Exponentially-fitted methods and their stability functions

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Abstract. Is it possible to determine the stability function of an exponentially-fitted Runge-Kutta method, without actually constructing the method itself? This question was answered in a recent paper and examples were given for one-stage methods. In this paper we summarize the results and we focus on two-stage methods.

Keywords: Exponential fitting; Stability functions
PACS: 02.60.Lj

EXPONENTIALLY-FITTED RUNGE-KUTTA METHODS

The most general form of an exponentially-fitted Runge-Kutta method for solving

$$y' = f(x,y)\,, \tag{1}$$

is

$$y_{n+1} = \gamma y_n + h\sum_{i=1}^{s} b_i\, f(x_n + c_i h, Y_i)$$

whereby

$$Y_i = \gamma_i y_n + h\sum_{j=1}^{s} a_{ij}\, f(x_n + c_j h, Y_j)\,, \qquad i = 1,\dots,s\,.$$

With such a method, a generalised Butcher tableau can be associated:

$$\begin{array}{c|c|cccc} c_1 & \gamma_1 & a_{11} & \dots & a_{1s} \\ c_2 & \gamma_2 & a_{21} & \dots & a_{2s} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ c_s & \gamma_s & a_{s1} & \dots & a_{ss} \\ \hline & \gamma & b_1 & \dots & b_s \end{array} \qquad \text{or} \qquad \begin{array}{c|c|c} c & \Gamma & A \\ \hline & \gamma & b^T \end{array}\,.$$

The coefficients of these EFRK methods in general depend upon the product $z_0 := \omega h$ where ω is a parameter that can be related to the solution of the problem to be solved. In fact, EF methods are designed to solve problems which have an exponential behaviour or (in the case ω is purely imaginary) a periodic behaviour. To construct such an EFRK method, a set of linear functionals can be introduced [1]:

$$\begin{cases} \mathscr{L}_i[y(x);h] = y(x+c_i h) - \gamma_i y(x) - h\sum_{j=1}^{s} a_{ij} y'(x+c_j h)\,, & i = 1,\dots,s \\ \mathscr{L}[y(x);h] = y(x+h) - \gamma y(x) - h\sum_{i=1}^{s} b_i y'(x+c_i h)\,. \end{cases}$$

Next, conditions are imposed onto these functionals. For each stage of the method, a so-called fitting space is determined. Each stage contains $s+1$ parameters and for each stage the same fitting space $\mathscr{S}$ of dimension $s+1$ can be considered.

It is well-known that collocation offers an alternative way to construct such methods: a function $P(x) \in \mathscr{S}$ is constructed such that

$$\begin{cases} P(x_n) = y_n \\ P(x_n + c_i h)' = f(x_n + c_i h, P(x_n + c_i h))\,, & i = 1,\dots,s\,. \end{cases} \tag{2}$$

The method is then defined by imposing $y_{n+1} := P(x_n + h)$.

Vanden Berghe et al. [2] and Calvo et al. [3] have constructed EFRK methods with $\mathscr{S} = \{x^q\,\mathrm{e}^{\pm\omega x}|q = 0, 1, \ldots, P\} \cup \{x^q|q = 0, 1, \ldots, K\}$ and $\mathscr{S} = \{\mathrm{e}^{\pm q\omega x}|q = 1, \ldots, P+1\} \cup \{x^q|q = 0, 1, \ldots, K\}$ resp. where $2\,(P+1)+K+1 = s+1$. Note that a generalisation of both approaches is to consider $\mathscr{S} = \{\mathrm{e}^{\omega_q x}|q = 1, \ldots, s+1\}$, where $\omega_1, \ldots, \omega_{s+1}$ take different values.

