Appendix H

Runge-Kutta Methods

In this appendix we will analyze the conditions on the coefficients of an explicit Runge-Kutta Method that are necessary and sufficient to guarantee convergence with accuracy of order P. In particular, we will establish the connection between these conditions and the set of rooted trees with no more than P nodes. As a consequence, we will be able to show that there are r-stage methods of order r for $r \leq 4$ but not for $r > 4$.

We begin by briefly considering more general one-step methods, $y_{n+1} = F(t_n, y_n, f, h)$, for approximating solutions of the scalar ODE $y' = f(t, y(t))$.

The local truncation error at t_n is the quantity ϵ_n defined by

$$y(t_{n+1}) := F(t_n, y(t_n), f, h) + \epsilon_n.$$

From our discussion following the convergence analysis of Euler's Method in the body of the text, we can show that a 0-stable one-step method will converge to a solution of the ODE $y \in C^{P+1}[t_o, t_o + T]$ with global order of accuracy P if $|\epsilon_n| \leq Ch^{P+1}$ for some $C > 0$ depending only on $\max_{t \in (t_o, t_o+T)} |y^{(P+1)}(t)|$.

One approach to constructing methods satisfying such an estimate is to define them using Taylor's Theorem with Remainder by letting $F(t_n, y_n, f, h) = \sum_{p=0}^{P} y^{(p)}(t_n)/p!\ h^p$ be the Taylor polynomial of degree p for $y(t)$ centered at t_n and evaluated at t_{n+1}. To implement this idea, we must be able to express $y^{(k)}(t_n)$ in terms of f and its derivatives evaluated at (t_n, y_n). The resulting one-step methods are known as *Taylor Methods*. Taylor Methods are an option

if the vector field that defines the ODE is given in a form that can be differentiated symbolically, which is not always the case.

To demonstrate how this would be carried out, and for later use, we examine the expressions for the first few derivatives of y in terms of f and its derivatives. We ignore the differential equation at first and differentiate $g(t) = f(t, y(t))$ and use multi-index notation for mixed partial derivatives,

$$f^{k,l} = \partial^{k,l} f(t, y) = \frac{\partial^{k+l} f}{\partial t^k \partial y^l}.$$

In this form, we can distinguish terms arising from differentiating f from those that arise by differentiating factors of y coming from the chain rule—terms that we will eventually also write in terms of f. Because of equality of mixed partial derivatives, these terms exhibit a binomial pattern,

$$\begin{aligned} y' &= f, \\ y'' &= f^{1,0} + f f^{0,1}, \\ y''' &= [f^{2,0} + 2 f f^{1,1} + f^2 f^{0,2}] + [(f^{1,0} + f f^{0,1}) f^{0,1}]. \end{aligned} \tag{H.1}$$

Even when this procedure is possible, by hand or with automatic symbolic differentiation, the number of terms required to carry the expansion to high order can yield diminishing returns with the growing cost of evaluation.

An alternate approach originally proposed and developed by Runge and Kutta only requires evaluation of f at arbitrary (t, y) values to match the terms of Taylor polynomial above to order p. Runge-Kutta Methods approximate $(\mathbf{y}(t_{n+1}) - \mathbf{y}(t_n))/h$ using a weighted average of samples of the vector field $f(t, y)$ that defines an ODE. For the method to be explicit, locations of the samples must be chosen based upon information obtained in previous samples. Because of this, the general form of an explicit one-stage Runge-Kutta Method is $y_{n+1} = y_n + h\gamma_0 f(t_n, y_n)$. For the right-hand side to match the first-order terms of the Taylor expansion above, we must have $\gamma_0 = 1$. This tells us that Euler's Method is the unique explicit one-stage Runge-Kutta Method that is convergent. No higher-order terms occur when a one-stage method is used.

The general form of an explicit two-stage Runge-Kutta Method is

$$\begin{aligned} y'_{n,1} &= f(t_n, y_n), \\ y'_{n,2} &= f(t_n + \beta_{21}h, y_n + h\beta_{21}y'_{n,1}), \\ y_{n+1} &= y_n + h(\gamma_1 y'_{n,1} + \gamma_2 y'_{n,2}). \end{aligned} \tag{H.2}$$

Two of the example methods in the text fit this pattern, the midpoint method ($\beta_{12} = 1/2$, $\gamma_1 = 0$, $\gamma_2 = 1$) and Heun's Method ($\beta_{12} = 1$, $\gamma_1 = \gamma_2 = 1/2$). Both solved the second-order accuracy model problem exactly and also appeared to converge to the solution of the absolute stability model problem with second-order accuracy.

To estimate the local truncation error of these methods, we perform Taylor expansions of the terms of the general explicit 2-stage Runge-Kutta Methods. Substituting $y'_{n,1}$ in the definition of $y'_{n,2}$,

$$y'_{n,2} = f(t_n + \beta_{21}h, y_n + h\beta_{21}f).$$

Then by Taylor expanding in powers of the perturbations (to first order to obtain hy' terms to second order),

$$y'_{n,2} = f + \beta_{21}h(f^{1,0} + ff^{0,1}) + O(h^2).$$

When this is inserted in the expression for y_{n+1}, we find

$$y_{n+1} = y_n + h(\gamma_1 + \gamma_2)f + \frac{h^2}{2}2\gamma_2\beta_{21}(f^{1,0} + ff^{0,1}) + O(h^3).$$

Comparing this with (H.1), the conditions for this expansion to match the first two terms of the Taylor series

$$y(t_{n+1}) = y(t_n) + hy'_n + \frac{h^2}{2}y''_n + O(h^3)$$

are

$$\begin{aligned} \gamma_1 + \gamma_2 &= 1, \\ 2\gamma_2\beta_{21} &= 1. \end{aligned}$$

We may use γ_2 to parametrize a family, $\gamma_1 = 1 - \gamma_2$, $\beta_{21} = 1/(2\gamma_2)$, of solutions of these equations. It is straightforward to check that the *midpoint* method and *Heun's* Method satisfy these conditions.

