Runge-Kutta Approximations of Arbitrary Order for $y' = f(x, y)$.

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July 12, 1995

1. Introduction.

It is the purpose of this paper to generalize the Runge-Kutta Method to Polynomial Approximations of Arbitrary Order. The essential tools that we use are composition of Lagrange Interpolation Formulas and the Inverse of the Vandermonde Matrix in the form (2.23).

We might term our method "Nonlinear Gaussian Quadratures" for it gives the same $2n^{\text{th}}$ order accuracy as the zeros of the nth Legendre Polynomial. We replace the orthogonality of the Legendre Polynomials by an admissibility condition applied to the mesh points $\nu_1, ..., \nu_n$. When $\nu_1 > 0$ we adjoin the root $\nu_0 = 0$ and consider the polynomials $P_k(t) = t(t - \nu_1), ..., (t - \nu_k)$ for each $k \leq n - 1$. These must satisfy the condition that γ_k, defined by 10.14, be non-vanishing for each mesh point $x = \nu_j$, $j = 1, ..., k + 1$ and for each $k = 1, ..., n - 1$. That this need not be satisfied at $x = 0$ follows from the fact that β_k, defined by 11.7 has the limit -1 as $x \to 0$.

We confine our attention to the case of a single first order non-autonomous ordinary differential equation. Once the formulas have been obtained, they extend immediately to systems, so the assumption that the equation be non-autonomous is not essential.

For approximation of even order $2n$ using the non-linear version of Gaussion Quadratures, the number of computations of f required is $p(p + 3)/2 + 2$. This

uses the zeros of an admissable mesh of $n = p + 1$ points. The complexity agrees with that of Butcher, $p = 2$ and Curtis, $p = 3$. It is one less that obtained by Hairer, $p = 4$.

The method is based on the fact that when adding up two or more numbers we can tolerate errors in the individual terms of the sum as long as they cancel. This fact is used to minimize the number of computations of f.

In Section 2, we introduce some notations regarding Lagrange Interpolation Polynomials. In Section 3, we show that in a Taylor Expansion of order $2p$ we may replace the coefficients of order greater than p by multiplies and retain the magnitude of the error by imposing a linear constraint. In Section 4, we change coordinates so that the constraint is given in terms of $f(x, y)$ evaluated at the mesh points. In Section 5, we show how the general solution of this system can be obtained from a particular solution. Section 6 is devoted to showing that the system has maximal rank. Section 7 obtains an identity which is used to simplify the forward elimination. It turns out that this system can be arranged in blocks with the right sides depending on variables already solved for. In Section 8, we apply forward elimination to these blocks and at the same time uncouple the systems so that each depends on only its own variables. In Section 9, we show that diagonal back substitution can be used to obtain a closed form solution of the system.

We prepare for the use of Lagrange Interpolation by polynomials with double roots in Section 10. In Section 11, we show that the results of Section 10 can be used as stated for linear differential equations or numerical integration. We then go on to show how to apply them to nonlinear equations.

Section 12 is devoted to modifying the averaging technique so that it may be applied to the perturbation errors of the constructable Runge, Kutta, Butcher Approximation and Section 13 is devoted to explaining the algorithm. In Section 14, we determine the form of the perturbation errors and, in Section 15, we explain how to deform the constructable approximation into the theoretical solution, then showing that they have the same error.

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2. Taylor Polynomials, Lagrange Interpolation Polynomials and the Vandermonde Matrix Applied to Numerical Integration.

Let $f \in C^{n+1}$ so that

$$(2.1) \qquad f(h) = \sum_{\ell=0}^{n} f_\ell h^\ell + O\left(h^{n+1}\right)$$

in a neighborhood of $h = 0$. Let us choose points

$$(2.2) \qquad 0 = \nu_0 < \nu_1 < ... < \nu_n \leq 1 \equiv \nu_{n+1}.$$

The point ν_{n+1} is unnecessary when $\nu_n = 1$, but it allows us to consider the classical Simpson approximation and Gaussion Quadrature as special cases of the same theory.

$$(2.3) \qquad \sum_{j=0}^{n} \nu_i^j \left(f_j h^i\right) = f(\nu_i h) + O\left(h^{n+1}\right), \quad i = 0, ..., n.$$

This is a linear system in the variables

$$(2.4) \qquad f_j h^j, \quad j = 0, ..., n$$

whose matrix is the Vandermonde matrix

$$(2.5) \qquad (\nu_i)^j, \quad 0 \leq i, \; j \leq n.$$

If we multiply (2.3) by its inverse

$$(2.6) \qquad W_{\ell,i}^n, \quad 0 = \ell, \; i \leq n$$

and sum we obtain

$$(2.7) \qquad f_\ell h^\ell = \sum_{j=0}^{n} W_{\ell,i}^n f(\nu_i h) + O\left(h^{n+1}\right).$$

Then by putting (2.7) into (2.1), we have

$$(2.8) \qquad f(h) = \sum_{j=0}^{n} C_j f(\nu_j h) + O\left(h^{n+1}\right)$$

where

$$(2.9) \qquad C_j = \sum_{\ell=0}^{n} W_{\ell,i}^{n}.$$

This reduces the problem of approximating the Taylor Polynomial of f in a neighborhood of zero to evaluation of f at $n+1$ points. Of course, the big O constant depends on the choice of the set of points.

We shall be working with consecutive subsets of the list (2.2). This leads to the arrays

$$(2.10) \qquad \nu_i^{j}, \quad q \le i \le r, \quad 0 \le j \le r - q$$

which may be regarded as a matrix whose rows and columns have different index sets. For the purpose of determining its inverse we introduce the polynomials

$$(2.11) \qquad p^{r,q}(x) = \prod_{j=q}^{r} (x - \nu_j),$$

the divided differences

$$(2.12) \qquad P_k^{r,q}(x) = \frac{p^{r,q}(x)}{(x - \nu_k)}, \quad q \le k \le r,$$

and the corresponding Lagrange interpolation polynomials

$$(2.13) \qquad \mathcal{P}_k^{r,q}(x) = \frac{P^{r,q}(x)}{P_k^{r,q}(\nu_k)}, \quad q \le k \le r.$$

The inverse of (2.10) is then

$$(2.14) \qquad W_{k,j}^{r,q} = (-1)^{r-q-j} \frac{S_{r-q-j}(\nu_q, ..., \nu_{k-1}, \nu_{k+1}, ...\nu_r)}{P_k^{r,q}(\nu_k)}$$

for $0 \le j \le r - q$ and $q \le k \le r$.

