Effective order of Partitioned Runge-Kutta Methods

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A thesis submitted in partial fulfillment of the requirements for the degree of **Master of Science** in **Mathematics**

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2018

FORM TH-4

National University of Sciences & Technology

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Dedication

To my beloved Parents and Siblings

Acknowledgements

In the name of Allah, the Gracious, the Benevolent. First of all, I am obliged to Allah Almighty who gave me confidence to complete my research and helped me to fulfill the expectations of elders. I would also like to thank the greatest person of the universe Prophet Mohammed (PBUH).

I want to express my heartfelt gratitude to my supervisor Assistant Professor Dr. Yousaf Habib for his constant support and motivation that has encouraged me to complete my thesis. I want to thank the New Zealand Mathematician J. C. Butcher for his worthy ideas and comments which helped me a lot throughout my research. I want to pay my gratitude for Guidance and Examination Committee (GEC) members, Dr. Muhammad Ishaq, Dr. Muhammad Asif Farooq for their support.

Lastly, I would not forget to appreciate the support of my beloved parents as without their support and love it would be a difficult task to complete my research.

Saba Shafiq

Abstract

In this thesis, we discuss about partitioned Runge-Kutta methods (PRK methods) and the algebraic properties of bi-color rooted trees associated with PRK methods i.e, groups of PRK methods, Hopf algebra of bi-color rooted trees and effective order of PRK methods. We will establish a connection between Hopf algebra of bi-color rooted trees and the group of PRK methods.

In this era, focus has been shifted towards the development of numerical methods which have low cost of implementation in finding the approximated solution of a large system of ODE's. In the sense of classical order, at least s stages are required for order s, thus for order two we require two stages and for order four we require four stages. The concept of effective order was introduced to overcome this barrier and construct method e.g RK-4 with three stages. Therefore, we will extend the concept of effective order to the PRK methods. We will construct an effective order three with two stages of PRK method and an effective order four with three stages of PRK method.

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Chapter 1

Introduction

Many physical problems of science and engineering can be modeled mathematically. These mathematical models can be represented by system of ordinary differential equations (ODE's). These ODE's have time as independent variable and other variables as dependent variable.

Definition 1.1 *An initial value problem $y' = f(x, y(x))$ with initial condition $y(x_0) = y_0$ is the first order ODE, where x is independent variable and y is dependent variable.*

Generally, we consider autonomous initial value problem which is independent of time variable given as $y' = f(y(x))$ with initial condition $y(x_0) = y_0$. The uniqueness and existence of the solution is definite if the function f justifies the Lipschitz condition [6].

Definition 1.2 *A function f justifies a Lipschitz condition, if $\forall$ Y,Z $\in \mathbb{R}^m$, $\exists$ a Lipschitz constant L such that*

$$\| f(Y) - F(Z) \| \leq L \| Y - Z \|$$

Sometimes ODE's cannot be solved analytically. So we need numerical methods to solve these ODE's. We have one-step methods, multi-step methods and general linear methods. One-step methods take our solution to y_{i+1} only using y_i leaving all other previously calculated values. An example of a one-step method is the Euler method,

$$y_{i+1} = y_i + hf(y_i), \qquad i = 0, 1, ..., n.$$

Euler method is order 1 method [1]. In this thesis, we will be focusing on higher order methods as Runge-Kutta (RK) methods. The RK methods were first developed by Runge (1895) and Kutta (1901).

1.1 Runge-Kutta methods

The problem $y' = f(y(x))$ with initial condition $y(x_0) = y_0$ can be solved by RK methods. The general s-stage RK method $S = [\mathrm{A}, \mathrm{b}^T, \mathrm{c}]$ can be defined as,

$$Y_i = y_n + h \sum_{j=1}^{s} \mathrm{a}_{ij} f(Y_j) \qquad\qquad i = 1, 2, ..., s, \tag{1.1}$$

$$y_{n+1} = y_n + h \sum_{i=1}^{s} \mathrm{b}_i f(Y_i). \tag{1.2}$$

The RK method can be expressed by a Butcher tableau as,

$$\begin{array}{c|cccc} \mathrm{c}_1 & \mathrm{a}_{11} & \mathrm{a}_{12} & \dots & \mathrm{a}_{1s} \\ \mathrm{c}_2 & \mathrm{a}_{21} & \mathrm{a}_{22} & \dots & \mathrm{a}_{2s} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ \mathrm{c}_s & \mathrm{a}_{s1} & \mathrm{a}_{s2} & \dots & \mathrm{a}_{ss} \\ \hline & \mathrm{b}_1 & \mathrm{b}_2 & \dots & \mathrm{b}_s \end{array}$$

where the method contains the coefficient matrix a_{ij} and the weight b_i's of the method. Moreover due to consistency,

$$\mathrm{c}_i = \sum_{j=1}^{s} \mathrm{a}_{ij} \qquad\qquad i = 1, 2, ..., s.$$

where c_i are the nodes, Y_i are the stages and y_{n+1} is the output value for the RK methods. RK methods can be explicit or implicit if $\mathrm{a}_{ij} = 0$ for $i \leq j$ and $\mathrm{a}_{ij} = 0$ for $i < j$ respectively. Explicit RK methods have low cost of implementation whereas implicit RK methods are used to solve stiff and conservative systems.

1.1.1 Order conditions

To obtain a particular order RK method, we need order conditions for RK method. For finding the order conditions of RK method, we compare the series expansion given by Taylor for approximated solution of the RK method with the series expansion given by Taylor for exact solution. The expanded numerical solution of the RK method is

$$y_{n+1} = y_n + h \sum_{i=1}^{s} \mathrm{b}_i y'(x_n) + h^2 \sum_{i=1}^{s} \mathrm{b}_i \mathrm{c}_i y''(x_n) + ... \tag{1.3}$$

Taylor series expansion of the exact solution is as follows,

$$y(x_n + h) = y(x_n) + hy'(x_n) + \frac{h^2}{2!} y''(x_n) + ... \tag{1.4}$$

Comparing eq (1.3) and eq (1.4), we obtain the order conditions for RK method which shows relationship between coefficients of RK method,

$$\sum_{i=1}^{s} \mathrm{b}_i = 1,$$

$$\sum_{i=1}^{s} \mathrm{b}_i \mathrm{c}_i = \frac{1}{2}.$$

It becomes difficult to find order conditions for higher order RK methods because the number of order conditions increases in higher order RK methods. Therefore, we use rooted trees for finding order conditions of RK method.

1.1.2 Some concepts from graph theory

For finding order conditions with the help of rooted trees, we need to know some basic definitions from graph theory.

Rooted Tree: *A non-cyclic connected graph having vertices (with a special vertex named as root) and edges is called a rooted tree.*

Order: *The total number of vertices of a rooted tree represented by $r(t)$ is known as the order of the rooted tree.*

Density: *Density of a rooted tree which is denoted by $\gamma(t)$ can be computed recursively by the product of order of tree and by the order of its subtrees after the pruning of the root.*

Symmetry: *Symmetry of a rooted tree is the order of a automorphism group of t which is defined as $\sigma(t) = (\sigma(t_1)^{n_1}\sigma(t_2)^{n_2}...\sigma(t_m)^{n_m})(n_1!n_2!...n_m!)$*

We can associate some combinatorial properties related with above defined concepts of rooted trees like $\alpha(t)$ and $\beta(t)$,

$$\alpha(t) = \frac{r(t)!}{\sigma(t)\gamma(t)},$$
$$\beta(t) = \frac{r(t)!}{\sigma(t)}.$$

Elementary differential:
We have,

$$y' = f(y) = f, \tag{1.5}$$
$$y'' = f'(y)y' = f'(y)f(y) = f'f, \tag{1.6}$$
$$y''' = f''ff + f'f'f, \tag{1.7}$$
$$y'''' = f'''fff + f''f'ff + f''ff'f + f''ff'f + f'f''ff + f'f'f'f. \tag{1.8}$$

where f, f' are elementary differentials. We can allot a specific rooted tree with every type of an elementary differential explicitly. For example: if we have a function f we can assign a vertex for it. Similarly, if we have an elementary differential $f'f$ we can first assign a vertex for the first f then one edge for the derivative and again a vertex on the other end of the edge for the second function f. Elementary differentials and their trees is shown in Table 1.1.

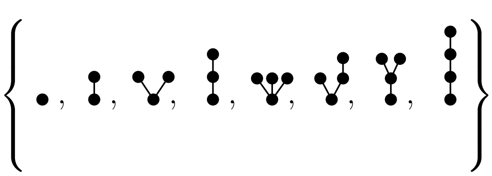
Elementary weights: *We can define an elementary weight of a rooted tree by*

$$\Phi(t) = \begin{cases} \sum_{i=1}^{s} \mathrm{b}_i & \text{if } t = \tau \\ \sum_{i=1}^{s} \mathrm{b}_i \Phi_i(t_1)\Phi_i(t_2)...\Phi_i(t_m) & \text{if } t = [t_1 t_2 ... t_m] \end{cases}$$

where $\Phi_i(t)$ is the elementary stage weight associated with i^{th}-stage defined as

$$\Phi_i(t) = \begin{cases} \sum_{i=j}^{s} \mathrm{a}_{ij} = \mathrm{c}_i & \text{if } t = \tau \\ \sum_{i=j}^{s} \mathrm{a}_{ij} \Phi_j(t_1)\Phi_j(t_2)...\Phi_i(t_m) & \text{if } t = [t_1 t_2 ... t_m] \end{cases}$$

Elementary weights are the functions related with the coefficients of the RK method depending upon trees of RK method. Let T denotes the set of trees up to order 4,

$T =$ 

As an example,

$t_5 =$ 

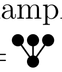
$r(t_5) = 4$

$\gamma(t_5) = 4 \times 1 \times 1 \times 1 = 4$

$\alpha(t_5) = \dfrac{r(t)!}{\sigma(t)\gamma(t)} = \dfrac{4!}{6 \times 4} = 1$

$\beta(t_5) = \dfrac{r(t)!}{\sigma(t)} = \dfrac{4!}{6} = 4$

$F(t_5) = f''' f f f$

Consider the above example to illustrate the construction of elementary weights $\Phi(t_5)$. For $t_5 =$ 

$$\Phi(t_5) = \sum_{i=1}^{s} \mathrm{b}_i \mathrm{c}_i^3$$

Elementary weights up to order 4 are represented in Table 1.1.
Now we can find the order conditions of RK method with the help of trees. Series expansion given by Taylor for the exact solution is [7],

$$y(x_n + h) = y(x_n) + \sum_{t \in T} \frac{\alpha(t)\, h^{r(t)}}{r(t)!} F(t)(y(x_n))$$

By putting the value of $\alpha(t)$ we get,

$$y(x_n + h) = y(x_n) + \sum_{t \in T} \frac{h^{r(t)}}{\sigma(t)\gamma(t)} F(t)(y(x_n)) \tag{1.9}$$

Series expansion given by Taylor for the numerical solution is [7],

$$y_{n+1} = y_n + \sum_{t \in T} \frac{\beta(t)\, h^{r(t)}}{r(t)!} \Phi(t) F(t)(y_n)$$

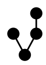
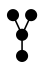
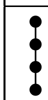
t	$r(t)$	$\gamma(t)$	$\sigma(t)$	$\alpha(t)$	$\beta(t)$	$F(t)$	$\Phi(t)$
	1	1	1	1	1	f	$\Sigma \mathrm{b}_i$
	2	2	1	1	1	$f'f$	$\Sigma \mathrm{b}_i \mathrm{c}_i$
	3	3	2	1	3	$f''ff$	$\Sigma \mathrm{b}_i \mathrm{c}_i^2$
	3	6	1	1	6	$f'f'f$	$\Sigma \mathrm{b}_i \mathrm{a}_{ij} \mathrm{c}_j$
	4	4	6	1	4	$f'''fff$	$\Sigma \mathrm{b}_i \mathrm{c}_i^3$
	4	8	1	3	24	$f''f'f$	$\Sigma \mathrm{c}_i \mathrm{b}_i \mathrm{a}_{ij} \mathrm{c}_j$
	4	12	2	1	12	$f'f''ff$	$\Sigma \mathrm{b}_i \mathrm{a}_{ij} \mathrm{c}_j^2$
	4	24	1	1	24	$f'f'f'f$	$\Sigma \mathrm{b}_i \mathrm{a}_{ij} \mathrm{a}_{jk} \mathrm{c}_k$

Table 1.1: Elementary weights of the rooted trees.

By putting the value of $\beta(t)$ we get [7],

$$y_{n+1} = y_n + \sum_{t \in T} \frac{h^{r(t)}}{\sigma(t)} \Phi(t) F(t)(y_n) \tag{1.10}$$

We can find order conditions by comparing exact and numerical solution of Taylor series expansion eq (1.9) and eq (1.10) respectively as,

$$\Phi(t) = \frac{1}{\gamma(t)} \tag{1.11}$$

Order conditions of an order 4 RK method is given as,

$$\begin{aligned} \Sigma \mathrm{b}_i &= 1, & \Sigma \mathrm{b}_i \mathrm{c}_i &= \frac{1}{2}, \\ \Sigma \mathrm{b}_i \mathrm{c}_i^2 &= \frac{1}{3}, & \Sigma \mathrm{b}_i \mathrm{a}_{ij} \mathrm{c}_j &= \frac{1}{6}, \\ \Sigma \mathrm{b}_i \mathrm{c}_i^3 &= \frac{1}{4}, & \Sigma \mathrm{c}_i \mathrm{b}_i \mathrm{a}_{ij} \mathrm{c}_j &= \frac{1}{8}, \\ \Sigma \mathrm{b}_i \mathrm{a}_{ij} \mathrm{c}_j^2 &= \frac{1}{12}, & \Sigma \mathrm{b}_i \mathrm{a}_{ij} \mathrm{a}_{jk} \mathrm{c}_k &= \frac{1}{24}. \end{aligned}$$

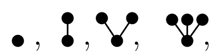
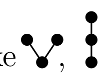
1.1.3 Simplifying assumptions

To obtain higher order RK methods, the number of order conditions increases. Therefore, there are some simplifying assumptions given by Butcher to decrease the number of order conditions to obtain a particular order RK method.

$$B(p) : \sum_{i=1}^{s} \mathrm{b}_i \mathrm{c}_i^{k-1} = \frac{1}{k}, \qquad k = 1, 2, ..., p$$

$$C(\eta) : \sum \mathrm{a}_{ij} \mathrm{c}_j^{k-1} = \frac{\mathrm{c}_i^k}{k}, \qquad i = 1, 2, ..., s, \quad k = 1, 2, ..., \eta$$

$$D(\xi) : \sum \mathrm{b}_i \mathrm{c}_i^{k-1} \mathrm{a}_{ij} = \frac{\mathrm{b}_j(1 - \mathrm{c}_j^k)}{k}, \qquad j = 1, 2, ..., s, \quad k = 1, 2, ..., \xi$$

- It is required that $B(p)$ satisfies, to obtain an order p method, because this condition only gives the order conditions associated to the trees ,...
- $C(\eta)$ gives same order conditions for $k \le \eta$ and for the pair of trees like .
- The $D(\xi)$ condition relates three types of trees in terms of their elementary weights such that the elementary weight of first tree has a factor $\mathrm{b}_i \mathrm{c}_i^{k-1} \mathrm{a}_{ij}$ and the elementary weight other two trees have factors b_j and $\mathrm{b}_j \mathrm{c}_j^k$ respectively.

