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Non-satisfiability of a positivity condition for commutator-free exponential integrators of order higher than four

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Abstract
We consider commutator-free exponential integrators as put forward in Alverman and Fehske (J Comput Phys 230:5930–5956, 2011). For parabolic problems, it is important for the well-definedness that such an integrator satisfies a positivity condition such that essentially it only proceeds forward in time. We prove that this requirement implies maximal convergence order of four for real coefficients, which has been conjectured earlier by other authors.

Mathematics Subject Classification 65L05

1 Introduction

Commutator-free exponential integrators are effective methods for the numerical solution of non-autonomous evolution equations of the form

$$u'(t) = A(t)u(t), \quad u(t_0) = u_0, \quad t \in [t_0, T], \tag{1}$$

where $A(t) \in \mathbb{C}^{d\times d}$, usually with large dimension d, see [1,2,7,8]. These methods compute approximations $\{u_n\}$ to the solution of (1) on a grid $\{t_n = t_0 + n\tau\}$ with step-size τ as

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$$u_{n+1} = \mathrm{e}^{\tau B_J(t_n,\tau)} \cdots \mathrm{e}^{\tau B_1(t_n,\tau)} u_n, \qquad n = 0, 1, \ldots. \tag{2}$$

Here,

$$B_j(t_n, \tau) = \sum_{k=1}^{K} a_{j,k} A(t_n + c_k \tau), \quad j = 1, \ldots, J \tag{3}$$

with coefficients $a_{j,k}, c_k \in \mathbb{R}$, $j = 1, \ldots, J$, $k = 1, \ldots, K$ chosen in such a way, that the exponential integrator has a certain convergence order $p \geq 1$,

$$\|u_n - u(t_n)\| = O(\tau^p).$$

Usually the nodes c_k are chosen as the nodes of a quadrature formula of order p. It is assumed that the matrix exponentials applied to some vector, $\mathrm{e}^{\tau B_j(t_n,\tau)} v$, can be evaluated efficiently. For large problems, this is commonly realized by Krylov methods like the Lanczos iteration, see for instance [20,21], or polynomial or rational approximations [18].

The numerical solution of large linear systems of the type (1) has been extensively studied in the literature. Attention has recently focussed on *commutator-free methods* (2), see for instance [9]. Earlier mathematical work has centered around the construction of commutator-free methods to supplement classical Magnus integrators based on commutators. Commutator-free methods are convenient to evaluate without storing excessive intermediate results, where the optimal balance between computational effort and accuracy is sought. Already in [9], the coefficients for high-order commutator-free methods were derived based on nonlinear optimization of the free parameters in the order conditions to minimize local error constants. With this objective, methods of orders 4–8 were constructed in [1].

Alternative approaches to the construction of favorable integrators based on the evaluation of exponentials rely on the Magnus expansion [16,17]. In [6] the algebraic framework underlying a systematic construction of classical Magnus integrators is discussed. Yet another interesting approach was applied to the Schrödinger equation in [3,4], where all the computations are performed in the Lie algebra. This leads to the derivation of exponential integrators in [4]. Unconventional schemes similar to (2) but containing in addition commutators have been proposed in [7]. Note that commutator-free methods were already considered in the context of Lie group methods for nonlinear problems on manifolds for example in [11,12,19]. Our analysis applies to the class of methods (2), a possible extension to other Lie group methods is not considered here, but may be a topic for future research.

For $A(t)$ with purely imaginary eigenvalues it does not matter whether some of the coefficients $a_{j,k}$ in (3) are negative. This holds for $A(t)$ anti-hermitian (i.e., for $\frac{1}{\mathrm{i}} A(t)$ hermitian), which usually is the case if (1) is a (space-discretized) Schrödinger equation, see [1,2].

