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Algebraic study on the coefficient set of the 4-stage, 4th-order explicit Runge-Kutta methods

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Abstract. In this paper, we study a set of conditions with 14 constants in the 4-stage, 4th-order explicit Runge-Kutta methods, which contain four weights, four nodes and six components of the Runge-Kutta matrix. For simplicity, we will simply call these constants as *coefficients* in the paper. We prove that the set of coefficients satisfying these conditions form an irreducible rational surface without a singular point.

1. Introduction

The Runge-Kutta method is one of the numerical analysis methods developed by mathematicians Carl David Tolme Runge and Martin Wilhelm Kutta around 1900 ([1, 11] are the original papers). For a first-order ordinary differential equation

$$\frac{dy}{dt} = f(t, y),$$

the p-th stage Runge-Kutta methods ($p = 1,\ 2, \dots$) is defined by

$$(1)\qquad \begin{aligned} y(t_0 + h) &= y(t_0) + h\Big(\sum_{i=1}^{p} b_i K_i\Big), \\ K_i &= f\big(t_0 + hc_i,\ y(t_0) + h(\sum_{j=1}^{p} a_{ij} K_j)\big). \end{aligned}$$

Here, t is a time parameter, h is a step size of time, a_{ij}, b_i, and c_i are constants independent of (t, y). Also b_i is called a weight, c_i is called a node, and a_{ij} is called a component of the Runge-Kutta matrix (a square matrix of order p). This method is one of the most used approaches among the one-step method of numerical analysis, and we know that a good approximation with less error can be obtained.

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Because of this, high-precision approximate solutions can be obtained for many kinds of complex differential equations, and they are used for research in various fields (see [3, 8]). In the recent past, the method "EVO-RUNGE-KUTTA" has been proposed that minimizes the local error of the Runge-Kutta method in connection with the problem of algebraic varieties (see [4]). On the other hand, there are not many literatures in which the definition of Runge-Kutta method has been mathematically considered. In this research, we focus on determinativeness of constants "weights, nodes, components of the Runge-Kutta matrix" appearing in this method, rather than estimation of the accuracy or errors of the Runge-Kutta method. Specifically, we determine the set of constants satisfying conditions in the 4-stage, 4th-order explicit Runge-Kutta methods, which contain four weights, four nodes and six components of the Runge-Kutta matrix. (Here we consider the explicit Runge-Kutta methods, we may assume that Runge-Kutta matrix (a_{ij}) satisfies $a_{ij} = 0$ for $i \leq j$.)* For simplicity, we will simply call these constants *coefficients* in the following. Moreover we investigate geometric characteristics of the space of constants satisfying conditions.

In Section 2, we compare the Taylor expansion of the approximate expression by the 4-stage, 4th-order explicit Runge-Kutta methods and that of the exact solution, and derive the conditions that coefficients should satisfy. In Section 3, we show that the set of coefficients is an irreducible rational surface by considering the closure of solution space that satisfies the conditions. In Sections 4, we prove that the set of coefficients has no singular points in two ways. In Section 5, we show that there is no coefficient that satisfies the condition derived in Section 2 when $c_1 \neq 0$.

The explicit Runge-Kutta methods having three or fewer stages can be obtained as a corollary in the 4-stage. For example, we know that the 3-stage explicit Runge-Kutta methods have 8 conditions to be satisfied for 9 coefficients. Also, we also know that each coefficient can be represented by two parameters. Derivation of conditions and geometric considerations are not as complicated as in the case of the 4-stage.

*We have another way of Runge-Kutta method, for example, implicit Runge-Kutta methods. Here each component a_{ij} of the Runge-Kutta matrix is given as an unconditional constant.

2. Coefficient conditions and values of each coefficient of the 4-stage, 4th-order explicit Runge-Kutta methods

The results in this section are recalculations of the results shown in Hairer [3].

The 4-stage explicit Runge-Kutta methods with $p = 4$ in (1) is[†]

$$
\begin{aligned}
\tilde{y}(t_0+h) &= y(t_0) + h\big(b_1K_1 + b_2K_2 + b_3K_3 + b_4K_4\big), \\
K_1 &= f\big(t_0 + hc_1,\ y\big), \\
K_2 &= f\big(t_0 + hc_2,\ y + ha_{21}K_1\big), \\
K_3 &= f\big(t_0 + hc_3,\ y + h(a_{31}K_1 + a_{32}K_2)\big), \\
K_4 &= f\big(t_0 + hc_4,\ y + h(a_{41}K_1 + a_{42}K_2 + a_{43}K_3)\big).
\end{aligned} \tag{2}
$$

Comparing an approximation $\tilde{y}(t_0+h)$ and the exact solution $y(t_0+h)$, we determine 14 coefficients b_i $(i = 1,\ 2,\ 3,\ 4)$, c_i $(i = 1,\ 2,\ 3,\ 4)$, and a_{ij} $(1 \le j < i \le 4)$ so that up to the fourth order terms of the Taylor expansions with respect to h of these two terms coincide.