The parameters of a Runge-Kutta Method are often displayed in the form of a so-called *Butcher tableau*:

$$\begin{array}{c|ccc} 0 & & & \\ \alpha_2 & \beta_{21} & & \\ \vdots & \vdots & \ddots & \\ \alpha_r & \beta_{r1} & \cdots & \beta_{r(r-1)} \\ \hline & \gamma_1 & \gamma_2 & \cdots \quad \gamma_r \end{array}$$

The Butcher tableau for the midpoint method is

$$\begin{array}{c|cc} 0 & & \\ \frac{1}{2} & \frac{1}{2} & \\ \hline & 0 & 1 \end{array}$$

The modified trapezoidal method is displayed in this format as

$$\begin{array}{c|cc} 0 & & \\ 1 & 1 & \\ \hline & \frac{1}{2} & \frac{1}{2} \end{array}$$

If we expanded $y'_{n,2}$ to higher order, we would discover that three parameters do not provide enough freedom to obtain a method of order 3. In order to satisfy the two additional h^3 conditions appearing in square brackets in the expression (H.1) for y''', another stage is needed.

The form of an explicit Runge-Kutta Method with $r = 3$ stages is

$$\begin{aligned} y'_{n,1} &= f(t_n, y_n), \\ y'_{n,2} &= f(t_n + \beta_{21}h, y_n + h\beta_{21}y'_{n,1}), \\ y'_{n,3} &= f(t_n + (\beta_{31} + \beta_{32})h, y_n + h(\beta_{31}y'_{n,1} + \beta_{32}y'_{n,2})), \\ y_{n+1} &= y_n + h(\gamma_1 y'_{n,1} + \gamma_2 y'_{n,2} + \gamma_3 y'_{n,3}). \end{aligned}$$

The coefficient of $\frac{h^4}{4!}$ in the Taylor expansion of $y(t+h)$ in terms of f and its derivatives is

$$\begin{aligned} y^{(4)} &= [f^{3,0} + 3ff^{2,1} + 3f^2f^{1,2} + f^3f^{0,3}] \\ &\quad + [3(f^{1,0} + ff^{0,1})(f^{1,1} + ff^{0,2})] \\ &\quad + [(f^{2,0} + 2ff^{1,1} + f^2f^{0,2} + (f^{1,0} + ff^{0,1})f^{0,1})f^{0,1}]. \end{aligned}$$

It clearly becomes worthwhile to find a framework to simplify the development and comparison of the Taylor and Runge-Kutta sides of these expansions to higher orders. The autonomous scalar case is exceptional, as can be seen by setting all t-derivatives to zero in the expressions above. For greater generality, we shift our setting and notation and now consider an $\mathbf{R}^D$ vector-valued $\mathbf{f}(\mathbf{y})$ and $\mathbf{y}(t)$ that is a solution of $\mathbf{y}' = \mathbf{f}(\mathbf{y})$. The nonautonomous case can be put into this form using the standard device of replacing t by additional dependent variables y_{D+1} satisfying $y'_{D+1} = 1$. In this setting, the general r-stage explicit Runge-Kutta Method takes the form

$$\mathbf{y}_{n+1} = \mathbf{y}_n + h\sum_{i=1}^{r} \gamma_i \mathbf{y}'_{n,i}, \tag{H.3}$$

where

$$\mathbf{y}'_{n,i} = \mathbf{f}(\mathbf{y}_{n,i}), \text{ with } \mathbf{y}_{n,i} = \mathbf{y}_n + h\sum_{j=1}^{i-1} \beta_{i,j}\mathbf{y}'_{n,j}. \tag{H.4}$$

An elegant formalism for organizing, visualizing, and understanding both the Taylor expansion of the solution $\mathbf{y}(t_n+h)$ and the *Runge-Kutta expansion* of $\mathbf{y}_{n+1}$ obtained by Taylor expanding the terms in (H.3) and (H.4) has been developed and advocated by Butcher [BJ], following on the work of Gill [GS] and Merson [MRH]. This approach associates terms in both expansions with *rooted trees*. To motivate it, we begin by reviewing the formal Taylor expansion to degree 5 for a function $\mathbf{y}(t) : \mathbf{R} \to \mathbf{R}^n$ satisfying $\mathbf{y}' = \mathbf{f}(\mathbf{y})$, where $\mathbf{f}$ is a smooth function from $\mathbf{R}^n$ to $\mathbf{R}^n$,

$$\mathbf{y}(t+h) = \mathbf{y}(t) + \mathbf{y}'(t)h + \mathbf{y}''(t)\frac{h^2}{2!} + \cdots + \mathbf{y}^{(k)}(t)\frac{h^k}{k!} + \cdots,$$

and then give the representation of its terms using rooted trees. We wish to represent the derivatives $\mathbf{y}^{(k)}(t)$ in terms of $\mathbf{f}$ and its derivatives. Here, in the column on the left, we list successive derivatives of the function $\mathbf{g}(t) = \mathbf{f}(\mathbf{y}(t))$ where again at first we ignore the differential equation:

$$\begin{aligned}
\mathbf{g}(t) &= \mathbf{f}(\mathbf{y}(t)) = \mathbf{f}, && \mathbf{y}', 1,\\
\mathbf{g}'(t) &= \mathbf{f}_{\mathbf{y}}\mathbf{y}', && \mathbf{y}'', 1,\\
\mathbf{g}''(t) &= \mathbf{f}_{\mathbf{yy}}\mathbf{y}'^2 + \mathbf{f}_{\mathbf{y}}\mathbf{y}'', && \mathbf{y}''', 1+1=2,\\
\mathbf{g}'''(t) &= \mathbf{f}_{\mathbf{yyy}}\mathbf{y}'^3 + 3\mathbf{f}_{\mathbf{yy}}\mathbf{y}'\mathbf{y}'' + \mathbf{f}_{\mathbf{y}}\mathbf{y}''', && \mathbf{y}^{(4)}, 1+1+2=4,\\
\mathbf{g}^{(4)}(t) &= \mathbf{f}_{\mathbf{yyyy}}\mathbf{y}'^4 + 6\mathbf{f}_{\mathbf{yyy}}\mathbf{y}'^2\mathbf{y}''\\
&\quad +3\mathbf{f}_{\mathbf{yy}}\mathbf{y}''\mathbf{y}''\\
&\quad +4\mathbf{f}_{\mathbf{yy}}\mathbf{y}'\mathbf{y}''' + \mathbf{f}_{\mathbf{y}}\mathbf{y}^{(4)}, && \mathbf{y}^{(5)}, 1+1+1+2+4=9.
\end{aligned}$$

In the column on the right, we list the correspondence between each derivative of $\mathbf{g}$ and the next higher derivative of y. We also list the number of terms that each row represents as a sum. The terms of the sum refer recursively to terms from previous rows that appear in subsequent rows and the numbers of terms they represent. Recall that the kth derivative of $\mathbf{f}$ with respect to $\mathbf{y}$ is a symmetric k-linear function from $(\mathbf{R}^n)^k \to \mathbf{R}^n$. For $k > 1$, the symmetry is nontrivial and decreases the number of its independent coefficients with respect to a basis from n^{k+1} accordingly. For example, when $k = 2$ there are $n(n(n+1))/2$ independent components.

