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A transformation relating explicit and diagonally-implicit general linear methods

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Abstract

Using the "inherent Runge–Kutta stability" property, it is possible to construct diagonally-implicit general linear methods with stability regions exactly the same as for Runge–Kutta methods. In addition to A-stable methods found in this way, it is also possible to construct explicit methods with stability regions identical to those of explicit Runge–Kutta methods. A transformation is introduced that links these two types of methods but with a modified form of the order conditions. This makes it possible to greatly widen the family of both explicit and diagonally-implicit methods possessing Runge–Kutta stability.

Keywords: General linear methods; Inherent Runge–Kutta stability; Transformation; Nordsieck form

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1. Introduction

General linear methods were originally introduced to provide a unifying framework to study consistency, stability and convergence of traditional methods [1]. More recently, attempts have been made to find members of this large class which might compete successfully with Runge–Kutta and linear multistep methods. One approach was to use the class of diagonally implicit multistage integration methods (DIMSIMs) [2]. The aim was to overcome the known disadvantages of traditional methods. These methods, for increasingly high orders, become very difficult to derive and another approach has been sought [3]. The new idea is to impose a property known as "inherent Runge–Kutta stability". This guarantees that the method has the same stability properties as a singly-implicit Runge–Kutta method. A slightly different construction enables inherent Runge–Kutta stability to be extended to explicit methods [6].

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Unlike DIMSIMs, the new methods possessing inherent Runge–Kutta stability can be constructed using only rational operations and it is possible, in a straightforward manner, to derive methods with acceptable stability regions, in the case of explicit methods, and possessing L-stability in the case of implicit methods. One of the aims of the present paper is the construction of improvements to existing methods. This goes beyond considerations such as the interplay between error constants and stability regions, which is now well understood. Rather, the aim is to see how choices that are at our disposal can be used to control the magnitudes of coefficients appearing in the matrices defining the methods. We want to be able to design robust and efficient algorithms based on these methods. Learning more about the dependence of coefficients on available parameters is intended as a step towards the characterization of all methods in these families. Here the emphasis will be on a transformation interrelating various implicit and explicit methods.

General linear methods in general do not have an order p in an absolute sense but only in relation to a starting procedure. This starting procedure could, for example, consist of the computation of an approximate Nordsieck vector. The order of the method, relative to this, is related to the ability of the method to adhere to a Nordsieck approximation from step to step without introducing errors that are not $O(h^{p+1})$. In the construction of DIMSIMs, the starting method is chosen freely but, in preparation for a practical implementation, the method can be transformed so that the starting data is in Nordsieck form. The advantage of the methods using inherent Runge–Kutta stability, is that instead of needing to satisfy order and stability conditions to find the methods, as required for DIMSIMs, certain conditions on the method are required which guarantees the stability conditions are satisfied. This allows the coefficients of the methods to be found using only linear operations. In carrying out the construction of methods in this way, there are sometimes free parameters, which can be selected in an attempt to improve numerical properties of the method.

Section 2 will be devoted to a review of general linear methods possessing inherent Runge–Kutta stability. Since it is intended to derive methods using only sequences of linear operations, we are constrained in the structure of the method. Furthermore, the nature of the constraint is different in the explicit and in the diagonally-implicit cases. This makes it difficult to decide where to look for the best methods that might have a chance of competing successfully with traditional methods.

The use of a transformation allows the explicit and implicit methods to be combined together into a unified structure. The specific transformation used is similar to the one used in [4]; this allowed implicit methods to be expressed in an explicit form by satisfying a modified form of the order conditions. For the methods in the present paper, explicit methods can be found from transformed implicit methods or, alternatively, implicit methods can be found from transformed explicit methods. Finally, implicit methods can be found from transformed implicit methods with different diagonal elements. This transformation and the inherent Runge–Kutta stability property will be discussed in Section 3. The specific details of each of these choices will be described and the derivation of the new methods using linear operations will be discussed in Section 4. Some low order methods which require the use of the transformation will be given in Section 5. Finally some concluding remarks and future plans will be outlined.

2. General linear methods and inherent RK stability

General linear methods are multistage and multivalue methods. Denote the stage values by $Y_1, Y_2, \dots, Y_s$ and the derivative evaluated at these steps by $F_1, F_2, \dots, F_s$. At the start of step number n,

r quantities denoted by $y_1^{[n-1]}, y_2^{[n-1]}, \dots, y_r^{[n-1]}$ are available as approximations computed in step $n-1$. Corresponding quantities $y_1^{[n]}, y_2^{[n]}, \dots, y_r^{[n]}$ are evaluated in the step along with the stage values and stage derivatives. For compactness of notation we introduce vectors Y, F, $y^{[n-1]}$ and $y^{[n]}$ given by

$$Y = \begin{bmatrix} Y_1 \\ Y_2 \\ \vdots \\ Y_s \end{bmatrix}, \qquad F = \begin{bmatrix} F_1 \\ F_2 \\ \vdots \\ F_s \end{bmatrix} = \begin{bmatrix} f(Y_1) \\ f(Y_2) \\ \vdots \\ f(Y_s) \end{bmatrix}, \qquad y^{[n-1]} = \begin{bmatrix} y_1^{[n-1]} \\ y_2^{[n-1]} \\ \vdots \\ y_r^{[n-1]} \end{bmatrix}, \qquad y^{[n]} = \begin{bmatrix} y_1^{[n]} \\ y_2^{[n]} \\ \vdots \\ y_r^{[n]} \end{bmatrix}.$$

Note that $f : \mathbb{R}^m \to \mathbb{R}^m$, in the definition of F, denotes the differential equation to be solved. That is, the function y, is a solution of

$$y'(x) = f\big(y(x)\big).$$

If h denotes the stepsize, then the quantities imported into and evaluated in step number n are related by

$$\begin{aligned} Y &= h(A \otimes I_m)F + (U \otimes I_m)y^{[n-1]}, \\ y^{[n]} &= h(B \otimes I_m)F + (V \otimes I_m)y^{[n-1]}. \end{aligned} \tag{2.1}$$

It is convenient to write the coefficients of the method, that is the elements of A, B, U and V, as a partitioned $(s+r) \times (s+r)$ matrix

$$\left[\begin{array}{c|c} A & U \\ \hline B & V \end{array}\right]. \tag{2.2}$$

The structure of A determines the implementation costs of these methods, just as in the special case of Runge–Kutta methods.