Up to the fourth order terms of the Taylor expansion of $y(t_0+h)$ is given as follows[‡].

$$
\begin{aligned}
y(t_0+h) = y(t_0) &+ hf + \frac{h^2}{2}(f_t + ff_y) \\
&+ \frac{h^3}{6}(f_{tt} + 2ff_{ty} + f_tf_y + ff_y^2 + f^2f_{yy}) \\
&+ \frac{h^4}{24}(f_{ttt} + 3ff_{tty} + 3f_tf_{ty} + 5ff_yf_{ty} + 3f^2f_{tyy} \\
&+ f_yf_{tt} + 3ff_tf_{yy} + f_tf_y^2 + ff_y^3 + 4f^2f_yf_{yy} + f^3f_{yyy}) + o(h^4).
\end{aligned} \tag{3}
$$

On the other hand, up to the third order terms of the Taylor expansion with respect to h of K_1, K_2, K_3, K_4 is

$$
\begin{aligned}
K_1 &= f + hc_1f_t + \tfrac{h^2}{2}c_1^2f_{tt} + \tfrac{h^3}{6}c_1^3f_{ttt}, \\
K_2 &= f + h\big(c_2f_t + a_{21}K_1f_y\big) + \tfrac{h^2}{2}\big(c_2^2f_{tt} + 2c_2a_{21}K_1f_{ty} + (a_{21}K_1)^2f_{yy}\big) \\
&\quad + \tfrac{h^3}{6}\big(c_2^3f_{ttt} + 3c_2^2a_{21}K_1f_{tty} + 3c_2(a_{21}K_1)^2f_{tyy} + (a_{21}K_1)^3f_{yyy}\big),
\end{aligned}
$$

[†]The corresponding term of $y(t_0+h)$ in Runge-Kutta method is expressed as $\tilde{y}(t_0+h)$ to distinguish from that in the Taylor expansion of the exact solution.

[‡]Let $f_t = \frac{\partial}{\partial t}f,\ f_y = \frac{\partial}{\partial y}f$, and so on.

$$\begin{aligned}
K_3 &= f + h\big(c_3 f_t + (a_{31}K_1 + a_{32}K_2) f_y\big) \\
&\quad + \tfrac{h^2}{2}\big(c_3^2 f_{tt} + 2c_3(a_{31}K_1 + a_{32}K_2) f_{ty} + (a_{31}K_1 + a_{32}K_2)^2 f_{yy}\big) \\
&\quad + \tfrac{h^3}{6}\big(c_3^3 f_{ttt} + 3c_3^2(a_{31}K_1 + a_{32}K_2) f_{tty} + 3c_3(a_{31}K_1 + a_{32}K_2)^2 f_{tyy} \\
&\quad + (a_{31}K_1 + a_{32}K_2)^3 f_{yyy}\big), \\
K_4 &= f + h\big(c_4 f_t + (a_{41}K_1 + a_{42}K_2 + a_{43}K_3) f_y\big) \\
&\quad + \tfrac{h^2}{2}\big(c_4^2 f_{tt} + 2c_4(a_{41}K_1 + a_{42}K_2 + a_{43}K_3) f_{ty} + (a_{41}K_1 + a_{42}K_2 + a_{43}K_3)^2 f_{yy}\big) \\
&\quad + \tfrac{h^3}{6}\big(c_4^3 f_{ttt} + 3c_4^2(a_{41}K_1 + a_{42}K_2 + a_{43}K_3) f_{tty} \\
&\quad + 3c_4(a_{41}K_1 + a_{42}K_2 + a_{43}K_3)^2 f_{tyy} + (a_{41}K_1 + a_{42}K_2 + a_{43}K_3)^3 f_{yyy}\big).
\end{aligned}$$

Substituting these $K_1,\ K_2,\ K_3,\ K_4$ into (2), and comparing the coefficients of each term with those of (3), the following 19 conditions are derived.

$$f : b_1 + b_2 + b_3 + b_4 = 1 \tag{4}$$

$$f_t : b_1c_1 + b_2c_2 + b_3c_3 + b_4c_4 = \tfrac{1}{2} \tag{5}$$

$$ff_y : b_2a_{21} + b_3(a_{31} + a_{32}) + b_4(a_{41} + a_{42} + a_{43}) = \tfrac{1}{2} \tag{6}$$

$$f_{tt} : b_1c_1^2 + b_2c_2^2 + b_3c_3^2 + b_4c_4^2 = \tfrac{1}{3} \tag{7}$$

$$ff_{ty} : b_2c_2a_{21} + b_3c_3(a_{31} + a_{32}) + b_4c_4(a_{41} + a_{42} + a_{43}) = \tfrac{1}{3} \tag{8}$$

$$f_tf_y : b_2c_1a_{21} + b_3(c_1a_{31} + c_2a_{32}) + b_4(c_1a_{41} + c_2a_{42} + c_3a_{43}) = \tfrac{1}{6} \tag{9}$$

$$ff_y^2 : b_3a_{21}a_{32} + b_4\big(a_{21}a_{42} + a_{43}(a_{31} + a_{32})\big) = \tfrac{1}{6} \tag{10}$$

$$f^2f_{yy} : b_2a_{21}^2 + b_3(a_{31} + a_{32})^2 + b_4(a_{41} + a_{42} + a_{43})^2 = \tfrac{1}{3} \tag{11}$$

$$f_{ttt} : b_1c_1^3 + b_2c_2^3 + b_3c_3^3 + b_4c_4^3 = \tfrac{1}{4} \tag{12}$$

$$ff_{tty} : b_2c_2^2a_{21} + b_3c_3^2(a_{31} + a_{32}) + b_4c_4^2(a_{41} + a_{42} + a_{43}) = \tfrac{1}{4} \tag{13}$$

$$f_tf_{ty} : b_2c_2c_1a_{21} + b_3c_3(c_1a_{31} + c_2a_{32}) + b_4c_4(c_1a_{41} + c_2a_{42} + c_3a_{43}) = \tfrac{1}{8} \tag{14}$$

$$\begin{aligned} ff_yf_{ty} : {}& b_3(c_2 + c_3)a_{21}a_{32} + b_4\big(c_2a_{21}a_{42} + c_3a_{43}(a_{31} + a_{32}) \\ & + c_4(a_{21}a_{42} + a_{43}(a_{31} + a_{32}))\big) = \tfrac{5}{24} \end{aligned} \tag{15}$$