Next we expand the rows recursively to write the Taylor expansion as a linear combination of *elementary differentials*. These are multilinear operator compositions that express $\mathbf{y}^{(k)}$ in terms of $\mathbf{f}$ and its derivatives evaluated at t. Since $\mathbf{f}_{\mathbf{y}\ldots\mathbf{y}}$ is an operator with k arguments, we will use a naturally related notation for lists that will be familiar to those who have encountered the artificial intelligence programming language LISP. For our purposes, a list begins with an open parentheses and the first element, the kth partial derivative of f with respect to y for some $k \geq 0$, followed by k sublists, then a close parentheses. If a sublist has zero sublists, we omit its parentheses, and we can close all open parentheses with a right square bracket. (Our convention will be to do so when more than two are open.)

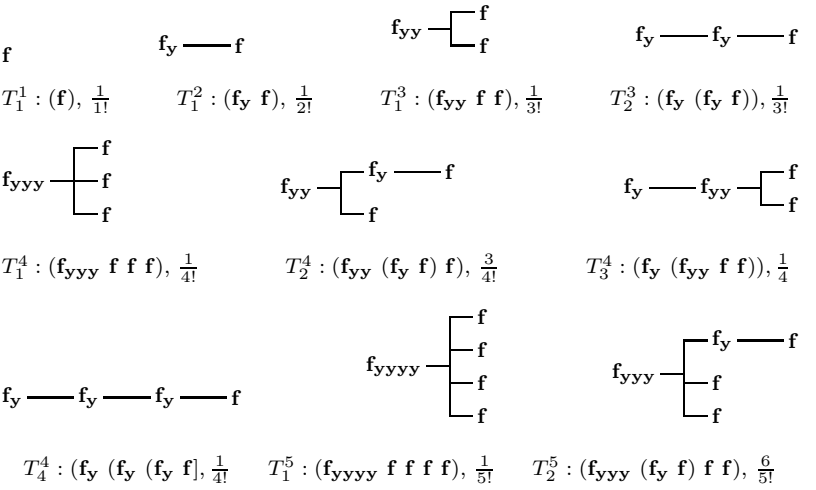
The internal representation of such a list in a LISP interpreter is in the form of a rooted tree data structure, the same algebraic structure that has been used to visualize and organize the terms of Taylor and Runge-Kutta expansions and their relationship. This suggests that LISP may be convenient for performing calculations involved in the derivation and analysis of Runge-Kutta Methods. A rooted tree is a set of nodes connected by edges oriented away from a distinguished node called the root, so it is a connected simple graph that contains no cycles, i.e., a tree. Graphically, we represent the lists associated with an elementary differential by a root node labeled by $\mathbf{f}_{\mathbf{y}\ldots\mathbf{y}}$ (k partial derivatives) attached to k subtrees corresponding to those sublists. Lists with no sublists are leaves—terminal nodes with no edges leaving them:

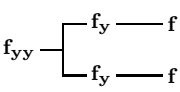
$$
\begin{aligned}
\mathbf{y}'(t) &= (\mathbf{f}) = \mathbf{f},\\
\mathbf{y}''(t) &= (\mathbf{f_y\ f}),\\
\mathbf{y}'''(t) &= (\mathbf{f_{yy}\ f\ f}) + (\mathbf{f_y\ (f_y\ f)}),\\
\mathbf{y}^{(4)}(t) &= (\mathbf{f_{yyy}\ f\ f\ f}) + 3(\mathbf{f_{yy}(f_y\ f)\ f}) + (\mathbf{f_y(f_{yy}\ f\ f)}) + (\mathbf{f_y(f_y(f_y\ f}],\\
\mathbf{y}^{(5)}(t) &= (\mathbf{f_{yyyy}\ f\ f\ f\ f}) + 6(\mathbf{f_{yyy}(f_y\ f)\ f\ f}) + 3(\mathbf{f_{yy}(f_y\ f)(f_y\ f)})\\
&\quad + 4(\mathbf{f_{yy}(f_{yy}\ f\ f)\ f}) + 4(\mathbf{f_{yy}(f_y(f_y\ f))\ f}) + (\mathbf{f_y(f_{yyy}\ f\ f\ f)})\\
&\quad + 3(\mathbf{f_y(f_{yy}(f_y\ f)\ f)}) + (\mathbf{f_y(f_y(f_{yy}\ f\ f}] + (\mathbf{f_y(f_y(f_y(f_y\ f}].
\end{aligned}
$$

We implicitly evaluate $\mathbf{f}$ and its derivatives at $\mathbf{y}(t)$. We will refer to the lth term of the kth-order (row) formal Taylor expansion above as T_l^k. Observe that each different term of a particular order arises from terms of the previous order from the vector-valued Leibniz rule and chain rule, through the addition of one derivative to each operator factor (we consider arguments $\mathbf{f}$ as preceded by a 0th-order identity operator) and adding a corresponding argument $\mathbf{y}' = \mathbf{f}$. In terms of rooted trees, this corresponds to the process of constructing all rooted trees with k nodes by attaching a new edge and leaf to each node (one at a time) of each rooted tree with $k-1$ nodes. The coefficients in the equations above represent the number of distinct ways each such tree can be built in this manner. Instead of expanding existing trees with new leaves, we will see that the new rooted trees that occur at the rth stage of a Runge-Kutta expansion are built by joining any number of

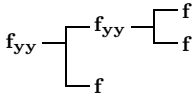
trees built at the $(r-1)$st stage to a new root node. By considering the multiplicities of ways the trees are built in both models and the coefficients that arise from the Runge-Kutta weighting coefficients, we will obtain the matching conditions that are necessary to achieve a certain order of accuracy.