The order conditions of general linear methods are very complicated. To overcome this difficulty simplifying assumptions are used on the stage values and the outgoing approximations see [2]. The stage values are required to have a specified order, that is approximate the solution at $x_{n-1} + c_i h$, to order q, and therefore

$$Y_i = \sum_{k=0}^{p} \frac{c_i^k}{k!} y^{(k)}(x_{n-1})h^k + \mathrm{O}\big(h^{q+1}\big), \quad i = 1, 2, \dots, s.$$

The outgoing approximations are chosen to have the special form

$$y_i^{[n]} = \sum_{k=0}^{p} \beta_{ik} h^k y^{(k)}(x_n) + \mathrm{O}\big(h^{p+1}\big), \quad i = 1, 2, \dots, r. \tag{2.3}$$

In [2] it was shown that when the stage order q is at least equal to $p-1$ and Y and $y^{[n]}$ are defined as above, the stage order and order conditions can be represented using functions of a complex variable, as follows

$$\begin{aligned} \exp(cz) &= zA\exp(cz) + Uw(z) + \mathrm{O}\big(z^{q+1}\big), \\ \exp(z)w(z) &= zB\exp(cz) + Vw(z) + \mathrm{O}\big(z^{p+1}\big), \end{aligned} \tag{2.4}$$

where the exp function is applied componentwise to a vector and $w(z)$ denotes a vector valued function with elements of the form

$$w_i(z) = \sum_{k=0}^{p} \beta_{ik} z^k, \quad i = 1, 2, \dots, r. \tag{2.5}$$

The stability behaviour of these methods is defined using the standard linear test problem $y' = \lambda y$, where λ is a complex parameter. If method (2.1) is applied to this problem, then the stability matrix is

$$M(z) = V + zB(I - zA)^{-1}U,$$

where $z = h\lambda$. Rearranging the first equation of (2.4) in terms of $\exp(cz)$ and substituting into the second equation, it follows that $\exp(z) + \mathrm{O}(z^{p+1})$ is an eigenvalue of $M(z)$.

Definition 2.1. If the characteristic polynomial of $M(z)$, known as the stability function, has the special form

$$p(w, z) = \det\bigl(wI - M(z)\bigr) = w^{r-1}\bigl(w - R(z)\bigr),$$

then the method is said to possess "Runge–Kutta stability".

In this case, the rational function $R(z)$ has the same role as the stability function of a Runge–Kutta method.

It was pointed out in [2] that if $p = q$, then asymptotically correct error estimates and continuous solutions can be found without extra stages needing to be computed. When the approximations passed from step to step have the form (2.3) then the most general choice for r is when $r = p + 1$. As pointed out in [3,6] when $s \geqslant p + 1$ there is sufficient freedom available to control higher order error coefficients. In this paper only the case when $p = q = r + 1 = s + 1$ will be investigated.

There is considerable freedom in the choice of coefficients β_{ik} which appear in (2.2). We will write the first row of coefficients as $\alpha_0, \alpha_1, \alpha_2, \ldots, \alpha_p$ and normalize these so that $\alpha_0 = 1$. Having made the choice of first row, we will restrict the successive rows to correspond to the derivatives of these quantities. That is

$$\begin{aligned}
y_1^{[n]} &= y(x_n) + \alpha_1 h y'(x_n) + \cdots + \alpha_p h^p y^{(p)}(x_n) + \mathrm{O}\bigl(h^{p+1}\bigr),\\
y_2^{[n]} &= h y'(x_n) + \alpha_1 h^2 y''(x_n) + \cdots + \alpha_{p-1} h^p y^{(p)}(x_n) + \mathrm{O}\bigl(h^{p+1}\bigr),\\
y_3^{[n]} &= h^2 y''(x_n) + \alpha_1 h^3 y'''(x_n) + \cdots + \alpha_{p-2} h^p y^{(p)}(x_n) + \mathrm{O}\bigl(h^{p+1}\bigr),\\
&\ \vdots\\
y_{p+1}^{[n]} &= h^p y^{(p)}(x_n) + \mathrm{O}\bigl(h^{p+1}\bigr).
\end{aligned}$$

Hence, the values of the β coefficients are given by

$$\beta_{ik} = \alpha_{k-i+1}, \quad i = 1, 2, \ldots, p+1,\ k = 0, 1, \ldots, p,$$

where $\alpha_j = 0$ if $j < 0$. This assumption is not restrictive, because it is always possible to change from one representation of the input and output quantities to another representation by using linear combinations. A transformation of this type makes no difference to the computational properties of the method but the convention we are adopting makes it easier to identify the requirements of Runge–Kutta stability.

With this particular choice of quantities passed from step to step the vector $w(z)$ has the special form

$$w(z) = \begin{bmatrix} \psi(z)^{-1} \\ z\psi(z)^{-1} \\ z^2\psi(z)^{-1} \\ \vdots \\ z^p\psi(z)^{-1} \end{bmatrix} = \psi(z)^{-1} Z, \tag{2.6}$$

where

$$Z = \begin{bmatrix} 1 & z & z^2 & \ldots & z^p \end{bmatrix}^{\mathrm{T}}.$$

The complex function $\psi(z)^{-1}$ has power series coefficients $1, \alpha_1, \alpha_2, \ldots, \alpha_p$ so that

$$\psi(z)^{-1} = 1 + \alpha_1 z + \alpha_2 z^2 + \cdots + \alpha_p z^p.$$

Hence, the coefficients in $\psi(z)$ are defined by

$$\begin{aligned} \psi(z) &= 1 + \psi_1 z + \psi_2 z^2 + \cdots + \psi_p z^p \\ &= \bigl(1 + \alpha_1 z + \alpha_2 z^2 + \cdots + \alpha_p z^p\bigr)^{-1} + \mathrm{O}\bigl(z^{p+1}\bigr). \end{aligned}$$

The order conditions now take the form

$$\begin{aligned} &\exp(cz) = zA\exp(cz) + U\psi(z)^{-1}Z + \mathrm{O}\bigl(z^{p+1}\bigr), \\ &\exp(z)\psi(z)^{-1}Z = zB\exp(cz) + V\psi(z)^{-1}Z + \mathrm{O}\bigl(z^{p+1}\bigr), \end{aligned} \tag{2.7}$$

or, as we will prefer to write them,

$$\begin{aligned} &\exp(cz)\psi(z) = zA\exp(cz)\psi(z) + UZ + \mathrm{O}\bigl(z^{p+1}\bigr), \\ &\exp(z)Z = zB\exp(cz)\psi(z) + VZ + \mathrm{O}\bigl(z^{p+1}\bigr). \end{aligned} \tag{2.8}$$

Notice that this implies that $Ve_1 = e_1$, where e_1 is the pre-consistency vector.