$$f^2f_{tyy} : b_2c_2a_{21}^2 + b_3c_3(a_{31} + a_{32})^2 + b_4c_4(a_{41} + a_{42} + a_{43})^2 = \tfrac{1}{4} \tag{16}$$

$$f_yf_{tt} : b_2c_1^2a_{21} + b_3(c_1^2a_{31} + c_2^2a_{32}) + b_4(c_1^2a_{41} + c_2^2a_{42} + c_3^2a_{43}) = \tfrac{1}{12} \tag{17}$$

$$\begin{aligned} ff_tf_{yy} : {}& b_2c_1a_{21}^2 + b_3(a_{31} + a_{32})(c_1a_{31} + c_2a_{32}) \\ & + b_4(a_{41} + a_{42} + a_{43})(c_1a_{41} + c_2a_{42} + c_3a_{43}) = \tfrac{1}{8} \end{aligned} \tag{18}$$

$$f_tf_y^2 : b_3c_1a_{21}a_{32} + b_4\big(c_1(a_{21}a_{42} + a_{31}a_{43}) + c_2a_{32}a_{43}\big) = \tfrac{1}{24} \tag{19}$$

$$ff_y^3 : b_4a_{21}a_{32}a_{43} = \tfrac{1}{24} \tag{20}$$

$$
\begin{aligned}
&f^2 f_y f_{yy} : b_3\bigl(a_{21}^2 a_{32} + 2a_{21}a_{32}(a_{31}+a_{32})\bigr) \\
&\qquad + b_4\Bigl(a_{21}^2 a_{42} + (a_{31}+a_{32})^2 a_{43} + 2\bigl(a_{21}a_{42}(a_{41}+a_{42}+a_{43}) \\
&\qquad + a_{43}(a_{31}+a_{32})(a_{41}+a_{42}+a_{43})\bigr)\Bigr) = \tfrac{1}{3}
\end{aligned} \tag{21}
$$

$$
f^3 f_{yyy} : b_2 a_{21}^3 + b_3(a_{31}+a_{32})^3 + b_4(a_{41}+a_{42}+a_{43})^3 = \tfrac{1}{4} \tag{22}
$$

Definition 2.1. *Let the set W be the solution space of the coefficients satisfying the conditions of the 4-stage, 4th-order explicit Runge-Kutta methods. That is,*

$$
W = \left\{ \begin{pmatrix} b_1,\ b_2,\ b_3,\ b_4,\ c_1,\ c_2,\ c_3,\ c_4, \\ a_{21},\ a_{31}\, a_{32},\ a_{41},\ a_{42},\ a_{43} \end{pmatrix} \middle| \begin{array}{l} b_i,\ c_i,\ a_{ij} \in \mathbb{R}, \\ \textit{which satisfy equations} \\ (4),\ \ldots,\ (22) \end{array} \right\} \subset \mathbb{R}^{14}.
$$

In the following, we will reduce these condition. From (20),

$$
b_4 \neq 0,\ a_{21} \neq 0,\ a_{32} \neq 0,\ a_{43} \neq 0
$$

holds. From (19), (20),

$$
c_1\bigl(a_{21}(b_3 a_{32} + b_4 a_{42} + b_4 a_{31} a_{43})\bigr) + b_4 a_{32} a_{43}(c_2 - a_{21}) = 0
$$

is derived. Here, Oliver [5] shows that there is no solution of (4) to (22) unless $c_1 = 0$. We will show in Section 5 that in case $c_1 \neq 0$ there exists no solution. In the following, the discussion will proceed under the assumption $c_1 = 0$ until Section 4. From this assumption, the relations

$$
c_2 = a_{21} \neq 0 \quad \bigl(\text{from (19), (20)}\bigr), \tag{23}
$$

$$
c_3 = a_{31} + a_{32} \quad \bigl(\text{from (9), (10)}\bigr), \tag{24}
$$

$$
c_4 = a_{41} + a_{42} + a_{43} \quad \bigl(\text{from (5), (6)}\bigr) \tag{25}
$$

of coefficients are obtained. Using these expressions on $c_2,\ c_3,\ c_4$, we have the followings§.

§Here, while finding the coefficients, we do not use a simplifying assumption

$$
\sum_{i=j+1}^{p} b_i a_{ij} = b_j(1 - c_j)
$$

described in [3, Chapter II Lemma1.3], etc.

(26) $$b_4(c_4-c_3)(c_2a_{42}+c_3a_{43}) = \tfrac{1}{8}-\tfrac{c_3}{6} \quad \bigl(\text{from } (14) - c_3\times(9)\bigr),$$

(27) $$b_4c_3a_{43}(c_2-c_3) = \tfrac{c_2}{6}-\tfrac{1}{12} \quad \bigl(\text{from } c_2\times(9)-(17)\bigr),$$

(28) $$b_4c_4(c_2-c_4)(c_3-c_4) = c_3\left(\tfrac{c_2}{2}-\tfrac{1}{3}\right)-\left(\tfrac{c_2}{3}-\tfrac{1}{4}\right)$$
$$\Bigl(\text{from } c_3\times\bigl(c_2\times(5)-(7)\bigr)-\bigl(c_2\times(7)-(12)\bigr)\Bigr),$$

(29) $$b_4\bigl(c_2c_4a_{32}(c_2-c_4)-c_3(c_2-c_3)(c_2a_{42}+c_3a_{43})\bigr)$$
$$= c_2a_{32}\left(\tfrac{c_2}{2}-\tfrac{1}{3}\right)-\tfrac{c_3(c_2-c_3)}{6}$$
$$\Bigl(\text{from } a_{32}c_2\times\bigl(c_2\times(5)-(7)\bigr)-c_3(c_2-c_3)\times(9)\Bigr).$$

Let (26) to (29) be simplified by $c_2 = t_1,\ c_3 = t_2$ as a parameter. Assuming $c_4 \neq 0,\ t_1 \neq c_4,\ t_2 \neq c_4$, we get