Below, we exhibit the rooted trees corresponding to each term T_l^k in the Taylor expansion above, along with their associated coefficients in that expansion. The coefficients in the numerators that represent multiplicities of the various terms in the expansion can be interpreted and determined directly in terms of the number of ways the corresponding trees can be constructed by repeatedly attaching an edge and leaf to any node of smaller trees, starting from an initial root node. For example, the factor 3 associated with T_2^4 corresponds to the fact that it can be obtained by attaching an edge and leaf to either of the two leaves of T_1^3 or by attaching an edge and leaf to the root node of T_2^3. Similarly, the factor 6 associated with T_2^5 corresponds to the fact that it can be obtained either by attaching an edge and leaf to any of the three leaves of T_1^4 or by attaching an edge and leaf to the root node of T_2^4 that itself has multiplicity 3.

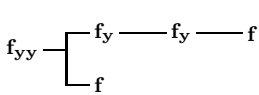




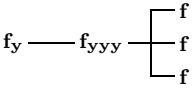
$T_3^5 : (\mathbf{f_{yy}}\ (\mathbf{f_y}\ \mathbf{f})(\mathbf{f_y}\ \mathbf{f})), \frac{3}{5!}$



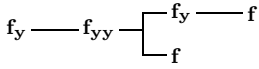
$T_4^5 : (\mathbf{f_{yy}}\ (\mathbf{f_{yy}}\ \mathbf{f}\ \mathbf{f})\ \mathbf{f}), \frac{4}{5!}$



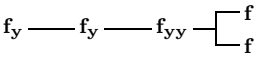
$T_5^5 : (\mathbf{f_{yy}}\ (\mathbf{f_y}\ (\mathbf{f_y}\ \mathbf{f}))\ \mathbf{f}), \frac{4}{5!}$



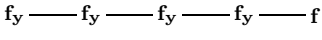
$T_6^5 : (\mathbf{f_y}\ (\mathbf{f_{yyy}}\ \mathbf{f}\ \mathbf{f}\ \mathbf{f})), \frac{1}{5!}$



$T_7^5 : (\mathbf{f_y}\ (\mathbf{f_{yy}}\ (\mathbf{f_y}\ \mathbf{f})\ \mathbf{f})), \frac{3}{5!}$



$T_8^5 : (\mathbf{f_y}\ (\mathbf{f_y}\ (\mathbf{f_{yy}}\ \mathbf{f}\ \mathbf{f}], \frac{1}{5!}$



$T_9^5 : (\mathbf{f_y}\ (\mathbf{f_y}\ (\mathbf{f_y}\ (\mathbf{f_y}\ \mathbf{f}], \frac{1}{5!}$

Below, we will perform Taylor expansions of the terms in the Runge-Kutta samples (H.4) for $r = 4$ stages through order h^3. When we form their weighted sum (H.3), this yields terms up to order h^4. These Runge-Kutta expansions very quickly become horrendous, but when they are interpreted in terms of rooted trees, another surprisingly simple pattern describing the terms present at each stage and their coefficients quickly emerges, just as we saw for Taylor expansion of $\mathbf{y}(t+h)$. Before we wade through the formulas, we preview the algebraic and analytical basis for this pattern and its consequences for determining the order of an r-stage Runge-Kutta Method. In (H.4) we have used $\mathbf{y}_{n,i}$ to denote the arguments of the sample of $\mathbf{f}$ that defines the $\mathbf{y}'_{n,i}$. The first stage of any explicit Runge-Kutta Method simply samples the vector field at the current time-step, $\mathbf{y}_{n,1} = \mathbf{y}_n$. Then for any method other than Euler's Method, another stage samples $\mathbf{f}$ at $\mathbf{y}_{n,2} = \mathbf{y}_n + h(\beta_{21}\mathbf{y}'_{n,1})$, and we can formally expand $\mathbf{f}(\mathbf{y}_{n,2})$ about $\mathbf{y}_n$ in a Taylor series of the form $\sum_{l=0}^{\infty}(\frac{\mathbf{f_{y\cdots y}}}{l!}(h\beta_{21}\mathbf{f})^l)$. If a third stage is used, it samples $\mathbf{f}$ at $\mathbf{y}_{n,3} = \mathbf{y}_n + h(\beta_{31}\mathbf{y}'_{n,1} + \beta_{32}\mathbf{y}'_{n,2})$. Expanding $\mathbf{f}(\mathbf{y}_{n,3})$ in powers of h involves substituting the prior expansion of $\mathbf{y}'_{n,2}$, combining like terms with $\mathbf{y}'_{n,1}$ in the perturbation of $\mathbf{y}_n$ in the argument (here just $\mathbf{f}$), and then expanding in powers

of the resulting power series. The lth power of this series results in terms of the form $\frac{\mathbf{f_{y\cdots y}}}{l!}$ operating on l-fold products of its terms. Any l terms whose orders in h sum to a particular order contribute to the overall result at that order, much like the convolution of coefficients that gives the coefficient of a certain order in a polynomial product.

Any subsequent stage can be expanded in the same manner. The description of this process in terms of rooted trees is simply that new trees are built by attaching any number of trees obtained at the prior stage to a new root node. In the ith stage we expand the evaluation of $\mathbf{f}$ at $\mathbf{y}_{n,i} = y + h(\beta_{i1}\mathbf{y}'_{n,1} + \cdots + \beta_{i(i-1)}\mathbf{y}'_{n,i-1})$. To do so, we first collect like terms in the expansions we have already obtained for $\mathbf{y}'_{n,1}, \ldots, \mathbf{y}'_{n,i-1}$ to obtain a single expansion $\mathbf{y}_{n,i} = \mathbf{y} + \sum(T_m h^m)^l$. This simply involves summing the parameters for the current stage times the corresponding coefficients obtained at the previous stage. Then the $(\frac{\mathbf{f_{y\cdots y}}}{l!}(\sum T_m h^m)^l)$ term of the Taylor expansion of $\mathbf{f}(\mathbf{y}_{n,i})$ is comprised of terms of the form $(\mathbf{f_{y\cdots y}}\ T_{i_1}\cdots T_{i_m})$. This is represented as a rooted tree whose root node is attached to the m trees corresponding to the terms $T_{i_1}, \ldots, T_{i_m}$ in the prior stage of the expansion. Now here is the expansion for $r = 4$.