On the other hand, for $A(t)$ with negative real eigenvalues of large modulus, which, e.g., is the case if (1) is a spatially semi-discretized sectorial operator associated with a parabolic equation, poor stability is to be expected if some of the coefficients $a_{j,k}$

are negative. More specifically, the analysis given in [8] shows that commutator-free exponential integrators applied to evolution equations of parabolic type are well-defined and stable only if their coefficients satisfy the *positivity condition*

$$b_j = \sum_{k=1}^{K} a_{j,k} > 0, \quad j = 1, \ldots, J. \tag{4}$$

In all examples of schemes given in [1,2,7,8], which involve real coefficients only and are of order higher than four, this condition is not satisfied. In [8] it is conjectured that no such schemes exist. However, no proof is given there. It is the purpose of this paper to give such a proof.[1]

2 Main result

Theorem 1 *If $p \geq 5$, then no commutator-free exponential integrator (2), (3) of convergence order p involving only real coefficients $a_{j,k}$ exists which satisfies the positivity condition (4).*

Proof It is sufficient to consider only problems of the special form

$$u'(t) = (A_0 + tA_1)u(t), \quad u(0) = u_0, \tag{5}$$

where $A_0, A_1 \in \mathbb{C}^{d\times d}$. For such problems we have

$$B_j(t_n, \tau) = b_j(A_0 + t_n A_1) + \tau y_j A_1 \quad \text{with} \quad y_j = \sum_{k=1}^{K} a_{j,k} c_k, \quad j = 1, \ldots, J, \tag{6}$$

and order conditions for the numerical solution to be of convergence order at least $p = 5$ are given by

$$\sum_{j=1}^{J} b_j = 1, \tag{7}$$

$$\sum_{j=1}^{J} y_j = \frac{1}{2}, \tag{8}$$

[1] Note that the situation is similar to that encountered for *exponential splitting methods*. For this class of time integrators, no methods of order greater than two exist with only positive real coefficients. This was first shown in [22], see also [13]. The ensuing instability can be avoided by splitting with complex coefficients [14], see also [10]. Splitting methods of high order with complex coefficients have been constructed for example in [5]. Similarly, for exponential commutator-free Magnus-type methods, stable high-order schemes with complex coefficients have been derived in [7]. Moreover, unconventional schemes involving additionally evaluation of some commutators are introduced there which are stable for parabolic problems. An error analysis of high-order commutator-free exponential integrators applied to semi-discretizations of parabolic problems is given in [8].

$$\sum_{j=1}^{J} \widehat{b}_j y_j = \frac{1}{3},$$

$$\sum_{j=1}^{J} \left(\widehat{b}_j^2 + \frac{1}{12} b_j^2 \right) y_j = \frac{1}{4},$$

$$\sum_{j=1}^{J} \left(\widehat{b}_j^3 + \frac{1}{4} \widehat{b}_j b_j^2 \right) y_j = \frac{1}{5}, \tag{9}$$

$$\sum_{j=1}^{J} \left(\widehat{y}_j^2 + \frac{1}{12} y_j^2 \right) b_j = \frac{1}{20}, \tag{10}$$

where

$$\widehat{b}_j = \sum_{k=1}^{j} b_k - \frac{1}{2} b_j \quad \text{and} \quad \widehat{y}_j = \sum_{k=1}^{j} y_k - \frac{1}{2} y_j, \quad j = 1, \dots, J.$$

A proof of these order conditions is given in "Appendix A". We will show that the system consisting of Eqs. (7)–(10) has no solution with $b_j \in \mathbb{R}_{>0}$ positive and $y_j \in \mathbb{R}$ arbitrary ($j = 1, \dots, J$). It is clear that these equations have no solution for $J = 1$, we thus assume $J \geq 2$. We will treat (8) and (9) as linear equations and (10) as a quadratic equation in the variables y_j and with coefficients depending on the parameters b_j subject to the constraint (7).

We define vectors

$$y = (y_1 \dots, y_J)^T, \quad e = (1, \dots, 1)^T, \quad d = \left(\widehat{b}_1^3 + \frac{1}{4} \widehat{b}_1 b_1^2, \dots, \widehat{b}_J^3 + \frac{1}{4} \widehat{b}_J b_J^2 \right)^T$$

in $\mathbb{R}^J$ and matrices

$$L = \begin{pmatrix} \frac{1}{2} & & & & \\ 1 & \frac{1}{2} & & \mathbf{0} & \\ 1 & 1 & \ddots & & \\ \vdots & \vdots & \ddots & \frac{1}{2} & \\ 1 & 1 & \cdots & 1 & \frac{1}{2} \end{pmatrix}, \quad D = \operatorname{diag}(b_1, \dots, b_J), \quad S = L^T D L + \frac{1}{12} D$$

in $\mathbb{R}^{J \times J}$. Then Eqs. (8)–(10) can be written as

$$e^T y = \frac{1}{2}, \quad d^T y = \frac{1}{5}, \quad y^T S y = \frac{1}{20}, \tag{11}$$

respectively. For the remainder of the proof we will assume that $b_j > 0$, $j = 1, \dots, J$. We will show that under this assumption the system of equations (11) has no solution