(30) $$b_4 = \tfrac{1}{c_4(t_1-c_4)(t_2-c_4)}\left(\tfrac{t_2(3t_1-2)}{6}-\tfrac{4t_1-3}{12}\right)$$

from (28). We derived

(31) $$a_{43} = \tfrac{2t_1-1}{12t_2(t_1-t_2)b_4}$$

from (27) assuming $t_2 \neq 0,\ t_1 \neq t_2$. (From the two above formulas, we need to assume $c_2 \neq \frac{4c_3-3}{2(3c_3-2)},\ c_2 \neq \frac{1}{2}$ for $b_4 \neq 0,\ a_{43} \neq 0$.) From (20),

(32) $$a_{32} = \tfrac{1}{24t_1b_4a_{43}}$$

is obtained. Substituting (30), (31), and (32) into formula (26)$\times t_2(t_1-t_2)$+(29)$\times(c_4-t_2)$ gives

$$t_1c_4(t_1-c_4)(c_4-t_2)b_4a_{32}$$
$$= (c_4-t_2)\left(t_1a_{32}\left(\tfrac{t_1}{2}-\tfrac{1}{3}\right)-\tfrac{t_1(t_1-t_2)}{6}\right)+t_2(t_1-t_2)\left(\tfrac{1}{8}-\tfrac{t_2}{6}\right),$$

$$\frac{t_1t_2(t_1-t_2)(c_4-1)}{12(2t_1-1)} = 0.$$

Here from $t_1 \neq 0,\ t_2 \neq 0,\ t_1 \neq t_2$ we derive $c_4 = 1$. Thus, the formulas of $b_4,\ a_{43},\ a_{32}$ are obtained by substituting c_4 for 1. Totally,

$$
\begin{aligned}
& b_1 = \tfrac{(6t_2-2)t_1-2t_2+1}{12t_1t_2}, \quad b_2 = \tfrac{2t_2-1}{12t_1(t_1-1)(t_1-t_2)}, \\
& b_3 = -\tfrac{2t_1-1}{12t_2(t_2-1)(t_1-t_2)}, \quad b_4 = \tfrac{(6t_2-4)t_1-4t_2+3}{12(t_1-1)(t_2-1)}, \\
& c_2 = t_1 \text{ (parameter)}, \quad c_3 = t_2 \text{ (parameter)}, \quad c_4 = 1, \\
& a_{21} = t_1, \quad a_{31} = \tfrac{t_2(4t_1^2-3t_1+t_2)}{2t_1(2t_1-1)}, \quad a_{32} = \tfrac{t_2(t_1-t_2)}{2t_1(2t_1-1)}, \\
& a_{41} = \tfrac{(12t_2^2-12t_2+4)t_1^2+(-12t_2^2+15t_2-6)t_1+4t_2^2-5t_2+2}{2t_1t_2\big((6t_2-4)t_1-4t_2+3\big)}, \\
& a_{42} = \tfrac{(t_1-1)(t_1-4t_2^2+5t_2-2)}{2t_1(t_1-t_2)\big((6t_2-4)t_1-4t_2+3\big)}, \ a_{43} = \tfrac{(t_1-1)(t_2-1)(2t_1-1)}{t_2(t_1-t_2)\big((6t_2-4)t_1-4t_2+3\big)}.
\end{aligned} \tag{33}
$$

Hence, we obtained[¶] that all the coefficients are rational formula by the parameter $t_1,\ t_2$ with the assumption

$$c_4 \neq 0,\ t_2 \neq 0,\ t_1 \neq c_4,\ t_2 \neq c_4,\ t_1 \neq t_2. \tag{34}$$

Definition 2.2. *Let W_m the space of coefficients determined by* (33) *and* (34)*. That is,*

$$W_m = \left\{ \begin{pmatrix} b_1,\ b_2,\ b_3,\ b_4,\ c_1,\ c_2,\ c_3,\ c_4, \\ a_{21},\ a_{31}\, a_{32},\ a_{41},\ a_{42},\ a_{43} \end{pmatrix} \middle|\ \begin{matrix} t_1,\ t_2 \in \mathbb{R}, \\ (33),\ (34) \end{matrix} \right\} \subset W.$$

We call W_m "the main part" of W.

Next, we examine solutions in the exceptional cases other than the condition (34). Here we consider the following seven cases :

case I : $c_2 = c_3$ and $c_2 \neq c_4$
case II : $c_2 = c_4$ and $c_2 \neq c_3$
case III : $c_3 = c_4$ and $c_3 \neq 0$
case IV : $c_3 = 0$ and $c_4 = 0$
case V : $c_2 = c_3$ and $c_3 = c_4$
case VI : $c_3 = 0$, $c_2 \neq 0$, $c_4 \neq 0$, and $c_2 \neq c_4$
case VII : $c_4 = 0$, $c_2 \neq 0$, $c_4 \neq 0$, and $c_2 \neq c_3$

[¶] As an auxiliary means, we used `Risa/Asir` to recalculation.

In cases (I), (II), and (VI), there exists a solution space with non-zero parameter s. In the other four cases, there is no solution. We omit the proof of this part, however the proof is shown in the master thesis [9] by the author.

(I) $c_2 = c_3$ and $c_2 \neq c_4$
$b_1 = \frac{1}{6},\ b_2 = \frac{2-s}{3},\ b_3 = \frac{s}{3},\ b_4 = \frac{1}{6},$
$c_2 = \frac{1}{2},\ c_3 = \frac{1}{2},\ c_4 = 1,$
$a_{21} = \frac{1}{2},\ a_{31} = \frac{s-1}{2s},\ a_{32} = \frac{1}{2s},\ a_{41} = 0,\ a_{42} = 1 - s,\ a_{43} = s$ (parameter, $s \neq 0$).