$$\mathbf{y}'_{n,1} = \mathbf{f}(\mathbf{y}_n) = \mathbf{f},$$

$$\begin{aligned}
\mathbf{y}'_{n,2} &= \mathbf{f}(\mathbf{y}_n + h(\beta_{21}\mathbf{y}'_{n,1})) = \mathbf{f}(\mathbf{y}_n + h(\beta_{21}\mathbf{f})) \\
&= \mathbf{f} + (\mathbf{f_y}\ (h\beta_{21}\mathbf{f})) \\
&\quad + (\frac{\mathbf{f_{yy}}}{2!}\ (h\beta_{21}\mathbf{f})^2) + (\frac{\mathbf{f_{yyy}}}{3!}\ (h\beta_{21}\mathbf{f})^3) + \cdots \\
&= \mathbf{f} + h\beta_{21}(\mathbf{f_y}\ \mathbf{f}) + \frac{h^2}{2!}\beta_{21}^2(\mathbf{f_{yy}}\ \mathbf{f}\ \mathbf{f}) + \frac{h^3}{3!}\beta_{21}^3\ (\mathbf{f_{yyy}}\ \mathbf{f}\ \mathbf{f}\ \mathbf{f}) + \cdots,
\end{aligned}$$

$$\begin{aligned}
\mathbf{y}'_{n,3} &= \mathbf{f}(\mathbf{y}_n + h(\beta_{31}\mathbf{y}'_{n,1} + \beta_{32}\mathbf{y}'_{n,2})) \\
&= \mathbf{f}(\mathbf{y}_n + h(\beta_{31} + \beta_{32})\mathbf{f} \\
&\qquad + h^2\beta_{32}\beta_{21}(\mathbf{f_y}\ \mathbf{f}) + \frac{h^3}{2!}\beta_{32}\beta_{21}^2(\mathbf{f_{yy}}\ \mathbf{f}\ \mathbf{f}) + \cdots)
\end{aligned}$$

$$
\begin{aligned}
&= \mathbf{f} + (\mathbf{f_y}\ (h(\beta_{31}+\beta_{32})\mathbf{f} \\
&\qquad + h^2\beta_{32}\beta_{21}(\mathbf{f_y}\ \mathbf{f}) + \frac{h^3}{2!}\beta_{32}\beta_{21}^2(\mathbf{f_{yy}}\ \mathbf{f}\ \mathbf{f}) + \cdots)) \\
&\quad + (\frac{\mathbf{f_{yy}}}{2!}\ (h(\beta_{31}+\beta_{32})\mathbf{f} + h^2\beta_{32}\beta_{21}(\mathbf{f_y}\ \mathbf{f}) + \cdots)^2) \\
&\quad + (\frac{\mathbf{f_{yyy}}}{3!}\ (h(\beta_{31}+\beta_{32})\mathbf{f} + \cdots)^3) + \cdots \\
&= \mathbf{f} + h(\beta_{31}+\beta_{32})(\mathbf{f_y}\ \mathbf{f}) + h^2\beta_{32}\beta_{21}(\mathbf{f_y}\ (\mathbf{f_y}\ \mathbf{f})) \\
&\quad + \frac{h^3}{2!}\beta_{32}\beta_{21}^2(\mathbf{f_y}\ (\mathbf{f_{yy}}\ \mathbf{f}\ \mathbf{f})) + \cdots \\
&\quad + \frac{h^2}{2!}(\beta_{31}+\beta_{32})^2(\mathbf{f_{yy}}\ \mathbf{f}\ \mathbf{f}) \\
&\quad + \frac{2h^3}{2!}(\beta_{31}+\beta_{32})\beta_{32}\beta_{21}(\mathbf{f_{yy}}\ (\mathbf{f_y}\ \mathbf{f})\ \mathbf{f}) \\
&\quad + \frac{h^3}{3!}(\beta_{31}+\beta_{32})^3(\mathbf{f_{yyy}}\ \mathbf{f}\ \mathbf{f}\ \mathbf{f}) + \cdots,
\end{aligned}
$$

$$
\begin{aligned}
\mathbf{y}'_{n,4} &= \mathbf{f}(\mathbf{y}_n + h(\beta_{41}\mathbf{y}'_{n,1} + \beta_{42}\mathbf{y}'_{n,2} + \beta_{43}\mathbf{y}'_{n,3})) \\
&= \mathbf{f}(\mathbf{y}_n + h(\beta_{41}+\beta_{42}+\beta_{43})\mathbf{f} + h^2(\beta_{42}\beta_{21} + \beta_{43}(\beta_{31}+\beta_{32}))(\mathbf{f_y}\ \mathbf{f}) \\
&\quad + \frac{h^3}{2!}(2\beta_{43}\beta_{32}\beta_{21}(\mathbf{f_y}\ (\mathbf{f_y}\ \mathbf{f})) \\
&\qquad + (\beta_{42}\beta_{21}^2 + \beta_{43}(\beta_{31}+\beta_{32})^2)(\mathbf{f_{yy}}\ \mathbf{f}\ \mathbf{f})) + \cdots) \\
&= \mathbf{f} + (\mathbf{f_y}(h(\beta_{41}+\beta_{42}+\beta_{43})\mathbf{f} + h^2(\beta_{42}\beta_{21}+\beta_{43}(\beta_{31}+\beta_{32}))(\mathbf{f_y}\ \mathbf{f}) \\
&\quad + \frac{h^3}{2!}(2\beta_{43}\beta_{32}\beta_{21}(\mathbf{f_y}\ (\mathbf{f_y}\ \mathbf{f})) \\
&\qquad + (\beta_{42}\beta_{21}^2 + \beta_{43}(\beta_{31}+\beta_{32})^2)(\mathbf{f_{yy}}\ \mathbf{f}\ \mathbf{f})) + \cdots)) \\
&\quad + (\frac{\mathbf{f_{yy}}}{2!}\ (h(\beta_{41}+\beta_{42}+\beta_{43})\mathbf{f} \\
&\qquad + h^2(\beta_{42}\beta_{21} + \beta_{43}(\beta_{31}+\beta_{32}))(\mathbf{f_y}\ \mathbf{f}) + \cdots))^2 \\
&\quad + (\frac{\mathbf{f_{yyy}}}{3!}\ (h(\beta_{41}+\beta_{42}+\beta_{43})\mathbf{f} + \cdots))^3 + \cdots
\end{aligned}
$$