THE STABILITY FUNCTION OF EFRK METHODS

In the case of initial value problems, the stability the method plays an important role and the stability properties of the methods should be examined. Therefore, the method is applied to the linear equation

$$y' = \lambda\, y \tag{3}$$

giving rise to a relation of the form $y_{n+1} = R(z,z_0)\,y_n$ with $z := \lambda\, h$. Independently of the specific choice for the space $\mathscr{S}$, the stability function $R(z,z_0)$ of an EFRK method can be written as

$$R(z,z_0) = \gamma + z\,b^T\,(I - zA)^{-1}\,\Gamma$$

where R is a rational function in z with coefficients that depend upon z_0. When the parameter(s) of an EFRK method tend(s) to 0, the classical RK method of collocation type is found. Its stability function is then given by (we omit the second argument, since it is not present in the expression)

$$R(z) = 1 + z\,b^T\,(I - zA)^{-1}\,e = \mathrm{e}^z + \mathscr{O}(z^{p+1})\,,$$

where e is the vector of length s with unit entries and $s \leq p \leq 2\,s$.

In [4] it is shown that for an EFRK method that is fitted to the functions $x^q\,\mathrm{e}^{\omega x}$, $q = 0, 1, \ldots, P$ the conditions that should be imposed, can be written down as

$$\frac{\partial^q}{\partial^q z} R(z,z_0)\big|_{z=z_0} = \mathrm{e}^{z_0} \qquad q = 0, 1, \ldots, P\,. \tag{4}$$

One notices that in the special case $\omega = 0$, i.e. z_0=0, the classical conditions $R^{(q)}(0) = 1$, $q = 0, 1, \ldots, P$, are obtained, which means that $R(z) - \exp(z) = \mathscr{O}(z^{P+1})$. The results can be extended to methods that are fitted so several parameters ω. For instance, suppose that a method is fitted for two values ω and ω'. We can then denote the corresponding stability function as $R(z,\{z_0,z_0'\})$ where $z_0 := \omega\,h$ and $z_0' = \omega'\,h$ and the method will be fitted to $\{x^q\,\mathrm{e}^{\omega x}, x^q\,\mathrm{e}^{\omega' x}\}$, $q = 0, \ldots, P$ iff

$$\frac{\partial^q}{\partial^q z} R(z,\{z_0,z_0'\})\big|_{z=z_0} = \mathrm{e}^{z_0} \qquad \text{and} \qquad \frac{\partial^q}{\partial^q z} R(z,\{z_0,z_0'\})\big|_{z=z_0'} = \mathrm{e}^{z_0'}\,, \qquad q = 0, \ldots, P\,.$$

In particular, an EFRK method that is fitted to the space of functions $\{1, x, \ldots, x^{P_1}\} \cup \{x^q\,\mathrm{e}^{\omega x}|q = 0, 1, \ldots, P_2\}$, has to satisfy:

$$\begin{cases} \frac{\partial^q}{\partial^q z} R(z,\{z_0,0\})\big|_{z=0} = 1 & q = 0, 1, \ldots, P_1 \\ \frac{\partial^q}{\partial^q z} R(z,\{z_0,0\})\big|_{z=z_0} = \mathrm{e}^{\pm z_0} & q = 0, 1, \ldots, P_2\,. \end{cases}$$

It was also shown in [4] that nice relations exist between stability functions and the order stars: suppose a method $M_{k,l}$ (the number of stages does not really matter here) is built to integrate exactly all functions in the space

$$\mathscr{S}_{k,l}(\omega) = \mathrm{Span}\{1, x, \ldots, x^{k-1}, \mathrm{e}^{\omega x}, x\,\mathrm{e}^{\omega x}, \ldots, x^{l-1}\mathrm{e}^{\omega x}\}\,.$$

For the equation (3), this gives rise to $y_{n+1} = R_{k,l}(z,z_0)\,y_n$.

On the other hand, following Lawson [5] and defining $u(x) = \mathrm{e}^{-\omega x}y(x)$ the equation (3) becomes $u' = (\lambda - \omega)\,u$. If $y \in \mathscr{S}_{k,l}(\omega)$, then $u \in \mathscr{S}_{l,k}(-\omega)$, and this then leads to $u_{n+1} = R_{l,k}(z - z_0, -z_0)\,u_n$, from which $y_{n+1} = \mathrm{e}^{z_0}\,R_{l,k}(z - z_0, -z_0)\,y_n$ is obtained. In general, we thus have

$$R_{k,l}(z,z_0) = \mathrm{e}^{z_0}\,R_{l,k}(z - z_0, -z_0)\,. \tag{5}$$

For the corresponding order star, this then means

$$\left|\frac{R_{k,l}(z,z_0)}{\mathrm{e}^z}\right| = \left|\frac{R_{l,k}(z - z_0, -z_0)}{\mathrm{e}^{z-z_0}}\right|\,. \tag{6}$$