(II) $c_2 = c_4$ and $c_2 \neq c_3$
$b_1 = \frac{1}{6},\ b_2 = \frac{1-6s}{6},\ b_3 = \frac{2}{3},\ b_4 = s$ (parameter, $s \neq 0$),
$c_2 = 1,\ c_3 = \frac{1}{2},\ c_4 = 1,$
$a_{21} = 1,\ a_{31} = \frac{3}{8},\ a_{32} = \frac{1}{8},\ a_{41} = \frac{4s-1}{4s},\ a_{42} = -\frac{1}{12s},\ a_{43} = \frac{1}{3s}.$

(VI) $c_3 = 0$, $c_2 \neq 0$, $c_4 \neq 0$, and $c_2 \neq c_4$
$b_1 = \frac{2s-1}{12s},\ b_2 = \frac{2}{3},\ b_3 = \frac{1}{12s},\ b_4 = \frac{1}{6},$
$c_2 = \frac{1}{2},\ c_3 = 0,\ c_4 = 1,$
$a_{21} = \frac{1}{2},\ a_{31} = -s,\ a_{32} = s$ (parameter, $s \neq 0$), $a_{41} = \frac{-s-1}{2s},\ a_{42} = \frac{3}{2},\ a_{43} = \frac{1}{2s}.$

DEFINITION 2.3. *Define the set $W_{e,I}$, $W_{e,II}$, and $W_{e,VI}$ as each solution space of (I), (II), and (VI) represented as above, and the union of these three spaces*

$$W_e = W_{e,I} \cup W_{e,II} \cup W_{e,VI} \subset W.$$

We call it "the exceptional part".

Thus, we find that main part W_m of the coefficient space of the 4-stage, 4th-order explicit Runge-Kutta methods can be represented by two parameters, and that there is exceptional part W_e where the coefficient space are represented by one parameter.

3. The limit point set of the main part of the coefficient space

In the previous section, we prove that the main part W_m can be expressed by two parameters. The closure $\overline{W_m}$ of the main part in $\mathbb{R}^{14}$ is a rational surface. Next, we prove that the exceptional part W_e is fully contained in $\overline{W_m}$. That is, this section shows the following proposition.

PROPOSITION 3.1.

$$W_e \subset \overline{W_m}$$

We consider a linear open path $t_1 = p + a\epsilon,\ t_2 = q + b\epsilon$, where $a,\ b$, and ϵ are arbitrary real numbers such that $(a, b) \neq (0, 0)$. Here p and q are the values of c_2 and c_3 in each case (I) or (II) or (VI). We obtain the limit of coefficients when $\epsilon \to 0$ and observe whether the limit is contained in an exceptional coefficient space.

At first, we consider the case (I). Let an open path be

$$t_1 = \tfrac{1}{2} + a\epsilon,\ t_2 = \tfrac{1}{2} + b\epsilon \tag{35}$$

where $a,\ b$ is a fixed constant such that $a \neq b$ and $a \neq 0$. Thus we have the followings after substituting (35) into the formulae (33).

$$\begin{aligned}
b_1 &= \tfrac{12ab\epsilon^2+(2a+2b)\epsilon+1}{6(2a\epsilon+1)(2b\epsilon+1)},\ b_2 = \tfrac{2b}{3(a-b)(2a\epsilon-1)(2a\epsilon+1)},\\
b_3 &= -\tfrac{2a}{3(a-b)(2b\epsilon-1)(2b\epsilon+1)},\ b_4 = \tfrac{12ab\epsilon^2+(-2a-2b)\epsilon+1}{6(2a\epsilon-1)(2b\epsilon-1)},\\
a_{31} &= \tfrac{(2b\epsilon+1)(4a^2\epsilon+a+b)}{4a(2a\epsilon+1)},\ a_{32} = \tfrac{(a-b)(2b\epsilon+1)}{4a(2a\epsilon+1)},\\
a_{41} &= \tfrac{2\epsilon(24a^2b^2\epsilon^3+(2a^2+6ba+2b^2)\epsilon-a+b)}{(2a\epsilon+1)(2b\epsilon+1)\left(12ab\epsilon^2+(-2a-2b)\epsilon+1\right)},\\
a_{42} &= -\tfrac{(4b^2\epsilon-a-b)(2a\epsilon-1)}{(a-b)(2a\epsilon+1)\left(12ab\epsilon^2+(-2a-2b)\epsilon+1\right)},\\
a_{43} &= \tfrac{2a(2a\epsilon-1)(2b\epsilon-1)}{(a-b)(2b\epsilon+1)\left(12ab\epsilon^2+(-2a-2b)\epsilon+1\right)}.
\end{aligned}$$

We consider the limit with $\epsilon \to 0$ and we have

$$\begin{aligned}
&b_1 = \tfrac{1}{6},\ b_2 = -\tfrac{2b}{3(a-b)},\ b_3 = \tfrac{2a}{3(a-b)},\ b_4 = \tfrac{1}{6},\\
&a_{31} = \tfrac{a+b}{4a},\ a_{32} = \tfrac{a-b}{4a},\ a_{41} = 0,\ a_{42} = -\tfrac{a+b}{a-b},\ a_{43} = \tfrac{2a}{a-b}.
\end{aligned}$$

