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ON THE DERIVATION OF EXPLICIT RUNGE – KUTTA METHODS BY MATRIX APPROACH

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ABSTRACT

This paper highlights the derivation of Explicit Runge-Kutta Method of order p≤ 4; stage m≤4 by matrix approach based on the order conditions proposed by Butcher (1964).

The matrix adopted is a square (m x m) matrix whose entries are the nodes, C_i 'S The set of, C_i 'S appearing in the mathematical expression for the determinant of the matrix are termed the free-parameters.

Each particular Explicit Runge-Kutta method constructed is dependent on the choice of the values of these free-parameters, , C_i 'S Usually the values of these free-parameters lie in the interval (0,1). Any arbitrary choice of the values of these free-parameters in the aforementioned interval leads to an Explicit Runge-Kutta method (Lambert,1973).

INTRODUCTION

Consider the initial value problem

$$Y^1 = f(t,y);\ y(t_0) = y_0,\ t \in (a,b) \qquad (1.1)$$

We shall partition (1.1) into two classes of initial value problems namely

$$Y^1 = f(t,y);\ y(t_0) = y_0,\ t \in (a,b) \qquad (1.2)$$

(I) Quadrature problem:

(ii) First Order Linear System with constant coefficient:

$$Y^1 = Ay + f(t);\ y(t_0) = y_0,\ t \in (a,b) \qquad (1.3)$$

Where A is nxn matrix

An Explicit Runge-Kutta (ERK) Method for solving the numerical problems (1.2) and (1.3) is based on the algorithm:

$$y_{n+1} = y_n + h_n \sum_{i=2}^{m+1} x_{i-1} k_{i-1} \quad ;\ n = 0(1)N-1 \qquad (1.4)$$

with steplength and number of iteration defined by

$$h_n = t_{n+1}' - t_n; n = 0(1)N-1$$

and

$$N = b - a / h_n \qquad \text{respectively}$$

For problems (1.3) :

$$k_{i-1} = f\langle t_n + c_{i-1}h_n, y_n + h_n \sum_{j=2}^{i-1} v_{i-1,j-1}; i = 2(1)m+1$$

with constraints

(i) $b_{i-1,j-1} = 0, \quad \text{for all} \quad j \geq i$

(ii) $c_{i-1} = \sum_{j=2}^{i-1} v_{i-1,j-1}, \quad for\ i = 2(1)m+1$ (1.5)

$= 0$ Otherwise

For Quadrature Problem(1.2)

$$k_{i-1} = f(t_n + c_{i-1}h_n); i = 2(1)m+1$$

with constraints

(i) $v_{i-1,j-1} = 0$, for all $j \geq i$

(ii) $c_{i-1} = \sum_{j-2}^{i-1} v_{i-1,j-1}$, for i = 2 (1) m+1 (1.6)

= 0 Otherwise

The k_i's are functions to be evaluated at given points and they are termed the slopes, x_i's, c_i's and v_{ij}'s are the weights, nodes and the entries of the matrix v associated with the method respectively .

The number of parameters of Explicit Runge-Kutta method is determined by the

$$N_P = \frac{m(m+1)}{2} \tag{1.7}$$

Where m is the number of function evaluations at every step of the integration. The parameters are given in the table below:-

C_2	V_{21}				
C_3	V_{31}	V_{32}			
C_4	V_{41}	V_{42}	V_{43}		
:	:	:	:		
:	:	:	:	. . .	
			.		
C_m	V_{m1}	V_{m2}	V_{m3}	. . . .	$V_{m,m-1}$
	X_1	X_2	X_3	. . . .	X

(1.8)

For the construction of Explicit Runge –Kutta Methods of Order P≤4; stage m≤4, we choose the nodes $\{c_{i-1}\}$ and the weights $\{X_{i-1}\}$ to be those of quadrature problem of degree of precision k.