At times we suppress the second superscript when it is zero.

We shall now apply the above material to the approximation of

$$(2.15) \qquad \int_0^h f(x)\, dx \equiv \int_0^{\nu_{n+1}h} f(x)\, dx$$

using the values of f at the points

$$(2.16) \qquad \nu_i h, \quad q \le i \le r, \quad \text{with } \nu_i \text{ defined by (2.2)}.$$

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Then, we have for $f \in C^{n+1}$

$$(2.17) \qquad f(x) = \sum_{k=q}^{r} f(\nu_k h) \, \mathcal{P}_k^{r,q}(x) + O\left(h^{r-q+1}\right).$$

It follows that if we define

$$(2.18) \qquad a_{\ell,k}^{n,q} = \int_0^{\nu_\ell} \mathcal{P}_k^n(x) \, dx$$

we have

$$(2.19) \qquad \int_0^{\nu_\ell h} f(x) \, dx = h \sum_{k=q}^{r} a_{\ell,k}^{r,q} f(\nu_k h) = 0\left(h^{r-q+2}\right)$$

for each $\ell = 0, ..., n+1$. The generalization of the classical Simpson approximation corresponds to even $n = 2p$, $q = 0$, $r = 2p$, $f \in C^{n+2}$ and the ν's satisfy the symmetry condition

$$(2.20) \qquad \nu_{2p-j} = \nu_j, \ j = 0, ..., 2p, \ \nu_{2p-1} = 1.$$

We then obtain an extra order of magnitude in the error

$$(2.21) \qquad \int_0^h f(x) \, dx = \sum_{k=0}^{n} a_{n+1,k}^{r,q} f(\nu_k h) + O\left(h^{n-q+3}\right)$$

The Gaussian Quadratures correspond to $n = p + 1$, $q = 1$ and the ν_i's being the zeros of the Legendine Polynomials translated to the interval $[0, 1]$. The orthogonality then gives the same error as above with half the number of mesh points. We also obtain extra stability from the fact that the coefficients $\mathcal{A}_{n+1,k}^{n,1}$ are positive. By contrast, the Uniform Mesh Simpson Formulas begins to develop negative coefficients at $n = 8$.

The coefficient $a_{\ell,k}^{r,q}$ are homogeneous of degree zero in k. We may, therefore, assume that $h = 1$ and use (2.12), (2.14) to deduce that

$$(2.22) \qquad a_{\ell,j}^{r,q} = \sum_{k=0}^{r-q} W_{j,k}^{r,q} \frac{\nu_\ell^{k+1}}{(k+1)}$$

for $j = 0, ..., n \ \ell = 0, ..., n+1$.

We shall make frequent use of the fact that

$$(2.23) \qquad \sum_{j=0}^{r-q} W_{k,j}^{r,q} (\nu_\ell)^j = \mathcal{P}_k^{r,q}(\nu_\ell)$$

for any $\ell, 0 \le \ell \le n$ and of course that)

$$(2.24) \qquad \mathcal{P}_k^{r,q}(\nu_\ell) = \delta_{k,\ell}, \ q \le k, \ \ell \le r.$$

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3. The Generalized Runge-Kutta System.

Let us approximate solutions of the first order ordinary differential initial value problem

(3.1) $$y' = f(x,y), \quad y(0) = b$$

by applying numerical integration to its integral representation

(3.2) $$y(h) = b + \int_0^h f(t, y(t)) \, dt.$$

In order to cover both cases of generalized Simpson Approximations and Gaussian Quadratures, let us consider the approximation, with q having a different significance than in Section 2.

(3.3) $$y(h) = b + h \sum_{j=0}^{m} a_j f(\nu_j h, y(\nu_j h))$$

$$+ O\left(h^{q+3}\right).$$

where

(3.4) $$p = [(q+1)/2],$$

the greatest integer in $(q+1)/2$.

Then we may obtain a usable numerical scheme by using the Taylor approximation

(3.5) $$y(h) = \sum_{i=0}^{q+1} y_i h^i + 0\left(h^{q+2}\right)$$

and substituting

(3.6) $$y(\nu_j h) = \sum_{i=0}^{q+1} y_i (\nu_j h)^i + 0\left(h^{q+2}\right).$$

Since it is

(3.7) $$v(h) = y'(h) = f(h, y(h))$$

that is most easily computed, we use the integrated form of

(3.8) $$v(h) = \sum_{i=0}^{q} v_i h^i + O\left(h^{q+1}\right)$$

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and replace (3.4), (3.5) by

$$(3.9) \qquad y(h) = b + h \sum_{i=0}^{q} \frac{v_i}{i+1} h^i + O\left(h^{q+2}\right)$$

and hence,

$$(3.10) \qquad y(\nu_j h) = b + h \sum_{i=0}^{q} \frac{v_i}{i+1} (\nu_j)^{i+1} h^i + O\left(h^{q+2}\right).$$

Then, if we approximate (3.10) by

$$(3.11) \qquad w_j(h) = b + h \sum_{i=0}^{q} \lambda_{j,i} v_i h^i$$

where w_j agrees with $y(\nu, h)$ to p terms in its Taylor Expansion, that is

$$(3.12) \qquad \lambda_{j,i} = \frac{(\nu_j)^{i+1}}{i+1}, \quad 0 \le i \le p-1,$$

we find that

$$f(\nu_j h, \, w_j(h)) - f(\nu_j h, \, y(\nu_j h))$$

$$(3.13) \qquad = f_y(\nu_j h, \, y(\nu_j h)) (w_j(h) - y(\nu_j h))$$

$$+ O\left(h^{2p+2}\right).$$

Hence, by using (3.12) and (3.13) in (3.3), we have

$$(3.14) \qquad y(h) = b + h \sum_{j=0}^{m} a_j f(\nu_j h, \, w_j(h))$$

$$+ E + O\left(h^{q+3}\right)$$

where

$$(3.15) \qquad E = -h^2 \sum_{j=1}^{m} a_j f_y(\nu_j h, \, y(\nu_j h)) [w_j(h) - y(\nu_j h)].$$