$y \in \mathbb{R}^J$. It is easily seen that for $b_j > 0$, S is symmetric positive definite and thus the equation $y^T Sy = \frac{1}{20}$ defines a bounded quadric (a "hyper-ellipsoid") in $\mathbb{R}^J$. Furthermore, a straightforward calculation shows that $\{e, d\}$ is linearly independent for $b_j > 0$ and $J \geq 2$, since in this case $d_1 \neq d_2$. From Lemma 1 in "Appendix B" it follows that the intersection of the two hyperplanes given by the equations $e^T y = \frac{1}{2}$ and $d^T y = \frac{1}{5}$ does not intersect the quadric defined by $y^T Sy = \frac{1}{20}$ if and only if

$$c^T \Gamma^{-1} c > \frac{1}{20}, \tag{12}$$

where $c = (\frac{1}{2}, \frac{1}{5})^T$ and Γ denotes the Gram matrix

$$\Gamma = \begin{pmatrix} e^T S^{-1} e & e^T S^{-1} d \\ e^T S^{-1} d & d^T S^{-1} d \end{pmatrix}.$$

Condition (12) is equivalent to

$$(2e - 5d)^T S^{-1} (2e - 5d) - 5 \det \Gamma > 0, \tag{13}$$

which is equivalent to

$$\frac{\big((e-d)^T S^{-1} (2e - 5d)\big)^2 + \big(9 - 5(e-d)^T S^{-1} (e-d)\big) \det \Gamma}{(e-d)^T S^{-1} (e-d)} > 0. \tag{14}$$

Indeed the left-hand-sides of (13) and (14) are equal, which is readily verified by a straightforward calculation. In (14) the denominator is positive because S and thus S^{-1} is positive definite. Clearly also the first term of the numerator is positive as is the Gram determinant $\det \Gamma$ for $J \geq 2$. Note that the positivity of these terms does not depend on the constraint (7).

We will now show that

$$(\sigma^3 e - d)^T S^{-1} (\sigma^3 e - d) < \frac{9}{5}\sigma^5, \quad \text{where} \quad \sigma = \sum_{j=1}^{J} b_j, \tag{15}$$

from which (14) follows for $\sigma = 1$ [i.e., if (7) is satisfied], which will conclude the proof of the theorem. We proceed using induction on the number J of exponentials.

Base case. For $J = 1$ we have

$$\sigma = b_1, \quad d = \frac{b_1^3}{4}, \quad S = \frac{b_1}{3}, \quad S^{-1} = \frac{3}{b_1},$$

such that

$$(\sigma^3 e - d)^T S^{-1} (\sigma^3 e - d) = \left(b_1^3 - \frac{b_1^3}{4}\right)^2 \cdot \frac{3}{b_1} = \frac{27}{16} b_1^5 < \frac{9}{5}\sigma^5.$$

Inductive step $J \to J+1$. Objects with a tilde belong to the $(J+1)$-case, those without a tilde to the J-case such that

$$\widetilde{\sigma} = \sigma + b_{J+1}, \quad \widetilde{e} = \begin{pmatrix} e \\ 1 \end{pmatrix}, \quad \widetilde{d} = \begin{pmatrix} d \\ d_{J+1} \end{pmatrix}, \quad \text{etc.}$$

Applying

$$\begin{pmatrix} A & u \\ u^T & \delta \end{pmatrix}^{-1} = \begin{pmatrix} (A - \frac{1}{\delta} u u^T)^{-1} & \dfrac{-1}{\delta - u^T A^{-1} u} A^{-1} u \\ \dfrac{-1}{\delta - u^T A^{-1} u} u^T A^{-1} & \dfrac{1}{\delta - u^T A^{-1} u} \end{pmatrix}$$