It becomes increasingly difficult to derive general linear methods with Runge–Kutta stability using a direct approach. It is therefore, desirable to look for interrelationships between the method parameters which guarantees Runge–Kutta stability and thus makes the task of finding methods easier. Before introducing such a relationship we first introduce some notation. For convenience, write "$\equiv$" to denote the equivalence relation between matrices that deems two matrices to be equivalent if and only if they "are identical except for the first row". If $Fe_1 = \lambda e_1$ then $D \equiv E$ implies $FD \equiv FE$. Moreover, for any G, $D \equiv E$ implies $DG \equiv EG$. Define the shifting matrix

$$J = \begin{bmatrix} 0 & 0 & \cdots & 0 & 0 \\ 1 & 0 & \cdots & 0 & 0 \\ 0 & 1 & \cdots & 0 & 0 \\ \vdots & \vdots & & \vdots & \vdots \\ 0 & 0 & \cdots & 1 & 0 \end{bmatrix},$$

which is used to shift rows and columns of a given matrix using either pre- or post-multiplication. Given a matrix R, RJ consists of the last p columns of R with an augmented column of zeros and JR consists of a row of zeros followed by the first p rows of R. For convenience write $K = J^{\mathrm{T}}$.

Definition 2.2. A general linear method satisfying (2.8) is said to have "inherent Runge–Kutta stability" if

$$BA \equiv JB, \tag{2.9}$$

$$BU \equiv JV - VJ, \tag{2.10}$$

and the matrix V has one eigenvalue equal to 1 and p eigenvalues equal to 0.

In [3,6] it was shown that if the above definition is satisfied and certain restrictions on the structure of the matrix V are satisfied, the nonlinear equations can be solved using only linear operations.

3. Derivation of methods using a transformation

Both implicit and explicit methods with inherent Runge–Kutta stability can be derived using slightly different approaches and the aim of this section is to draw these methods closer together using a transformation. This will also widen the classes of known methods.

Denote by A, B, U, V the original method and by $\widehat{A}$, $\widehat{B}$, $\widehat{U}$, $\widehat{V}$ the transformed method. In order to construct the original method, we will derive the transformed method using modified order conditions and then transform back to find the original method. The particular transformation we will use leaves the elements of A unchanged, except for the diagonal elements. This allows us to find an original stiff method by satisfying the order conditions of the transformed non-stiff method but it also works in the other direction. Furthermore one stiff method can be found from another stiff method, using modified order conditions. It is therefore, possible to construct L-stable methods in this way, even though the coefficients in the transformed method are not consistent with L-stability. The extra flexibility that then becomes available, is used to exert more control over the coefficients of the method.

In the analysis of the original method, write z for the complex variable used in the order conditions and $\hat{z} = z/(1-\theta z)$. This means that $z = \hat{z}/(1+\theta\hat{z})$ and that $(1+\theta\hat{z})(1-\theta z) = 1$. The transformation can also be expressed as $\hat{z} = -1/\theta + 1/(\theta - \theta^2 z)$ so that, when $z = \infty$, $\hat{z} = -1/\theta$. Also write $\hat{\psi}(\hat{z})$ in place of $\psi(z)$ in the formulation of the original method. First note that the relationship between Z and $\widehat{Z}$ can be written in the form

$$Z = \left(1+\theta\hat{z}\right)^{-p} T(\theta)\widehat{Z},$$

where the transformation matrix $T(\theta)$ is

$$T(\theta) = \begin{bmatrix} 1 & t_{1,2}\theta & \cdots & t_{1,p}\theta^{p-1} & t_{1,p+1}\theta^{p} \\ 0 & 1 & \cdots & t_{2,p}\theta^{p-2} & t_{2,p+1}\theta^{p-1} \\ \vdots & \vdots & & \vdots & \vdots \\ 0 & 0 & \cdots & 1 & t_{p,p+1}\theta \\ 0 & 0 & \cdots & 0 & 1 \end{bmatrix},$$

with coefficients $t_{i,j}$, given by the binomial coefficients

$$t_{i,j} = \binom{p+1-i}{j-i}.$$

Substitute $A = \widehat{A} + \theta I$, z and Z in terms of $\hat{z}$ and $\widehat{Z}$ into (2.8); it turns out that

$$\left(1+\theta\hat{z}\right)\exp\left(\frac{c\hat{z}}{1+\theta\hat{z}}\right)\hat{\psi}\left(\hat{z}\right) = \hat{z}\left(\widehat{A}+\theta I\right)\exp\left(\frac{c\hat{z}}{1+\theta\hat{z}}\right)\hat{\psi}\left(\hat{z}\right) + UT(\theta)\widehat{Z} + \mathrm{O}\left(\hat{z}^{p+1}\right),$$

$$\exp\left(\frac{\hat{z}}{1+\theta\hat{z}}\right)T(\theta)\widehat{Z} = \hat{z}B\exp\left(\frac{c\hat{z}}{1+\theta\hat{z}}\right)\hat{\psi}\left(\hat{z}\right) + VT(\theta)\widehat{Z} + \mathrm{O}\left(\hat{z}^{p+1}\right),$$

where

$$\hat{\psi}\left(\hat{z}\right) = \left(1+\theta\hat{z}\right)^{p-1}\psi\left(\frac{\hat{z}}{1+\theta\hat{z}}\right).$$