These parameters $\{c_{i-1}\}$ and $\{X_{i-1})$ must satisfy the of order equations.

$$\sum_{i=2}^{m+1} X_{i=1}\, C_{i-1}^{k} - \frac{1}{k+1} = 0; k = 0\,(1)\,m-1 \tag{1.9}$$

and for the first order Linear System with constant coefficient, the parameters $\{c_{i-1}\}$
$\{x_{i-1}\}$ and $\{V_{i-1,j-1}\}$ must satisfy the following set of order equations;

(a) $$\sum_{j=2}^{m}\sum_{i=2}^{m+1} X_{i-1} V_{i-1\,j-1}\, C_{i-1}^{k} - \frac{1}{(k+1)(k+2)} = 0, k = 0(1)\,m-2$$

(b) $$\sum_{L=2}^{m-1}\sum_{i=2}^{m}\sum_{j=2}^{m+1} X_{l-1}\, V_{i-1,j-1}\, V_{j-1,l-1}\, C_{l,-1}^{k}\left(\frac{1}{(k+1)(k+2)(k+3)}\right) = 0; \tag{1.10}$$

$$k = 0\,(1)\,m-3$$

(c) $$\sum_{j=2}^{m}\sum_{i=2}^{m+1} X_{i=1}\, C_{i=1}^{k-1}\, V_{i-1\,j-1}\, C_{j=1}^{k-1} - \frac{1}{2k^2} = 0; k = 2$$

With set of order equations for the quadrature problem, we construct an m x m matrix, B_m whose entries are the nodes C_i'S,

That is

$$\begin{bmatrix} 1 & 1 & 1 & \cdots & 1 \\ 0 & C_2 & C_3 & \cdots & C_m \\ 0 & C_2^2 & C_3^2 & \cdots & C_m^2 \\ \cdot & \cdot & \cdot & \cdots & \cdot \\ 0 & C_2^m & C_3^m & \cdots & C_m^m \end{bmatrix}$$

Hence $B_m W_m = T_m$ (1·11)

Where

$$W_m = \begin{bmatrix} X_1 \\ X_2 \\ \cdot \\ \cdot \\ X_m \end{bmatrix} \text{ and } T_m = \begin{bmatrix} 1 \\ ½ \\ \cdot \\ \cdot \\ 1/m \end{bmatrix}$$

The solution set

$\{X_1, X_2, X_3, \ldots X_m\}$

of equation (1.11) must satisfy the set of order equations (1.10).
Adopting the set of order equations (1.10) and using (1.5) or (1.6). other parameters W_{1j},s can be obtained.

To determine <u>free parameter</u>(s), we obtain the determinant of matrix B_m. That is:

$|B_m| = f(c_2, c_3, \ldots c_m)$ (1.12)

The variable (s) that appear(s) in (1.12) is /are termed the free parameter(s), we choose $x_3 = \varnothing;\ o < \varnothing < 1$

By proper substitution of $\varnothing$ and the free – parameters into the matrix B_m and vector W_m respectively, we have some rows of matrix B_m dependent. This reduces column vector W_m to (m-1) column vector, W_{m-1}. That is:

$$W_m = 1 \begin{bmatrix} X_1 \\ X_2 \\ \cdot \\ \cdot \\ \cdot \\ \cdot \\ Xm-1 \end{bmatrix} \quad (1.13)$$

Since some rows of matrix B_m are dependent, we shall drop the last row (which is redundant) and the corresponding term in column vector T_m. This reduces matrix B_m and vector T_m to (m −1) by (m-1) matrix Bm-1 and (m-1) column vector T_{m-1} respectively such that

$$B_{m-1} W_{m-1} = T_{m-1} \quad (1.14)$$

Hence the solution set $\{x_1, x_2 \ldots\ldots x_{m-1}\}$ of (1.14) with $x_3 = \varnothing$ must satisfy the set of order equations (1.10).

Other parameters Vij 'S can be obtained from (1.5) and (1.10) Butcher (1964) suggested the simplifying assumptions:

$$\sum_{i=j+1}^{m+1} X_{i-1} V_{i-1\,j-1} = X_{j-1}(1-C_{j-1}) \; ; j = 2\ (1)\ m+1 \quad (1.15)$$

Which we found useful in obtaining the values of the parameters V_{ij}'s and X_i's of the methods

Definition 1.15: The method is said to be of order P if P is the largest integer for which

$$\left|\, \left| y(t_{n+1}) - y(t_n) - h_n \sum_{i=2}^{m+1} X_{i-1} k_{i-1} \right| \right| \le C h_n^{p+1} \quad (1.16)$$

Where $K_1 = f(t_n{'}\ y(t_n))$

$$\text{and } k_{i-1} = f\left(t_n + C_{i-1} h_n,\ Y(t_n) + h_n \sum_{j=2}^{i-1} V_{i-1} K_{j-1}\right); \quad i = 3(1)(m+1) \quad (1.17)$$

C is a constant.