(see [15, eq. (7.7.5)]) and the Sherman-Morrison formula

$$(A + u v^T)^{-1} = A^{-1} - \frac{1}{1 + v^T A^{-1} u} A^{-1} u v^T A^{-1}$$

(see [15, §0.7.4)]) to

$$\widetilde{S} = \begin{pmatrix} S + b_{J+1} e e^T & \frac{1}{2} b_{J+1} e \\ \frac{1}{2} b_{J+1} e^T & \frac{1}{3} b_{J+1} \end{pmatrix}$$

we obtain

$$\widetilde{S}^{-1} = \begin{pmatrix} S^{-1} - \dfrac{b_{J+1}}{4 + b_{J+1} e^T S^{-1} e} S^{-1} e e^T S^{-1} & \dfrac{-6}{4 + b_{J+1} e^T S^{-1} e} S^{-1} e \\ \dfrac{-6}{4 + b_{J+1} e^T S^{-1} e} e^T S^{-1} & \dfrac{12}{b_{J+1}} \cdot \dfrac{1 + b_{J+1} e^T S^{-1} e}{4 + b_{J+1} e^T S^{-1} e} \end{pmatrix}.$$

It follows

$$\begin{aligned} (\widetilde{\sigma}^3 \widetilde{e} - \widetilde{d})^T \widetilde{S}^{-1} (\widetilde{\sigma}^3 \widetilde{e} - \widetilde{d}) \; &= \; (\widetilde{\sigma}^3 e - d)^T S^{-1} (\widetilde{\sigma}^3 e - d) \\ &+ \frac{b_{J+1}}{4 + b_{J+1} e^T S^{-1} e} \left(- \left(e^T S^{-1} (\widetilde{\sigma}^3 e - d) \right)^2 - 12 \frac{\widetilde{\sigma}^3 - d_{J+1}}{b_{J+1}} e^T S^{-1} (\widetilde{\sigma}^3 e - d) \right. \\ &\left. + 12 \frac{(\widetilde{\sigma}^3 - d_{J+1})^2}{b_{J+1}^2} (1 + b_{J+1} e^T S^{-1} e) \right). \end{aligned} \tag{16}$$

Substituting

$$\widetilde{\sigma}^3 = \sigma^3 + b_{J+1}^3 + 3 b_{J+1}^2 (\widetilde{\sigma} - b_{J+1}) + 3 b_{J+1} (\widetilde{\sigma} - b_{J+1})^2$$

in the first term $(\widetilde{\sigma}^3 e - d)^T S^{-1}(\widetilde{\sigma}^3 e - d)$ only, and

$$d_{J+1} = \widetilde{\sigma}^3 - \frac{3}{2}\widetilde{\sigma}^2 b_{J+1} + \widetilde{\sigma} b_{J+1}^2 - \frac{1}{4} b_{J+1}^3$$

(which follows by substituting $\widehat{b}_{J+1} = \widetilde{\sigma} - \frac{1}{2} b_{J+1}$ in $d_{J+1} = \widehat{b}_{J+1}^3 + \frac{1}{4}\widehat{b}_{J+1} b_{J+1}^2$) in the other terms we obtain (to be verified using a computer algebra system, see "Appendix C")

$$\begin{aligned}
(\widetilde{\sigma}^3 \widetilde{e} - \widetilde{d})^T \widetilde{S}^{-1}(\widetilde{\sigma}^3 \widetilde{e} - \widetilde{d}) \;&=\; (\sigma^3 e - d)^T S^{-1}(\sigma^3 e - d) \\
&+ \frac{b_{J+1}}{4}\left(7b_{J+1}^4 - 36 b_{J+1}^3 \widetilde{\sigma} + 72 b_{J+1}^2 \widetilde{\sigma}^2 - 72 b_{J+1}\widetilde{\sigma}^3 + 36\widetilde{\sigma}^4\right) \\
&- \frac{b_{J+1}}{4+b_{J+1} e^T S e}\left(\left((\widetilde{\sigma} - b_{J+1})^3 e - d\right)^T S^{-1} e - \frac{1}{2}\left(5b_{J+1}^2 - 12 b_{J+1}\widetilde{\sigma} + 6\widetilde{\sigma}^2\right)\right)^2.
\end{aligned} \tag{17}$$