In terms of the transformation $T(\theta)$, the transformed matrices can be written as follows

$$\widehat{U} = UT(\theta), \qquad \widehat{B} = T(-\theta)B, \qquad \widehat{V} = T(-\theta)VT(\theta). \tag{3.1}$$

The order conditions now take the form

$$\begin{aligned}\exp\left(\frac{c\hat{z}}{1+\theta\hat{z}}\right)\hat{\psi}(\hat{z}) &= \hat{z}\widehat{A}\exp\left(\frac{c\hat{z}}{1+\theta\hat{z}}\right)\hat{\psi}(\hat{z}) + \widehat{U}\widehat{Z} + \mathrm{O}\big(\hat{z}^{p+1}\big),\\ \exp\left(\frac{\hat{z}}{1+\theta\hat{z}}\right)\widehat{Z} &= \hat{z}\widehat{B}\exp\left(\frac{c\hat{z}}{1+\theta\hat{z}}\right)\hat{\psi}(\hat{z}) + \widehat{V}\widehat{Z} + \mathrm{O}\big(\hat{z}^{p+1}\big).\end{aligned} \tag{3.2}$$

Note that $\widehat{V}e_1 = e_1$, where e_1 is the pre-consistency vector. The transformation we have used takes no account of inherent Runge–Kutta stability. We will show that with the form of the transformation we have used, this property is preserved. First notice that

$$\hat{z}J\widehat{Z} \equiv \widehat{Z}. \tag{3.3}$$

Now substituting the first equation of (3.2) into the second, gives

$$\begin{aligned}\exp\left(\frac{\hat{z}}{1+\theta\hat{z}}\right)\widehat{Z} &= \hat{z}^2\widehat{B}\widehat{A}\exp\left(\frac{c\hat{z}}{1+\theta\hat{z}}\right)\hat{\psi}(\hat{z}) + \big(\hat{z}\widehat{B}\widehat{U} + \widehat{V}\big)\widehat{Z} + \mathrm{O}\big(\hat{z}^{p+1}\big)\\ &\equiv \hat{z}^2\widehat{B}\widehat{A}\exp\left(\frac{c\hat{z}}{1+\theta\hat{z}}\right)\hat{\psi}(\hat{z}) + \hat{z}\big(\widehat{B}\widehat{U} + \widehat{V}J\big)\widehat{Z} + \mathrm{O}\big(\hat{z}^{p+1}\big).\end{aligned} \tag{3.4}$$

Now multiply the second equation of (3.2) on the left by $\hat{z}J$ and make use of (3.3), to find that

$$\exp\left(\frac{\hat{z}}{1+\theta\hat{z}}\right)\widehat{Z} \equiv \hat{z}^2J\widehat{B}\exp\left(\frac{c\hat{z}}{1+\theta\hat{z}}\right)\hat{\psi}(\hat{z}) + \hat{z}J\widehat{V}\widehat{Z} + \mathrm{O}\big(\hat{z}^{p+1}\big). \tag{3.5}$$

Compare (3.4) and (3.5), and we see that the coefficients of the transformed method are interrelated by

$$\widehat{B}\widehat{A} \equiv J\widehat{B}, \tag{3.6}$$

$$\widehat{B}\widehat{U} \equiv J\widehat{V} - \widehat{V}J. \tag{3.7}$$

In the relationship between a method and its transformed counterpart, we need to consider the connection between their stability functions. Consider the stability matrix of the original method

$$\begin{aligned}M(z) &= V + zB(I-zA)^{-1}U\\ &= V + \frac{z}{1-\theta z}B\left(\frac{1}{1-\theta z}I - \frac{z}{1-\theta z}A\right)^{-1}U\\ &= V + \frac{z}{1-\theta z}B\left(I - \frac{z}{1-\theta z}(A-\theta I)\right)^{-1}U,\\ M\left(\frac{\hat{z}}{1+\theta\hat{z}}\right) &= V + \hat{z}B\big(I-\hat{z}\widehat{A}\big)^{-1}U.\end{aligned}$$

This is related to $\widehat{M}(\hat{z})$ by a similarity. That is

$$\begin{aligned}T(-\theta)M\left(\frac{\hat{z}}{1+\theta\hat{z}}\right)T(\theta) &= T(-\theta)VT(\theta) + \hat{z}T(-\theta)B\big(I-\hat{z}\widehat{A}\big)^{-1}UT(\theta)\\ &= \widehat{V} + \hat{z}\widehat{B}\big(I-\hat{z}\widehat{A}\big)^{-1}\widehat{U} = \widehat{M}\big(\hat{z}\big).\end{aligned}$$

This leads to the following theorem.

Theorem 3.1. *A transformed general linear method satisfying* (3.2) *has inherent Runge–Kutta stability if*

$$\widehat{B}\widehat{A} \equiv J\widehat{B}, \qquad \widehat{B}\widehat{U} \equiv J\widehat{V} - \widehat{V}J$$

and the matrix $\widehat{V}$ *has one eigenvalue equal to* 1 *and* p *eigenvalues equal to* 0.

Proof. A similar result has been proved in [3]. □

The transformed stability function $\widehat{R}(\hat{z})$ is the $(1,1)$ element of $(I - \hat{z}J)\widehat{M}(\hat{z})(I - \hat{z}J)^{-1}$. Therefore,

$$\widehat{R}(\hat{z}) = e_1^{\mathrm{T}}\big(\widehat{V} + \hat{z}\widehat{B}\big(I - \hat{z}\widetilde{A}\big)^{-1}\widehat{U}\big)\widehat{Z}, \tag{3.8}$$

which approximates $\exp(\hat{z}/(1+\theta\hat{z}))$ up to order p. If A-stability is required it is possible to satisfy $|\widehat{R}(\hat{z})| < 1$ for all $\hat{z}$ on the circle, centred at $-1/2\theta$ with radius $1/2\theta$. If L-stability is required, it is sufficient to ensure that $\widehat{R}(-1/\theta) = 0$.