Definition 1.16 The stage, m of the method is the number of function evaluations at every step of integration in the interval.

$[\,t_n, t_{n+1}]$, n = O(1) N − 1.

Definition 1.17 The method is consistent iff

$$\sum_{i=2}^{m+1} X_{i-1} f\left(t_n + C_{i-1} h_n, Y_n + h_n \sum_{j=2}^{i-1} V_{i-1\,j-1} K_{j-1}\right) = f(t_n, Y_n) \quad (1.18)$$

(1.18) is attainable only when

(a) $h_n = O$ (b) $\sum_{i=2}^{m+1} X_{i-1} = 1$

2. (2.2) **EXPLICIT RUNGE- KUTTA METHOD**

For the construction of this method we shall adopt 2 x 2 matrix:

$$B_2\begin{bmatrix} 1 & 1 \\ 0 & C_2 \end{bmatrix} \qquad (2.1)$$

and the column vectors

$$W_2 = \begin{bmatrix} X_1 \\ X_2 \end{bmatrix}, \quad T_2 = \begin{bmatrix} 1 \\ \frac{1}{2} \end{bmatrix}$$

Such that

$$B_2 W_2 = T_2 \qquad (2.2$$

Equation (2.2) has a solution if

$$|B_2| \neq 0$$

and this holds only when

$$f(C_2) = C_2 \neq 0 \qquad (2.3)$$

From (2.3) we obtain the free – parameter C_2. The solution set x_1 , x_2 which are the weights are obtained as:

$$\begin{bmatrix} X_1 \\ X_2 \end{bmatrix} = \begin{bmatrix} \frac{1}{f(C_2)}(C_2 - \frac{1}{2}) \\ \frac{1}{2} f(C_2) \end{bmatrix} = \begin{bmatrix} 1 - \frac{1}{2C_2} \\ \frac{1}{2C_2} \end{bmatrix} \qquad (2.4)$$

Adopting equation (1.5), we obtain

$$V_{21} = C_2 \qquad (2.5)$$

The parameters of the method are given in terms of the free – parameter C_2
The table below
Displays the parameters:

(2.6)

C_2	C_2	
	$1 - \frac{1}{2}C_2$	$\frac{1}{C_2}$

It follows that the method depends solely on the free parameter C_2

Any arbitrary choice of the C_2 in (0,1] will yield a (2,2) method. The slopes of the method is given as:

$k_i = f(t_n, Y_n)$ and $k_2 = f(t_n + C_n h_n, Y_2 + h_n C_2 k_1)$

In particular, if we adopt (1.14) for j = 2 we have

$$V_{21} = \frac{X_1}{X_2} \quad (2.7)$$

Which implies that

$$V_{21} = 2C_2 - 1 \quad (2.8)$$

Solving (2.5) and (2.8) we have

$C_2 = 1$

This yields a (2,2) method given by the table

1	1	
	½	½

(2.9)

(2.9) is called modified Euler's method.

(3.3) EXPLICIT RUNGE-KUTTA METHOD

In this particular case the matrix adopted is 3x3 matrix defined by

$$B_3 \begin{bmatrix} 1 & 1 & 1 \\ 0 & C_2 & C_3 \\ 0 & C_2 & C_3 \end{bmatrix}$$

and its corresponding column vectors are

$$W_2 \begin{bmatrix} X_1 \\ X_2 \\ X_3 \end{bmatrix} \quad and\ T_3 = \begin{bmatrix} 1 \\ \frac{1}{2} \\ \frac{1}{3} \end{bmatrix}$$

We seek the values of the weights x_1, x_2, x_3

Such that

$$B_3 W_3 = T_3 \quad (3.1)$$

To obtain the solution of (3.1). We sought the determinant of the matrix B_3.