Disregarding the last term (which is negative) and using the inductive assumption $(\sigma^3 e - d)^T S^{-1}(\sigma^3 e - d) < \frac{9}{5}\sigma^5 = \frac{9}{5}(\widetilde{\sigma} - b_{J+1})^5$ we obtain

$$\begin{aligned}
&(\widetilde{\sigma}^3 \widetilde{e} - \widetilde{d})^T \widetilde{S}^{-1}(\widetilde{\sigma}^3 \widetilde{e} - \widetilde{d}) \\
&\quad < \frac{9}{5}(\widetilde{\sigma} - b_{J+1})^5 \\
&\qquad + \frac{b_{J+1}}{4}\left(7b_{J+1}^4 - 36 b_{J+1}^3 \widetilde{\sigma} + 72 b_{J+1}^2 \widetilde{\sigma}^2 - 72 b_{J+1}\widetilde{\sigma}^3 + 36\widetilde{\sigma}^4\right) \\
&\quad = \frac{9}{5}\widetilde{\sigma}^5 - \frac{1}{2} b_{J+1}^5 \;<\; \frac{9}{5}\widetilde{\sigma}^5,
\end{aligned}$$

which completes the inductive step for the proof of (15). □

Remark Note that the theorem also covers the situation where (some) $a_{j,k} \in \mathbb{C}$, but $b_j,\ y_j \in \mathbb{R}$.

A Proof of the order conditions (7)–(10)

For the global error to have order $p = 5$ it is required that the local error have convergence order $p + 1 = 6$. If, without restriction of generality, we consider only the first integration step for the special problem (5), this condition for the local error is written as

$$\mathrm{e}^{\tau b_J A_0 + \tau^2 y_J A_1} \cdots \mathrm{e}^{\tau b_1 A_0 + \tau^2 y_1 A_1} u_0 = u(\tau) + O(\tau^6). \tag{18}$$

A Taylor expansion of the left-hand side leads to (let $\mathbf{k} = (k_1, \ldots, k_m)$, $|\mathbf{k}| = \sum_{l=1}^m k_l$)

$$
\begin{aligned}
&\mathrm{e}^{\tau b_J A_0+\tau^2 y_J A_1}\cdots \mathrm{e}^{\tau b_1 A_0+\tau^2 y_1 A_1}u_0 = c_{\emptyset}^{(J)}u_0\\
&\quad+\sum_{\substack{\mathbf{k}=(k_1,\dots k_m)\\ m\ge 1,k_l\in\{0,1\},|\mathbf{k}|+m\le 5}} \tau^{|\mathbf{k}|+m}c_{k_1\dots k_m}^{(J)}A_{k_1}\cdots A_{k_m}u_0+O(\tau^6).
\end{aligned}
$$

Here for $J=1$ we have [note that already a subset of coefficients suffices to derive the order conditions (7)–(10)],

$$
\begin{aligned}
&c_{\emptyset}^{(1)}=1,\quad c_0^{(1)}=b_1,\quad c_1^{(1)}=y_1,\quad c_{01}^{(1)}=\frac{1}{2}b_1y_1,\quad c_{11}^{(1)}=\frac{1}{2}y_1^2,\\
&c_{001}^{(1)}=\frac{1}{6}b_1^2y_1,\quad c_{011}^{(1)}=\frac{1}{6}b_1y_1^2,\quad c_{0001}^{(1)}=\frac{1}{24}b_1^3y_1,
\end{aligned}
$$

and for $J\ge 2$ the coefficients can be computed recursively,

$$
\begin{aligned}
&c_{\emptyset}^{(J)}=c_{\emptyset}^{(J-1)},\quad c_0^{(J)}=c_0^{(J-1)}+b_Jc_{\emptyset}^{(J-1)},\quad c_1^{(J)}=c_1^{(J-1)}+y_Jc_{\emptyset}^{(J-1)},\\
&c_{01}^{(J)}=c_{01}^{(J-1)}+b_Jc_1^{(J-1)}+\frac{1}{2}b_Jy_Jc_{\emptyset}^{(J-1)},\\
&c_{11}^{(J)}=c_{11}^{(J-1)}+y_Jc_1^{(J-1)}+\frac{1}{2}y_J^2c_{\emptyset}^{(J-1)},\\
&c_{001}^{(J)}=c_{001}^{(J-1)}+b_Jc_{01}^{(J-1)}+\frac{1}{2}b_J^2c_1^{(J-1)}+\frac{1}{6}b_J^2y_Jc_{\emptyset}^{(J-1)},\\
&c_{011}^{(J)}=c_{011}^{(J-1)}+b_Jc_{11}^{(J-1)}+\frac{1}{2}b_Jy_Jc_1^{(J-1)}+\frac{1}{6}b_Jy_J^2c_{\emptyset}^{(J-1)},\\
&c_{0001}^{(J)}=c_{0001}^{(J-1)}+b_Jc_{001}^{(J-1)}+\frac{1}{2}b_J^2c_{01}^{(J-1)}+\frac{1}{6}b_J^3c_1^{(J-1)}+\frac{1}{24}b_J^3y_Jc_{\emptyset}^{(J-1)}.
\end{aligned}
$$