The error $O\left(h^{q+3}\right)$ can therefore be preserved by imposing the constraint $E = O\left(h^{q+3}\right)$. To this end we expand

$$(3.16) \qquad f_y(h, y(h)) = \sum_{k=0}^{q-p} b_k h^k + O\left(h^{q-p+1}\right).$$

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It follows that

$$(3.17) \qquad E = -h^2 \sum_{j=1}^{m} a_j \sum_{k=0}^{q-p} b_k \sum_{i=p}^{q} \left(\lambda_{j,i} - \frac{\nu_j^{i+1}}{i+1} \right) \nu_j^k v_i h^{i+k}.$$

Hence, the error $O\left(h^{2q+3}\right)$ is preserved if we impose the linear constraints

$$(3.18) \qquad \sum_{j=1}^{m} a_j \left(\nu_j\right)^k \left[\lambda_{j,i} - \frac{\left(\nu_j\right)^{i+1}}{i+1} \right] = 0$$

for
$$(3.19) \qquad p \le i \le q, \quad 0 \le k \le q - p$$

or equivalently
$$(3.20) \qquad 0 \le k \le q - i, \quad p \le i \le q.$$

The number of constraints is therefore

$$(3.21) \qquad \sum_{k=0}^{q-p} (q+1-p-k) = \sum_{j=1}^{q+1-p} j = \frac{(q+1-p)(q+2-p)}{2}.$$

Then, the number of unknowns is

$$(3.22) \qquad m\left(q+1-p\right)$$

and the number of unknowns exceed the number of equations by

$$(3.23) \qquad \left(q+1-p\right)\left(2m+p-q-2\right).$$

4. A Change of Variables in the Generalized Runge-Kutta System.

Since it is $v\left(h\right) = f\left(h, y\left(h\right)\right)$ that is most easily computed, we now express

$$(4.1) \qquad \omega_j\left(h\right) = b + h \sum_{\ell=0}^{q} \varphi_{j,\ell} v\left(\nu_\ell h\right) + O\left(h^{q+2}\right).$$

By substituting the power series of v into (4.1) and equating coefficients with (3.10), we find that

$$(4.2) \qquad \lambda_{j,k} = \sum_{i=0}^{q} \varphi_{j,i}\left(\nu_i\right)^k, \quad k = 0, ..., q, \quad j = 1, ..., m.$$

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Our task now is to express the Generalized Runge-Kutta System using the φ's instead of the λ's. It turns out that we can use

$$(4.3) \qquad \varphi_{j,i}, \quad i = p, ..., q, \quad j = 1, ..., m$$

as the independent variables. Note that this is the same index set as we used for the λ's. In order to eliminate the variables $\varphi_{j,\ell}, \ell, < p$ we note that for $k \leq q$

$$(4.4) \qquad \lambda_{j,k} = \frac{(\nu_j)^{k+1}}{(k+1)} = \int_0^{\nu_j} x^k dx.$$

We now put (3.4) with $k < p$ into (3.2) split the sum on the right at p and multiply by the inverse Vandermonde matrix $W_{\ell,k}^{p-1}$ and sum to obtain

$$(4.5) \qquad \varphi_{j,\ell} - \int_0^{\nu_j} \mathcal{P}_\ell^{p-1}(x)\, dx - \sum_{i=p}^q \mathcal{P}_\ell^{p-1}(\nu_j)\, \varphi_{j,i}$$

for $\ell = 0, ..., p-1, \quad j = 0, ..., m$. After expressing the polynomials $\mathcal{P}_\ell^{p-1}(x)$ in terms of the Lagrange interpolation formula for the polynomial $P^q(x)$ we obtain from (3.5)

$$(4.6) \qquad \varphi_{j,\ell} = \mathcal{A}_{j,\ell}^q + \sum_{i=p}^q \mathcal{P}_\ell^{p-1}(\nu_j) \left[\mathcal{A}_{j,i}^q - \varphi_{j,i} \right]$$

for $O \leq \ell \leq p-1, \quad 1 \leq j \leq m$.

Next, using the Lagrange Interpolation representation of x^k with respect to $P^q(x)$, we find that it follows from (4.4) that

$$(4.7) \qquad \lambda_{j,r} - \frac{\nu^{r+1}}{(r+1)} = \lambda_{j,r} - \sum_{i=0}^q \nu_i^r \mathcal{A}_{j,i}^q.$$

We now define the matrix

$$(4.8) \qquad \xi_{r,i}^p = \nu_i^r - \sum_{\ell=0}^{p-1} \nu_\ell^r \mathcal{P}_\ell^{p-1}(\nu_i).$$

After putting (4.6) into (4.2) and then substituting the result into the right side of (4.7) and then (4.7) into (3.18), we find that the Generalized Runge-Kutta System takes the form

$$(4.9) \qquad \sum_{j=1}^m \alpha_j \nu_j^k \sum_{i=p}^q \xi_{\ell,i}^p \left[\varphi_{j,i} - \mathcal{A}_{j,i}^q \right] = 0$$

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for $k + \ell \leq q$, $\ell \geq p$. After introducing the notational simplification

(4.10) $$\psi_{j,i} = \alpha_j \Phi_{j,i}, \quad b_{j,i} = \alpha_j \; \mathcal{A}^q_{j,i}, \quad \delta = m - q$$

we may rewrite (4.9) as

(4.11)
$$\sum_{j=\ell+\delta}^{m} \nu_j^k \sum_{i=p}^{q} \xi_{\ell,i}^p \left[\psi_{j,i} - b_{j,i} \right]$$
$$+ \sum_{j=0}^{\ell+\delta-1} \nu_j^k \sum_{i=p}^{q} \xi_{\ell,i}^p \left[\psi_{j,i} - b_{j,i} \right] = 0$$

for $k + \ell \leq q$, $\ell \geq p$. Now for each fixed ℓ, $p \leq \ell \leq q$, we multiply (4.11) by the Vandermonde inverse $W_{r,k}^{m,\ell+\delta}$ and sum from $k = 0, ..., q$ to obtain

(4.12)
$$\sum_{i=p}^{q} \xi_{r,i}^p \left[\psi_{r,i} - b_{r,i} \right]$$
$$= - \sum_{j=1}^{\ell+\delta-1} \mathcal{P}_r^{m,\delta+\ell} \left(\nu_j \right) \sum_{i=p}^{q} \left[\psi_{j,i} - b_{j,i} \right]$$

for $r = \ell + \delta, ..., m$, $\ell = p, ..., q$.