That is

$$B_3 = f(C_2, C_3) = C_2 C_3 [C_3 \ \ C_2] \quad (3.2)$$

The free – parameters for the method are c_2 and c_3. Equation (3.1) has a solution if

$f(c_2, c_3) \neq f(c_2, c_3) \neq 0$

and this is true only when

$c_2 \neq c_3$

From (3.1), we obtain the solution set x_1, x_2, x_3 given by

$$W_3 = \frac{1}{f(C_2, C_3)} \begin{bmatrix} C_2C_3(C_3 - C_3) & (C_2 - C_3)(C_2 + C_3) & C_3 - C_2 \\ 0 & C_3^2 & C_3 \\ 0 & -C_2^2 & -C_2 \end{bmatrix} \begin{bmatrix} 1 \\ ½ \\ 1/3 \end{bmatrix}$$

Thus the weight are given by the following expressions:

$$X_1 = \frac{2 - 3(C_2 + C_3) + 6C_2C_3}{6C_2C_3}$$

$$X_2 = \frac{2 - 3C_3}{6C_2(C_2 - C_3)}; C_2 \neq C_3$$

$$X_3 = \frac{2 - 3C_2}{6C_3(C_3 - C_2)}; C_2 \neq C_3$$

Implementing equations (1.10a) and (1.9)
Simultaneously, we have expressions for v_{ij}'s
That is:

$$V_{21} = C_2$$

$$V_{31} = \frac{C_3[3C_2(1 - C_2) - C_3]}{C_2(2 - 3C_2)}; C_2 \neq ⅔$$

$$V_{32} = \frac{C_3(C_3 - C_2)}{C_2(2 - 3C_2)}; C_2 \neq ⅔$$

The table below displays the parameters of the method in terms of the free – parameters c_2 and C_3 (nodes).

C_2	C_2		
C_3	$\frac{C_3[3C_2(1-C)-C_3]}{C_2(2-3C_2)}$	$\frac{C_3(C_3 - C_2)}{C_2(2-3C_2)}$	
	$\frac{2 - 3[C_2 + C_3] + 6C_2C_3}{6C_2C_3}$	$\frac{2-3C_3}{6C_2(C_2 - C_3)}$	$\frac{2-3C_2}{6C_3(C_3 - C_2)}$

(3.3)

The method (3.3) described above is suitable for unequal free – parameters. This is when the following conditions are satisfied:

$$\text{(i)} \quad C_3 \neq C_2 \qquad\qquad (3.4)$$

$$\text{(ii)} \quad C_2 \neq C_3$$

Tableau (3.3) with the condition (3.4) gives a (3,3) Explicit Runge – Kutta for equal free – parameters.

For equal nodes, $C_2 = C_3 = k$, say; we choose $x_3 = \theta$, $o < \theta \leq 1$. The parameter k is a constant, and clearly $k \neq o$. Adopting the matrix

$$B_2 = \begin{bmatrix} 1 & 1 \\ 0 & k \end{bmatrix}$$

and column vectors

$$W_2 = \begin{bmatrix} X_1 \\ X_2 \end{bmatrix} \; and \; T_2 = \begin{bmatrix} 1 & - & \theta \\ ½ & - & k\theta \end{bmatrix}$$

we have that

$$B_2 W_2 = T_2 \qquad (3.5)$$

The solution vector (x_1, x_2) is obtained by solving equation (3.5)

That is:

$$\begin{bmatrix} X_1 \\ X_2 \end{bmatrix} = \begin{bmatrix} k & - & ½ \\ ½ & - & k\theta \end{bmatrix}$$

We obtain the weights

$$X_1 = 1 - \frac{1}{2k}$$

$$X_2 = \frac{1}{2K} - \theta; \; k \neq 0$$

and $X_3 = \theta$

Imposing the condition that

$$X_2 = X_3 \tag{3.6}$$

We obtain

$$\theta = \frac{1}{4k}$$

$$V_{21} = k$$

$$V_{31} = k - \frac{2}{3} \qquad (3.7)$$

$$V_{32} = \frac{2}{3}$$

Hence, with equal free – parameters ($C_2 = C_3 = k$) the method is described by the tableau below

$$\begin{array}{c|ccc} K & K & & \\ K & K - \frac{2}{3} & \frac{2}{3} & ;k \in (0,1) \\ \hline & 1 - \frac{1}{2k} & \frac{1}{4k} & \frac{1}{4k} \end{array}$$