From the above formula, we found that all the coefficients converge. In particular, if and only if we set $s = \frac{2a}{a-b}$, then (33) converges to a point in $W_{e,I}$. In the case $W_{e,II}$, if we set $t_1 = 1 + a\epsilon,\ t_2 = \frac{1}{2} + b\epsilon,\ (a \neq 2b,\ a \neq 0)$ and $s = \frac{a-2b}{6a}$, then (33) converges to a point in $W_{e,II}$. In fact,

$$\begin{aligned}
&b_1 = \tfrac{1}{6},\ b_2 = \tfrac{b}{3a},\ b_3 = \tfrac{2}{3},\ b_4 = \tfrac{a-2b}{6a},\\
&a_{31} = \tfrac{3}{8},\ a_{32} = \tfrac{1}{8},\ a_{41} = -\tfrac{a+4b}{2(a-2b)},\ a_{42} = -\tfrac{a}{2(a-2b)},\ a_{43} = \tfrac{2a}{a-2b}.
\end{aligned}$$

In the same way, if we set $t_1 = \frac{1}{2} + a\epsilon,\ t_2 = b\epsilon,\ (a \neq 0,\ b \neq 0)$ and $s = \frac{b}{4a}$, then (33) converges to a point in $W_{e,VI}$. In fact,

$$b_1 = -\tfrac{2a-b}{6b},\ b_2 = \tfrac{2}{3},\ b_3 = \tfrac{a}{3b},\ b_4 = \tfrac{1}{6},$$
$$a_{31} = -\tfrac{b}{4a},\ a_{32} = \tfrac{b}{4a},\ a_{41} = -\tfrac{4a+b}{2b},\ a_{42} = \tfrac{3}{2},\ a_{43} = \tfrac{2a}{b}.$$

Hence, we showed that the case of all point in W_e can be expressed by limits of paths in W_m. Since $W_m \subset W = W_m \cup W_e \subset \overline{W_m}$ and W is closed, we have the following proposition.

PROPOSITION 3.2. *The closure $\overline{W_m}$ of W_m in $\mathbb{R}^{14}$ satisfies*

$$\overline{W_m} = W_m \cup W_e = W.$$

LEMMA 3.3. *If k is an infinite field and V is a variety defined by the rational parametrization*

$$x_1 = \frac{f_1(t_1, \ldots, t_m)}{g_1(t_1, \ldots, t_m)},$$
$$\vdots$$
$$x_n = \frac{f_n(t_1, \ldots, t_m)}{g_n(t_1, \ldots, t_m)}$$

where $f_1,\ \ldots,\ f_n,\ g_1,\ \ldots,\ g_n \in k[t_1,\ \ldots,\ t_m]$, then V is irreducible.

proof. See [2, p.208, Proposition 6]. □

PROPOSITION 3.4. *The algebraic variety formed by W is the irreducible rational surface.*

proof. From the previous section, it was found that all coefficients in W_m are represented by a rational formula whose denominator is not 0 by two parameters $t_1,\ t_2$. Hence, Lemma 3.3 shows that the algebraic variety formed by W_m is irreducible. Since W_m is irreducible, closure $\overline{W_m} = W$ is also irreducible from Proposition 3.2.

□

4. Non-existence of singular points in *W*

Next, we show non-existence of singular points in W in two ways[‖].

4.1. Proof using a Jacobian matrix

m and n are natural numbers. Let V be an algebraic variety defined by

$$V = \{(x_1, \ldots, x_n) \in \mathbb{R}^n \mid f_1(x_1, \ldots, x_n) = \cdots = f_m(x_1, \ldots, x_n) = 0\},$$

and let p be a point in V. p is a non-singular point if and only if the rank of the Jacobi matrix

$$J = \left\{ \left(\frac{\partial f_i}{\partial x_j} \right)(p) \middle| \, 1 \leq i \leq m, 1 \leq j \leq n \right\}$$

satisfies

$$\operatorname{rank}(J) = n - \dim(V).$$

PROPOSITION 4.1. *For any point $p \in W$, p is a non-singular point.*

proof. In our case, there are 14 variables, $b_1, \ldots, b_4, c_1, \ldots, c_4, a_{21}, \ldots, a_{43}$. However, we assume $c_1 = 0$ and we consider 13 variables. And there are 19 functions from (4) to (22). The Jacobi matrix J is a 19×13 matrix and it is hard to calculate the rank of J by hand. We uses `Risa/Asir`, a famous CAS in Japan and checks that $\operatorname{rank}(J) = 11$. This implies that J is a non-singular variety.

First, any point in W_m is a non-singular point since for all the coefficients is represented by the rational formulae of t_1 and t_2 whose denominators is not 0. Thus, it is sufficient to consider the point in W_e. As a result of consideration rank in point of W_e, we showed that all points were $\operatorname{rank}(J) = 11$. For the source code of `Asir` and the calculation result, see [9].

Hence we show that any point in W is a non-singular point. □

4.2. Proof by a parameter replacement

In this section we show Proposition 4.1 by changing two parameters of the main part. When we change parameters, it is important to take new parameters such that points in W_e are contained in the new main part. Geometrically, we may suppose changing the view of a rational surface.

First, we take (c_2, b_2) in place of (c_2, c_3) for parameters of the main part. We

[‖]We don't consider singularity at infinite points here.