THE TWO STAGE-CASE

The one-stage case has been discussed in detail in [4]. In this paper, we will focus on the two-stage case. For a two-stage method, the stability function will be a rational approximation of degree at most two in both the numerator and the denominator, i.e.

$$R(z,z_0)=\frac{a_0+a_1\,z_+a_2\,z^2}{1+b_1\,z+b_2\,z^2}\,,$$

where a_0, a_1, a_2, b_1 and b_2 can depend upon z_0. There are five degrees of freedom, so we can impose $i+j=5$ conditions: $\frac{\partial^q}{\partial^q z}R(z,z_0)\big|_{z=0}=1$, $q=1,\ldots,i$ and $\frac{\partial^q}{\partial^q z}R(z,z_0)\big|_{z=z_0}=\mathrm{e}^{z_0}$, $q=1\ldots,j$, i.e. we consider the stability functions that are obtained by fitting to $\{1,x,\ldots,x^{i-1}\}\cup\{\mathrm{e}^{\omega x},x\,\mathrm{e}^{\omega x},\ldots,x^{j-1}\,\mathrm{e}^{\omega x}\}$. Then we obtain six different stability functions that are denoted as $\hat{R}_{i,j}(z,z_0)$

- $\hat{R}_{5,0}$: $a_0=1$, $b_1=a_1-1$, $b_2=a_2-a_1+\frac{1}{2}$, $a_1=\frac{1}{2}$, $a_2=\frac{1}{12}$
- $\hat{R}_{4,1}$: $a_0=1$, $b_1=a_1-1$, $b_2=a_2-a_1+\frac{1}{2}$, $a_1=\frac{1}{2}+\phi$, $a_2=\frac{1}{12}+\frac{\phi}{2}$

$$\phi=\frac{\left(12+{z_0}^2-6\,z_0\right)e^{z_0}-12-{z_0}^2-6\,z_0}{12\,z_0\,\left((z_0-2)\,e^{z_0}+z_0+2\right)}$$

- $\hat{R}_{3,2}$: $a_0=1$, $b_1=a_1-1$, $b_2=a_2-a_1+\frac{1}{2}$,

$$a_1=\frac{\left(z_0^3-2\,z_0^2+2\,z_0-8\right)e_0^z+4+(4-2\,z_0)\,e^{2\,z_0}}{2\,z_0\,\left(z_0^2+2\right)e_0^z-2\,z_0e^{2\,z_0}-2\,z_0}\qquad a_2=\frac{\left(4-4\,z_0-z_0^2-z_0^3\right)e_0^z-2+\left(-2+4\,z_0-z_0^2\right)e^{2\,z_0}}{2\,z_0^2\,\left(z_0^2+2\right)e_0^z-2\,z_0^2e^{2\,z_0}-2\,z_0^2}$$

Making use of (5), the explicit form of the functions $\hat{R}_{2,3}$, $\hat{R}_{1,4}$ and $\hat{R}_{0,5}$ can be determined. All these functions reduce to $\hat{R}_{5,0}(z)$, the Padé approximant of order $[2/2]$ of e^z, for $z_0\to 0$.

In Figure 1 the stability regions, the order stars and the deviation from e^z along the real axis for these functions have been shown for the case $z_0=-3$. Starting at the left side with $\hat{R}_{5,0}$, which is exactly A-stable, and going to the right, we see that the stability region (i.e. the gray area) grows. From the corresponding order stars, we can learn how well the stability function approximates e^z for $z=0$ and $z=z_0$. Indeed, we can see that an approximation of order p in $z=z_0$ or $z=0$ results in an order star in that point with $2\,(p+1)$ equal sectors. Also the relations (6) that exist between the different order stars are clearly illustrated. The bottom row, which shows the differences $\mathrm{e}^z-\hat{R}_{i,j}(z,z_0)$ also shows the orders of approximation in $z=z_0$ and $z=0$.