1.2 Group of Runge-Kutta methods

It is of much importance to study the groups of RK methods. An important application of the groups of RK methods is the introduction of "Effective order" which we will study later. Firstly, we will see how RK methods form a group.

Definition 1.3 *A group* $(\mathrm{G}, *)$ *is a non-empty set having a binary operation* $*$ *satisfies the given properties,*

1) *If* $\forall\ \upsilon, \nu \in \mathrm{G}$*, then* $\upsilon * \nu \in \mathrm{G}$*,*

2) $\forall\ \upsilon \in \mathrm{G}, \exists\ e \in \mathrm{G}\ s.t\ \upsilon * e = e * \upsilon = \upsilon,$

3) $\forall\ \upsilon, \nu, \omega \in G\ s.t\ \upsilon * (\nu * \omega) = (\upsilon * \nu) * \omega,$

4) $\forall\ \upsilon \in G, \exists\ \upsilon^{-1} \in \mathrm{G}\ s.t\ \upsilon * \upsilon^{-1} = \upsilon^{-1} * \upsilon = e.$

Definition 1.4 *A group* G *is called an abelian group if* $\forall\ \upsilon, \nu \in \mathrm{G}\ s.t\ \upsilon*\nu = \nu * \upsilon.$

The group of RK methods under the composition is elaborated by considering two RK methods $\breve{M} = [\breve{A}, \breve{b}^T, \breve{c}]$ and $\bar{M} = [\bar{A}, \bar{b}^T, \bar{c}]$ given as,

$$Y_i = y_0 + h \sum_{j=1}^{s} \breve{a}_{ij} f(Y_j) \qquad i = 1, 2, ..., s, \tag{1.12}$$

$$y_1 = y_0 + h \sum_{j=1}^{s} \breve{b}_j f(Y_j). \tag{1.13}$$

$$\bar{Y}_i = y_1 + h \sum_{j=1}^{\bar{s}} \bar{a}_{ij} f(\bar{Y}_j) \qquad i = 1, 2, ..., \bar{s}, \tag{1.14}$$

$$y_2 = y_1 + h \sum_{j=1}^{\bar{s}} \bar{b}_j f(\bar{Y}_j). \tag{1.15}$$

The composed RK method is,

$$\begin{aligned} Y_i &= y_0 + h \sum_{j=1}^{s} \breve{a}_{ij} f(Y_j) \\ \bar{Y}_i &= y_0 + h \sum_{j=1}^{s} \breve{b}_j f(Y_j) + h \sum_{j=1}^{\bar{s}} \bar{a}_{ij} f(\bar{Y}_j) \\ y_2 &= y_0 + h \sum_{j=1}^{s} \breve{b}_j f(Y_j) + h \sum_{j=1}^{\bar{s}} \bar{b}_j f(\bar{Y}_j) \end{aligned}$$

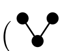
The Butcher tableau of composed RK method is shown in Table 1.2.

We can define an algebraic group G from rooted trees to elementary weights. Its elements are functions acting on rooted trees. We can define function $\alpha \in G$ corresponding to the RK method $M = [A, b^T, c]$ which map trees to

$\breve{c}_1$	$\breve{a}_{11}$	$\breve{a}_{12}$	$\cdots$	$\breve{a}_{1s}$	0	0	$\cdots$	0
$\breve{c}_2$	$\breve{a}_{21}$	$\breve{a}_{22}$	$\cdots$	$\breve{a}_{2s}$	0	0	$\cdots$	0
$\vdots$	$\vdots$	$\vdots$	$\ddots$	$\vdots$	$\vdots$	$\vdots$	$\ddots$	$\vdots$
$\breve{c}_s$	$\breve{a}_{s1}$	$\breve{a}_{s2}$	$\cdots$	$\breve{a}_{ss}$	0	0	$\cdots$	0
$\bar{c}_1 + \sum_{i=1}^{s} \breve{b}_i$	$\breve{b}_1$	$\breve{b}_2$	$\cdots$	$\breve{b}_s$	$\bar{a}_{11}$	$\bar{a}_{12}$	$\vdots$	$\bar{a}_{1\bar{s}}$
$\bar{c}_2 + \sum_{i=1}^{s} \breve{b}_i$	$\breve{b}_1$	$\breve{b}_2$	$\cdots$	$\breve{b}_s$	$\bar{a}_{21}$	$\bar{a}_{22}$	$\cdots$	$\bar{a}_{2\bar{s}}$
$\vdots$	$\vdots$	$\vdots$	$\ddots$	$\vdots$	$\vdots$	$\vdots$	$\ddots$	$\vdots$
$\bar{c}_{\bar{s}} + \sum_{i=1}^{s} \breve{b}_i$	$\breve{b}_1$	$\breve{b}_2$	$\cdots$	$\breve{b}_s$	$\bar{a}_{\bar{s}1}$	$\bar{a}_{\bar{s}2}$	$\cdots$	$\bar{a}_{\bar{s}\bar{s}}$
	$\breve{b}_1$	$\breve{b}_2$	$\cdots$	$\breve{b}_s$	$\bar{b}_1$	$\bar{b}_2$	$\cdots$	$\bar{b}_{\bar{s}}$

Table 1.2: Butcher tableau for composition of 2 Runge-Kutta methods.

elementary weights of the RK method. Thus $\alpha(t_i) = \alpha_i$ represents elementary weights corresponding to the tree t. As an example,

$\alpha($  $) = \alpha_3 = \sum_i b_i c_i^2$

The composition of two RK methods can be also defined in terms of their functions from group G. Let α, β are the functions corresponding to the methods M, S. We can define the multiplicative group operation given as,

$$(\beta\alpha)(t) = \alpha(\phi)\beta(t) + \alpha(t) + \sum \beta(t \setminus u)\alpha(u) \tag{1.16}$$

In the computation of $\beta\alpha$, the tree u is the subtree of a tree t and $t \setminus u$ is the remaining tree when u is chopped off tree t. Calculation for the term of $(\beta\alpha)(t_4)$ is shown in Table 1.3.

- **Closure:** It is obvious that the RK method satisfies the closure property which means that if we compose two RK methods then the resulting method is again an RK method.

- **Associative:** RK method also satisfies the associative proprty.

- **Identity:** The identity of the RK method is the method which maps y_0 to y_0 and it is the identity map.

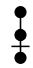
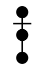
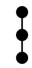
t				
u				
$t \setminus u$				
term	β_4	$\beta_2\alpha_1$	$\beta_1\alpha_2$	α_4

Table 1.3: Calculation of $(\beta\alpha)(t_4)$.

- **Inverse:** RK method maps the solution from y_0 to y_1. The inverse of an RK method maps the solution from y_1 to y_0. The inverse of RK method $\bar{S} = [\bar{\mathrm{A}}, \bar{\mathrm{b}}^T, \bar{\mathrm{c}}]$ is

$$\bar{Y}_i = y_1 - h \sum_{j=1}^{\bar{s}} \bar{\mathrm{b}}_j f(\bar{Y}_j) + h \sum_{j=1}^{\bar{s}} \bar{\mathrm{a}}_{ij} f(\bar{Y}_j),$$
$$y_0 = y_1 - h \sum_{j=1}^{\bar{s}} \bar{\mathrm{b}}_j f(\bar{Y}_j).$$

The Butcher tableau for the inverse RK method is given in Table 1.4 [6].

$$\begin{array}{c|cccc}
\bar{\mathrm{c}}_1 - \Sigma_{i=1}^{\bar{s}} \bar{\mathrm{b}}_i & \bar{\mathrm{a}}_{11} - \bar{\mathrm{b}}_1 & \bar{\mathrm{a}}_{12} - \bar{\mathrm{b}}_2 & \cdots & \bar{\mathrm{a}}_{1\bar{s}} - \bar{\mathrm{b}}_{\bar{s}} \\
\bar{\mathrm{c}}_2 - \Sigma_{i=1}^{\bar{s}} \bar{\mathrm{b}}_i & \bar{\mathrm{a}}_{21} - \bar{\mathrm{b}}_1 & \bar{\mathrm{a}}_{22} - \bar{\mathrm{b}}_2 & \cdots & \bar{\mathrm{a}}_{2\bar{s}} - \bar{\mathrm{b}}_{\bar{s}} \\
\vdots & \vdots & \vdots & \ddots & \vdots \\
\bar{\mathrm{c}}_{\bar{s}} - \Sigma_{i=1}^{\bar{s}} \bar{\mathrm{b}}_i & \bar{\mathrm{a}}_{\bar{s}1} - \bar{\mathrm{b}}_1 & \bar{\mathrm{a}}_{\bar{s}2} - \bar{\mathrm{b}}_2 & \cdots & \bar{\mathrm{a}}_{\bar{s}\bar{s}} - \bar{\mathrm{b}}_{\bar{s}} \\
\hline
 & -\bar{\mathrm{b}}_1 & -\bar{\mathrm{b}}_2 & \cdots & -\bar{\mathrm{b}}_{\bar{s}}
\end{array}$$

Table 1.4: Butcher tableau for inverse of Runge-Kutta methods.

1.3 Hopf algebra of rooted trees

Before defining Hopf algebra of rooted trees, we need to look at some basic definitions of algebra.

Definition 1.5 *A ring* R *be a non-empty set having binary operations '+' and '×' satisfies the given properties,*

1) *The set* $(\mathrm{R}, +)$ *is an abelian group,*

2) *If* $\forall\ \upsilon, \nu \in \mathrm{R}$*, then* $\upsilon \times \nu \in \mathrm{R}$*,*

3) $\upsilon \times (\nu \times \omega) = (\upsilon \times \nu) \times \omega$*, where* $\upsilon, \nu, \omega \in \mathrm{R}$*,*

4) *Left and right distributive law holds, i.e*
$\upsilon \times (\nu + \omega) = \upsilon \times \nu + \upsilon \times \omega$,
$(\upsilon + \nu) \times \omega = \upsilon \times \omega + \nu \times \omega,\ \forall\ \upsilon, \nu, \omega \in \mathrm{R}.$

Definition 1.6 *If* R *and* S *are two rings, then the ring homomorphism is the function* $\eta : \mathrm{R} \longrightarrow \mathrm{S}$ *such that,*

1) $\eta(\upsilon + \nu) = \eta(\upsilon) + \eta(\nu)$,

2) $\eta(\upsilon\nu) = \eta(\upsilon)\eta(\nu)$,

3) $\eta(1_{\mathrm{R}}) = 1_{\mathrm{S}}$.

Definition 1.7 *A field is a non-empty set having binary operations '+' and '×' satisfies the given properties,*

1) *The set* $(\mathrm{F}, +)$ *is an abelian group,*

2) *The set* $(\mathrm{F} \setminus \{0\}, \times)$ *is an abelian group,*

3) *Left and right distributive law holds, i.e*
$\upsilon \times (\nu + \omega) = \upsilon \times \nu + \upsilon \times \omega$,
$(\upsilon + \nu) \times \omega = \upsilon \times \omega + \nu \times \omega,\ \forall\ \upsilon, \nu, \omega \in F.$

Definition 1.8 *A vector space over a field* F *is the set* V *together with scalar addition and scalar multiplication. Let* $\upsilon, \nu, \omega \in V$ *and* $\kappa, \mu \in \mathrm{F}$*.*

1) *The set* $(\mathrm{V}, +)$ *is an abelian group,*

2) $\kappa(\mu\nu) = (\kappa\mu)\nu$,

3) $1\nu = \nu$, *where* $1 \in \mathrm{F}$,

4) $\kappa(\upsilon + \nu) = \kappa\upsilon + \kappa\nu$,

5) $(\kappa + \mu)\upsilon = \kappa\upsilon + \mu\upsilon$.

Definition 1.9 *Let* R *is a ring. A left* R*-Module is a set* M *with properties,*

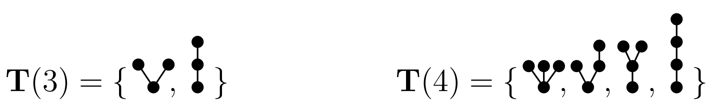
1) *The set* $(\mathrm{M}, +)$ *is an abelian group,*

2) $\mathrm{R} \times \mathrm{M} \longrightarrow \mathrm{M}$ *denoted by* $\kappa\mu$, $\forall\ \kappa \in \mathrm{R}$, *and* $\mu \in \mathrm{M}$,

- **a)** $(\kappa + \mu) \times \nu = \kappa\nu + \mu\nu$, $\forall\ \kappa, \mu \in \mathrm{R}$ *and* $\nu \in \mathrm{M}$
- **b)** $(\kappa\mu)\nu = \kappa(\mu\nu)$, $\forall\ \kappa, \mu \in \mathrm{R}$ *and* $\nu \in \mathrm{M}$
- **c)** $\kappa(\mu + \nu) = \kappa\mu + \kappa\nu$, $\forall\ \kappa \in \mathrm{R}$ *and* $\mu, \nu \in \mathrm{M}$

3) *If* R *has a unit element 1, then*
$1\kappa = \kappa$, $\forall\ \kappa \in \mathrm{M}$.

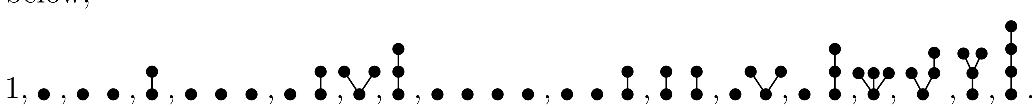
Hopf algebra $\mathcal{H}_R$ of rooted trees is introduced in Connes and Kreimer [1998]. The set of rooted trees will be denoted by $\mathbf{T}(n)$.



Definition 1.10 *Let* R *is a commutative ring with* 1_{R}. *Ring* A *with* 1_{A} *and ring homomorphism* $\eta : \mathrm{R} \to \mathrm{A}$ *mapping* 1_{R} *to* 1_{A} *s.t subring* $\eta(\mathrm{R})$ *of* A *is contained in the center of* A.

Definition 1.11 *Hopf algebra* $\mathcal{H}_R$ *is the unital associative* $\boldsymbol{K}$*-algebra having a coproduct, a counit and an antipode generated by* $\boldsymbol{T}$.

K-basis of Hopf algebra is given by rooted forests. Each component of rooted forest **F** is a rooted tree. The rooted forest for the trees upto order 4 is given below,



Now, we can define the coproduct, counit and antipode of Hopf algebra for rooted trees.