have

$$
(36)\quad
\begin{aligned}
&b_1=\frac{36s_1^3s_2-60s_1^2s_2+30s_1s_2-6s_2+1}{6(12s_1^3s_2-12s_1^2s_2+1)},\ b_2=s_2\ \text{(parameter)},\\
&b_3=\frac{-2(6s_1^2s_2-6s_1s_2+1)^3}{3(12s_1^3s_2-24s_1^2s_2+12s_1s_2-1)(12s_1^3s_2-12s_1^2s_2+1)},\\
&b_4=\frac{36s_1^3s_2-48s_1^2s_2+18s_1s_2-1}{6(12s_1^3s_2-24s_1^2s_2+12s_1s_2-1)},\\
&c_2=s_1\ \text{(parameter)},\ c_3=\frac{12s_1^3s_2-12s_1^2s_2+1}{2(6s_1^2s_2-6s_1s_2+1)},\ c_4=1,\ a_{21}=s_1,\\
&a_{31}=\frac{(12s_1^3s_2-12s_1^2s_2+1)(24s_1^3s_2-24s_1^2s_2+4s_1-1)}{8s_1(6s_1^2s_2-6s_1s_2+1)^2},\\
&a_{32}=\frac{12s_1^3s_2-12s_1^2s_2+1}{8s_1(6s_1^2s_2-6s_1s_2+1)^2},\\
&a_{41}=\frac{(2s_1-1)\left(432s_1^6s_2^2-1080s_1^5s_2^2+1152s_1^4s_2^2-648s_1^3s_2^2+(144s_2^2+30s_2)s_1^2-18s_1s_2+1\right)}{2s_1(12s_1^3s_2-12s_1^2s_2+1)(36s_1^3s_2-48s_1^2s_2+18s_1s_2-1)},\\
&a_{42}=-\frac{\left(144s_1^5s_2^2-432s_1^4s_2^2+432s_1^3s_2^2+(-144s_2^2-18s_2)s_1^2+18s_1s_2-1\right)}{2s_1(36s_1^3s_2-48s_1^2s_2+18s_1s_2-1)},\\
&a_{43}=\frac{2(6s_1^2s_2-6s_1s_2+1)^2(12s_1^3s_2-24s_1^2s_2+12s_1s_2-1)}{(12s_1^3s_2-12s_1^2s_2+1)(36s_1^3s_2-48s_1^2s_2+18s_1s_2-1)}.
\end{aligned}
$$

Here, s_1 and s_2 are parameters with conditions $s_1\neq 0$, and let W'_m be the new main part with respect to s_1 and s_2. We check that a point in W_e can be represented by (36) of parameters s_1 and s_2. In fact, if we set $s_1=\frac{1}{2},\ s_2=\frac{2-s}{3}$ then a point in $W_{e,I}$ is contained in W'_m (result of substituting $s_1=\frac{1}{2},\ s_2=\frac{2-s}{3}$ for (36) is the same as (I)), if we set $s_1=1,\ s_2=\frac{1-6s}{6}$ then a point in $W_{e,II}$ is included in W'_m (result of substitution is the same as (II)). However, all of the points in $W_{e,VI}$ are not contained in W'_m. Because, $c_2,\ b_2$ at points in $W_{e,VI}$ is $c_2=\frac{1}{2},\ b_2=\frac{2}{3}$, but the points in W'_m diverges at this value.

Hence, if we take parameters $(c_2,\ b_2)$, any point in (I) and (II) is included in the main part W'_m of new parameters. Therefore, we showed that any points in $W_{e,I}$ and $W_{e,II}$ are non-singular.

Next, we take $(c_3,\ b_3)$ in place of $(c_2,\ c_3)$ for parameters of the main part. Then,

(37)

$$
\begin{aligned}
&b_1=\frac{36r_1^3r_2-60r_1^2r_2+30r_1r_2-6r_2+1}{6(12r_1^3r_2-12r_1^2r_2+1)},\ b_2=-\frac{2(6r_1^2r_2-6r_1r_2+1)^3}{3(12r_1^3r_2-24r_1^2r_2+12r_1r_2-1)(12r_1^3r_2-12r_1^2r_2+1)},\\
&b_3=r_2\ \text{(parameter)},\ b_4=\frac{36r_1^3r_2-48r_1^2r_2+18r_1r_2-1}{6(12r_1^3r_2-24r_1^2r_2+12r_1r_2-1)},\\
&c_2=\frac{12r_1^3r_2-12r_1^2r_2+1}{2(6r_1^2r_2-6r_1r_2+1)},\ c_3=r_1\ \text{(parameter)},\ c_4=1,\ a_{21}=\frac{12r_1^3r_2-12r_1^2r_2+1}{2(6r_1^2r_2-6r_1r_2+1)},
\end{aligned}
$$

$$a_{31}=\frac{144r_1^5r_2^2-288r_1^4r_2^2+144r_1^3r_2^2+18r_1^2r_2^2-18r_1r_2+1}{12r_2(r_1-1)(12r_1^3r_2-12r_1^2r_2+1)},\ a_{32}=-\frac{(6r_1^2r_2-6r_1r_2+1)}{12r_2(r_1-1)(12r_1^3r_2-12r_1^2r_2+1)},$$

$$a_{41}=\frac{(2r_1-1)\left(432r_1^6r_2^2-1512r_1^5r_2^2+2232r_1^4r_2^2-1800r_1^3r_2^2+(792r_2^2+30r_2)r_1^2+(-144r_2^2-42r_2)r_1+12r_2+1\right)}{2(r_1-1)(12r_1^3r_2-12r_1^2r_2+1)(36r_1^3r_2-48r_1^2r_2+18r_1r_2-1)},$$

$$a_{42}=\frac{(6r_1^2r_2-6r_1r_2+1)(12r_1^3r_2-24r_1^2r_2+12r_1r_2-1)\left(24r_1^3r_2-48r_1^2r_2+(24r_2+4)r_1-3\right)}{2(r_1-1)(12r_1^3r_2-12r_1^2r_2+1)(36r_1^3r_2-48r_1^2r_2+18r_1r_2-1)},$$

$$a_{43}=-\frac{6r_2(r_1-1)(12r_1^3r_2-24r_1^2r_2+12r_1r_2-1)}{36r_1^3r_2-48r_1^2r_2+18r_1r_2-1}.$$

Here, r_1 and r_2 are parameters with conditions $r_1 \neq 1$ and $r_2 \neq 0$. Let W''_m be the main part with respect to r_1 and r_2. Substituting $r_1 = 0,\ r_2 = \frac{1}{12s}$ for (37) result the same result as (VI), and we derive that if we set $r_1 = 0,\ r_2 = \frac{1}{12s}$ then a point in $W_{e,VI}$ is contained in W''_m.

