_1 &= f(x_{n-1}+\tfrac{1}{4}h, Y_1),\\
Y_2 &= y_{n-1} + \tfrac{1}{10}hy'_{n-1} + \tfrac{1}{40}h^2y''_{n-1} + \tfrac{2}{5}hF_1, & F_2 &= f(x_{n-1}+\tfrac{1}{2}h, Y_2),\\
Y_3 &= y_{n-1} - \tfrac{3}{640}hy'_{n-1} - \tfrac{69}{1280}h^2y''_{n-1} + \tfrac{27}{160}hF_1 + \tfrac{75}{128}hF_2, & F_3 &= f(x_{n-1}+\tfrac{3}{4}h, Y_3),\\
Y_4 &= y_{n-1} - \tfrac{41}{140}hy'_{n-1} + \tfrac{17}{280}h^2y''_{n-1} + \tfrac{69}{35}hF_1 - \tfrac{51}{28}hF_2 + \tfrac{8}{7}hF_3, & F_4 &= f(x_{n-1}+h, Y_4),\\
Y_5 &= y_{n-1} + \tfrac{7}{90}hy'_{n-1} + \tfrac{16}{45}hF_1 + \tfrac{2}{15}hF_2 + \tfrac{16}{45}hF_3 + \tfrac{7}{90}hF_4, & F_5 &= f(x_{n-1}+h, Y_5),\\
y_n &= Y_5, & &\\
hy'_n &= hF_5, & &\\
h^2y''_n &= \tfrac{242}{75}hy'_{n-1} - \tfrac{1352}{225}hF_1 + \tfrac{34}{15}hF2 - \tfrac{256}{75}hF_3 - \tfrac{196}{225}hF_4 + \tfrac{24}{5}hF_5. & &
\end{aligned}$$

Try it, using starting values $hy'_0 = hf(x_0, y_0)$ and $h^2y''_0 = hf(x_0+h, y_0+hy'_0) - hy'_0$, and see how it compares with a classical Runge-Kutta method.

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