Definition 1.12 *The linear map $\Delta : \mathcal{H}_R \rightarrow \mathcal{H}_R \otimes \mathcal{H}_R$ such that $\forall$ rooted trees $t \in T$ is known as coproduct of $\mathcal{H}_R$.*

$$\Delta(t) = \sum_{c \in Adm_*(t)} P^c(t) \otimes R^c(t) = t \otimes 1 + 1 \otimes t + \sum_{c \in Adm(t)} P^c(t) \otimes R^c(t)$$

and Δ is an algebra morphism [9],

$$\Delta(t_1 t_2) = \Delta(t_1)\Delta(t_2).$$

Definition 1.13 *The choice of edges of tree t is a non total cut c for a tree t.*

Definition 1.14 *If a tree t have at most one cut in an edge for any oriented path, then such a cut is called an admissible cut c.*

Definition 1.15 *$W^c(t)$ is the forest after deleting a chosen edge in any cut c for the tree t.*

Definition 1.16 *The $R^c(t)$ is a subtree of $W^c(t)$ which consists of the root of t.*

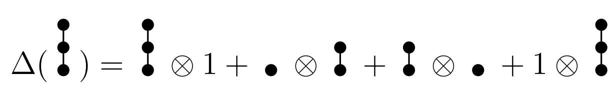
Definition 1.17 *$P^c(t)$ is the product of other subtrees of $W^c(t)$ except $R^c(t)$, for any admissible cut c.*

Definition 1.18 *A total cut is also an admissible cut i.e, $W^c(t) = P^c(t) = t$ and $R^c(t) = 1$.*

Now, we can find the coproduct of rooted trees as follows,

$$\Delta(\bullet) = \bullet \otimes 1 + 1 \otimes \bullet$$

From the Table 1.5



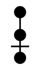
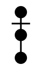
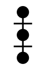
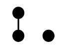
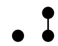
Cut					total
Admissible	y	y	y	n	y
$W^c(t)$					
$R^c(t)$				$\times$	1
$P^c(t)$	1			$\times$	

Table 1.5: Calculations of terms for Δ of t_4.

Definition 1.19 *The linear map $\varepsilon : \mathcal{H} \to K$ such that for all $t \in T$*

$$\epsilon(1) = 1,$$
$$\epsilon(t) = 0$$

is known as counit and it is an algebra morphism [2]

$$\varepsilon(t_1 t_2) = \varepsilon(t_1)\varepsilon(t_2).$$

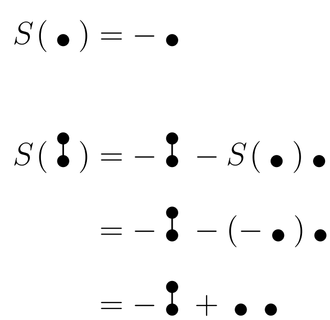
Definition 1.20 *An antipode is a linear map $S : \mathcal{H}_R \to \mathcal{H}_R$ such that*

$$S(1) = 1$$
$$S(t) = -t - \sum_{c \in Adm(t)} S(P^c(t))R^c(t)$$

and antipode is an algebra antimorphism [2]

$$S(t_1 t_2) = S(t_2)S(t_1).$$

We can calculate S(t) for rooted trees as follows,



1.4 Isomorphism

There is a one-one correspondence between the coproduct of the Hopf algebra of rooted trees and the composition rule of the RK method. As an example, let t= $\bullet$.

The coproduct for t= $\bullet$ is,

$$\Delta(\bullet) = \bullet \otimes 1 + 1 \otimes \bullet$$

and the composition rule for t= $\bullet$ is

$$\bullet + \bullet$$

which shows one-one correspondence between them.
There is one-one correspondence between the antipode of the Hopf algebra of rooted trees and the inverse of composed RK method. As an example, let t= $\bullet$.

The antipode for $\bullet$ is

$$S(\bullet) = -\bullet$$

and the inverse of composed RK method for $\bullet$ is

$$-\sum_{i=1}^{s} \mathrm{b}_i = -\bullet$$

which shows one-one correspondence between them [8].

1.5 Effective order of Runge-Kutta methods

The idea of effective order was introduced by J.C. Butcher in (1969) [3]. Later, it was rediscovered by L*ó*pez-Marcos, Sanz-Serna and Skeel in 1996 and now a days more results on the idea of effective order is introduced in [6, 4, 5]. This idea was used to construct order five RK method with five stages. The method α has an "effective order" p if there exist another method β such that the composition $\beta\alpha\beta^{-1}$ has an order p. The method β used once at the beginning and the β^{-1} at the last. According to another definition of "effective order" by J. C. Butcher, we can obtain the order conditions of an effective order by equating the composition $\beta\alpha$ to the composition $E\beta$, where E represents the exact solution i.e, $E = \dfrac{1}{\gamma(t)}$ [4].

1.5.1 Two stage effective order three Runge-Kutta methods

For the trees of order up to 3, the composition of $\beta\alpha$ and $E\beta$ is shown in Table 1.6. By equating composition $(\beta\alpha)$ and $(E\beta)$ given in Table 1.6 and

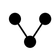
t_i	$(\beta\alpha)(t_i)$	$(E\beta)(t_i)$
	$\beta_1 + \alpha_1$	$1 + \beta_1$
	$\beta_2 + \beta_1\alpha_1 + \alpha_2$	$\frac{1}{2} + \beta_1 + \beta_2$
	$\beta_3 + \beta_1^2\alpha_1 + 2\beta_1\alpha_2 + \alpha_3$	$\frac{1}{3} + \beta_1 + 2\beta_2 + \beta_3$
	$\beta_4 + \beta_2\alpha_1 + \beta_1\alpha_2 + \alpha_4$	$\frac{1}{6} + \frac{1}{2}\beta_1 + \beta_2 + \beta_4$

Table 1.6: $\beta\alpha$ and $E\beta$ for the trees up to order 3.

taking $\beta_1 = 0$, we got the following equations,

$$\alpha_1 = 1, \tag{1.17}$$

$$\alpha_2 = \frac{1}{2}, \tag{1.18}$$

$$\alpha_3 = \frac{1}{3} + 2\beta_2, \tag{1.19}$$

$$\alpha_4 = \frac{1}{6}. \tag{1.20}$$

Eq (1.17) to eq (1.20) can be converted in terms of elementary weights as,

$$b_1 + b_2 = 1, \tag{1.21}$$

$$b_1 c_1 + b_2 c_2 = \frac{1}{2}, \tag{1.22}$$

$$b_1 c_1^2 + b_2 c_2^2 = \frac{1}{3} + 2\beta_2, \tag{1.23}$$

$$b_1 a_{11} c_1 + b_2 a_{21} c_1 + b_2 a_{22} c_2 = \frac{1}{6}. \tag{1.24}$$

Solving equations eq (1.21), eq (1.22), eq (1.24) together with consistency conditions $\sum_{i,j} a_{ij} = c_i$ and choosing $c_1 = \frac{1}{3}$ and $c_2 = \frac{2}{3}$, we get the following Butcher tableau,

$$\begin{array}{c|cc} \frac{1}{3} & \frac{1}{3} & 0 \\ \frac{2}{3} & \frac{2}{3} & 0 \\ \hline & \frac{1}{2} & \frac{1}{2} \end{array}$$

For perturbation method, we have

$$\beta_1 = 0 \tag{1.25}$$

For finding condition on β_2 we need to find α_3,

$$\alpha_3 = \sum b_i c_i^2 = b_1 c_1^2 + b_2 c_2^2 = \frac{1}{2}(\frac{1}{9} + \frac{4}{9}) = \frac{5}{18}$$

Putting the value of α_3 in eq (1.23), we get,

$$\beta_2 = -\frac{1}{36}. \tag{1.26}$$

Eq (1.25) and eq (1.26) can be converted in the form of elementary weights and expanding them for explicit 2-stage RK method in coefficient form taking $C_2 = \frac{1}{2}$, we get the following β perturbation method.

$$\begin{array}{c|cc} 0 & 0 & 0 \\ \frac{1}{2} & \frac{1}{2} & 0 \\ \hline & \frac{1}{18} & -\frac{1}{18} \end{array}$$

We can finally find suitable ending β^{-1} method using the method explained by Butcher in [6] for finding inverse of the RK method.

$$\begin{array}{c|cc} 0 & -\frac{1}{18} & \frac{1}{18} \\ \frac{1}{2} & \frac{4}{9} & \frac{1}{18} \\ \hline & -\frac{1}{18} & \frac{1}{18} \end{array}$$

Chapter 2

Partitioned Runge Kutta methods and associated Hopf algebra

The differential system

$$\begin{pmatrix} p \\ q \end{pmatrix}' = \begin{pmatrix} f(q) \\ g(p) \end{pmatrix} \qquad p(x_0) = p_0, \quad q(x_0) = q_0. \tag{2.1}$$

can be solved using partitioned Runge-Kutta (PRK) methods, where the solution for above differential system is (p_{n+1}, q_{n+1}). The PRK method can be defined as following [12],

$$P_i = p_n + h \sum_{j=1}^{s} a_{ij} f(Q_j) \qquad i = 1, 2, ..., s, \tag{2.2}$$

$$p_{n+1} = p_n + h \sum_{j=1}^{s} b_j f(Q_j) \tag{2.3}$$

$$Q_i = q_n + h \sum_{j=1}^{s} \widetilde{a}_{ij} g(P_j) \qquad i = 1, 2, ..., s, \tag{2.4}$$

$$q_{n+1} = q_n + h \sum_{j=1}^{s} \widetilde{b}_j g(P_j). \tag{2.5}$$

The first component of the system eq (2.1) is solved by one RK method defind in eq (2.2) and eq (2.3) and the other component of the system (2.1) is solved by another RK method defined in eq (2.4) and eq (2.5). The PRK method can be shown by Butcher tableaux as,

$$
\begin{array}{c|cccc}
c_1 & a_{11} & a_{12} & \dots & a_{1s} \\
c_2 & a_{21} & a_{22} & \dots & a_{2s} \\
\vdots & \vdots & \vdots & \ddots & \vdots \\
c_s & a_{s1} & a_{s2} & \dots & a_{ss} \\
\hline
 & b_1 & b_2 & \dots & b_s
\end{array}
\qquad
\begin{array}{c|cccc}
\widetilde{c}_1 & \widetilde{a}_{11} & \widetilde{a}_{12} & \dots & \widetilde{a}_{1s} \\
\widetilde{c}_2 & \widetilde{a}_{21} & \widetilde{a}_{22} & \dots & \widetilde{a}_{2s} \\
\vdots & \vdots & \vdots & \ddots & \vdots \\
\widetilde{c}_s & \widetilde{a}_{s1} & \widetilde{a}_{s2} & \dots & \widetilde{a}_{ss} \\
\hline
 & \widetilde{b}_1 & \widetilde{b}_2 & \dots & \widetilde{b}_s
\end{array}
$$

P_i and Q_i are the stages, a_{ij} and $\widetilde{a}_{ij}$ are the coefficient matrices, b_j and $\widetilde{b}_j$ are the weights. p_{n+1} and q_{n+1} are the output values of the system eq (2.1) taking p_n and q_n as initial values respectively. Moreover,

$$
\begin{aligned}
c_i &= \sum_{j=1}^{s} a_{ij} \qquad i = 1, 2, ..., s, \\
\widetilde{c}_i &= \sum_{j=1}^{s} \widetilde{a}_{ij} \qquad i = 1, 2, ..., s.
\end{aligned}
$$

are the consistency conditions of the PRK method. Order conditions related to PRK method can be found using the concept of rooted trees. Therefore, we will first evaluate the elementary differentials of eq (2.1). Take

$$p^{(1)} = f(q) \tag{2.6}$$

Differentiating eq (2.6) again and again, we obtain higher order elementary differentials.

$$p^{(2)} = \frac{\partial f}{\partial q} g \tag{2.7}$$

$$p^{(3)} = \frac{\partial^2 f}{\partial q \partial q}(g, g) + \frac{\partial f}{\partial q}\frac{\partial g}{\partial p} f \tag{2.8}$$

$$
\begin{aligned}
p^{(4)} = {} & \frac{\partial^3 f}{\partial q \partial q \partial q}(g, g, g) + \frac{\partial^2 f}{\partial q \partial q}\frac{\partial g}{\partial p}(f, g) + \frac{\partial^2 f}{\partial q \partial q} g \frac{\partial g}{\partial p} f + \\
& \frac{\partial^2 f}{\partial q \partial q} g \frac{\partial g}{\partial p} f + \frac{\partial f}{\partial q}\frac{\partial^2 g}{\partial p \partial p}(f, f) + \frac{\partial f}{\partial q}\frac{\partial g}{\partial p}\frac{\partial f}{\partial q} g
\end{aligned} \tag{2.9}
$$

Take

$$q^{(1)} = g(p) \tag{2.10}$$

Differentiating eq (2.10) again and again, we obtain higher order elementary differentials.

$$q^{(2)} = \frac{\partial g}{\partial p} f \tag{2.11}$$

$$q^{(3)} = \frac{\partial^2 g}{\partial p \partial p}(f, f) + \frac{\partial g}{\partial p}\frac{\partial f}{\partial q} g \tag{2.12}$$

$$q^{(4)} = \frac{\partial^3 g}{\partial p \partial p \partial p}(f, f, f) + \frac{\partial^2 g}{\partial p \partial p}\frac{\partial f}{\partial q}(g, f) + \frac{\partial^2 g}{\partial p \partial p} f \frac{\partial f}{\partial q} g + \frac{\partial^2 g}{\partial p \partial p} f \frac{\partial f}{\partial q} g + \frac{\partial f}{\partial p}\frac{\partial^2 f}{\partial q \partial q}(g, g) + \frac{\partial g}{\partial p}\frac{\partial f}{\partial q}\frac{\partial g}{\partial p} f \tag{2.13}$$

With the help of elementary differentials defined in eq (2.7) to eq (2.9) and eq (2.11) to eq (2.12), we can find bi-color rooted trees. Order conditions can be determined using the bi-color rooted trees with their densities and elementary weights shown in Table 2.1 and Table 2.2.

Order conditions for PRK method can be found using following condition,

$$\Phi(t) = \frac{1}{\gamma(t)}$$

Order conditions for the PRK method is shown in Table 2.1 and Table 2.2.

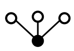
t	$\gamma(t)$	$F(t)$	$\Phi(t)$	$\Phi(t) = \dfrac{1}{\gamma(t)}$
	1	f	$\sum_{i=1}^{s} b_i$	$\sum_{i=1}^{s} b_i = 1$
	2	$\dfrac{\partial f}{\partial q} g$	$\sum_{i=1}^{s} b_i \widetilde{c}_i$	$\sum_{i=1}^{s} b_i \widetilde{c}_i = \dfrac{1}{2}$
	3	$\dfrac{\partial^2 f}{\partial q \partial q}(g, g)$	$\sum_{i=1}^{s} b_i \widetilde{c}_i^2$	$\sum_{i=1}^{s} b_i \widetilde{c}_i^2 = \dfrac{1}{3}$
	6	$\dfrac{\partial f}{\partial q} \dfrac{\partial g}{\partial p} f$	$\sum_{i,j=1}^{s} b_i \widetilde{a}_{ij} c_j$	$\sum_{i,j=1}^{s} b_i \widetilde{a}_{ij} c_j = \dfrac{1}{6}$
	4	$\dfrac{\partial^3 f}{\partial q \partial q \partial q}(g, g, g)$	$\sum_{i=1}^{s} b_i \widetilde{c}_i^3$	$\sum_{i=1}^{s} b_i \widetilde{c}_i^3 = \dfrac{1}{4}$
	8	$\dfrac{\partial^2 f}{\partial q \partial q} \dfrac{\partial g}{\partial p}(f, f)$	$\sum_{i,j=1}^{s} \widetilde{c}_i b_i \widetilde{a}_{ij} c_j$	$\sum_{i,j=1}^{s} \widetilde{c}_i b_i \widetilde{a}_{ij} c_j = \dfrac{1}{8}$
	12	$\dfrac{\partial f}{\partial q} \dfrac{\partial^2 g}{\partial p \partial p}(f, f)$	$\sum_{i,j=1}^{s} b_i \widetilde{a}_{ij} c_j^2$	$\sum_{i,j=1}^{s} b_i \widetilde{a}_{ij} c_j^2 = \dfrac{1}{12}$
	24	$\dfrac{\partial f}{\partial q} \dfrac{\partial g}{\partial p} \dfrac{\partial f}{\partial q} g$	$\sum_{i,j,k=1}^{s} b_i \widetilde{a}_{ij} a_{jk} \widetilde{c}_k$	$\sum_{i,j,k=1}^{s} b_i \widetilde{a}_{ij} a_{jk} \widetilde{c}_k = \dfrac{1}{24}$

Table 2.1: Order conditions for the bi-color rooted trees with black vertex as root.