5. A Particular Solution and the General Solution of the Generalized Runge-Kutta System.

If we add to the system (3.12) the constraints

(5.1) $$\psi_{r,i} = 0, \quad r = 1, ..., i + \delta - 1, \quad i = p, ..., q$$

the number of new constraints is equal to the excess of the number of unknowns over the number of equations. This gives us the system

(5.2)
$$\sum_{i=p}^{r-\delta} \xi_{\ell,i}^p \, \psi_{r,i} = \sum_{i=p}^{q} \xi_{\ell,i}^p \, b_{r,i}$$
$$- \sum_{j=0}^{\ell+\delta-1} \mathcal{P}_r^{m,\ell+\delta} \left(\nu_i \right) \left[\sum_{i=p}^{j-\delta} \xi_{\ell,i}^p \, \psi_{j,i} - \sum_{i=p}^{q} \xi_{\ell,i}^p b_{j,i} \right]$$

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for $\ell = p, ..., r - \delta$, $r = p + \delta, ..., m$. For each fixed r this is a square system with the right hand sides depending on the variables $\psi_{j,i}$, $j < r$. Hence, if we can prove the matrix $\zeta_{\ell,i}^p$ is non-singular for $p \leq \ell$, $i \leq r - \delta$, we have a unique solution. This we shall prove in Section 5.

We shall find a closed form solution of the system (5.2) for any choice of the matrix $(b_{j,i})$. The numerical use of this solution is provisional since it depends on being able to construct a solution with the computed values of the φ's. Therefore, it would be nice to have the general solution of the system (4.12). To do so we need only to replace the $b_{j,i}$'s by

$$(5.3) \qquad b_{j,i} = b_{j,i} - \psi_{j,i}, \quad r - \delta < i < q.$$

6. Forward Elimination Applied to the Matrix $\xi_{r,i}^p$.

In this section we shall show that after k forward Gaussian Elimination steps, without dividing out the pivots the matrix has rows defined by

$$(6.1) \qquad P^{p+k-1}(\nu_i), \quad p = j < k$$

and

$$(6.2) \qquad \xi_{j,i}^{p+k}, \quad j \geq k.$$

It suffices to consider the case $k = 1$, hence $j = 0$.

If we define

$$(6.3) \qquad f_r^p(x) = x^r - \sum_{\ell=0}^{p-1} \nu_\ell^r P_\ell^{p-1}(x)$$

then $\xi_{r,i}^p = f_r^b(\nu_i)$.

In particular $f_p^p(x)$ has p zeros $\nu_0, ..., \nu_{p-1}$ and since it is a monic polynomial

$$(6.4) \qquad f_p^p(x) = P^{p-1}(x).$$

It follows that (6.1) is true when $j = 0$. For $r > p$ we have, after one forward Gaussian Elimination step the matrix with elements

$$(6.5) \qquad \xi_{r,i}^p - \frac{\xi_{p,i}^p}{\xi_{p,p}^p} \xi_{r,p}^p.$$

After using (6.1) with $j = 0$ this is $Q_r(\nu_i)$ with

$$(6.6) \qquad Q_r(x) = f_r^p(x) - \frac{P^{p-1}(x)}{P^{p-1}(\nu_p)} f_r^p(\nu_p).$$

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The difference

(6.7)
$$Q_r(x) - P^{p+1}(x)$$

is a polynomial of degree at most p with $p+1$ zeros $\nu_0, \nu_1, ..., \nu_p$. This establishes (6.2).

It now follows from (6.1) that the matrix of our Generalized Runge-Kutta system is non-singular.

7. A Useful Identity.

We have seen that forward elimination applied to the left side of our system is quite simple. Applying it to the right sides requires a bit more work. Specifically the proof uses iterations that make it appear the products of the matrices defined by $\mathcal{P}$ will arise. The following identity shows that these all collapse to a single factor.

Theorem 7.1. *If $\sigma < \rho \leq m$ then*

(7.1)
$$\mathcal{P}_k^{m,\rho}(x) = \sum_{\ell=\sigma}^{q} \mathcal{P}_k^{q,\rho}(\nu_\ell)\mathcal{P}_\ell^{q,\sigma}(x)$$

for any k, $\sigma \leq k \leq m$.

Proof. This is just the Lagrange Interpolation Polynomial Representation of the lower degree polynomial in terms of the higher.

8. Uncoupling the System to Upper Triangular Form.

Let us define

(8.1)
$$\Omega_{\ell,r}^{\mu} = \sum_{i=\mu}^{r-\delta} \xi_{\ell i}^{\mu}\Psi_{r,i} - \sum_{i=\mu}^{q} \xi_{\ell,i}^{\mu}b_{r,i}.$$

Note that, when $\mu > r - \delta$, the first sum vanishes.