It might seem possible to use slightly different transformations and still come to the same conclusion. That this is not possible can be seen by carrying out a further transformation with an upper triangular Toeplitz matrix

$$S = \begin{bmatrix} 1 & s_1 & \cdots & s_{r-2} & s_{r-1} \\ 0 & 1 & \cdots & s_{r-3} & s_{r-2} \\ \vdots & \vdots & & \vdots & \vdots \\ 0 & 0 & \cdots & 1 & s_1 \\ 0 & 0 & \cdots & 0 & 1 \end{bmatrix}.$$

The reason that S must be an upper triangular Toeplitz matrix is that Z must be expressed in terms of $\widehat{Z}$. When (3.6) is pre-multiplied by S,

$$S\widehat{B}\widehat{A} \equiv SJS^{-1}S\widehat{B}.$$

If this still preserves the stability condition (3.6) then $SJS^{-1} \equiv J$, which is equivalent to $SJ \equiv JS$. Calculate $SJ - JS$ and we find

$$SJ - JS = \begin{bmatrix} s_1 & s_2 & \cdots & s_{r-1} & 0 \\ 0 & 0 & \cdots & 0 & -s_{r-1} \\ \vdots & \vdots & & \vdots & \vdots \\ 0 & 0 & \cdots & 0 & -s_2 \\ 0 & 0 & \cdots & 0 & -s_1 \end{bmatrix},$$

which is only non-zero in the first row if

$$s_1 = s_2 = \cdots = s_{r-1} = 0.$$

Thus $S = I$ and the additional transformation has no effect. The following lemma is needed for analyzing stability.

Lemma 3.2. *Let* x *and* θ *denote real numbers, then for* u *satisfying* $|\theta u| < 1$,

$$\exp\left(\frac{xu}{1+\theta u}\right) = 1 + \sum_{i=1}^{\infty} N_i(x,\theta)u^i, \tag{3.9}$$

where

$$N_i(x,\theta)=\sum_{k=0}^{i-1}\binom{i-1}{k}\frac{(-\theta)^k x^{i-k}}{(i-k)!}.$$

Proof. Write (3.9) in the form

$$\sum_{j=0}^{\infty} a_j\frac{x^j}{j!}=\sum_{j=0}^{\infty} b_j\frac{x^j}{j!}, \tag{3.10}$$

so that it is only necessary to prove that $a_j=b_j$, for $j=0,1,2,\ldots$. This will hold if

$$\sum_{j=0}^{\infty} a_j t^j=\sum_{j=0}^{\infty} b_j t^j,$$

for sufficiently small $|t|$. However, (3.10) holds for $|tu|<|1+\theta u|$, because

$$\begin{aligned}\sum_{j=0}^{\infty}\left(\frac{tu}{1+\theta u}\right)^j &= \left(1-\frac{tu}{1+\theta u}\right)^{-1}=\frac{1+\theta u}{1+u(\theta-t)}=1+\frac{tu}{1-u(t-\theta)}\\ &= 1+\sum_{j=1}^{\infty}\bigl(t(t-\theta)^{j-1}\bigr)u^j=1+\sum_{j=1}^{\infty}\left(\sum_{k=0}^{j-1}\binom{j-1}{k}(-\theta)^k t^{j-k}\right)u^j. \qquad \square\end{aligned}$$

An alternative proof is based on the negative binomial expansion

$$(1+\theta u)^{-l}=\sum_{k=0}^{\infty}\binom{k+l-1}{k}(-\theta u)^k.$$

Substitute this into the exponential series

$$\exp\left(\frac{xu}{1+\theta u}\right)=1+\sum_{l=1}^{\infty}\frac{1}{l!}(xu)^l(1+\theta u)^{-l},$$

and write $j=l+k$. The result is

$$1+\sum_{i=1}^{\infty}\sum_{k=0}^{i-1}\binom{i-1}{k}\frac{1}{(i-k)!}(xu)^{i-k}(-\theta u)^k=1+\sum_{i=1}^{\infty}\left(\sum_{k=0}^{i-1}\binom{i-1}{k}\frac{(-\theta)^k x^{i-k}}{(i-k)!}\right)u^i.$$

This result of Lemma 3.2 can be extended to the case that x is a vector if powers of x are interpreted in a component by component sense. With this in mind, the $\widehat{U}$ and $\widehat{V}$ matrices can be found using the identity

$$\exp\left(\frac{c\hat{z}}{1+\theta\hat{z}}\right)\hat{\psi}(\hat{z})=\widehat{\Phi}\widehat{Z}+\mathrm{O}(\hat{z}^{p+1}),$$

where

$$\widehat{\Phi}=\bigl[\,\widehat{\Phi}_0\quad \widehat{\Phi}_1\quad \widehat{\Phi}_2\quad \ldots\quad \widehat{\Phi}_p\,\bigr]$$

and the vector valued function $\widehat{\Phi}_j$, has the form

$$\widehat{\Phi}_j = \sum_{i=0}^{j} \hat{\psi}_i N_{j-i}(c,\theta),$$

with the convention that $\widehat{\Phi}_{-1} = 0$. The order conditions (3.2) can be expressed as follows

$$\bigl(I - \hat{z}\widehat{A}\bigr)\widehat{\Phi}\widehat{Z} = \widehat{U}\widehat{Z} + \mathrm{O}\bigl(\hat{z}^{p+1}\bigr), \tag{3.11}$$

$$\exp\left(\frac{\hat{z}}{1+\theta\hat{z}}\right)\widehat{Z} - \hat{z}\widehat{B}\widehat{\Phi}\widehat{Z} = \widehat{V}\widehat{Z} + \mathrm{O}\bigl(\hat{z}^{p+1}\bigr). \tag{3.12}$$

Therefore, from (3.11), the $\widehat{U}$ matrix is given by

$$\widehat{U} = \widehat{\Phi} - \widehat{A}\widehat{\Phi}K, \tag{3.13}$$

since $\hat{z}\widehat{Z} = K\widehat{Z} + \mathrm{O}(\hat{z}^{p+1})$. From (3.12) the $\widehat{V}$ matrix is

$$\widehat{V} = \exp\bigl(K(I+\theta K)^{-1}\bigr) - \widehat{B}\widehat{\Phi}K, \tag{3.14}$$

where $\exp(K(I+\theta K)^{-1})Z = \exp(\hat{z}/(1+\theta\hat{z}))\widehat{Z} + \mathrm{O}(\hat{z}^{p+1})$. This is natural since K is nilpotent.