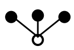
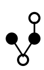
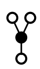
$\widetilde{t}$	$\gamma(\widetilde{t})$	$F(\widetilde{t})$	$\Phi(\widetilde{t})$	$\Phi(\widetilde{t}) = \dfrac{1}{\gamma(\widetilde{t})}$
	1	g	$\sum_{i=1}^{s} \widetilde{b}_i$	$\sum_{i=1}^{s} \widetilde{b}_i = 1$
	2	$\dfrac{\partial g}{\partial p} f$	$\sum_{i=1}^{s} \widetilde{b}_i c_i$	$\sum_{i=1}^{s} \widetilde{b}_i c_i = \dfrac{1}{2}$
	3	$\dfrac{\partial^2 g}{\partial p \partial p}(f, f)$	$\sum_{i=1}^{s} \widetilde{b}_i c_i^2$	$\sum_{i=1}^{s} \widetilde{b}_i c_i^2 = \dfrac{1}{3}$
	6	$\dfrac{\partial g}{\partial p} \dfrac{\partial f}{\partial q} g$	$\sum_{i,j=1}^{s} \widetilde{b}_i a_{ij} \widetilde{c}_j$	$\sum_{i,j=1}^{s} \widetilde{b}_i a_{ij} \widetilde{c}_j = \dfrac{1}{6}$
	4	$\dfrac{\partial^3 g}{\partial p \partial p \partial p}(f, f, f)$	$\sum_{i=1}^{s} \widetilde{b}_i c_i^3$	$\sum_{i=1}^{s} \widetilde{b}_i c_i^3 = \dfrac{1}{4}$
	8	$\dfrac{\partial^2 g}{\partial p \partial p} \dfrac{\partial f}{\partial q}(g, f)$	$\sum_{i,j=1}^{s} c_i \widetilde{b}_i a_{ij} \widetilde{c}_j$	$\sum_{i,j=1}^{s} c_i \widetilde{b}_i a_{ij} \widetilde{c}_j = \dfrac{1}{8}$
	12	$\dfrac{\partial g}{\partial p} \dfrac{\partial^2 f}{\partial q \partial q}(g, g)$	$\sum_{i,j=1}^{s} \widetilde{b}_i a_{ij} \widetilde{c}_j^2$	$\sum_{i,j=1}^{s} \widetilde{b}_i a_{ij} \widetilde{c}_j^2 = \dfrac{1}{12}$
	24	$\dfrac{\partial g}{\partial p} \dfrac{\partial f}{\partial q} \dfrac{\partial g}{\partial p} f$	$\sum_{i,j,k=1}^{s} \widetilde{b}_i a_{ij} \widetilde{a}_{jk} c_k$	$\sum_{i,j,k=1}^{s} \widetilde{b}_i a_{ij} \widetilde{a}_{jk} c_k = \dfrac{1}{24}$

Table 2.2: Order conditions for the bi-color rooted trees with white vertex as root.

2.1 Group of partitioned Runge-Kutta methods

The group of PRK methods under the composition is elaborated by considering two PRK methods $M = [A, b^T, c]$, $\widetilde{M} = [\widetilde{A}, \widetilde{b}^T, \widetilde{c}]$ and $S = [\mathcal{A}, \mathcal{B}^T, \mathcal{C}]$, $\widetilde{S} = [\widetilde{\mathcal{A}}, \widetilde{\mathcal{B}}^T, \widetilde{\mathcal{C}}]$, given as

$$P_i = p_0 + h \sum_{j=1}^{s} a_{ij} f(Q_j) \qquad i = 1, 2, ..., s, \tag{2.14}$$

$$p_1 = p_0 + h \sum_{j=1}^{s} b_j f(Q_j), \tag{2.15}$$

$$Q_i = q_0 + h \sum_{j=1}^{s} \widetilde{a}_{ij} g(P_j) \qquad i = 1, 2, ..., s, \tag{2.16}$$

$$q_1 = q_0 + h \sum_{j=1}^{s} \widetilde{b}_j g(P_j), \tag{2.17}$$

$$\mathcal{P}_i = p_1 + h \sum_{j=1}^{s} \mathcal{A}_{ij} f(\mathcal{Q}_j) \qquad i = 1, 2, ..., s, \tag{2.18}$$

$$p_2 = p_1 + h \sum_{j=1}^{s} \mathcal{B}_j f(\mathcal{Q}_j), \tag{2.19}$$

$$\mathcal{Q}_i = q_1 + h \sum_{j=1}^{s} \widetilde{\mathcal{A}}_{ij} g(\mathcal{P}_j) \qquad i = 1, 2, ..., s, \tag{2.20}$$

$$q_2 = q_1 + h \sum_{j=1}^{s} \widetilde{\mathcal{B}}_j g(\mathcal{P}_j). \tag{2.21}$$

The composed PRK method is

$$
\begin{aligned}
P_i &= p_0 + h\sum_{j=1}^{s} a_{ij} f(Q_j) && i = 1, 2, ..., s,\\
\mathcal{P}_i &= p_0 + h\sum_{j=1}^{s} b_j f(Q_j) + h\sum_{j=1}^{s} \mathcal{A}_{ij} f(Q_j) && i = 1, 2, ..., s,\\
p_2 &= p_0 + h\sum_{j=1}^{s} b_j f(Q_j) + h\sum_{j=1}^{s} \mathcal{B}_j f(Q_j), &&\\
Q_i &= q_0 + h\sum_{j=1}^{s} \widetilde{a}_{ij} g(P_j) && i = 1, 2, ..., s,\\
\mathcal{Q}_i &= q_0 + h\sum_{j=1}^{s} \widetilde{b}_j g(P_j) + h\sum_{j=1}^{s} \widetilde{\mathcal{A}}_{ij} g(P_j) && i = 1, 2, ..., s,\\
q_2 &= q_0 + h\sum_{j=1}^{s} \widetilde{b}_j g(P_j) + h\sum_{j=1}^{s} \widetilde{\mathcal{B}}_j g(P_j).
\end{aligned}
\tag{2.22}
$$

The Butcher tableaux for composed PRK methods are,

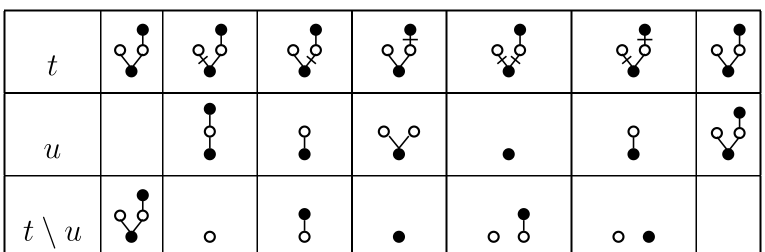
c_1	a_{11}	a_{12}	$\cdots$	a_{1s}	0	0	$\cdots$	0
c_2	a_{21}	a_{22}	$\cdots$	a_{2s}	0	0	$\cdots$	0
$\vdots$	$\vdots$	$\vdots$	$\ddots$	$\vdots$	$\vdots$	$\vdots$	$\ddots$	$\vdots$
c_s	a_{s1}	a_{s2}	$\cdots$	a_{ss}	0	0	$\cdots$	0
$\mathcal{C}_1 + \sum_{i=1}^{s} b_i$	b_1	b_2	$\cdots$	b_s	$\mathcal{A}_{11}$	$\mathcal{A}_{12}$	$\vdots$	$\mathcal{A}_{1s}$
$\mathcal{C}_2 + \sum_{i=1}^{s} b_i$	b_1	b_2	$\cdots$	b_s	$\mathcal{A}_{21}$	$\mathcal{A}_{22}$	$\cdots$	$\mathcal{A}_{2s}$
$\vdots$	$\vdots$	$\vdots$	$\ddots$	$\vdots$	$\vdots$	$\vdots$	$\ddots$	$\vdots$
$\mathcal{C}_s + \sum_{i=1}^{s} b_i$	b_1	b_2	$\cdots$	b_s	$\mathcal{A}_{s1}$	$\mathcal{A}_{s2}$	$\cdots$	$\mathcal{A}_{ss}$
	b_1	b_2	$\cdots$	b_s	$\mathcal{B}_1$	$\mathcal{B}_2$	$\cdots$	$\mathcal{B}_s$

Table 2.3: Butcher tableau for composition of PRK methods SM.

$$
\begin{array}{c|cccccccc}
\widetilde{c}_1 & \widetilde{a}_{11} & \widetilde{a}_{12} & \cdots & \widetilde{a}_{1s} & 0 & 0 & \cdots & 0 \\
\widetilde{c}_2 & \widetilde{a}_{21} & \widetilde{a}_{22} & \cdots & \widetilde{a}_{2s} & 0 & 0 & \cdots & 0 \\
\vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots & \ddots & \vdots \\
\widetilde{c}_s & \widetilde{a}_{s1} & \widetilde{a}_{s2} & \cdots & \widetilde{a}_{ss} & 0 & 0 & \cdots & 0 \\
\widetilde{\mathcal{C}}_1 + \sum_{i=1}^{s} \widetilde{b}_i & \widetilde{b}_1 & \widetilde{b}_2 & \cdots & \widetilde{b}_s & \widetilde{\mathcal{A}}_{11} & \widetilde{\mathcal{A}}_{12} & \vdots & \widetilde{\mathcal{A}}_{1s} \\
\widetilde{\mathcal{C}}_2 + \sum_{i=1}^{s} \widetilde{b}_i & \widetilde{b}_1 & \widetilde{b}_2 & \cdots & \widetilde{b}_s & \widetilde{\mathcal{A}}_{21} & \widetilde{\mathcal{A}}_{22} & \cdots & \widetilde{\mathcal{A}}_{2s} \\
\vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots & \ddots & \vdots \\
\widetilde{\mathcal{C}}_s + \sum_{i=1}^{s} \widetilde{b}_i & \widetilde{b}_1 & \widetilde{b}_2 & \cdots & \widetilde{b}_s & \widetilde{\mathcal{A}}_{s1} & \widetilde{\mathcal{A}}_{s2} & \cdots & \widetilde{\mathcal{A}}_{ss} \\
\hline
 & \widetilde{b}_1 & \widetilde{b}_2 & \cdots & \widetilde{b}_s & \widetilde{\mathcal{B}}_1 & \widetilde{\mathcal{B}}_2 & \cdots & \widetilde{\mathcal{B}}_s
\end{array}
$$

Table 2.4: Butcher tableau for composition of PRK methods $\widetilde{S}\widetilde{M}$.

Let G be the group as mappings from trees to real numbers of corresponding elementary weights of the PRK method. We can define the multiplication operation for the group G. If $\alpha, \beta, \widetilde{\alpha}, \widetilde{\beta} \in G$, then the terms of $(\beta\alpha)(t_6)$ is shown in Table 2.5. Similarly, we can calculate the terms of $\widetilde{\beta}\widetilde{\alpha}$ only by replacing β with $\widetilde{\beta}$ and α with $\widetilde{\alpha}$.



term	β_6	$\widetilde{\beta}_1\alpha_4$	$\widetilde{\beta}_2\alpha_2$	$\beta_1\alpha_3$	$\widetilde{\beta}_1\widetilde{\beta}_2\alpha_1$	$\widetilde{\beta}_1\beta_1\alpha_2$	α_6

Table 2.5: Calculation for the term $\beta\alpha(t_6)$.

Hence,

$$\beta\alpha(t_6) = \beta_6 + \widetilde{\beta}_1\alpha_4 + \widetilde{\beta}_2\alpha_2 + \beta_1\alpha_3 + \widetilde{\beta}_1\widetilde{\beta}_2\alpha_1 + \widetilde{\beta}_1\beta_1\alpha_2 + \alpha_6$$

- **Closure:** It is obvious that the PRK method satisfies the closure property which means that if we compose two PRK methods then the resulting method is again an PRK method.

- **Associative:** PRK methods also satisfy associative property.

- **Identity:** The identity of the PRK method is the method which maps p_0 to p_0 and q_0 to q_0 and it is the identity map.

- **Inverse:** PRK method maps the solution from p_0 to p_1 and q_0 to q_1. The inverse of PRK method maps the solution from p_1 to p_0 and q_1 to q_0. The inverse of PRK method $S = [\mathcal{A}, \mathcal{B}^T, \mathcal{C}]$, $\widetilde{S} = [\widetilde{\mathcal{A}}, \widetilde{\mathcal{B}}^T, \widetilde{\mathcal{C}}]$ is given as,

$$\begin{aligned}
\mathcal{P}_i &= p_{n+1} + h\sum_{j=1}^{s}\mathcal{A}_{ij}f(\mathcal{Q}_j) - h\sum_{j=1}^{s}\mathcal{B}_j f(\mathcal{Q}_j) \quad i = 1, 2, ..., s,\\
p_n &= p_{n+1} - h\sum_{j=1}^{s}\mathcal{B}_j f(\mathcal{Q}_j),\\
\mathcal{Q}_i &= q_{n+1} + h\sum_{j=1}^{s}\widetilde{\mathcal{A}}_{ij}g(\mathcal{P}_j) - h\sum_{j=1}^{s}\widetilde{\mathcal{B}}_j g(\mathcal{P}_j) \quad i = 1, 2, ..., s,\\
q_n &= q_{n+1} - h\sum_{j=1}^{s}\widetilde{\mathcal{B}}_j g(\mathcal{P}_j).
\end{aligned} \tag{2.23}$$

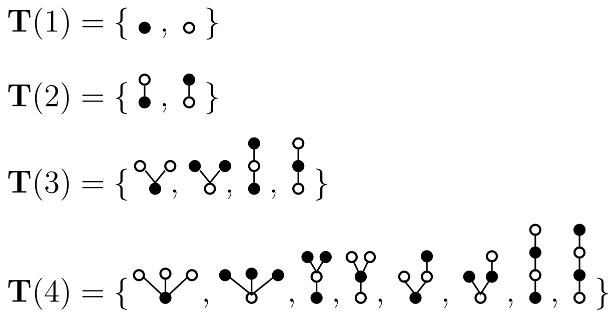
Butcher tableaux for inverse of PRK method are,

$$\begin{array}{c|cccc}
\mathcal{C}_1 - \Sigma_{i=1}^{s}\mathcal{B}_i & \mathcal{A}_{11} - \mathcal{B}_1 & \mathcal{A}_{12} - \mathcal{B}_2 & \cdots & \mathcal{A}_{1s} - \mathcal{B}_s\\
\mathcal{C}_2 - \Sigma_{i=1}^{s}\mathcal{B}_i & \mathcal{A}_{21} - \mathcal{B}_1 & \mathcal{A}_{22} - \mathcal{B}_2 & \cdots & \mathcal{A}_{2s} - \mathcal{B}_s\\
\vdots & \vdots & \vdots & \ddots & \vdots\\
\mathcal{C}_s - \Sigma_{i=1}^{s}\mathcal{B}_i & \mathcal{A}_{s1} - \mathcal{B}_1 & \mathcal{A}_{s2} - \mathcal{B}_2 & \cdots & \mathcal{A}_{ss} - \mathcal{B}_s\\
\hline
 & -\mathcal{B}_1 & -\mathcal{B}_2 & \cdots & -\mathcal{B}_s
\end{array}$$