We shall show that, after k Forward Elimination Steps, the system has the form

(8.2)
$$\sum_{j=p+k+\delta}^{m} \mathcal{P}_r^{m,\ell+\delta}(\nu_j)\Omega_{\ell,j}^{p+k} - \Gamma_\ell^{r,k} = 0$$

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for $\ell = p + k, ..., r - \delta, \ \ r = p + k + \delta, ..., m$ with $\Gamma_\ell^{r,k}$ defined by

$$(8.3) \qquad \Gamma_\ell^{r,k} = \sum_{j=\sigma}^{p+k+\delta-1} \mathcal{P}_r^{m,\ell+k+\delta}(\nu_i) \sum_{i=p+k}^{q} \xi_{\ell,i}^{p+k} b_{j,i}.$$

Since $\mathcal{P}_r^{m,\ell+\delta}(\nu_j) = \delta_{r,j}$ for $\ell + \delta \leq r \leq m$, this agrees exactly with the system (5.2) when $k = 0$. In any case, the pivot row corresponds to $\ell = p + k$. The sum in (8.1) then vanishes and we are left with

$$(8.4) \qquad \Omega_{p+k,r}^{p+k} - \Gamma_{p+k}^{r,k} = 0.$$

Let us express the Gaussian Elimination step (6.5) in the form

$$(8.5) \qquad \xi_{\ell,i}^{p+k+1} = \xi_{\ell,i}^{p+k} - \eta_{p+k,\ell}\, \xi_{p+k,i}^{p+k}.$$

Then, after multiplying (8.4) by $\eta_{p+k,\ell}$ and subtracting from $\Omega_{\ell,r}^{p+k}$, we obtain the identity

$$(8.6) \qquad \Omega_{\ell,r}^{p+k} = \Omega_{\ell,r}^{p+k+1} + \eta_{p+k}\,, \ \Gamma_{p+k}^{r,k}.$$

We may assume this to be true with r replaced by j for any j, $p + k + \delta \leq j < r$. Hence, after substituting (8.6) with (8.2), we have

$$(8.7) \qquad \sum_{j=p+k+\delta}^{m} \mathcal{P}_r^{m,\ell+\delta}(\nu_j) \left[\Omega_{\ell,j}^{p+k+1} + \eta_{p+k,\ell}\, \Gamma_{p+k}^{j,k} \right] - \Gamma_\ell^{\ell,k} = 0.$$

By substituting for $\Gamma_{k+p}^{j,k}$ from (8.3) using the identity (7.1) and combining this result with the representation (8.3) of $\Gamma_\ell^{r,k}$ with the help of (8.5), we obtain the terms in the representaitons of $\Gamma_\ell^{r,k+1}$ except for the summand corresponding to $j = p + k + \delta$. This one comes from the contribution of this value of j in the first sum in (8.7). Thus we have derived the system (8.2) with k replaced by $k + 1$.

Now let us rewrite the system (8.2) in the form

$$(8.8) \qquad \Omega_{\ell,r}^{p+k} - \Gamma_\ell^{r,k} + \sum_{j=p+k+\delta}^{\ell+k+\delta-1} \mathcal{P}_r^{m,\ell+\delta}(\nu_i)\, \Omega_{\ell,j}^{p+k} = 0$$

for $\ell = p + k, ..., r - \delta, \ r = p + k + \delta, ..., m$. When $k = p - \ell$, the sum vanishes. This gives us the desired upper triangular form.

9. Diagonal Back-Substituting to a Closed-Form Solution of the Generalized Runge-Kutta System.

Let us define

$$(9.1) \qquad \mathcal{P}_\gamma^{\alpha,\beta}(x) = \frac{P^{\alpha,\beta}(x)}{(x - \nu_\gamma)}, \quad \beta \leq \beta \leq \alpha$$

and introduce the matrices

$$(9.2) \qquad \zeta_{\ell,i}^k = \frac{P^{\ell+k,0}}{P_\ell^{\ell+k,0}(\nu_\ell)}.$$

Note that when $k = 0$ amounts to giving constant polynomial 1 the factor $x - \nu_\ell$ and then dividing it out. This device is used to make the following formula valid on the diagonal. When $k = 0$, in a slightly different notation our upper triangular form is

$$(9.3) \qquad \sum_{i=\ell}^{r-\delta} \psi_{r,i} \, \zeta_{\ell,i}^k = w_{r,\ell}^k$$

with

$$(9.4) \qquad w_{r,\ell}^0 = \sum_{j=1}^m \mathcal{P}_{r,j}^{m,\ell+\delta} \sum_{i=\ell}^q b_{j,i} \, \zeta_{\ell,i}^0$$

and with

$$(9.5) \qquad \Pi_\ell^k = \frac{\zeta_{\ell,\ell+k+1}^k}{\zeta_{\ell+k+1,\ell+k+1}^0},$$

$\zeta_{\ell,i}^{k+1}$ and $w_{r,\ell}^{k+1}$ satisfying the recursion formulas

$$(9.6) \qquad \zeta_{\ell,i}^{k+1} = \zeta_{\ell,i}^k - \Pi_\ell^k \, \zeta_{\ell+k+1,i}^\ell$$

and

$$(9.7) \qquad w_{r,\ell}^{k+1} = w_{r,\ell}^k - \Pi_\ell^k \, w_{r,\ell+k+1}^0.$$

The above recursion formulas amount to using the system corresponding to $k = 0$ to eliminate one super diagonal at a time. At the end of the elimination, we have the closed form solution.

$$(9.8) \qquad \psi_{r,\ell} = \sum_{k=\ell}^{r-\delta} \sum_{j=1}^m \frac{\mathcal{P}_r^{m,k+\delta}(\nu_i) \sum_{i=k}^q b_{j,i} \, \zeta_{\ell,i}^0}{P_\ell^{k,0}(\nu_i)},$$

$$\ell = p, ..., r - \delta, \quad r = p + \delta, ..., m.$$

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10. Application of the Residue Theorem to Lagrange Interpolation.

What remains of our task is to find suitable p^{th} order approximations to use with our previous work. The success of completing our effort depends on finding the Taylor Coefficients of order higher than p of these approximations.

Since polynomial approximations involve only the finite part of the Taylor Expansion, there is no loss of generality in assuming that we are finding approximations of an entire analytic function f. Thus consider the polynomial

$$(10.1) \qquad P(x) = \prod_{j=1}^{n} (x - \nu_j)$$

and the function

$$(10.2) \qquad \tilde{f}(hx) = \frac{1}{2\pi i} \int_\gamma \frac{P(x) f(hz) \, dz}{(x - z) P(z)}$$

where γ is a contour containing the roots of P in its interior and excluding x. If these roots are distinct, we see by evaluating the residues that $\tilde{f}(hz)$ is the Lagrange Interpolation Polynomial of $f(hz)$ with respect to the polynomial P. It is clear that the roots ν_i may be deformed into any set of n numbers in the interior of γ without changing the fact that

$$(10.3) \qquad \tilde{f}(hz) - f(hz) = 0 \, (h^n) \, .$$

Hence it is not necessary to assume that the roots ν_j of P are distinct. When they are multiple, the expansion will involve derivatives of f.