Hence, if we take the parameter $(c_3,\ b_3)$, any point in (VI) is included in the main part W''_m of new parameters. Thus, we showed that any point in $W_{e,VI}$ are non-singular.

Now, we complete the proof of non-singularity of W by taking parameters in three ways $(c_2,\ c_3)$, $(c_2,\ b_2)$, and $(c_3,\ b_3)$.

5. The 4-stage, 4th-order explicit Runge-Kutta methods with $c_1 \neq 0$

Oliver [5] describes that "there is no solution that satisfies all conditions in the 4-stage, 4th-order explicit Runge-Kutta methods when $c_1 \neq 0$". However, the proof was partially omitted due to complexity of the calculation. Here based on [5], we show that non-existence of solution that satisfies the conditions (4) to (22) when $c_1 \neq 0$.

[5, (5.1)] describes as the followings.

$$c_2 = a_{21},\ c_3 = a_{31}+a_{32},\ c_4 = a_{41}+a_{42}+a_{43},\ b_1 = 0.$$

Applying the above relations from (4) to (22), we obtain the following 12 conditions.

(38) $\quad b_2+b_3+b_4 = 1$

(39) $\quad b_2c_2+b_3c_3+b_4c_4 = \frac{1}{2}$

(40) $\quad b_2c_2^2+b_3c_3^2+b_4c_4^2 = \frac{1}{3}$

(41) $\quad b_2c_1c_2+b_3(c_1a_{31}+c_2a_{32})+b_4(c_1a_{41}+c_2a_{42}+c_3a_{43}) = \frac{1}{6}$

(42) $\quad b_3c_2a_{32}+b_4(c_2a_{42}+c_3a_{43}) = \frac{1}{6}$

(43) $\quad b_2c_2^3+b_3c_3^3+b_4c_4^3 = \frac{1}{4}$

(44) $\quad b_2c_2^2c_1+b_3c_3\big(c_1a_{31}+c_2a_{32}+b_4c_4(c_1a_{41}+c_2a_{42}+c_3a_{43})\big) = \frac{1}{8}$

(45) $\quad b_3(c_2+c_3)c_2a_{32}+b_4\big(c_2^2a_{42}+c_3^2a_{43}+c_4(c_2a_{42}+c_3a_{43})\big) = \frac{5}{24}$

(46) $$b_2c_1^2c_2 + b_3\big(c_1^2a_{31} + c_2^2a_{32} + b_4(c_1^2a_{41} + c_2^2a_{42} + c_3^2a_{43})\big) = \tfrac{1}{12}$$

(47) $$b_3c_1c_2a_{32} + b_4\big(c_1(c_2a_{42} + a_{31}a_{43} + c_2a_{32}a_{43})\big) = \tfrac{1}{24}$$

(48) $$b_4c_2a_{32}a_{43} = \tfrac{1}{24}$$

(49) $$b_3c_2a_{32}(c_2 + 2c_3) + b_4\big(c_2^2a_{42} + c_3^2a_{43} + 2(c_2c_4a_{42} + c_3c_4a_{43})\big) = \tfrac{1}{3}$$

By combining the above equations, five equations

(50) $$c_1(b_3a_{32} + b_4a_{42} + b_4a_{43} - \tfrac{1}{2}) = 0 \quad \big(\text{from}(39),\ (41),\ (42)\big),$$

(51) $$b_3c_2^2a_{32} + b_4c_2^2a_{42} + b_4c_3^2a_{43} = \tfrac{1}{12} \quad \big(\text{from } (41),\ (42),\ (46)\big),$$

(52) $$b_3c_2c_3a_{32} + b_4c_2c_4a_{42} + b_4c_3c_4a_{43} = \tfrac{1}{8} \quad \big(\text{from } (49),\ (51)\big),$$

(53) $$c_1(b_3c_3a_{32} + b_4c_4a_{42} + b_4c_4a_{43} - \tfrac{1}{3}) = 0 \quad \big(\text{from } (40),\ (44),\ (52)\big),$$

(54) $$c_1(b_4a_{32}a_{43} - \tfrac{1}{6}) = 0 \quad \big(\text{from } (42),\ (47),\ (48)\big)$$

are derived. We consider each coefficient using equations from (38) to (54).

First,

$$a_{32} \neq 0,\ a_{43} \neq 0,\ b_4 = \frac{1}{6a_{32}a_{43}},\ c_2 = \frac{1}{4}$$

holds from (48) and (54). From (52), (53),

(55) $$b_4c_4a_{43}(c_2 - c_3) = \frac{c_2}{3} - \frac{1}{8} \iff a_{32} = c_4(4c_3 - 1)$$

can be derived. On the other side,

(56) $$b_4c_3a_{43}(c_2 - c_3) = \frac{c_2}{6} - \frac{1}{12} \iff a_{32} = c_3(4c_3 - 1)$$

is obtained from (42), (51). Since a_{32} of (55) and (56) is uniquely determined and $a_{32} \neq 0$, $c_3 = c_4$ holds. From (53),

$$c_1c_4(b_3a_{32} + b_4a_{42} + b_4a_{43} - \tfrac{1}{3}) = 0$$

is obtained. Here, $\frac{c_1c_4}{6} = 0$ by $b_3a_{32} + b_4a_{42} + b_4a_{43} = \frac{1}{2}$ from (50). The assumption $c_1 \neq 0$ implies $c_4 = 0$. However, this contradicts $a_{32} \neq 0$ in (55).

Therefore, we showed that there was not a solution that satisfies the condition of the 4-stage, 4th-order explicit Runge-Kutta methods when $c_1 \neq 0$.

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