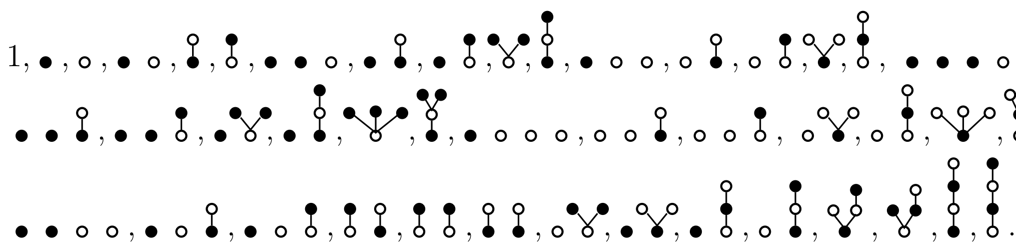
$$\begin{array}{c|cccc}
\widetilde{\mathcal{C}}_1 - \Sigma_{i=1}^{s}\widetilde{\mathcal{B}}_i & \widetilde{\mathcal{A}}_{11} - \widetilde{\mathcal{B}}_1 & \widetilde{\mathcal{A}}_{12} - \widetilde{\mathcal{B}}_2 & \cdots & \widetilde{\mathcal{A}}_{1s} - \widetilde{\mathcal{B}}_s\\
\widetilde{\mathcal{C}}_2 - \Sigma_{i=1}^{s}\widetilde{\mathcal{B}}_i & \widetilde{\mathcal{A}}_{21} - \widetilde{\mathcal{B}}_1 & \widetilde{\mathcal{A}}_{22} - \widetilde{\mathcal{B}}_2 & \cdots & \widetilde{\mathcal{A}}_{2s} - \widetilde{\mathcal{B}}_s\\
\vdots & \vdots & \vdots & \ddots & \vdots\\
\widetilde{\mathcal{C}}_s - \Sigma_{i=1}^{s}\widetilde{\mathcal{B}}_i & \widetilde{\mathcal{A}}_{s1} - \widetilde{\mathcal{B}}_1 & \widetilde{\mathcal{A}}_{s2} - \widetilde{\mathcal{B}}_2 & \cdots & \widetilde{\mathcal{A}}_{ss} - \widetilde{\mathcal{B}}_s\\
\hline
 & -\widetilde{\mathcal{B}}_1 & -\widetilde{\mathcal{B}}_2 & \cdots & -\widetilde{\mathcal{B}}_s
\end{array}$$

2.2 Hopf algebra of bi-color rooted trees

The set of bi-color rooted trees for the elementary differentials of eq (2.1) of weight $n \leq 4$ will be denoted by $\mathbf{T}(n)$.



The rooted forest for the bi-color rooted trees upto order 4 is given below,



Now, we can move towards to see that how bi-color rooted trees can form the Hopf algebra. We can similarly define the coproduct, counit and antipode for the Hopf algebra of bi-color rooted trees as we have defined the Hopf algebra of rooted trees.

Definition 2.1 *The linear map $\Delta : \mathcal{H}_R \to \mathcal{H}_R \otimes \mathcal{H}_R$ such that for all bi-color rooted trees $t \in T$ is known as the coproduct of $\mathcal{H}_R$.*

$$\Delta(t) = \sum_{c \in Adm_*(t)} P_c(t) \otimes R_c(t) = t \otimes 1 + 1 \otimes t + \sum_{c \in Adm(t)} P^c(t) \otimes R^c(t)$$

and Δ is an algebra morphism,

$$\Delta(t_1 t_2) = \Delta(t_1)\Delta(t_2)$$

.

The notation of admissible cuts, $W^c(t)$, $P^c(t)$ and $R^c(t)$ is defined in 1.3.

$\Delta(\bullet)$, $\Delta(\circ)$ is given below,

$$\Delta(\bullet) = \bullet \otimes 1 + 1 \otimes \bullet$$

$$\Delta(\circ) = \circ \otimes 1 + 1 \otimes \circ$$

Calculating Δ for $t = \genfrac{}{}{0pt}{}{\bullet}{\circ}$

Cut	$\genfrac{}{}{0pt}{}{\bullet}{\circ}$	$\genfrac{}{}{1pt}{}{\bullet}{\circ}$	total
Admissible	y	y	y
$W^c(t)$	$\genfrac{}{}{0pt}{}{\bullet}{\circ}$	$\bullet\ \circ$	$\genfrac{}{}{0pt}{}{\bullet}{\circ}$
$R^c(t)$	$\genfrac{}{}{0pt}{}{\bullet}{\circ}$	$\circ$	1
$P^c(t)$	1	$\bullet$	$\genfrac{}{}{0pt}{}{\bullet}{\circ}$

$$\Delta(\genfrac{}{}{0pt}{}{\bullet}{\circ}) = \genfrac{}{}{0pt}{}{\bullet}{\circ} \otimes 1 + 1 \otimes \genfrac{}{}{0pt}{}{\bullet}{\circ} + \bullet \otimes \circ$$

Similarly, we can calculate Δ for $t = \genfrac{}{}{0pt}{}{\circ}{\bullet}$

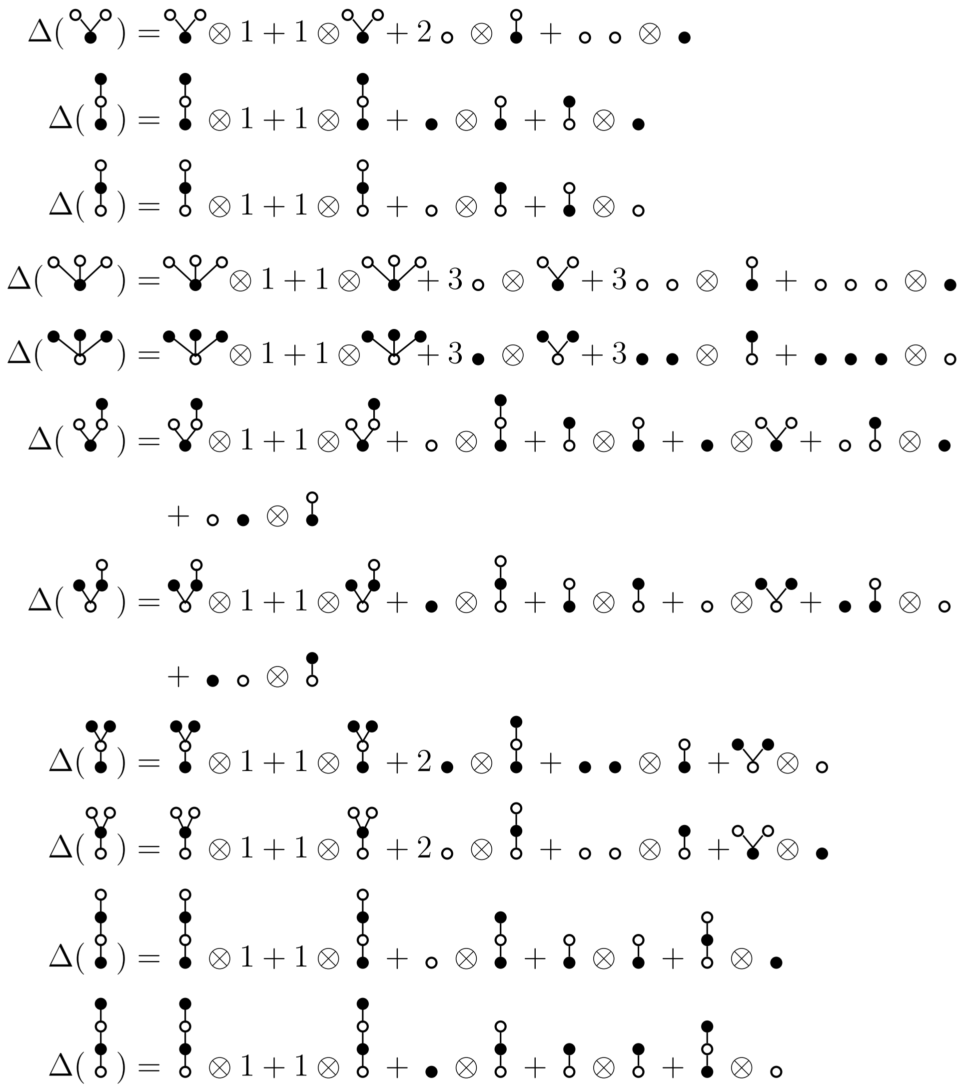
$$\Delta(\genfrac{}{}{0pt}{}{\circ}{\bullet}) = \genfrac{}{}{0pt}{}{\circ}{\bullet} \otimes 1 + 1 \otimes \genfrac{}{}{0pt}{}{\circ}{\bullet} + \circ \otimes \bullet$$

Calculating Δ for $t = \genfrac{}{}{0pt}{}{\bullet\ \bullet}{\circ}$

Cut	$\genfrac{}{}{0pt}{}{\bullet\ \bullet}{\circ}$	$\genfrac{}{}{0pt}{}{\bullet_{\times}\ \bullet}{\circ}$	$\genfrac{}{}{0pt}{}{\bullet\ {}_{\times}\bullet}{\circ}$	$\genfrac{}{}{0pt}{}{\bullet_{\times\times}\bullet}{\circ}$	total
Admissible	y	y	y	y	y
$W^c(t)$	$\genfrac{}{}{0pt}{}{\bullet\ \bullet}{\circ}$	$\bullet\ \genfrac{}{}{0pt}{}{\bullet}{\circ}$	$\genfrac{}{}{0pt}{}{\bullet}{\circ}\ \bullet$	$\bullet\ \bullet\ \circ$	$\genfrac{}{}{0pt}{}{\bullet\ \bullet}{\circ}$
$R^c(t)$	$\genfrac{}{}{0pt}{}{\bullet\ \bullet}{\circ}$	$\genfrac{}{}{0pt}{}{\bullet}{\circ}$	$\genfrac{}{}{0pt}{}{\bullet}{\circ}$	$\circ$	1
$P^c(t)$	1	$\bullet$	$\bullet$	$\bullet\ \bullet$	$\genfrac{}{}{0pt}{}{\bullet\ \bullet}{\circ}$

$$\Delta(\genfrac{}{}{0pt}{}{\bullet\ \bullet}{\circ}) = \genfrac{}{}{0pt}{}{\bullet\ \bullet}{\circ} \otimes 1 + 1 \otimes \genfrac{}{}{0pt}{}{\bullet\ \bullet}{\circ} + 2\,\bullet \otimes \genfrac{}{}{0pt}{}{\bullet}{\circ} + \bullet\ \bullet \otimes \circ$$

Similarly, we can calculate Δ for other trees of order 3 and 4,



Definition 2.2 *The counit is a linear map $\varepsilon : \mathcal{H} \to K$ such that for all $t \in T$*

$$\epsilon(1) = 1$$
$$\epsilon(t) = 0$$

and it is an algebra morphism

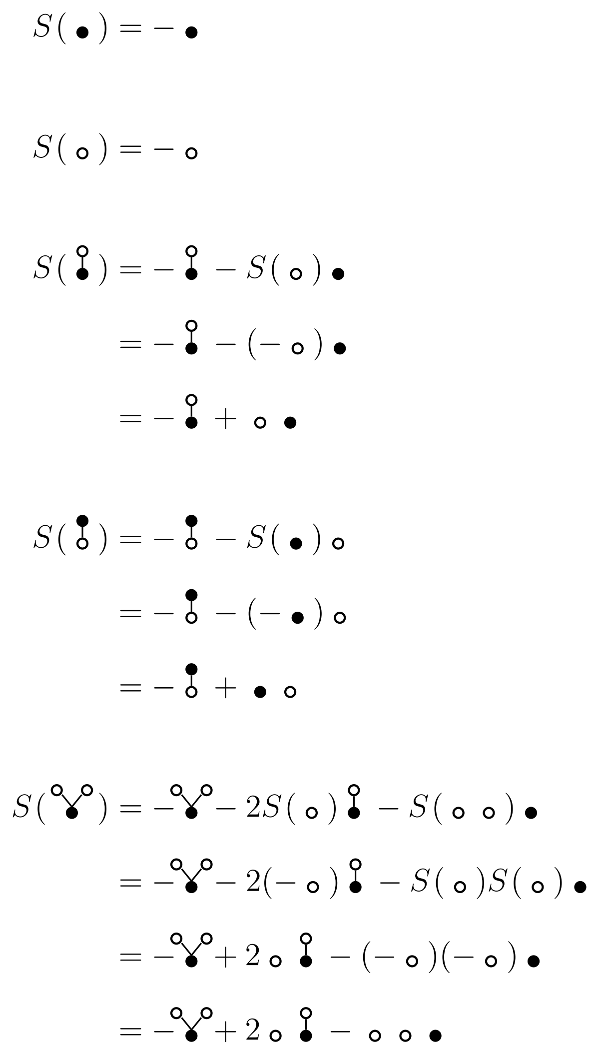
$$\varepsilon(t_1 t_2) = \varepsilon(t_1)\varepsilon(t_2).$$

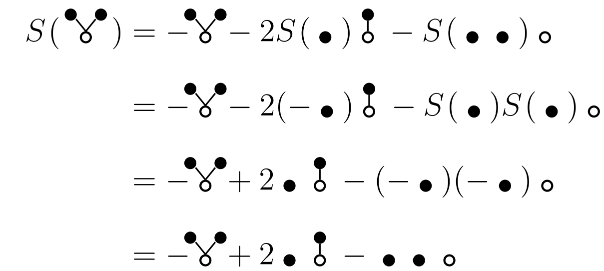
Definition 2.3 *An antipode is a linear map* $S : \mathcal{H}_R \to \mathcal{H}_R$ *such that*

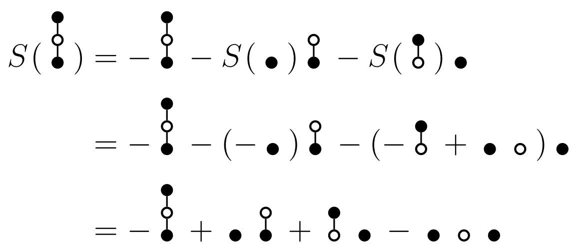
$$\begin{aligned} S(1) &= 1 \\ S(t) &= -t - \sum_{c \in Adm(t)} S(P^c(t))R^c(t) \end{aligned}$$