Now, let us note that the integrand of (10.2) has residue - $f(hz)$ at the point $z = x$. Hence, if γ' is a contour containing γ and x in its interior, we have the formula for the error

$$(10.4) \qquad \tilde{f}(hx) - f(hx) = \frac{1}{2\pi i} \int_{\gamma'} \frac{P(x) f(hz)}{(x - z) P(z)} dz.$$

Now we may assume that γ' is a circle of arbitrarily large radius. There is then no problem in integrating and determining a formula for

$$(10.5) \qquad \int_0^x \left[\tilde{f}(ht) - f(ht) \right] dt$$

and, since there is no problem in integrating a finite Taylor Polynomial, we may determine the higher expansion coefficients of

$$(10.6) \qquad \int_0^x \tilde{f}(ht) \, dt.$$

Let us now write

(10.7)
$$f(z) = \sum_{j=0}^{\infty} f_n z^n.$$

Then we may write

(10.8)
$$\tilde{f}(hx) - f(hx) = P(x) \sum_{j=n}^{\infty} E_j f_j h^j$$

where

(10.9)
$$E_j = \frac{1}{2\pi i} \int_{p'} \frac{z^j}{(x-z)P(z)} dz.$$

Now, let us define

(10.10)
$$Q(z) = (z-x)P(z) = \sum_{j=0}^{n} (-1)^j S_i z^{n+1-i}$$

where $S_i \equiv S_i(x, \nu_1, ..., \nu_n)$ are the elementary symmetric functions of $(x, \nu_1, ..., \nu_n)$.
By evaluating the residue at $z = \alpha$, we find that

(10.11)
$$E_j = 0, \quad j \le n,$$

(10.12)
$$E_n = -1$$

and, for $j > n$,

(10.13)
$$E_j = \sum_{i=1}^{n+1} (-1)^i E_{j-i} S_i.$$

Now let us define

(10.14)
$$\alpha_j = \int_0^x E_j(t, \nu) P(t) dt, \quad \gamma_j = \frac{x^j}{j} + \alpha_j.$$

We may use the techniques used in proving (10.3) – (10.6) to deduce that

(10.15)
$$\int_0^x \tilde{f}(ht) dt \quad \text{and} \quad \int_0^x \left[\tilde{f}(ht) - f(t) \right] dt$$

have coefficients indexed by $j \ge n + 1$

(10.16)
$$\alpha_j f_{j-1} \quad \text{and} \quad \gamma_j f_{j-1}$$

respectively.

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11. Averaging: Real of Superficial

Let us suppose that f_1, f_2 are two different n^{th} order approximations of a function f and consider the function

$$(11.1) \qquad f_3(x) = \mu f_1(x) + (1 - \mu) f_2(x)$$

We see that, if the $(n+1)^{\text{st}}$ order coefficients of f_1 and f_2 are different, we can choose μ so that f_3 is an $(n+1)^{\text{st}}$ order approximation.

Now suppose that we apply the above remarks to the Lagrange interpolation polynomial representations corresponding to the polynomials $(x - x_1) P(x)$ and $(x - x_2) P(x)$ where P is a polynomial of degree $(n+1)$. It is clear from the error forms (10.4) that the $(n+1)^{\text{st}}$ order coefficients will be different whenever $x_1 \neq x_2$ and x is not a root of either polynomial. In fact, the choice

$$(11.2) \qquad \mu = \frac{(x_2 - x)}{(x_2 - x_1)}, \ (1 - \mu) = \frac{(x_1 - x)}{(x_1 - x_2)}$$

is the choice which achieves $(n+1)^{\text{st}}$ order accuracy. By computing this linear combination from the representation given by (10.2), we see that this is the Lagrange Interpolation Polynomial representation corresponding to the polynomial

$$(11.3) \qquad (x - x_1)(x - x_2) P(x).$$

Thus, with the solution $y' = f(x, y)$, we get accuracy of order $(n+1)$ at all mesh points. The actual accuracy then depends on the accuracy of the approximation of y that are substituted into $f(x_j, y(x_j))$. This can be different at different mesh points. In any case, we do not actually have to compute the linear combination corresponding to the pair μ and $(1 - \mu)$.

But the above remarks do not apply to substituting approximations of y at the mesh points. One way of getting approximations that depend only on $f(\nu_j h, y(\nu_j h))$ is to let $\tilde{y}$ be the approximation corresponding to the integrated version of the representation with respect to $P(x) = (x - \nu_1) \dots (x - \nu_n)$. Then $\tilde{y}(\nu_i h) - y(\nu_i h) = O(h^{n+1})$. The same accuracy can be obtained by using the Lagrange Interpolation Polynomial Representative with respect to the polynomial $(x - \nu_i) P(x)$. Now if we substitute $\tilde{y}$ into this representation and call the result $\tilde{\tilde{y}}_i$, we have n more representations of accuracy $O(h^{n+1})$. By applying the

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averaging process to $\overset{\approx}{y}_i$ and $\overset{\approx}{y}_2$ we obtain the $O\left(h^{n+2}\right)$ approximation

$$\overset{\approx}{y}_{ij}\left(xh\right) = \frac{1}{2\pi_i}\int_\gamma \frac{\left(x-\nu_1\right)\left(x-\nu_2\right)P\left(x\right)}{\left(z-\nu_1\right)\left(z-\nu_2\right)P\left(z\right)}\frac{\hat{f}\left(zh\right)}{\left(x-z\right)}$$

(11.4)

$$+\frac{\int_0^x P\left(t\right)dt}{\frac{x^{n+1}}{n+i}-\int_0^x P\left(t\right)dt}\cdot\frac{1}{2\pi_i}\int\frac{\tilde{y}\left(zh\right)}{\left(z-\nu_1\right)\left(z-\nu_2\right)P\left(z\right)}dz.$$

This is a perturbation of the representation with respect to $\left(x-\nu_1\right)\left(x-\nu_2\right)P\left(x\right)$ which can't be valid unless

(11.5)
$$\int_0^x P\left(t\right)dt \neq \frac{x^{n+1}}{\left(n+1\right)}.$$

If $0 \leq \nu_1 \leq \nu_2... \leq \nu_n \leq x$, it follows from the inequality between geometric and arithmetic means that

(11.6)
$$\left|\int_0^x P\left(t\right)dt\right| \leq \frac{x^{n+1}}{n+1}$$

with equality only if all the ν_j's are zero or all equal to x.