An inductive argument involving straightforward but laborious calculations gives

$$
\begin{aligned}
&c_{\emptyset}^{(J)}=1,\quad c_0^{(J)}=\sum_{j=1}^J b_j,\quad c_1^{(J)}=\sum_{j=1}^J y_j,\\
&c_{01}^{(J)}=c_0^{(J)}c_1^{(J)}-\sum_{j=1}^J\widehat{b}_jy_j,\quad c_{11}^{(J)}=\frac{1}{2}(c_1^{(J)})^2,\\
&c_{001}^{(J)}=c_0^{(J)}c_{01}^{(J)}-\frac{1}{2}(c_0^{(J)})^2c_1^{(J)}-\frac{1}{2}\sum_{j=1}^J\left(\widehat{b}_j^2+\frac{1}{12}b_j^2\right)y_j,\\
&c_{011}^{(J)}=\frac{1}{2}\sum_{j=1}^J\left(\widehat{y}_j^2+\frac{1}{12}y_j^2\right)b_j,\\
&c_{0001}^{(J)}=c_0^{(J)}c_{001}^{(J)}-\frac{1}{2}(c_0^{(J)})^2c_{01}^{(J)}+\frac{1}{6}(c_0^{(J)})^3c_1^{(J)}-\frac{1}{6}\sum_{j=1}^J\left(\widehat{b}_j^3+\frac{1}{4}\widehat{b}_jb_j^2\right)y_j. \qquad (19)
\end{aligned}
$$

Repeated differentiation of the differential equation (5) yields

$$\begin{aligned}
&u(0) = u_0, \quad u'(0) = A_0 u_0, \quad u''(0) = (A_1 + A_0^2)u_0, \\
&u'''(0) = (A_0 A_1 + 2A_1 A_0 + A_0^3)u_0, \\
&u^{(4)}(0) = (3A_1^2 + A_0^2 A_1 + 2A_0 A_1 A_0 + A_1 A_0^2 + A_0^4)u_0, \\
&u^{(5)}(0) = (3A_0 A_1^2 + 4A_1 A_0 A_1 + 8A_1^2 A_0 + A_0^3 A_1 \\
&\qquad\qquad + 2A_0^2 A_1 A_0 + 3A_0 A_1 A_0^2 + 4A_1 A_0^3 + A_0^5)u_0.
\end{aligned}$$

Thus for the Taylor expansion of the right-hand side of (18) we obtain

$$\begin{aligned}
u(\tau) = \sum_{q=0}^{5} \frac{\tau^q}{q!} u^{(q)}(0) + O(\tau^6) = s_\emptyset u_0 \\
+ \sum_{\substack{\mathbf{k}=(k_1,\ldots k_m) \\ m\geq 1, k_l \in \{0,1\}, |\mathbf{k}|+m\leq 5}} \tau^{|\mathbf{k}|+m} s_{k_1\ldots k_m} A_{k_1} \cdots A_{k_m} u_0 + O(\tau^6)
\end{aligned}$$

with coefficients [only those corresponding to the subset of coefficients as in (19)]

$$\begin{aligned}
&s_\emptyset = \frac{1}{0!} = 1, \quad s_0 = \frac{1}{1!} = 1, \quad s_1 = \frac{1}{2!} = \frac{1}{2}, \quad s_{01} = \frac{1}{3!} = \frac{1}{6}, \quad s_{11} = \frac{3}{4!} = \frac{1}{8}, \\
&s_{001} = \frac{1}{4!} = \frac{1}{24}, \quad s_{011} = \frac{3}{5!} = \frac{1}{40}, \quad s_{0001} = \frac{1}{5!} = \frac{1}{120}.
\end{aligned} \tag{20}$$

Equating corresponding coefficients in (19) and (20) leads to the order conditions (7)–(10).