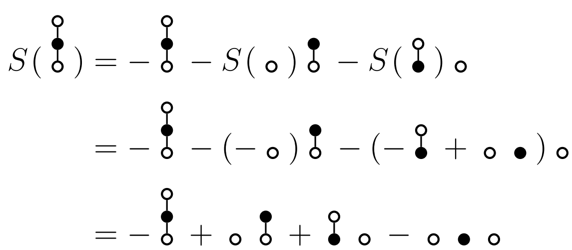
and antipode is an algebra antimorphism

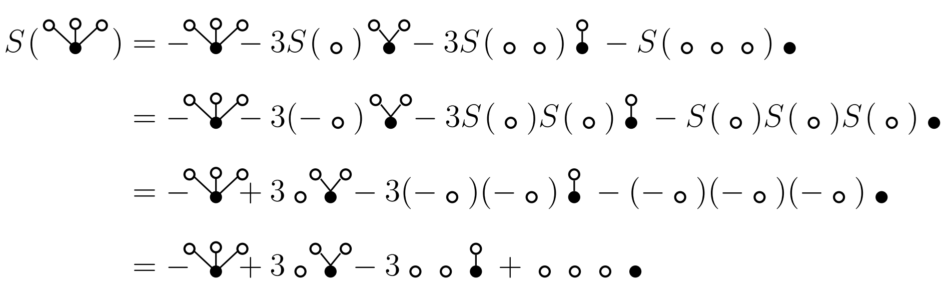
$$S(t_1 t_2) = S(t_2)S(t_1).$$

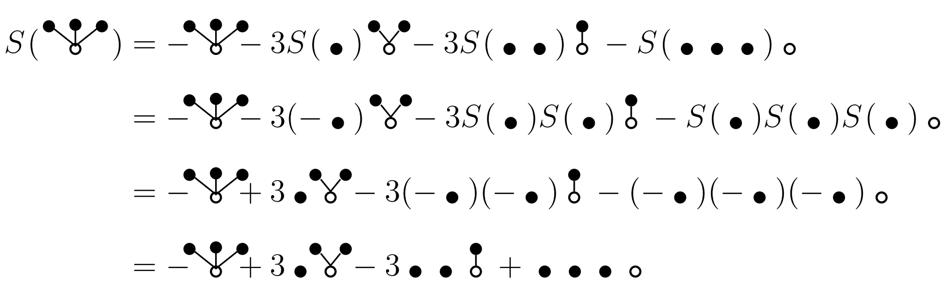


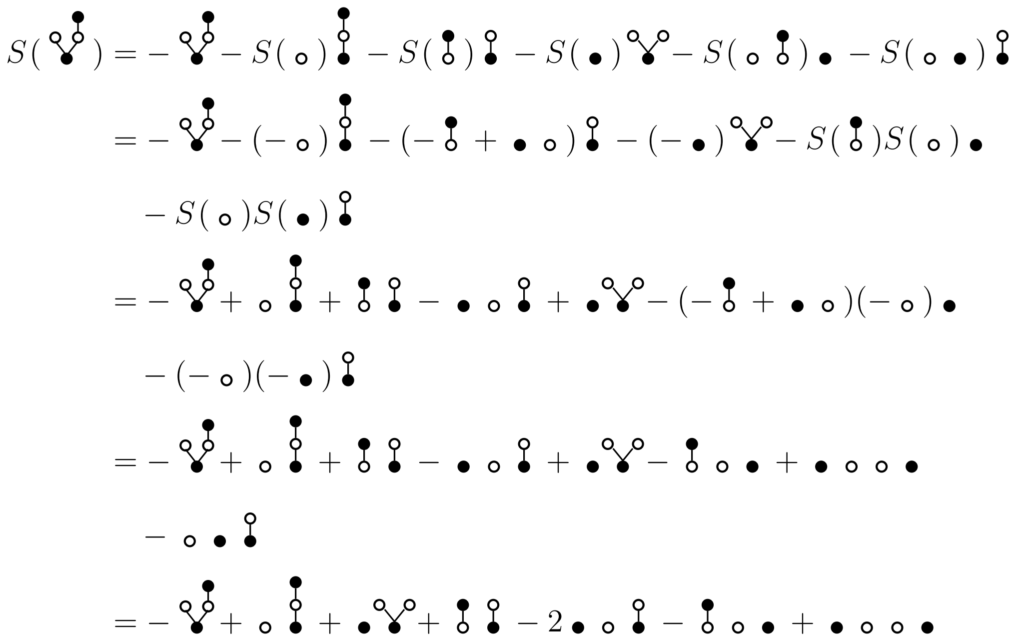


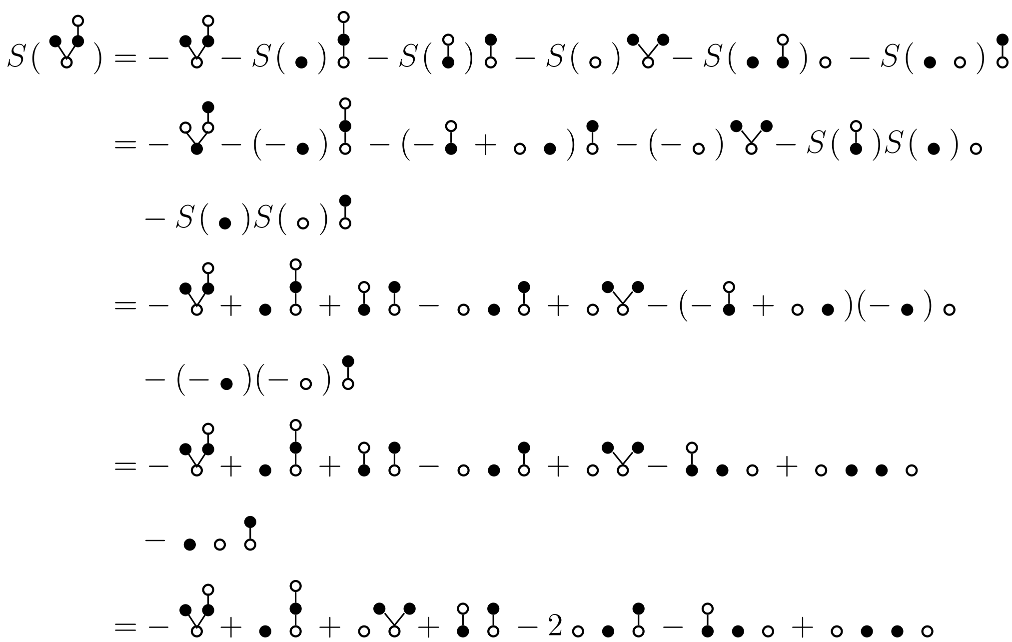


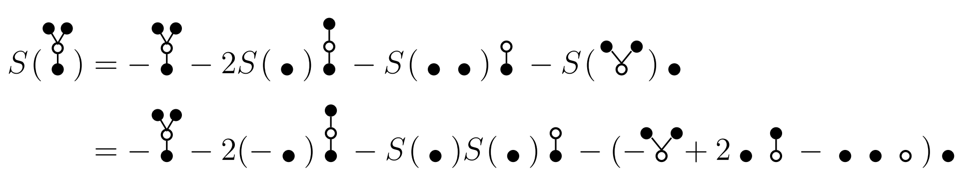


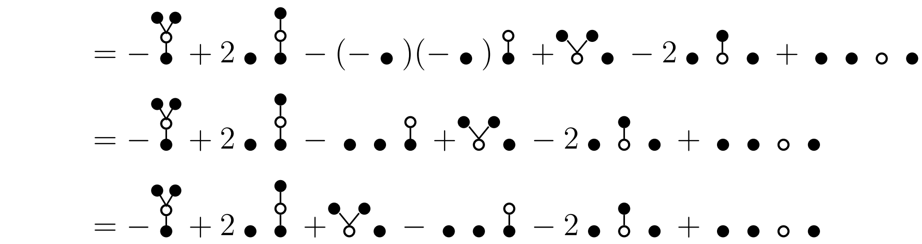


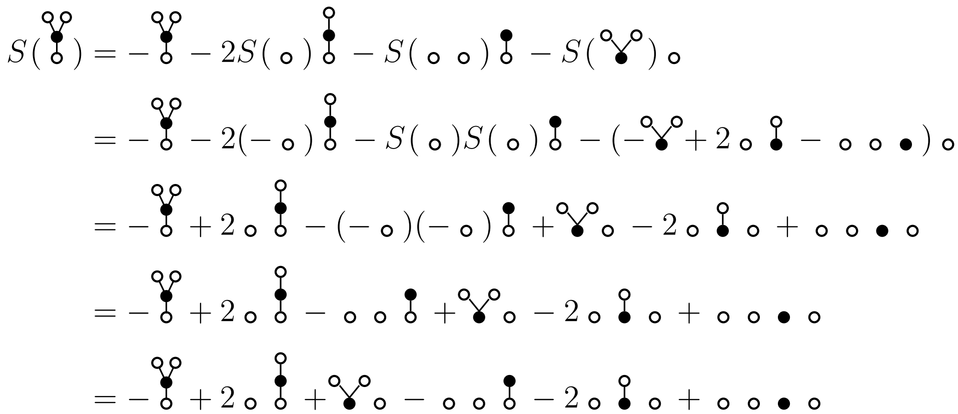


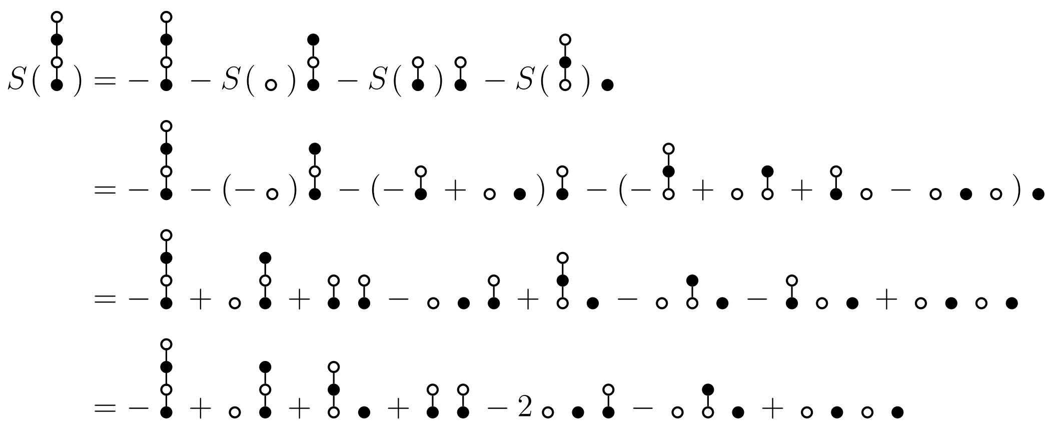


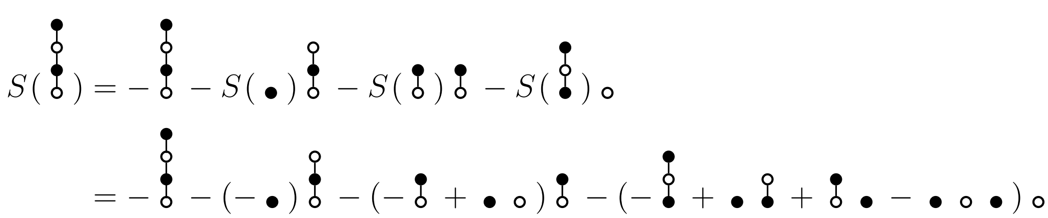


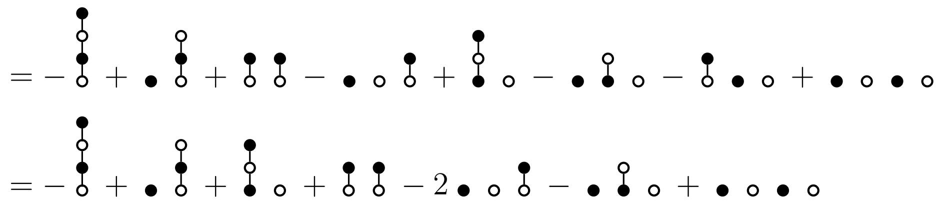








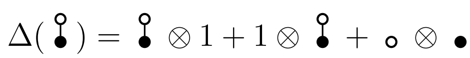




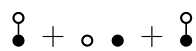
2.3 Isomorphism

There is a one-one correspondence between the coproduct of the Hopf algebra of bi-color rooted trees and the composition rule of the PRK methods. As an example, let t= .

The coproduct for t=  is,

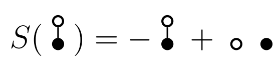


and the composition rule for t=  is

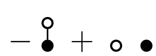


which shows one-one correspondence between them.
There is one-one correspondence between the antipode of the Hopf algebra of bi-color rooted trees and the inverse of composed PRK method. As an example, let t= .

The antipode for  is



and the inverse of composed PRK method for  is



which shows one-one correspondence between them.

Chapter 3

Effective order of partitioned Runge-Kutta methods

A brief review of effective order for RK method is given in Chapter 1. In this chapter, we will try to extend the idea of effective order to PRK methods. The main aim of this thesis is to obtain higher effective order PRK methods using less number of stages as requires by classical order. Consider the problem

$$\begin{pmatrix} p \\ q \end{pmatrix}' = \begin{pmatrix} f(q) \\ g(p) \end{pmatrix} \qquad\qquad p(x_0) = p_0, \quad q(x_0) = q_0. \tag{3.1}$$

We can find its solution using the PRK method $\alpha = [A, b^T, c]$ and $\widetilde{\alpha} = [\widetilde{A}, \widetilde{b}^T, \widetilde{c}]$ defined below:

$$\begin{aligned} P_i &= p_n + h\sum_{j=1}^{s} a_{ij} f(Q_j) \quad i = 1, 2, ..., s, \\ Q_i &= q_n + h\sum_{j=1}^{s} \widetilde{a}_{ij} g(P_j) \quad i = 1, 2, ..., s, \\ p_{n+1} &= p_n + h\sum_{j=1}^{s} b_j f(Q_j), \\ q_{n+1} &= q_n + h\sum_{j=1}^{s} \widetilde{b}_j g(P_j). \end{aligned} \tag{3.2}$$

P_i and Q_i are the stages, a_{ij} and $\widetilde{a}_{ij}$ are the coefficient matrices, b_j and $\widetilde{b}_j$ are the weights. p_{n+1} and q_{n+1} are the output values of the system eq (3.2)

taking p_n and q_n as initial values respectively. Moreover, $c_i = \sum a_{ij}$ and $\widetilde{c}_i = \sum \widetilde{a}_{ij}$ are the consistency conditions of the PRK method.
Now, the PRK method α and $\widetilde{\alpha}$ has an "effective order" p if there exist two starting methods $\beta = [\mathcal{A}, \mathcal{B}^T, \mathcal{C}]$ and $\widetilde{\beta} = [\widetilde{\mathcal{A}}, \widetilde{\mathcal{B}}^T, \widetilde{\mathcal{C}}]$ with two ending methods β^{-1} and $\widetilde{\beta}^{-1}$ such that the composition $\beta\alpha\beta^{-1}$ and $\widetilde{\beta}\widetilde{\alpha}\widetilde{\beta}^{-1}$ has an order p. The method β and $\widetilde{\beta}$ used once at the beginning and the β^{-1} and $\widetilde{\beta}^{-1}$ at the end. We can obtain the order conditions of an effective order for PRK method by equating the composition $\beta\alpha$ to the composition $E\beta$ and the composition $\widetilde{\beta}\widetilde{\alpha}$ to the composition $E\widetilde{\beta}$, where E represents the exact solution i.e, $E = \dfrac{1}{\gamma(t)}$.
The Butcher tableaux

$$\alpha = \begin{array}{c|c} \mathrm{c} & A \\ \hline & b^T \end{array} \qquad \widetilde{\alpha} = \begin{array}{c|c} \widetilde{c} & \widetilde{A} \\ \hline & \widetilde{b}^T \end{array}$$

$$\beta = \begin{array}{c|c} \mathcal{C} & \mathcal{A} \\ \hline & \mathcal{B}^T \end{array} \qquad \widetilde{\beta} = \begin{array}{c|c} \widetilde{\mathcal{C}} & \widetilde{\mathcal{A}} \\ \hline & \widetilde{\mathcal{B}}^T \end{array}$$

We can write their product as $\alpha\beta$ and $\widetilde{\alpha}\widetilde{\beta}$:

$$\alpha\beta : \begin{array}{c|cc} c & A & 0 \\ \mathcal{C} + \sum_{i=1}^{s} b & b & \mathcal{A} \\ \hline & b^T & \mathcal{B}^T \end{array} \qquad \widetilde{\alpha}\widetilde{\beta} : \begin{array}{c|cc} \widetilde{c} & \widetilde{A} & 0 \\ \widetilde{\mathcal{C}} + \sum_{i=1}^{s} \widetilde{b} & \widetilde{b} & \widetilde{\mathcal{A}} \\ \hline & \widetilde{b}^T & \widetilde{\mathcal{B}}^T \end{array}$$

Trees of order 4 are given in in Table 3.1 and Table 3.2. We have black and white vertices as the root of the rooted trees. We will denote the tree with black vertex as a root with t_i and the tree with white vertex as a root with $\widetilde{t}_i$.