Let us define, using (10.14),

(11.7)
$$\beta_j = \frac{-\alpha_j}{\gamma_j}$$

and assume that $\gamma_j \neq 0$. We also define

(11.8)
$$P_{n+j} = \left(x-\nu_i\right)...\left(x-\nu_j\right)P\left(x\right).,\ j=1,...,n.$$

The formula (11.4) generalizes to

$$\overset{\approx}{y}_r = \frac{1}{2\pi_i}\int_\gamma \frac{P_{n+j}\left(x\right)\tilde{y}\left(hz\right)dt}{\left(x-z\right)P_{n+j}\left(z\right)}$$

(11.9)

$$+\sum_{\ell=0}^r \frac{\beta_{n+\ell+i}}{2\pi_i}\int_\gamma \frac{\displaystyle\sum_{i=0}^{r-\ell}\left(-1\right)^i S_i\left(\nu_i,...,\nu_r\right)z^{r-\ell-i}\tilde{y}\left(hz\right)dz}{P_{n+r+2}\left(z\right)}$$

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That $\overset{\approx}{y}_r$ approximates the solution y of $y' = f(x,y)$ to order $n + r + 1$ is seen by using the identity

$$(11.10) \qquad \frac{1}{2\pi i} \int_\gamma \sum_{i=0}^{n-r} \frac{(-1)^i S_i z^{r-\ell-i} z^{n+1+q}}{P_{n+r+z}(z)} dt = \delta_{\ell,q}$$

for $0 \le \ell$, $q \le r$. This is proved in the cases $\ell \ge q$ and $0 < \ell \le q$ by computing the residue at $z = \infty$ by inspection. This leaves the case $\ell = 0$, $q > 0$ which is proved by separating off the term corresponding to $i = 0$ and using the analogue of the identity (10.13) for the present polynomial. The proof then follows by substituting the power series expansion of $\overset{\approx}{y}_j - \tilde{y}$ and $\tilde{y} - y$.

One can arrive at (11.9) in a better motivated fashion by writing the two approximations corresponding to $\nu_1, ..., \nu_{r-1}, \nu_r$ and $\nu_1, ..., \nu_{r-1}, \nu_{r+1}$ and taking to linear combination corresponding to

$$(11.11) \qquad \frac{x - \nu_{r+1}}{\nu_r - \nu_{r+1}} + \sigma \text{ and } \frac{x - \nu_r}{\nu_{r+1} - \nu_r} - \sigma.$$

This leads to the correct identity plus the term

$$(\nu_{r+1} - \nu_r)\,\sigma\left[P_{n+r+1}(x) + \sum_{\ell=0}^{r} \beta_{n+1+r}(-1)^{r-\ell} S_{r-\ell}\right]$$

$$+ \sum_{\ell=0}^{r} \beta_{n+1+r}(-1)^{r-\ell}[S_{r+1-\ell} + x S_{r-\ell}]$$

This term can then be eliminated when the coefficient of σ is not zero. But this fails to be true only at isolated points x and by continuity must be true there also.

12. Higher Order Averaging.

Now suppose that we replace the variables λ_{ji} in (2.17) by $\lambda_{ji} + \chi_{ji}$ and subject the χ_{ji} to the constraint

$$(12.1) \qquad \sum_{j=1}^{m} \alpha_j (\nu_j)^k \chi_{ji} = 0$$

for $i + k \le q - \rho$, $p - \rho \le i \le q - \rho$. Then for each $i = p - \rho, ..., q - \rho$ and $r = i + \delta, ..., m$ we may break the sum at $i + \delta$. Then after multiplying by the Van

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der Monde inverse $w_{r,k}^{m,i+\delta}$ and sum from $k = 0$ to $m - i - \delta$ we obtain

$$\alpha_r \chi_{ri} + \sum_{j=1}^{i+\delta-1} \alpha_j \mathcal{P}_r^{m,i+\delta}(\nu_j)\chi_{ji} = 0$$

for $r = i + \delta, ..., m$, $i + \rho = p$ to q. This serves to shift terms from above the diagonal $r = i + \delta$ to below.

13. The Generalized Runge, Kutta, Butcher Algorithm.

We start with
(13.1)
$$\tilde{y}_i^0 = b + h\,\nu_i\,f\,(0,b)\,.$$

Then we compute

(13.2)
$$\tilde{y}_0^1 = b + h\left[\mathcal{A}_{i,0}^1 f\,(0,b) + \mathcal{A}_{i,1}^1 f\left(\nu, h_j \tilde{y}_i^0\right)\right]\,.$$

If n is even, we make the additional computation

(13.3)
$$\tilde{\tilde{y}}_i' = b + h\left[\mathcal{A}_{i,0}^1 f\,(0,b) + \mathcal{A}_{i,1}^1 f\,(\nu, h_j \tilde{y}_1')\right]\,.$$

Then we define
$$y_i' = \tilde{y}_i \quad \text{if } n \text{ is odd,}$$
(13.4)
$$= \tilde{\tilde{y}}_i \quad \text{if } n \text{ is even.}$$

Now, for each $k > 1$, we compute approximation g_i^h of $f'\,(\nu_i h)$, $i = 1, ..., k$ and y_i' of $y\,(\nu_i h)$ for $i = 1, ..., k + 1$. To achieve these we define

(13.5)
$$\mathcal{A}_{i,j}^{k,0} = \mathcal{A}_{i,j}^k$$

with the right side defined by (2.18) and

(13.6)
$$\mathcal{A}_{i,j}^{k,\ell}, \quad \ell \geq 1$$

to be the coefficient as obtained in Section 10 with the roots $\nu_0, \nu_1, ..., \nu_\ell$ doubled. Note that in (13.5), the superscript 0 is not doubled. Then we define for $k \geq 2$, $i \geq 1$.