For k = ½, ¼, ²/₃ ¾ and 1 ; we have the following (3,3) E-R-K methods namely:

$$\begin{array}{c|ccc} \frac{1}{2} & \frac{1}{2} & & \\ \frac{1}{2} & -\frac{1}{6} & & \\ \hline & 0 & \frac{1}{2} & \frac{1}{2} \end{array} \qquad \begin{array}{c|ccc} \frac{1}{4} & \frac{2}{3} & & \\ \frac{1}{4} & -\frac{5}{12} & \frac{2}{3} & \\ \hline & -1 & 1 & 1 \end{array} \qquad \begin{array}{c|ccc} \frac{2}{3} & \frac{2}{3} & & \\ \frac{2}{3} & 0 & \frac{2}{3} & \\ \hline & \frac{1}{4} & \frac{3}{8} & \frac{3}{8} \end{array}$$

$$\begin{array}{c|ccc} \frac{3}{4} & \frac{3}{4} & & \\ \frac{3}{4} & 1/12 & \frac{2}{3} & \\ \hline & \frac{1}{3} & \frac{1}{3} & \frac{1}{3} \end{array} \quad \text{and} \quad \begin{array}{c|ccc} 1 & 1 & & \\ 1 & \frac{1}{3} & \frac{2}{3} & \\ \hline & \frac{1}{2} & \frac{1}{4} & \frac{1}{4} \end{array}$$

There are more E-R-K methods with different choices of k in the interval (0.1)}.

(4.4) Explicit Runge Kutta Method

The derivation of this particular method involves the adaptation of the matrix.

$$B_4 \begin{bmatrix} 1 & 1 & 1 & 1 \\ 0 & C_2 & C_3 & C_4 \\ 0 & C_2 & C_3^2 & C_4^2 \\ 0 & C_2^3 & C_3^3 & C_4^3 \end{bmatrix}$$

and the corresponding column vectors

$$W_4 \begin{bmatrix} X_1 \\ X_2 \\ X_3 \\ X_4 \end{bmatrix} \text{ and } T_4 = \begin{bmatrix} 1 \\ \frac{1}{2} \\ \frac{1}{3} \\ \frac{1}{4} \end{bmatrix}$$

Such that

$$B_4 W_4 = T_4 \qquad (4.1)$$

It was shown by Butcher (1964) that for the construction of the method, $C_4 = 1$

Implementing the condition that $C_4 = 1$, we observe that

$$B_4 \begin{bmatrix} 1 & 1 & 1 & 1 \\ 0 & C_2 & C_3 & 1 \\ 0 & C_2^2 & C_3^2 & 1 \\ 0 & C_2^3 & C_3^3 & 1 \end{bmatrix}$$

The matrix B_4 is non – singular and hence

$| B_4 | = f(c_2, c_3)$ where

$$f(C_2, C_3) = C_2\, C_3^2\,(1 - C_3)\; - C_3 C_2^2\,(1 - C) + C_2^2 C_3^2 (C_3 - C_2)$$

It follows that the free parameters are c_2 and c_3

The minors of the matrix B_4 are

$$M_{11} = C_2\, C_3^2\,(1 - C_3) - C_3 C_2^2\,(1 - C_2) + C_2^2 C_3^2\,(C_3 - C_2)$$

$M_{12} = 0$

$M_{13} = 0$

$M_{14} = 0$

$$M_{21} = \left(C_3^2 - C_3^3\right) - \left(C_2^2 - C_2^3\right) + (C_2^2 C_3^3 - C_2^3 - C_2^3\, C_3^2)$$

$$M_{22} = - C_3^2 + C_3^3$$

$$M_{23} = C_2^2 - C_2^3$$

$$M_{24} = (C_2^3 C_3^2 - C_2^2\, C_3^3)$$

$$M_{31} = \left(C_3 - C_3^3\right) - \left(C_2 - C_2^3\right) + (C_2 C_3^3 - C_3^2\, C_2^3)$$

$$M_{32} = - C_3 + C_3^3$$

$$M_{33} = C_2 - C_2^3$$

$$M_{34} = (C_2^3 C_3 - C_2\, C_3^3)$$

$$M_{41} = \left(C_3 - C_3^2\right) - \left(C_2 - C_2^2\right) + (C_2 C_3^2 - C_3 C_2^2)$$

$$M_{42} = - C_3^2 + C_3^2$$

$$M_{43} = C_2 - C_2^2$$

$$M_{44} = (C_3 C_2^2 - C_2\, C_3^2)$$

From above we obtain the matrix

$$M = \begin{bmatrix} M_{11} & M_{12} & M_{13} & M_{14} \\ M_{21} & M_{22} & M_{23} & M_{24} \\ M_{31} & M_{32} & M_{33} & M_{34} \\ M_{41} & M_{42} & M_{43} & M_{44} \end{bmatrix} \quad (4.2)$$