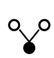
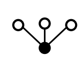
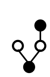
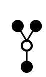
Name	t_1	t_2	t_3	t_4	t_5	t_6	t_7	t_8
trees								

Table 3.1: Bi-color rooted trees with black vertex as root.

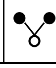
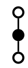
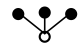
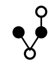
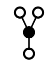
Name	$\widetilde{t}_1$	$\widetilde{t}_2$	$\widetilde{t}_3$	$\widetilde{t}_4$	$\widetilde{t}_5$	$\widetilde{t}_6$	$\widetilde{t}_7$	$\widetilde{t}_8$
trees								

Table 3.2: Bi-color rooted trees with white vertex as root.

3.1 Two stage effective order of partitioned Runge-Kutta methods

In this section, we want to construct effective order 3 method with two stages. For the trees of order up to 3, the composition of $\beta\alpha$ and $E\beta$ is shown in Table 3.3 and the composition of $\widetilde{\beta}\widetilde{\alpha}$ and $E\widetilde{\beta}$ is shown in Table 3.4.

t_i	$(\beta\alpha)(t_i)$	$(E\beta)(t_i)$
	$\beta_1 + \alpha_1$	$1 + \beta_1$
	$\beta_2 + \widetilde{\beta}_1\alpha_1 + \alpha_2$	$\frac{1}{2} + \beta_1 + \beta_2$
	$\beta_3 + \widetilde{\beta}_1^2\alpha_1 + 2\widetilde{\beta}_1\alpha_2 + \alpha_3$	$\frac{1}{3} + \beta_1 + 2\beta_2 + \beta_3$
	$\beta_4 + \widetilde{\beta}_2\alpha_1 + \beta_1\alpha_2 + \alpha_4$	$\frac{1}{6} + \frac{1}{2}\beta_1 + \beta_2 + \beta_4$

Table 3.3: $\beta\alpha$ and $E\beta$ for the trees up to order 3.

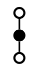
$\widetilde{t}_i$	$(\widetilde{\beta}\widetilde{\alpha})(\widetilde{t}_i)$	$(E\widetilde{\beta})(\widetilde{t}_i)$
	$\widetilde{\beta}_1 + \widetilde{\alpha}_1$	$1 + \widetilde{\beta}_1$
	$\widetilde{\beta}_2 + \beta_1\widetilde{\alpha}_1 + \widetilde{\alpha}_2$	$\frac{1}{2} + \widetilde{\beta}_1 + \widetilde{\beta}_2$
	$\widetilde{\beta}_3 + \beta_1^2\widetilde{\alpha}_1 + 2\beta_1\widetilde{\alpha}_2 + \widetilde{\alpha}_3$	$\frac{1}{3} + \widetilde{\beta}_1 + 2\widetilde{\beta}_2 + \widetilde{\beta}_3$
	$\widetilde{\beta}_4 + \beta_2\widetilde{\alpha}_1 + \widetilde{\beta}_1\widetilde{\alpha}_2 + \widetilde{\alpha}_4$	$\frac{1}{6} + \frac{1}{2}\widetilde{\beta}_1 + \widetilde{\beta}_2 + \widetilde{\beta}_4$

Table 3.4: $\widetilde{\beta}\widetilde{\alpha}$ and $E\widetilde{\beta}$ for the trees up to order 3.

By equating $(\beta\alpha) = (E\beta)$, $(\widetilde{\beta}\widetilde{\alpha}) = (E\widetilde{\beta})$ and taking $\beta_1 = \widetilde{\beta}_1 = 0$, we got have following equations,

$$\alpha_1 = 1, \tag{3.3}$$
$$\widetilde{\alpha}_1 = 1, \tag{3.4}$$
$$\alpha_2 = \frac{1}{2}, \tag{3.5}$$
$$\widetilde{\alpha}_2 = \frac{1}{2}, \tag{3.6}$$
$$\alpha_3 = \frac{1}{3} + 2\beta_2, \tag{3.7}$$
$$\widetilde{\alpha}_3 = \frac{1}{3} + 2\widetilde{\beta}_2, \tag{3.8}$$
$$\alpha_4 + \widetilde{\beta}_2 = \frac{1}{6} + \beta_2, \tag{3.9}$$
$$\widetilde{\alpha}_4 + \beta_2 = \frac{1}{6} + \widetilde{\beta}_2. \tag{3.10}$$

We can find values of β_2 and $\widetilde{\beta}_2$ from eq (3.7) and eq (3.8),

$$\beta_2 = \frac{3\alpha_3 - 1}{6},$$
$$\widetilde{\beta}_2 = \frac{3\widetilde{\alpha}_3 - 1}{6}.$$

After substituting the values of β_2 and $\widetilde{\beta}_2$ in eq (3.9) and eq (3.10), we have the following eq's independent of β values.

$$\begin{aligned} \alpha_1 =& 1, \\ \widetilde{\alpha}_1 =& 1, \\ \alpha_2 =& \frac{1}{2}, \\ \widetilde{\alpha}_2 =& \frac{1}{2}, \\ 6\alpha_4 + 3\widetilde{\alpha}_3 - 3\alpha_3 =& 1, \\ 6\widetilde{\alpha}_4 + 3\alpha_3 - 3\widetilde{\alpha}_3 =& 1. \end{aligned} \tag{3.11}$$

Writing the set of equations (3.11) in terms of elementary weights with usual indices,

$$\begin{aligned} \sum b_i &= 1, \\ \sum \widetilde{b}_i &= 1, \\ \sum b_i \widetilde{c}_i &= \frac{1}{2}, \\ \sum \widetilde{b}_i c_i &= \frac{1}{2}, \\ 6(\sum b_i \widetilde{a}_{ij} c_j) + 3(\sum \widetilde{b}_i c_i^2) - 3(\sum b_i \widetilde{c}_i^2) &= 1, \\ 6(\sum \widetilde{b}_i a_{ij} \widetilde{c}_j) + 3(\sum b_i \widetilde{c}_i^2) - 3(\sum \widetilde{b}_i c_i^2) &= 1. \end{aligned} \tag{3.12}$$

Expanding the set of equations (3.12) in terms of coefficients of the following Butcher tableaux,

$$\begin{array}{c|cc} 0 & 0 & 0 \\ c_2 & a_{21} & 0 \\ \hline & b_1 & b_2 \end{array} \qquad \begin{array}{c|cc} \widetilde{c}_1 & \widetilde{a}_{11} & 0 \\ \widetilde{c}_2 & \widetilde{a}_{21} & \widetilde{a}_{22} \\ \hline & \widetilde{b}_1 & \widetilde{b}_2 \end{array}$$

we get the following equations.

$$\begin{aligned} b_1 + b_2 =& 1, \\ \widetilde{b}_1 + \widetilde{b}_2 =& 1, \\ b_1\widetilde{c}_1 + b_2\widetilde{c}_2 =& \frac{1}{2}, \\ \widetilde{b}_2 c_2 =& \frac{1}{2}, \\ 6b_2\widetilde{a}_{22}c_2 + 3\widetilde{b}_2 c_2^2 - 3b_1\widetilde{c}_1^2 - 3b_2\widetilde{c}_2^2 =& 1, \\ 6\widetilde{b}_2 c_2 \widetilde{c}_1 + 3b_1\widetilde{c}_1^2 + 3b_2 c_2^2 - 3\widetilde{b}_2 c_2^2 =& 1. \end{aligned} \tag{3.13}$$

Solving the 6 equations (3.13) for 6 unknowns $b_1, b_2, \widetilde{b}_1, \widetilde{b}_2, \widetilde{a}_{22}, c_2$ taking $\widetilde{c}_1, \widetilde{c}_2$ as parameters, we get

$$
\begin{aligned}
b_1 &= \frac{-1+2\widetilde{c}_2}{2(-\widetilde{c}_1+\widetilde{c}_2)},\\
b_2 &= \frac{-1+2\widetilde{c}_1}{2(\widetilde{c}_1-\widetilde{c}_{2)}},\\
\widetilde{b}_1 &= \frac{7-18\widetilde{c}_1-6\widetilde{c}_2+12\widetilde{c}_1\widetilde{c}_2}{4-18\widetilde{c}_1-6\widetilde{c}_2+12\widetilde{c}_1\widetilde{c}_2},\\
\widetilde{b}_2 &= -\frac{3}{2(2-9\widetilde{c}_1-3\widetilde{c}_2+6\widetilde{c}_1\widetilde{c}_2)},\\
\widetilde{a}_{22} &= \frac{(-2+3\widetilde{c}_1)(\widetilde{c}_1-\widetilde{c}_2)}{(-1+2\widetilde{c}_1)(2-9\widetilde{c}_1-3\widetilde{c}_2+6\widetilde{c}_1\widetilde{c}_2)},\\
c_2 &= \frac{1}{3}(-2+9\widetilde{c}_1+3\widetilde{c}_2-6\widetilde{c}_1\widetilde{c}_2).
\end{aligned}
$$

Using consistency conditions, we can find the values of $\widetilde{a}_{11}, \widetilde{a}_{21}$ and a_{21}.

$$
\begin{aligned}
\widetilde{a}_{11} &= \widetilde{c}_1,\\
\widetilde{a}_{21} &= \widetilde{c}_2 - \widetilde{a}_{22},\\
&= \widetilde{c}_2 - \frac{(-2+3\widetilde{c}_1)(\widetilde{c}_1-\widetilde{c}_2)}{(-1+2\widetilde{c}_1)(2-3\widetilde{c}_2+\widetilde{c}_1(-9+6\widetilde{c}_2))},\\
a_{21} &= c_2,\\
&= \frac{1}{3}(-2+9\widetilde{c}_1+3\widetilde{c}_2-6\widetilde{c}_1\widetilde{c}_2).
\end{aligned}
$$

Choosing $\widetilde{c}_1 = \frac{1}{3}$ and $\widetilde{c}_2 = \frac{2}{3}$, we get the following two Butcher tableaux α and $\widetilde{\alpha}$ method respectively.

$$
\begin{array}{c|cc}
0 & 0 & 0\\
\frac{5}{9} & \frac{5}{9} & 0\\
\hline
 & \frac{1}{2} & \frac{1}{2}
\end{array}
\qquad
\begin{array}{c|cc}
\frac{1}{3} & \frac{1}{3} & 0\\
\frac{2}{3} & \frac{1}{15} & \frac{3}{5}\\
\hline
 & \frac{1}{10} & \frac{9}{10}
\end{array}
$$

For perturbation method β and $\widetilde{\beta}$, we have

$$\beta_1 = 0, \tag{3.14}$$

$$\widetilde{\beta}_1 = 0. \tag{3.15}$$

For finding β_2 and $\widetilde{\beta}_2$ condition, we need to find the values of α_3 and $\widetilde{\alpha}_3$.

$$\begin{aligned}\alpha_3 &= \sum b_i\widetilde{c}_i^2 = b_1\widetilde{c}_1^2 + b_2\widetilde{c}_2^2\\ &= \frac{1}{2}(\frac{1}{9} + \frac{4}{9})\\ &= \frac{5}{18}\\ \widetilde{\alpha}_3 &= \sum \widetilde{b}_i c_i^2 = \widetilde{b}_2 c_2^2\\ &= \frac{9}{10}\left(\frac{5}{9}\right)^2\\ &= \frac{5}{18}\end{aligned}$$

Putting the values of α_3 and $\widetilde{\alpha}_3$ in eq (3.7) and eq (3.8), we will have:

$$\beta_2 = -\frac{1}{36}, \tag{3.16}$$

$$\widetilde{\beta}_2 = -\frac{1}{36}. \tag{3.17}$$

We can write eq (3.14) to eq (3.17) in elementary form,

$$\begin{aligned}\sum B_i &= 0,\\ \sum \widetilde{B}_i &= 0,\\ \sum B_i\widetilde{C}_i &= -\frac{1}{36},\\ \sum \widetilde{B}_i C_i &= -\frac{1}{36}.\end{aligned} \tag{3.18}$$

Writing equations (3.18) in coefficient form for the Butcher tableaux.

$$\begin{array}{c|cc} 0 & 0 & 0\\ C_2 & A_{21} & 0\\ \hline & B_1 & B_2\end{array} \qquad \begin{array}{c|cc} 0 & 0 & 0\\ \widetilde{C}_2 & \widetilde{A}_{21} & 0\\ \hline & \widetilde{B}_1 & \widetilde{B}_2\end{array}$$

as follows,

$$\begin{aligned}B_1 + B_2 &= 0,\\ \widetilde{B}_1 + \widetilde{B}_2 &= 0,\\ B_2\widetilde{C}_2 &= -\frac{1}{36},\\ \widetilde{B}_2 C_2 &= -\frac{1}{36}.\end{aligned} \tag{3.19}$$

Solving the equations (3.19), we get the following perturbation method $\beta=\widetilde{\beta}$ because $C_2 = \widetilde{C}_2$, $A_{21} = \widetilde{A}_{21}$, $B_1 = \widetilde{B}_1$ and $B_2 = \widetilde{B}_2$.

$$
\begin{array}{c|cc}
0 & 0 & 0 \\
\frac{1}{6} & \frac{1}{6} & 0 \\
\hline
 & \frac{1}{6} & -\frac{1}{6}
\end{array}
$$

Now, we will finally find suitable ending beta inverse (β^{-1}) method. By combining ($\beta\alpha\beta^{-1}$), we get the following Butcher table.