After computing the following for $i \leq k - 1$, $g_0^k \equiv f(0, b)$,

$$(13.7) \qquad \bar{y}_i^k = b + h \left\{ \sum_{j=0}^{i-1} \mathcal{A}_{ij}^{k-1,i} g_i^k + \sum_{j=1}^{k-1} \mathcal{A}_{ij}^{k-1,i} g_j^{k-1} \right\},$$

$$(13.8) \qquad g_i^k = f\left(\nu_i h, \bar{y}_i^k\right),$$

and

$$(13.9) \qquad y_i^k = b + h \left\{ \sum_{j=0}^{i} \mathcal{A}_{ij}^{k-1,i} g_i^k + \sum_{j=i+1}^{k-1} \mathcal{A}_{ij}^{k-1,i} g_j^{k-1} \right\}$$

for $i \leq k - 1$, we compute (13.7) and (13.8) for $i = k$ and then replace (13.9) by

$$y_i^k = b + h \sum_{j=0}^{k} \mathcal{A}_{ij}^{k,k-1} g_j^k,$$

and then loop to the next k.

Note that the computation of the $\bar{y}_i^k$'s require no new computation of f so that exactly k computations of f are used in each k-loop.

When $k = p - 1$, we have the initial p^{th} order approximation of y.

In order to complete the algorithm, we use the independent φ_{ji}, (9.8), obtained by setting the free variables (5.1) equal to zero. The dependent φ_{ji}'s are obtained from the recursion formula (4.6). Then we define

$$(13.10) \qquad \mu_{ij} = - \sum_{\ell=1}^{j+\delta-1} \frac{\alpha_j}{\alpha_r} \cdot \frac{\varphi_{j\ell}}{\varphi_{i\ell}} \mathcal{P}_i^{m,j+\delta}(v_j).$$

For $i \leq p + \delta$, we use
$$(13.11) \qquad w_i = y_i^{p-1}$$

and compute
$$(13.12) \qquad f(\nu_i h, \ w_i).$$

For each $i > p + \delta$, we run the recursion formula (13.7) for $k = p$ but substituting w_j for g_j^k when $j < i$. Then, after computing (13.8), we compute w_i using

$$(13.13) \qquad \mu_{ij} w_j + \left(1 - \mu_{ij}\right) g_i^p$$

to approximate $y'(\nu_j h)$ when $j < i$ and g_i^p to approximate $y'(\nu_i h)$. Then we loop to the next i.

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14. The Theoretical Runge, Kutta, Butcher Initial Approximation.

The recursion formula of the previous section is written exactly as it will be used in practice. In this form though, it is difficult to determine the magnitude of the errors. For this purpose we use, at every opportunity,

(14.1)
$$f\left(x, z\left(x\right)\right) - f\left(x, y\left(x\right)\right) = \tfrac{\partial f}{\partial y}\left(x, y\left(x\right)\right)\left(z\left(x\right) - y\left(x\right)\right)$$
$$+ 0\left(\left(z\left(x\right) - y\left(x\right)\right)^2\right)$$

where z is an approximation of the exact solution $y\left(x\right)$. Then the g's are replaced by the derivative y' and the formula (??) takes either of the forms

(14.2)
$$y_i^k = y\left(\nu_i h\right) + E_i^k$$

or
(14.3)
$$y_i^k = P_{k+i}\left(\nu_i h\right) + E_i^k$$

where P_ℓ is the ℓth Taylor Polynomial of y and E_i^k is of the form

(14.4)
$$E_i^k = \sum_{\rho=0}^{2k+1} \sum_{\ell=k+1-\min\{\rho,k\}}^{\infty} P_{i\ell}^{k,\rho} v_\ell h^{\ell+\rho+1}$$

where $P_{i\ell}^{k,n}$ is a homogeneous polynomial of degree k in the variable

(14.5)
$$b\left(\nu_i h\right) = \frac{\partial f}{\partial y}\left(\nu_i h, y\left(\nu_i h\right)\right), \quad i = 1, ..., k.$$

The E_i^k's differ between (14.2) and (14.3) only in the constant terms of these polynomials, there being obtained from Section 10.

In other words, the approximations (14.2) and (14.3) keep track of the form of the error up to approximately twice the order where we know it exactly. In particular, it is order $0\left(h^{2k+3}\right)$ when q is odd and $0\left(h^{2k+4}\right)$ when q is even. The reader will note that it does not depend explicitly on the partial derivatives of f of order greater than one.

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15. Deformation of the Constructed Solution into the Theoretical Solution.

We first note that the terms in the error (14.4) with $i + \rho = $ const. all have the same order of magnitude. We also note that dependence on h in X_{ji}^p may be regarded as a parameter since the only dependence on h is obtained from the Taylor expansion of $f(v_i h, y(v_i h))$ which accounts for the factor $(v_i)^k$ which is eliminated by the inverse Vandermonde matrix. Then we add the negatives of the terms in the order we wish to eliminate and the choice of the μ_{ri}'s shows that the contribution of g_i^p is cancelled. The term g_{i+1}^p is then replaced by a derivative plus an error. Actually, this is only an artiface. The second order averaging technique is used only to determine the μ_{ri} and the constribution of g_i^p. After we have eliminated all of the error terms, we are left with the theoretical solution. Hence, the constructed solutio has the same error.

This is most easily seen by writing the error (??) in the form

$$(15.1) \qquad \mu_{ij} \left[w_j - y'(x, k) \right] - 1 \left(1 - \mu_{ij} \right) \left[g_i^h - y'(x_i h) \right].$$

If we eliminate errors in increasing order, the first term in (15.1) represents the terms currently being eliminated and the second of one higher order.

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