Substituting the expressions (3.13) and (3.14) into (3.7) and simplifying yields

$$\widehat{B}\widehat{\Phi}(I - KJ) \equiv J\exp\bigl(K(I+\theta K)^{-1}\bigr) - \exp\bigl(K(I+\theta K)^{-1}\bigr)J,$$

which results in the following consistency conditions

$$\hat{b}_i^{\mathrm{T}}\widehat{\Phi}_p = N_{p-i+2}(1,\theta), \quad 2 \leqslant i \leqslant p+1. \tag{3.15}$$

Given the $\widehat{A}$, $\widehat{B}$ matrices are known then the $\widehat{U}$, $\widehat{V}$ matrices are known. Given $\widehat{A}$ or $\widehat{B}$ the other can be found from the (3.6) condition as was done in [3,6].

4. Relating the original and transformed methods

If the original method is explicit, the freedom in the stability function is used to control the error constant and possibly the stability region. If the original method is implicit, the freedom in the numerator of the stability function is used to guarantee L-stability. These conditions on the original method must be interpreted into conditions on the transformed method. To simplify the discussion, denote by $\langle z^n, \phi(z)\rangle$ the coefficient of z^n in the polynomial, or Taylor series expansion of, $\phi(z)$. Consider the stability function of the original method as the rational approximation

$$R(z) = \frac{N(z)}{(1-\lambda z)^{p+1}} = \exp(z) + \sigma z^{p+1} + \mathrm{O}\bigl(z^{p+2}\bigr),$$

with the stability function of the transformed method given as

$$\widehat{R}\bigl(\hat{z}\bigr) = \frac{\widehat{N}(\hat{z})}{(1-\hat{\lambda}\hat{z})^{p+1}} = \exp\left(\frac{\hat{z}}{1+\theta\hat{z}}\right) + \sigma\hat{z}^{p+1} + \mathrm{O}\bigl(\hat{z}^{p+2}\bigr).$$

In these rational functions, $N(z)$ and $\widehat{N}(\hat{z})$ are polynomials of degree $p+1$; note that $R(z)$ and $\widehat{R}(\hat{z})$ are related by $z = \hat{z}/(1+\theta\hat{z})$. Let

$$\rho = \langle z^{p+1}, N(z)\rangle = \sigma + \langle z^{p+1}, (1-\lambda z)^{p+1}\exp(z)\rangle,$$
$$\hat\rho = \langle \hat z^{p+1}, \widehat N(\hat z)\rangle = \sigma + \left\langle \hat z^{p+1}, (1-\hat\lambda\hat z)^{p+1}\exp\left(\frac{\hat z}{1+\theta\hat z}\right)\right\rangle.$$

Since, the two adjustments will be identical, it follows that

$$\rho = \hat\rho + \left\langle z^{p+1}, (1-\lambda z)^{p+1}\exp(z) - (1-\hat\lambda z)^{p+1}\exp\left(\frac{z}{1+\theta z}\right)\right\rangle. \tag{4.1}$$

A further order condition can be to found by determining a relationship between the matrices of the transformed method and the desired value for ρ.

To analyze the possible methods available using the transformation, consider two cases. In the case $\hat\lambda = 0$, derive the transformed explicit method, using modified order conditions in a manner similar to that described in [6]. The second case $\hat\lambda \neq 0$ is treated as in [3].

4.1. Case 1

When $\hat\lambda = 0$ the transformed method is explicit, but the transformation allows the original method to be explicit or implicit. If $\lambda = 0$ the original method is explicit and no transformation is used, that is $\theta = 0$. Methods of this type correspond to the ones derived in [6]. If $\lambda \neq 0$ the original method is implicit but formed using a transformed explicit method. DIMSIMs using this approach were constructed in [4]. It is not possible to construct these methods using the results from [3].

To represent the additional order condition, the coefficient of the $\hat z^{p+1}$ in $\widehat R(\hat z)$ must be found using the matrices of the transformed method. This is found by expanding (3.8). First notice that

$$(I - \hat z\widehat A)^{-1}\widehat U\widehat Z = \sum_{i=0}^{p-1}\widehat\Phi_i\hat z^i + \widehat\Phi_p\hat z^p.$$

The stability function is given by

$$\widehat R(\hat z) = e_1^{\mathrm T}\widehat V\widehat Z + \hat z\hat b_1^{\mathrm T}(I - \hat z\widehat A)^{-1}\widehat U\widehat Z = \hat v_1^{\mathrm T}\widehat Z + \hat b_1^{\mathrm T}\sum_{i=0}^{p-1}\widehat\Phi_i\hat z^{i+1} + \hat b_1^{\mathrm T}\widehat\Phi_p\hat z^{p+1}. \tag{4.2}$$

Compare the first two terms in this expression with the order conditions for the first output approximation. The additional condition is therefore given by

$$\hat b_1^{\mathrm T}\widehat\Phi_p = \hat\rho.$$

When the original method is explicit this condition reveals the error constant, whereas in the implicit case L-stability is guaranteed. This can be shown by comparing (4.1) to (4.2) with $\hat z = -1/\theta$.

To find the methods as an equivalent linear system the matrix formed from deleting the first row and column of $\widehat V$ must be strictly upper triangular. This pattern allows the final conditions required and the methods are found using the same procedure as outlined in [6].

4.2. Case 2

When $\hat\lambda \neq 0$ both explicit and implicit methods can be constructed. If $\hat\lambda = \lambda$ the original method is implicit and no transformation is used. Methods of this type correspond to those derived in [3]. If $\lambda \neq 0$

the original implicit method is formed using a transformed implicit method. Therefore, methods can be constructed with a diagonal component which would not normally allow A-stability. If $\lambda = 0$ the original method is explicit formed using a transformed implicit method. Methods constructed in this way are not available using the approach outlined in [6]. These methods are in some sense a high stage order generalization of the Almost Runge–Kutta methods studied in [5].