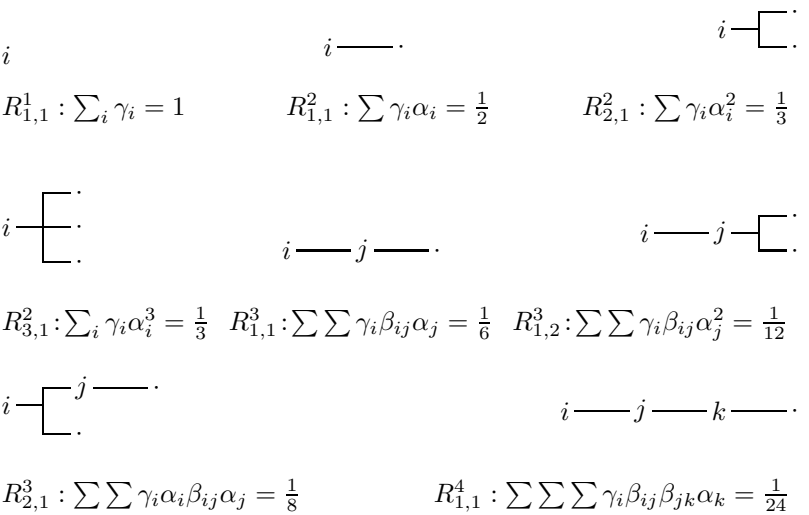
$$
\begin{aligned}
&= \mathbf{f} + h(\beta_{41}+\beta_{42}+\beta_{43})(\mathbf{f_y}\ \mathbf{f}) \\
&\quad + h^2(\beta_{42}\beta_{21}+\beta_{43}(\beta_{31}+\beta_{32}))(\mathbf{f_y}\ (\mathbf{f_y}\ \mathbf{f})) \\
&\quad + \frac{h^3}{2!}(2\beta_{43}\beta_{32}\beta_{21}(\mathbf{f_y}\ (\mathbf{f_y}\ (\mathbf{f_y}\ \mathbf{f}))) \\
&\qquad\qquad + (\beta_{42}\beta_{21}^2+\beta_{43}(\beta_{31}+\beta_{32})^2)(\mathbf{f_y}\ (\mathbf{f_{yy}}\ \mathbf{f}\ \mathbf{f})+\cdots)) \\
&\quad + \frac{h^2}{2!}(\beta_{41}+\beta_{42}+\beta_{43})^2(\mathbf{f_{yy}}\ \mathbf{f}\ \mathbf{f}) \\
&\quad + \frac{2h^3}{2!}(\beta_{41}+\beta_{42}+\beta_{43})(\beta_{42}\beta_{21}+\beta_{43}(\beta_{31}+\beta_{32}))(\mathbf{f_{yy}}(\mathbf{f_y}\ \mathbf{f})\ \mathbf{f})+\cdots \\
&\quad + \frac{h^3}{3!}((\beta_{41}+\beta_{42}+\beta_{43})^3(\mathbf{f_{yyy}}\ \mathbf{f}\ \mathbf{f}\ \mathbf{f})+\cdots).
\end{aligned}
$$

Below is a summary of the elementary differential terms that appeared in the expansion, according to their order in h. The notation $R^i_{l,m}$ identifies the order h^i, the order l of the leading derivative of $\mathbf{f}$, and the index m among such terms. Next to this is the T^k_j of the corresponding term in the Taylor expansion, followed by the equation of coefficients from the respective expansions. Recall the notation $\alpha_i = \sum_{j=1}^{i-1}\beta_{ij}$ for expressions that appear repeatedly in the expansion.

h^k, Elementary Differential	$R^i_{l,m}$	T^k_j	RK coefficient $= T$ coefficient
$h^1(\mathbf{f})$	$R^1_{1,1}$	T^1_1	$\gamma_1+\gamma_2+\gamma_3+\gamma_4 = \frac{1}{1!}$
$h^2(\mathbf{f_y}\ \mathbf{f})$	$R^2_{1,1}$	T^2_1	$\gamma_2\alpha_2+\gamma_3\alpha_3+\gamma_4\alpha_4 = \frac{1}{2!}$
$h^3(\mathbf{f_{yy}}\ \mathbf{f}\ \mathbf{f})$	$R^2_{2,1}$	T^3_1	$\frac{1}{2!}(\gamma_2\alpha_2^2+\gamma_3\alpha_3^2+\gamma_4\alpha_4^2) = \frac{1}{3!}$
$h^3(\mathbf{f_y}\ (\mathbf{f_y}\ \mathbf{f}))$	$R^3_{1,1}$	T^3_2	$\gamma_3\beta_{32}\alpha_2+\gamma_4(\beta_{42}\alpha_2+\beta_{43}\alpha_3) = \frac{1}{3!}$
$h^4(\mathbf{f_{yyy}}\ \mathbf{f}\ \mathbf{f}\ \mathbf{f})$	$R^2_{3,1}$	T^4_1	$\frac{1}{3!}(\gamma_2\alpha_2^3+\gamma_3\alpha_3^3+\gamma_4\alpha_4^3) = \frac{1}{4!}$
$h^4(\mathbf{f_y}\ (\mathbf{f_{yy}}\ \mathbf{f}\ \mathbf{f}))$	$R^3_{1,2}$	T^4_3	$\frac{1}{2!}(\gamma_3\beta_{32}\alpha_2^2+\gamma_4(\beta_{42}\alpha_2^2+\beta_{43}\alpha_3^2)) = \frac{1}{4!}$
$h^4(\mathbf{f_{yy}}\ (\mathbf{f_y}\ \mathbf{f})\ \mathbf{f})$	$R^3_{2,1}$	T^4_3	$\gamma_3\alpha_3\beta_{32}\alpha_2+\gamma_4\alpha_4(\beta_{42}\alpha_2+\beta_{43}\alpha_3) = \frac{3}{4!}$
$h^4(\mathbf{f_y}\ (\mathbf{f_y}\ (\mathbf{f_y}\ \mathbf{f}]$	$R^4_{1,1}$	T^4_4	$\gamma_4\beta_{43}\beta_{32}\alpha_2 = \frac{1}{4!}$

The rooted trees $R^i_{l,m}$ corresponding to elementary differentials up to order $k=4$ are shown below in order of their occurrence in stages $i = 1,\ldots,4$ of the Runge-Kutta approximation. Within a

stage, we have listed trees by the order l of the l-fold product that produces them, i.e., by how many previously existing trees are attached to a new root node in order to construct the tree.