On the other hand, given two nodes c_1 and c_2 we can construct 2-stage EFRK methods and then we obtain the following stability functions

- $\mathscr{S}_{3,0}(\omega)=\mathrm{Span}\{1,x,x^2\}$

$$R_{3,0}^{\{c_1,c_2\}}(z)=\frac{P_{3,0}^{\{c_1-1,c_2-1\}}(z)}{P_{3,0}^{\{c_1,c_2\}}(z)}\ \text{ with }\ P_{3,0}^{\{c_1,c_2\}}(z)=1-\frac{1}{2}\,(c_1+c_2)\,z+\frac{1}{2}\,c_1\,c_2\,z^2$$

- $\mathscr{S}_{2,1}(\omega)=\mathrm{Span}\{1,x,\mathrm{e}^{\omega x}\}$

$$R_{2,1}^{\{c_1,c_2\}}(z,z_0)=\frac{P_{2,1}^{\{c_1-1,c_2-1\}}(z,z_0)}{P_{2,1}^{\{c_1,c_2\}}(z,z_0)}\qquad\text{with}$$

$$P_{2,1}^{\{c_1,c_2\}}(z,z_0)=1-\frac{(c_1z_0+1)\,e^{c_2z_0}-(c_2z_0+1)\,e^{c_1z_0}}{z_0\,(e^{c_2z_0}-e^{c_1z_0})}z+\frac{c_1\,(e^{c_2z_0}-1)-c_2\,(e^{c_1z_0}-1)}{z_0\,(e^{c_2z_0}-e^{c_1z_0})}z^2$$

- $\mathscr{S}_{1,2}(\omega)=\mathrm{Span}\{1,\mathrm{e}^{\omega x},x\,\mathrm{e}^{\omega x}\}$:

$$R_{1,2}^{\{c_1,c_2\}}(z,z_0)=\mathrm{e}^{z_0}\,R_{2,1}^{\{c_1,c_2\}}(z-z_0,-z_0)$$

- $\mathscr{S}_{0,3}(\omega)=\mathrm{Span}\{\mathrm{e}^{\omega x},x\,\mathrm{e}^{\omega x},x^2\,\mathrm{e}^{\omega x}\}$:

$$R_{0,3}^{\{c_1,c_2\}}(z,z_0)=\mathrm{e}^{z_0}\,R_{3,0}^{\{c_1,c_2\}}(z-z_0)$$

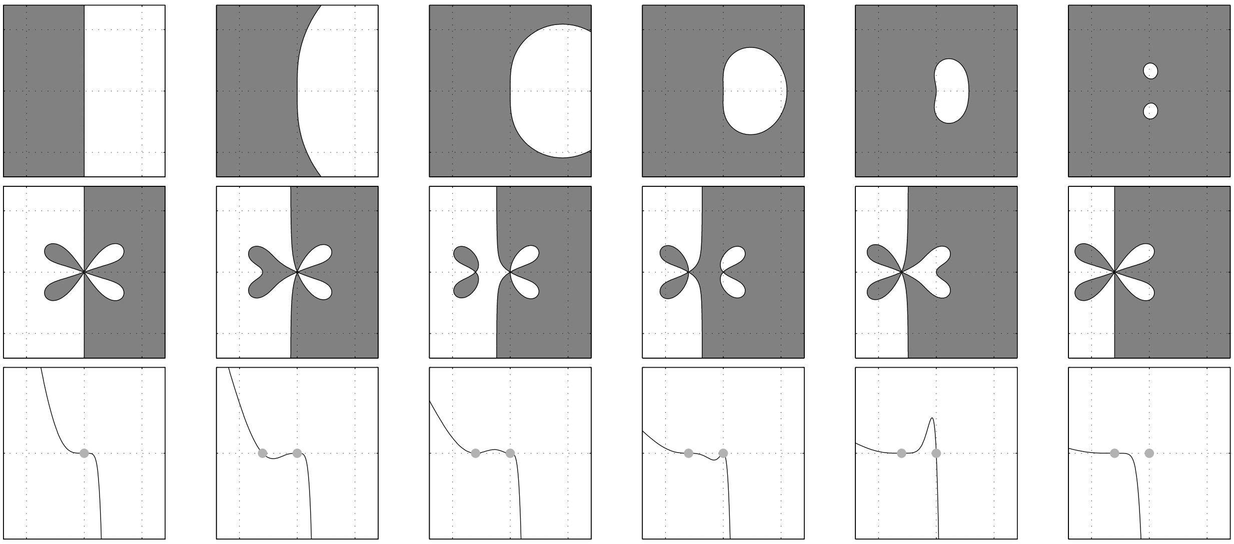

FIGURE 1. The stability regions (top) and the order stars (middle) for the functions $\hat{R}_{5-i,i}(z,z_0)$, $i = 0, \ldots, 5$, for $z_0 = -3$. For each picture, both axes vary between -7 en 75. In the lower part, the difference with e^z along the real axis is shown. Again the x-axis covers the interval $[-7,7]$, the y-axis shows the interval $[-0.05, 0.05]$.

We thus have two sets of stability functions : functions $\hat{R}_{j,5-j}(z,z_0)$, $j = 0,\ldots,5$ that are determined by imposing 5 conditions on a rational function and functions $R^{\{c_1,c_2\}}_{i,3-i}(z,z_0)$, $i = 0,\ldots,3$ that are obtained by constructing 2 stages EFRK methods fitted to 3 dimensional set. One could wonder whether it is possible to choose c_1 and c_2 in such a way that $R^{\{c_1,c_2\}}_{i,3-i}(z,z_0)$ coincides with $\hat{R}_{j,5-j}(z,z_0)$ for some j with $i \leq j \leq i+2$. E.g. it is well-known that $R^{\{c_1,c_2\}}_{3,0}(z,z_0)$ coincides with $\hat{R}_{5,0}(z,z_0)$ iff $\{c_1,c_2\} = \{\frac{3-\sqrt{3}}{6}, \frac{3+\sqrt{3}}{6}\}$, but is it also possible to coincide with $\hat{R}_{4,1}(z,z_0)$ or $\hat{R}_{3,2}(z,z_0)$. Yes it is possible, but in that case c_1 and c_2 depend upon z_0, as shown in the left part of Figure 2.

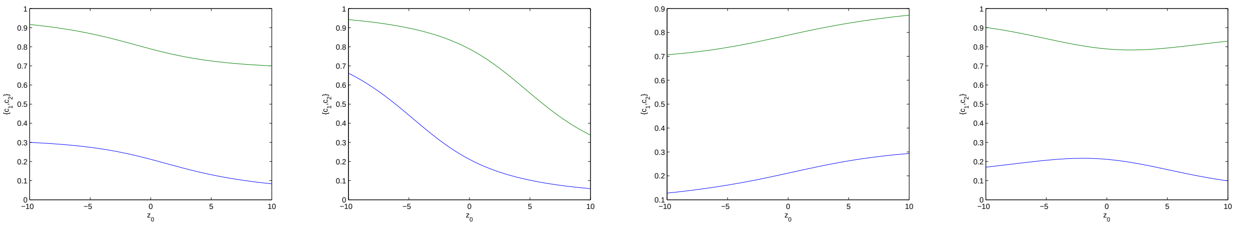

FIGURE 2. Behavior of the coefficients c_1 and c_2 to satisfy (from left to right) $R^{\{c_1,c_2\}}_{3,0}(z,z_0) = \hat{R}_{4,1}(z,z_0)$, $R^{\{c_1,c_2\}}_{3,0}(z,z_0) = \hat{R}_{3,2}(z,z_0)$, $R^{\{c_1,c_2\}}_{2,1}(z,z_0) = \hat{R}_{4,1}(z,z_0)$, $R^{\{c_1,c_2\}}_{2,1}(z,z_0) = \hat{R}_{3,2}(z,z_0)$.

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