To represent the additional order condition, the coefficient of the $\hat{z}^{p+1}$ in $\widehat{N}(\hat{z})$ must be found using the matrices of the transformed method. This is achieved by expanding (3.8) as follows

$$\begin{aligned}
\widehat{R}(\hat{z}) &= e_1^{\mathrm{T}}\left(\widehat{V} - \widehat{B}\widehat{A}^{-1}\left(I - \frac{1}{\hat{z}}\widehat{A}^{-1}\right)^{-1}\widehat{U}\right)\widehat{Z} \\
&= \sum_{i=0}^{p}\big(N_i(1,-\theta) - \hat{b}_1^{\mathrm{T}}\widehat{\Phi}_{i-1}\big)\hat{z}^i - \hat{b}_1^{\mathrm{T}}\sum_{i=0}^{p}\frac{1}{\hat{z}^i}\widehat{A}^{-i-1}\widehat{U}\widehat{Z} \\
&= \sum_{i=0}^{p}\left[\big(N_i(1,-\theta) - \hat{b}_1^{\mathrm{T}}\widehat{\Phi}_{i-1}\big)\hat{z}^i - \hat{b}_1^{\mathrm{T}}\widehat{A}^{-i-1}\sum_{j=0}^{p}\big(\widehat{\Phi}_j - \widehat{A}\widehat{\Phi}_{j-1}\big)\hat{z}^{j-i}\right].
\end{aligned}$$

It is now sufficient to check that the coefficients of $\widehat{R}(\hat{z})$, satisfy $\hat{z}^i = 0$ for $i > 0$. These are given by

$$N_i(1,-\theta) - \hat{b}_1^{\mathrm{T}}\widehat{\Phi}_{i-1} - \hat{b}_1^{\mathrm{T}}\sum_{j=i}^{p}\widehat{A}^{i-j-1}\big(\widehat{\Phi}_j - \widehat{A}\widehat{\Phi}_{j-1}\big) = 0,$$

which simplifies to

$$N_i(1,-\theta) - \hat{b}_{p+1-i}^{\mathrm{T}}\widehat{\Phi}_p = 0,$$

which is equivalent to the consistency conditions (3.15). The additional condition required is

$$\hat{b}_p^{\mathrm{T}}\widehat{A}^{-1}\widehat{\Phi}_p = 1 - \big(-\hat{\lambda}\big)^{-(p+1)}\hat{\rho}.$$

When the original method is explicit this condition reveals the error constant, whereas in the implicit case L-stability is guaranteed. This can be shown by comparing (4.1) to (4.2) with $\hat{\rho} = 0$.

To find the methods as an equivalent linear system the matrix formed from deleting the first row and column of $\widehat{V}$ must be strictly lower triangular. This pattern allows the final conditions required and the methods are found using the same procedure as outlined in [3].

5. Methods

In summary the transformed methods are derived as follows. If the transformed method is explicit, then $\widehat{B}$ is derived using the results from [6]; the free parameters available take care of the error constant and the stability region. The matrix $\widehat{A}$ is then found from (3.6). The stage order and order conditions are therefore, satisfied by choosing $\widehat{U}$, $\widehat{V}$ according to (3.13), (3.14). On the other hand if the transformed method is implicit, then the $\widehat{A}$ is derived using the results from [3] the free parameters available are used to guarantee L-stability. The matrix $\widehat{B}$ is then found from modifying (3.6) slightly. The stage order and order conditions are again satisfied by requiring (3.13), (3.14). The original method is then found by reversing the transformations (3.1). The methods given in this section are not supposed to be in any sense optimal. They are rather displayed as examples of methods which cannot be derived using the techniques developed in [3,6].

Even though Nordsieck vectors were originally proposed for linear multistep methods they have a natural role in general linear methods because of the ease of stepsize changing. This is also a convenient representation because the data is standardized. All the following methods are expressed in traditional Nordsieck form. Representing the method in this form does destroy the (3.6) condition, this is because the matrix J is not the most general matrix available for this situation. This will be discussed in future work.

The first example is of an order 3 explicit method generated using a transformed implicit method, with $c = [\frac{1}{4}, \frac{1}{2}, \frac{3}{4}, 1]^{\mathrm{T}}$ and $R(z) = 1 + z + z^2/2 + z^3/6 + z^4/24$. Because $R(z) = \exp(z) + \mathrm{O}(z^5)$, the error constant is zero and it is possible with careful implementation to obtain fourth order performance from the method. The choice $\beta = [0, 0, 0, 1]$ means that the method has a structure which resembles the FSAL property of some Runge–Kutta methods. The method was constructed from $\hat{\lambda} = 1/4$. This means that many of the coefficients have smaller rational values than could be obtained without a transformation as well as smaller magnitudes. Notice that the matrix formed by deleting the first row and column of V is not strictly upper triangular but of course does have zero spectral radius. The coefficient matrices are

$$\left[\begin{array}{cccc|cccc}
0 & 0 & 0 & 0 & 1 & \frac{1}{4} & \frac{1}{16} & \frac{1}{64} \\
\frac{224}{403} & 0 & 0 & 0 & 1 & -\frac{45}{806} & -\frac{45}{1612} & \frac{67}{3224} \\
\frac{1851}{2170} & \frac{93}{280} & 0 & 0 & 1 & -\frac{3777}{8680} & -\frac{681}{3472} & \frac{891}{69440} \\
\frac{305}{364} & \frac{5}{28} & \frac{5}{12} & 0 & 1 & -\frac{473}{1092} & -\frac{81}{364} & \frac{17}{2912} \\
\hline
\frac{305}{364} & \frac{5}{28} & \frac{5}{12} & 0 & 1 & -\frac{473}{1092} & -\frac{81}{364} & \frac{17}{2912} \\
0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 \\
-\frac{78}{7} & \frac{94}{7} & -10 & 4 & 0 & \frac{26}{7} & \frac{1}{7} & -\frac{3}{28} \\
-\frac{256}{21} & \frac{292}{21} & -\frac{80}{9} & \frac{8}{3} & 0 & \frac{284}{63} & \frac{4}{21} & -\frac{1}{7}
\end{array}\right].$$