The solution vector (X_1, X_2, X_3, X_4) of equation (4.1) is given by

$$W = \frac{M^T . T_4}{f\,(C_2, C_3)} \quad (4.3)$$

Where M^T is the transpose of M.

Equation (4.3) exists iff

$F(C_2, C_3) \neq 0$ (4.4)

and this is true only when the following conditions are satisfied:

(i) $C_2 \neq C_3$

(ii) $C_2 \neq 1$ and $C_3 \neq 1$

From (4.3) we obtain expressions for the weights namely
Adopting the simplifying condition for j = 4, 3, and 2; and using equation (1.10), we obtain

(i) $$V_{43} = \frac{X_3}{X_4}(1-C_3)$$

$$= \frac{(1-2C_2)(1-C_2)(1-C_3)}{C_3(C_3-C_2)(6C_2C_3-4C_2-4C_3+3)}$$

$X_1 = \frac{P}{Q}$, Where

$$P = 18C_2^2C_3^3 - 12C_2^3C_3^3 - 6C_2^3C_3^2$$
$$+16C_2^3C_3 - 16C_2C_3^3 + 3C_2C_3^2$$

$$-15C_2^2 + 12C_2C_3 - 3C_3^2 + 4C_3^3$$

$$-3C_2^2 + C_2 + C_3$$

$$Q = 12C_2C_3(1-C_2)(C_3-C_2)(1-C_3)$$

$$X_2 = \frac{2C_3-1}{12C_2(1-C_2)(C_3-C_2)}$$

$$X_3 = \frac{1-2C_2}{12C_3}(1-C_2)(C_3-C_2)$$

and

$$X_4 = \frac{6C_2C_3-4C_2-4C_3+3}{12(1-C_2)(1-C_3)}$$

$$X_4 = \frac{6C_2C_3 - 4C_2 - 4C_3 + 3}{12\,(1-C_2)\,(1-C_3)}$$

(*ii*) $$V_{32} = \frac{1}{24C_2V_{43}X_4} = \frac{C_3\,(C_3 - C_2)}{2C_2\,(1-2C_2)}$$

(*iii* $$V_{31} = C_3 - V_{32} \quad \frac{2C_2C_3(1-2C_2) - C_3(C_3 - C_2}{C_2^2\,(1-2C_2)}$$

(*iv*) $$\frac{X_3}{24C_2V_{43}X_4} + X_4V_{42} = X_2\,(1-C_2)$$

From (iv), we have

$$V_{42} = \frac{2(1-C_2)\,(2C_3-1)\,(1-C_3) - (1-C_2)\,(C_3 - C_2)}{2C_2\,(C_3 - C_2)\,(6C_2C_3 - 4C_2 - 4C_3 + 3)}$$

(v) $V_{21} = C_2$

vi) $$V_{41} = 1 - \left[\frac{X_2(1-C_2)}{X_4} - \frac{1}{24C_2X_4(1-C_3)} + \frac{X_2(1-C_2)}{X_4}\right]$$

The parameters of the method are described above and hence the tableau below gives the method

C_2	V_{21}			
C_3	V_{31}	V_{32}		
C_4	V_{41}	V_{42}	V_{43}	
	X_1	X_2	X_3	X_4

With

$k_i = f(t_n\, y_n)$

and

$$k_{i-1} = f(t_n + C_{i-1}\,h_n, Y_n + h_n \sum_{j=1}^{i-1} V_{i-1,j-1}\, k_{j-1});$$

CONCLUSION

It becomes clear that in the construction of Explicit Runge – Kutta method, the variables which appeared in the expression for determinant of the square matrix adopted are the free parameters

These free – parameters are the ingredients of every Explicit Runge – Kutta constructed. We mean here that every method constructed is dependent on these free – parameters. All possible choice of these parameters are within the interval (0,1}.

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