B A geometric lemma

Lemma 1 *Let $\{a_1, \ldots, a_m\}$ be a linearly independent set of vectors in $\mathbb{R}^n$ and $S \in \mathbb{R}^{n\times n}$ symmetric positive definite. Further let $c = (\gamma_1, \ldots, \gamma_m)^T \in \mathbb{R}^m$ and $\delta \in \mathbb{R}$. Then the intersection $\mathcal{I}$ of the m hyperplanes in $\mathbb{R}^n$ given by the equations $a_1^T x = \gamma_1, \ldots, a_m^T x = \gamma_m$ intersects the hyper-ellipsoid $\mathcal{Q}$ given by the equation $x^T S x = \delta$ if and only if it holds*

$$c^T \Gamma^{-1} c \leq \delta, \tag{21}$$

where $\Gamma = (a_i^T S^{-1} a_j)_{i,j=1}^m$ denotes the Gram matrix of the vectors $a_1, \ldots, a_m$ with respect to the scalar product $x^T S^{-1} y$.

Proof First we consider the special case $S = I_n$ (identity matrix), where $\mathcal{Q}$ is a hypersphere. In this case $\mathcal{I}$ intersects $\mathcal{Q}$ if and only if the point $x_* \in \mathcal{I}$ of minimal norm satisfies

$$\|x_*\|^2 = x_*^T x_* \leq \delta. \tag{22}$$

It is easy to see that this point x_* lies in the linear subspace of $\mathbb{R}^n$ spanned by $a_1, \dots a_m$ (the normal vectors to the given hyperplanes), i.e., there exists $b = (\beta_1, \dots, \beta_m)^T \in \mathbb{R}^m$ such that

$$x_* = \beta_1 a_1 + \cdots + \beta_m a_m = Ab,$$

where $A = [a_1 \ \cdots \ a_m] \in \mathbb{R}^{n\times m}$. Because $x_* \in \mathcal{I}$ it holds

$$\Gamma b = A^T A b = A^T x_* = c,$$

and thus

$$x_*^T x_* = b^T A^T A b = b^T \Gamma b = c^T \Gamma^{-1} c,$$

which shows that (22) is equivalent to (21). This completes the proof for the special case $S = I_n$.

For the general case, the symmetric positive definite matrix S can be written as

$$S = X \Lambda X^T$$

with $\Lambda = \mathrm{diag}(\lambda_1, \dots, \lambda_n)$, where $\lambda_j > 0$ are the eigenvalues of S, and X orthogonal. We define $\widetilde{a}_j = \Lambda^{-1/2} X^T a_j$, $j = 1, \dots, m$. Then under the transformation of variables $\widetilde{x} = \Lambda^{1/2} X^T x$, the equation $\widetilde{a}_j^T \widetilde{x} = \gamma_j$ is equivalent to $a_j^T x = \gamma_j$ and $\widetilde{x}^T \widetilde{x} = \delta$ is equivalent to $x^T S x = \delta$. For these transformed equations the special case from above is applicable. Using $\widetilde{A} = [\widetilde{a}_1 \ \cdots \ \widetilde{a}_m] = \Lambda^{-1/2} X^T A$ with $A = [a_1 \ \cdots \ a_m]$ it follows that for the transformed equations the corresponding Gram matrix satisfies $\widetilde{\Gamma} = \widetilde{A}^T \widetilde{A} = A^T X \Lambda^{-1} X^T A = A^T S^{-1} A = \Gamma$ as claimed. □

C Maple code for checking (16)=(17)

Here, the Maple identifiers `s`, `s1`, `bb`, `dd`, `eSe`, `eSd`, `dSd` correspond to σ, $\widetilde{\sigma}$, b_{J+1}, d_{J+1}, $e^T S^{-1} e$, $e^T S^{-1} d$, $d^T S^{-1} d$, respectively.

```
> expr3 := s1^6*eSe-2*s1^3*eSd+dSd+bb*(-(eSe*s1^3-eSd)^2
           -(12*(s1^3-dd))*(eSe*s1^3-eSd)/bb
           +12*(s1^3-dd)^2*(bb*eSe+1)/bb^2)/(bb*eSe+4):
> expr4 := s^6*eSe-2*s^3*eSd+dSd
           +(1/4)*bb*(7*bb^4-36*bb^3*s1+72*bb^2*s1^2
           -72*bb*s1^3+36*s1^4)-bb*((s1-bb)^3*eSe-eSd
           -1/2*(5*bb^2-12*bb*s1+6*s1^2))^2/(bb*eSe+4):
> simplify( subs(dd = s1^3-(3/2)*s1^2*bb+s1*bb^2-(1/4)
          *bb^3, expr3)
           -subs(s = s1-bb, expr4));
                                             0
```

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