$R^1_{1,1} : \sum_i \gamma_i = 1$ $\quad R^2_{1,1} : \sum \gamma_i \alpha_i = \frac{1}{2}$ $\quad R^2_{2,1} : \sum \gamma_i \alpha_i^2 = \frac{1}{3}$

$R^2_{3,1} : \sum_i \gamma_i \alpha_i^3 = \frac{1}{3}$ $\quad R^3_{1,1} : \sum \sum \gamma_i \beta_{ij} \alpha_j = \frac{1}{6}$ $\quad R^3_{1,2} : \sum \sum \gamma_i \beta_{ij} \alpha_j^2 = \frac{1}{12}$

$R^3_{2,1} : \sum \sum \gamma_i \alpha_i \beta_{ij} \alpha_j = \frac{1}{8}$ $\quad R^4_{1,1} : \sum \sum \sum \gamma_i \beta_{ij} \beta_{jk} \alpha_k = \frac{1}{24}$

Just as for the first-order Taylor expansion of $\mathbf{y}(t+h)$, there is only one tree at the first stage of the Runge-Kutta expansion, the tree corresponding to $\mathbf{f}$ itself. However, at the second stage, there is already an infinite family of trees corresponding to the infinite series of terms $(\mathbf{f}_{\mathbf{y}\cdots\mathbf{y}}\ \mathbf{f} \cdots \mathbf{f})$ with l $\mathbf{y}$'s and operands $\mathbf{f}$ for $l = 0, 1, \ldots$. So while the third-order tree corresponding to $(\mathbf{f}_{\mathbf{yy}}\ \mathbf{f}\ \mathbf{f})$ appears at the second stage, the other third-order tree corresponding to $(\mathbf{f}_{\mathbf{y}}\ (\mathbf{f}_{\mathbf{y}}\ \mathbf{f}))$ does not. This tree only appears in the first-order term of the expansion of this series at the third stage when $(\mathbf{f}_{\mathbf{y}}$ is added in front of existing terms including $(\mathbf{f}_{\mathbf{y}}\ \mathbf{f})$, or in tree form, the tree corresponding to $(\mathbf{f}_{\mathbf{y}}\ \mathbf{f})$ is attached to a new root node. Carrying this further, we can see that the tree with r nodes having depth $r-1$ corresponding to the elementary differential of the form $(\mathbf{f}_{\mathbf{y}}\ (\mathbf{f}_{\mathbf{y}} \ldots (\mathbf{f}_{\mathbf{y}}\ \mathbf{f}]$ does not occur until the rth stage of a Runge-Kutta expansion. Note that the tree corresponding to $(\mathbf{f}_{\mathbf{yy}}\ \mathbf{f}\ \mathbf{f})$, and in fact every tree that occurs at the second stage, also recurs as the first term in each order at every subsequent stage.

Conversely, since every tree with r nodes arises by attaching some number of trees with strictly fewer nodes to its root, every tree with r nodes does occur by the rth stage. This shows that r stages are necessary for a Runge-Kutta expansion to match a Taylor expansion to order r, because at least one term is missing with fewer stages. It also shows that all of the terms necessary for matching are present at the rth stage, but sufficiency depends upon the relation between the number of parameters, $r(r+1)/2$, that define an r stage method and the number of coefficient equations corresponding to the elementary differential (or rooted tree) up to a given order. In particular, we have seen that there is one parameter for one-stage methods and one tree for first-order agreement, and one method, Euler's Method, satisfies the matching conditions. There are three parameters for two-stage methods, and only two trees of order two or less, resulting in a one-parameter family of explicit two-stage Runge-Kutta Methods of order two. There are three more parameters for three-stage methods, and with two more trees at order three with conditions to match, we reach a two-parameter family of three-stage methods of order three. With four more parameters for a four-stage method, but also four additional trees with four nodes, there will again be a two-parameter family of four-stage methods of order four. But since there are nine rooted trees having five nodes, two free fourth-stage parameters plus five new fifth-stage parameters are still deficient by two. Six stages are required to achieve a fifth-order method.

The conditions for matching the Runge-Kutta and Taylor expansion terms involving an elementary differential can be obtained directly from the structure of the corresponding rooted tree. For this purpose, we relabel the nonleaf nodes with index symbols for summation. Note that the earlier labeling with $\mathbf{y}$-derivatives of $\mathbf{f}$ was helpful but not actually necessary to recover the elementary differential, and the same holds here for recovering coefficients. The coefficients developed in successive stages arose from summing over the β parameters of the method times corresponding coefficients of previous elementary differential terms. Therefore, each time we attach an existing node to a new root node, we contribute a sum of the corresponding β coefficients to the coefficient corresponding to the resulting tree. Each leaf

node contributes $\alpha_i = \beta_{ij}$ for the stage it represents and therefore does not need to be indexed. Though the purposes are slightly different, the form in which β coefficients appear is the same as that of the γ coefficients. The β's are used to construct evaluation points for $\mathbf{f}$, $y'_{n,i} = \mathbf{f}(\mathbf{y}_{n,i})$, with $\mathbf{y}_{n,i} = \mathbf{y}_n + \beta_{n,1}\mathbf{y}'_{n,1} + \cdots + \beta_{n,i}\mathbf{y}'_{n,i-1}$. When we have obtained sufficiently many (i.e., r) of these evaluations, the γ's are used to obtain $\mathbf{y}_{n+1} = \mathbf{y}_n + \gamma_{n,1}\mathbf{y}'_{n,1} + \cdots + \gamma_{n,r}\mathbf{y}'_{n,r}$. Because of this, the form of the coefficient formula associated with a particular tree is the same regardless of the number of stages of the method in which it appears. In other words, the coefficient formulas and corresponding matching conditions for a four-stage method reduce to those for a three-stage method simply by eliminating all terms involving coefficients whose first index is ≥ 4. If we only retain terms involving coefficients whose first index is ≤ 2, we recover the two conditions we found for a two-stage method to be second-order.