The second method which is an implicit order 4 method is L-stable with $\hat{\lambda} = \frac{1}{2}$, abscissae vector $c = [1, \frac{3}{4}, \frac{1}{4}, \frac{1}{2}, 1]^{\mathrm{T}}$ and $\beta = [0, 0, 0, 0, 1]$. It is generated using a transformed implicit method, the extra freedom was used to find what appears to be a better method. Using the direct approach the coefficient with the largest magnitude of the method is $-\frac{608}{27}$, using the transformation this decreases to $-\frac{3364}{549}$ which can be counted as an advantage. The coefficient matrices for this method are

$$A = \begin{bmatrix}
\frac{1}{4} & 0 & 0 & 0 & 0 \\
-\frac{513}{54272} & \frac{1}{4} & 0 & 0 & 0 \\
\frac{3706119}{69088256} & -\frac{488}{3819} & \frac{1}{4} & 0 & 0 \\
\frac{32161061}{197549232} & -\frac{111814}{232959} & \frac{134}{183} & \frac{1}{4} & 0 \\
-\frac{135425}{2948496} & -\frac{641}{10431} & \frac{73}{183} & \frac{1}{2} & \frac{1}{4}
\end{bmatrix},$$

$$U=\begin{bmatrix} 1 & \frac{3}{4} & \frac{1}{2} & \frac{1}{4} & 0 \\ 1 & \frac{27649}{54272} & \frac{5601}{27136} & \frac{1539}{54272} & -\frac{459}{6784} \\ 1 & \frac{15366379}{207264768} & \frac{756057}{34544128} & \frac{1620299}{69088256} & -\frac{4845}{454528} \\ 1 & -\frac{32609017}{197549232} & \frac{929753}{32924872} & \frac{4008881}{32924872} & \frac{174981}{3465776} \\ 1 & -\frac{367313}{8845488} & -\frac{22727}{1474248} & \frac{40979}{982832} & \frac{323}{25864} \end{bmatrix},$$

$$B=\begin{bmatrix} -\frac{135425}{2948496} & -\frac{641}{10431} & \frac{73}{183} & \frac{1}{2} & \frac{1}{4} \\ 0 & 0 & 0 & 0 & 1 \\ \frac{2255}{2318} & -\frac{47125}{20862} & \frac{447}{122} & -\frac{11}{4} & \frac{7}{4} \\ \frac{12620}{10431} & -\frac{96388}{31293} & \frac{3364}{549} & -\frac{10}{3} & \frac{4}{3} \\ \frac{414}{1159} & -\frac{29954}{31293} & \frac{130}{61} & -1 & \frac{1}{3} \end{bmatrix},$$

$$V=\begin{bmatrix} 1 & -\frac{367313}{8845488} & -\frac{22727}{1474248} & \frac{40979}{982832} & \frac{323}{25864} \\ 0 & 0 & 0 & 0 & 0 \\ 0 & -\frac{28745}{20862} & -\frac{1937}{13908} & \frac{351}{18544} & \frac{65}{976} \\ 0 & -\frac{70634}{31293} & -\frac{2050}{10431} & -\frac{187}{2318} & \frac{113}{366} \\ 0 & -\frac{27052}{31293} & -\frac{113}{10431} & -\frac{491}{4636} & \frac{161}{732} \end{bmatrix}.$$

The final method is derived from a transformed explicit method. It is an L-stable order 3 implicit method, which has $\hat{\lambda}=\frac{1}{4}$, abscissae vector $c=[\frac{1}{4},\frac{1}{2},\frac{3}{4},1]^{\mathrm{T}}$ and $\psi(z)=1+\frac{1}{4}z+\frac{1}{4}z^2+\frac{1}{4}z^3$. Note that the matrix formed by deleting the first row and column of V is strictly upper triangular. This means that this method will be zero-stable for any choice of variable mesh. The coefficient matrices are

$$\left[\begin{array}{cccc|cccc} \frac{1}{4} & 0 & 0 & 0 & 1 & 0 & -\frac{1}{16} & -\frac{1}{32} \\ \frac{11}{2124} & \frac{1}{4} & 0 & 0 & 1 & \frac{130}{531} & -\frac{11}{4248} & -\frac{719}{11328} \\ \frac{117761}{23364} & -\frac{189}{44} & \frac{1}{4} & 0 & 1 & -\frac{130}{531} & \frac{183437}{93456} & \frac{283675}{124608} \\ \frac{312449}{23364} & -\frac{4525}{396} & \frac{1}{36} & \frac{1}{4} & 1 & -\frac{650}{531} & \frac{121459}{23364} & \frac{130127}{20768} \\ \hline -\frac{58405}{7788} & \frac{4297}{132} & -\frac{475}{12} & 15 & 1 & \frac{125}{236} & \frac{1020}{649} & -\frac{2199}{10384} \\ -\frac{64}{33} & \frac{746}{33} & -\frac{95}{3} & 12 & 0 & 0 & \frac{85}{22} & \frac{677}{176} \\ -\frac{4}{3} & \frac{2}{3} & \frac{2}{3} & 0 & 0 & 0 & 0 & \frac{13}{8} \\ -\frac{16}{3} & \frac{56}{3} & -\frac{64}{3} & 8 & 0 & 0 & 0 & 0 \end{array}\right].$$

6. Concluding remarks

We have attempted to widen the range of available general linear methods possessing “inherent Runge–Kutta stability” by applying a transformation to the order conditions for these methods. Previously, implicit methods were based on the style of [3] and explicit methods on [6]. The new transformation enables explicit and alternative implicit methods to be found with a close relationship to [3]. Furthermore, the transformation enables the approach used in [6] to yield implicit as well as explicit methods. Now that a wide family of methods exists for various orders, the question remains as to how the new freedom can be used to best advantage. We intend to examine this question and at the same time to obtain the most general situation possible for which the property of inherent Runge–Kutta stability holds. We believe we can obtain a full classification of methods with inherent Runge–Kutta stability and this will be the subject of a later paper. It is also intended, that methods with $s > p+1$ be investigated. This will determine which choice of s versus p is most likely to lead to optimal methods.

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