The rooted trees corresponding to exactness of the solution of the polynomial accuracy model problems $y' = (t^P)'$ are the depth-one trees with P nodes, $R^2_{P-1,1} = T^P_1$, that occur at the second stage. These are the only rooted trees of order $P \leq 2$. Therefore, exactness on equations whose solutions are polynomials of degree P is necessary and sufficient for general Pth-order accuracy of an explicit Runge-Kutta Method when $P \leq 2$. Even though these trees occur at the second stage, for $P > 2$, P stages are required to match the Taylor coefficient. The rooted trees corresponding to Pth-order accuracy for the absolute stability model problem $y' = \lambda y$ are the maximal depth trees with P nodes, $R^P_{1,1} = T^P_P$, i.e., the trees with one edge leaving every node except the leaf. For this problem, all derivatives of $\mathbf{f}(\mathbf{y})$ beyond the first are zero. This tree does not occur until the Pth stage. Therefore, P stages are necessary for general Pth-order accuracy.

Below the trees representing eight elementary differentials of order ≤ 4, we have collected the factors from the two sides of the matching conditions in the table into one of the form $1/d(T)$. Here $d(T)$ arises as the ratio of the multiplicity of ways the tree can be constructed by addition of edges and leaves on the Taylor side and a combination of lth-order expansion factorials and multinomial coefficients on the Runge-Kutta side. These factors can also be computed

directly from their trees using the following simple algorithm. The density of any leaf, a rooted tree of order one arising from evaluating $\mathbf{f}$ in the first stage, is 1. At every subsequent stage, at which we attach one or more trees to a new root node, the density of the resulting trees is the product of the densities of the trees being attached, times the order of the resulting tree. For example, the tree $R^3_{2,1}$ is a rooted tree with four nodes corresponding to the elementary differential $(\mathbf{f_{yy}}\ (\mathbf{f_y}\ \mathbf{f})\ \mathbf{f})$. It is first obtained at the $i = 3$rd stage of the Runge-Kutta expansion in the $l = 2$nd-order term of the expansion, by joining the trees corresponding to $(\mathbf{f_y}\ \mathbf{f})$ and $\mathbf{f}$. The former has density $1 \cdot 2$ and the latter has density 1, so since the resulting tree has order 4, its density is $1 \cdot 2 \cdot 4 = 8$.

For $r = 4$ stages, the eight fourth-order matching conditions are

$$\gamma_1 + \gamma_2 + \gamma_3 + \gamma_4 = 1, \qquad \gamma_2\alpha_2 + \gamma_3\alpha_3 + \gamma_4\alpha_4 = \tfrac{1}{2},$$
$$\gamma_2\alpha_2^2 + \gamma_3\alpha_3^2 + \gamma_4\alpha_4^2 = \tfrac{1}{3}, \qquad \gamma_3\beta_{32}\alpha_2 + \gamma_4(\beta_{42}\alpha_2 + \beta_{43}\alpha_3) = \tfrac{1}{6},$$
$$\gamma_2\alpha_2^3 + \gamma_3\alpha_3^3 + \gamma_4\alpha_4^3 = \tfrac{1}{4}, \qquad \gamma_3\beta_{32}\alpha_2^2 + \gamma_4(\beta_{42}\alpha_2^2 + \beta_{43}\alpha_3^2) = \tfrac{1}{12},$$
$$\gamma_3\alpha_3\beta_{32}\alpha_2 + \gamma_4\alpha_4(\beta_{42}\alpha_2 + \beta_{43}\alpha_3) = \tfrac{1}{8}, \qquad \gamma_4\beta_{43}\beta_{32}\alpha_2 = \tfrac{1}{24}.$$

The recommended procedure for solving the equations is to choose $\alpha_2, \ldots, \alpha_r$ and then solve the r equations, $\sum_{i=1}^r \gamma_i\alpha_i^k,\ k = 0, \ldots, r-1$, for $\gamma_1, \ldots, \gamma_r$. Next, solve for the β_{ij} that are determined by linear equations. In this case, the fourth, sixth, and seventh equations above allow us to solve for β_{32}, β_{42}, and β_{43}. The classical fourth-order Runge-Kutta Method corresponds to the solution obtained by setting $\alpha_2 = \alpha_3 = \frac{1}{2}$, $\alpha_4 = 1$, given in tableau form as

$$\begin{array}{c|cccc} 0 & & & & \\ \frac{1}{2} & \frac{1}{2} & & & \\ \frac{1}{2} & 0 & \frac{1}{2} & & \\ 1 & 0 & 0 & 1 & \\ \hline & \frac{1}{6} & \frac{2}{6} & \frac{2}{6} & \frac{1}{6} \end{array}$$

For the scalar ODE with $f_y = 0$, i.e., $y' = f(t)$, this method reduces to the Simpson-parabolic quadrature method.

Among the methods satisfying the matching equations of a given order, optimal methods can be obtained by minimizing local truncation error bounds. A well-known example of this is the two-stage method of order 2 known as *Ralston's Method*, given in tableau form as

$$\begin{array}{c|cc} 0 & & \\ \frac{3}{4} & \frac{3}{4} & \\ \hline & \frac{1}{3} & \frac{2}{3} \end{array}$$

Pairs of closely related Runge-Kutta Methods can be used for automatic step-size control in the same manner that pairs of multistep methods are used for error estimation and step-size modification. A well-known example of this technique is the Runge-Kutta-Fehlberg pair consisting of a five-stage and six-stage method of orders 4 and 5, respectively. Further details on these and other topics, including special cases for scalar, autonomous, and constant coefficient systems of equations, methods based on extrapolation, methods to treat second- and higher-order equations directly, etc., can be found in [BJ].

The region of absolute stability for an explicit r-stage method is determined by one step of the method applied to the absolute stability model problem, $y' = \lambda y$. For $r \leq 4$, we know that the coefficients can be chosen so that the method has order of accuracy $P = 4$. In this case the region of absolute stability is $\{w \in \mathbf{C} \mid |p_r(w)| \leq 1\}$ where $p_r(z) = \sum_{k=0}^{r} z^k/k!$, the truncation to degree r of the exact exponential series solution of the model problem (Figure 5.14). For $r > 4$, we must replace p_r by some polynomial of degree $\leq r$ that depends on the specifics of the method.

Implicit Runge-Kutta Methods can be employed if larger stability regions are required. See [IA1] for a discussion of these methods and their relation to Gauss-Legendre quadrature and collocation methods. Of particular relevance to the topic of this appendix are several publications on Runge-Kutta Methods for Hamiltonian systems. Explicit symplectic Runge-Kutta Methods only exist for general Hamiltonians that are separable, but the implicit Gauss-Legendre Runge-Kutta Methods are symplectic and they are optimal for general Hamiltonians. See [IA2], [SJM], [CS], [HLW], [YH], [CP].