$$
\begin{array}{c|cccccc}
0 & 0 & 0 & 0 & 0 & 0 & 0 \\
\frac{1}{6} & \frac{1}{6} & 0 & 0 & 0 & 0 & 0 \\
0 & \frac{1}{6} & -\frac{1}{6} & 0 & 0 & 0 & 0 \\
\frac{5}{9} & \frac{1}{6} & -\frac{1}{6} & \frac{5}{9} & 0 & 0 & 0 \\
1 & \frac{1}{6} & -\frac{1}{6} & \frac{1}{2} & \frac{1}{2} & 0 & 0 \\
1+\mathcal{A}_{21} & \frac{1}{6} & -\frac{1}{6} & \frac{1}{2} & \frac{1}{2} & \mathcal{A}_{21} & 0 \\
\hline
 & \frac{1}{6} & -\frac{1}{6} & \frac{1}{2} & \frac{1}{2} & \mathcal{B}_1 & \mathcal{B}_2
\end{array}
$$

We can obtain the order conditions for β^{-1} method of 2-stage effective order 3 from the above Butcher table to construct β^{-1} method. Order conditions for β^{-1} method in the form of elementary weights are,

$$
\begin{aligned}
\sum \mathcal{B}_i &= 1, \\
\sum \mathcal{B}_i \widetilde{\mathcal{C}}_i &= \frac{1}{2}, \\
\sum \mathcal{B}_i \widetilde{\mathcal{C}}_i^2 &= \frac{1}{3}, \\
\sum \mathcal{B}_i \widetilde{\mathcal{A}}_{ij} \mathcal{C}_j &= \frac{1}{6}.
\end{aligned}
\tag{3.20}
$$

Order conditions for β^{-1} method are

$$\mathcal{B}_1 + \mathcal{B}_2 = 0, \tag{3.21}$$

$$\mathcal{B}_1 + \mathcal{B}_2 + \mathcal{B}_2\mathcal{A}_{21} = \frac{1}{36}, \tag{3.22}$$

$$\mathcal{B}_1 + \mathcal{B}_2 + \mathcal{B}_2(\mathcal{A}_{21}^2 + 2\mathcal{A}_{21}) = \frac{13}{216}, \tag{3.23}$$

$$\frac{17}{36}(\mathcal{B}_1 + \mathcal{B}_2) + \mathcal{B}_2\mathcal{A}_{21} = 1/36. \tag{3.24}$$

After solving eq (3.21) to eq (3.24), we get the following suitable finishing method β^{-1}.

$$\begin{array}{c|cc} 0 & 0 & 0 \\ \frac{1}{6} & \frac{1}{6} & 0 \\ \hline & -\frac{1}{6} & \frac{1}{6} \end{array}$$

Since, $\beta = \widetilde{\beta}$. Therefore, $\beta^{-1} = \widetilde{\beta}^{-1}$

3.2 Three stage effective order of partitioned Runge-Kutta methods

In this section, we want to construct effective order 4 method with three stages. For the trees of order up to 4, the composition of $\beta\alpha$ and $E\beta$ is shown in Table 3.5 and the composition of $\widetilde{\beta}\widetilde{\alpha}$ and $E\widetilde{\beta}$ is shown in Table 3.6.

By equating $(\beta\alpha) = (E\beta)$, $(\widetilde{\beta}\widetilde{\alpha}) = (E\widetilde{\beta})$ and taking $\beta_1 = \widetilde{\beta}_1 = 0$, we got the

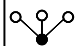
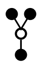
t_i	$(\beta\alpha)(t_i)$	$(E\beta)(t_i)$
	$\beta_1 + \alpha_1$	$1 + \beta_1$
	$\beta_2 + \widetilde{\beta}_1\alpha_1 + \alpha_2$	$\frac{1}{2} + \beta_1 + \beta_2$
	$\beta_3 + \widetilde{\beta}_1^2\alpha_1 + 2\widetilde{\beta}_1\alpha_2 + \alpha_3$	$\frac{1}{3} + \beta_1 + 2\beta_2 + \beta_3$
	$\beta_4 + \beta_1\alpha_2 + \widetilde{\beta}_2\alpha_1 + \alpha_4$	$\frac{1}{6} + \frac{1}{2}\beta_1 + \beta_2 + \beta_4$
	$\beta_5 + 3\widetilde{\beta}_1\alpha_3 + 3\widetilde{\beta}_1^2\alpha_2 + \widetilde{\beta}_1^3\alpha_1 + \alpha_5$	$\frac{1}{4} + \beta_1 + 3\beta_2 + 3\beta_3 + \beta_5$
	$\beta_6 + \widetilde{\beta}_1\alpha_4 + \widetilde{\beta}_2\alpha_2 + \beta_1\alpha_3 + \widetilde{\beta}_1\widetilde{\beta}_2\alpha_1 + \widetilde{\beta}_1\beta_1\alpha_2 + \alpha_6$	$\frac{1}{8} + \frac{1}{2}\beta_1 + \frac{3}{2}\beta_2 + \beta_3 + \beta_4 + \beta_6$
	$\beta_7 + \widetilde{\beta}_3\alpha_1 + 2\beta_1\alpha_4 + \beta_1^2\alpha_2 + \alpha_7$	$\frac{1}{12} + \frac{1}{3}\beta_1 + \beta_2 + 2\beta_4 + \beta_7$
	$\beta_8 + \widetilde{\beta}_4\alpha_1 + \beta_2\alpha_2 + \widetilde{\beta}_1\alpha_4 + \alpha_8$	$\frac{1}{24} + \frac{1}{6}\beta_1 + \frac{1}{2}\beta_2 + \beta_4 + \beta_8$

Table 3.5: $\beta\alpha$ and $E\beta$ for the trees up to order 4.

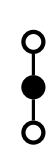
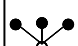
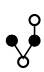
$\widetilde{t}_i$	$(\widetilde{\beta}\widetilde{\alpha})(\widetilde{t}_i)$	$(E\widetilde{\beta})(\widetilde{t}_i)$
	$\widetilde{\beta}_1 + \widetilde{\alpha}_1$	$1 + \widetilde{\beta}_1$
	$\widetilde{\beta}_2 + \beta_1\widetilde{\alpha}_1 + \widetilde{\alpha}_2$	$\frac{1}{2} + \widetilde{\beta}_1 + \widetilde{\beta}_2$
	$\widetilde{\beta}_3 + \beta_1^2\widetilde{\alpha}_1 + 2\beta_1\widetilde{\alpha}_2 + \widetilde{\alpha}_3$	$\frac{1}{3} + \widetilde{\beta}_1 + 2\widetilde{\beta}_2 + \widetilde{\beta}_3$
	$\widetilde{\beta}_4 + \beta_2\widetilde{\alpha}_1 + \widetilde{\beta}_1\widetilde{\alpha}_2 + \widetilde{\alpha}_4$	$\frac{1}{6} + \frac{1}{2}\widetilde{\beta}_1 + \widetilde{\beta}_2 + \widetilde{\beta}_4$
	$\widetilde{\beta}_5 + 3\beta_1\widetilde{\alpha}_3 + 3\beta_1^2\widetilde{\alpha}_2 + \beta_1^3\widetilde{\alpha}_1 + \widetilde{\alpha}_5$	$\frac{1}{4} + \widetilde{\beta}_1 + 3\widetilde{\beta}_2 + 3\widetilde{\beta}_3 + \widetilde{\beta}_5$
	$\widetilde{\beta}_6 + \beta_1\widetilde{\alpha}_4 + \beta_2\widetilde{\alpha}_2 + \widetilde{\beta}_1\widetilde{\alpha}_3 + \beta_1\beta_2\widetilde{\alpha}_1 + \widetilde{\beta}_1\beta_1\widetilde{\alpha}_2 + \widetilde{\alpha}_6$	$\frac{1}{8} + \frac{1}{2}\widetilde{\beta}_1 + \frac{3}{2}\widetilde{\beta}_2 + \widetilde{\beta}_3 + \widetilde{\beta}_4 + \widetilde{\beta}_6$
	$\widetilde{\beta}_7 + \beta_3\widetilde{\alpha}_1 + 2\widetilde{\beta}_1\widetilde{\alpha}_4 + \widetilde{\beta}_1^2\widetilde{\alpha}_2 + \widetilde{\alpha}_7$	$\frac{1}{12} + \frac{1}{3}\widetilde{\beta}_1 + \widetilde{\beta}_2 + 2\widetilde{\beta}_4 + \widetilde{\beta}_7$
	$\widetilde{\beta}_8 + \beta_4\widetilde{\alpha}_1 + \widetilde{\beta}_2\widetilde{\alpha}_2 + \beta_1\widetilde{\alpha}_4 + \widetilde{\alpha}_8$	$\frac{1}{24} + \frac{1}{6}\widetilde{\beta}_1 + \frac{1}{2}\widetilde{\beta}_2 + \widetilde{\beta}_4 + \widetilde{\beta}_8$

Table 3.6: $\widetilde{\beta}\widetilde{\alpha}$ and $E\widetilde{\beta}$ for the trees up to order 4.

following equations,

$$\alpha_1 = 1, \tag{3.25}$$
$$\widetilde{\alpha}_1 = 1, \tag{3.26}$$
$$\alpha_2 = \frac{1}{2}, \tag{3.27}$$
$$\widetilde{\alpha}_2 = \frac{1}{2}, \tag{3.28}$$
$$\alpha_3 = \frac{1}{3} + 2\beta_2, \tag{3.29}$$
$$\widetilde{\alpha}_3 = \frac{1}{3} + 2\widetilde{\beta}_2, \tag{3.30}$$
$$\alpha_4 + \widetilde{\beta}_2 = \frac{1}{6} + \beta_2, \tag{3.31}$$
$$\widetilde{\alpha}_4 + \beta_2 = \frac{1}{6} + \widetilde{\beta}_2, \tag{3.32}$$
$$\alpha_5 = \frac{1}{4} + 3\beta_2 + 3\beta_3, \tag{3.33}$$
$$\widetilde{\alpha}_5 = \frac{1}{4} + 3\widetilde{\beta}_2 + 3\widetilde{\beta}_3, \tag{3.34}$$
$$\alpha_6 + \frac{1}{2}\widetilde{\beta}_2 = \frac{1}{8} + \frac{3}{2}\beta_2 + \beta_3 + \beta_4, \tag{3.35}$$
$$\widetilde{\alpha}_6 + \frac{1}{2}\beta_2 = \frac{1}{8} + \frac{3}{2}\widetilde{\beta}_2 + \widetilde{\beta}_3 + \widetilde{\beta}_4, \tag{3.36}$$
$$\alpha_7 + \widetilde{\beta}_3 = \frac{1}{12} + \beta_2 + 2\beta_4, \tag{3.37}$$
$$\widetilde{\alpha}_7 + \beta_3 = \frac{1}{12} + \widetilde{\beta}_2 + 2\widetilde{\beta}_4, \tag{3.38}$$
$$\alpha_8 + \widetilde{\beta}_4 = \frac{1}{24} + \beta_4, \tag{3.39}$$
$$\widetilde{\alpha}_8 + \beta_4 = \frac{1}{24} + \widetilde{\beta}_4. \tag{3.40}$$

From eq (3.29) and eq (3.30),we can find the values of β_2 and $\widetilde{\beta}_2$,

$$\beta_2 = \frac{3\alpha_3 - 1}{6},$$
$$\widetilde{\beta}_2 = \frac{3\widetilde{\alpha}_3 - 1}{6}.$$

Putting values of β_2 and $\widetilde{\beta}_2$ in eq (3.31) and eq (3.32), we get the reduced equation's independent of beta,

$$
\begin{aligned}
6\alpha_4 + 3\widetilde{\alpha}_3 - 3\alpha_3 =& 1, \\
6\widetilde{\alpha}_4 + 3\alpha_3 - 3\widetilde{\alpha}_3 =& 1.
\end{aligned}
$$

Now, we can find the values of β_3 and $\widetilde{\beta}_3$ by putting β_2 and $\widetilde{\beta}_2$ in eq (3.33) and eq (3.34),

$$
\begin{aligned}
\beta_3 &= \frac{1}{12} + \frac{1}{3}\alpha_5 - \frac{1}{2}\alpha_3, \\
\widetilde{\beta}_3 &= \frac{1}{12} + \frac{1}{3}\widetilde{\alpha}_5 - \frac{1}{2}\widetilde{\alpha}_3.
\end{aligned}
$$

We can find the values of β_4 and $\widetilde{\beta}_4$ from eq (3.35) and eq (3.36) by putting values of β_2, $\widetilde{\beta}_2$, β_3 and $\widetilde{\beta}_3$ in them,

$$
\begin{aligned}
\beta_4 &= -\frac{1}{24} + \alpha_6 + \frac{1}{4}\widetilde{\alpha}_3 - \frac{1}{4}\alpha_3 - \frac{1}{3}\alpha_5, \\
\widetilde{\beta}_4 &= -\frac{1}{24} + \widetilde{\alpha}_6 + \frac{1}{4}\alpha_3 - \frac{1}{4}\widetilde{\alpha}_3 - \frac{1}{3}\widetilde{\alpha}_5.
\end{aligned}
$$

Finally, putting β_2, $\widetilde{\beta}_2$, β_3, $\widetilde{\beta}_3$, β_4 and $\widetilde{\beta}_4$ in eq (3.37) as well as in eq (3.38). Also put β_4 and $\widetilde{\beta}_4$ in eq (3.39) and eq (3.40), we get the following equations,

$$
\begin{aligned}
-12\alpha_7 + 24\alpha_6 - 4\widetilde{\alpha}_5 - 8\alpha_5 + 12\widetilde{\alpha}_3 =& 3, \\
-12\widetilde{\alpha}_7 + 24\widetilde{\alpha}_6 - 4\alpha_5 - 8\widetilde{\alpha}_5 + 12\alpha_3 =& 3, \\
144\alpha_8 + 144\widetilde{\alpha}_6 - 144\alpha_6 - 48\widetilde{\alpha}_5 + 48\alpha_5 - 72\widetilde{\alpha}_3 + 72\alpha_3 =& 6, \\
144\widetilde{\alpha}_8 + 144\alpha_6 - 144\widetilde{\alpha}_6 - 48\alpha_5 + 48\widetilde{\alpha}_5 - 72\alpha_3 + 72\widetilde{\alpha}_3 =& 6.
\end{aligned}
$$

So equations from eq (3.25) to eq (3.40) has been reduced to 10 equations independent of β values written below.

$$\alpha_1 = 1, \tag{3.41}$$
$$\widetilde{\alpha}_1 = 1, \tag{3.42}$$
$$\alpha_2 = \frac{1}{2}, \tag{3.43}$$
$$\widetilde{\alpha}_2 = \frac{1}{2}, \tag{3.44}$$
$$6\alpha_4 + 3\widetilde{\alpha}_3 - 3\alpha_3 = 1, \tag{3.45}$$
$$6\widetilde{\alpha}_4 + 3\alpha_3 - 3\widetilde{\alpha}_3 = 1, \tag{3.46}$$
$$-12\alpha_7 + 24\alpha_6 - 4\widetilde{\alpha}_5 - 8\alpha_5 + 12\widetilde{\alpha}_3 = 3, \tag{3.47}$$
$$-12\widetilde{\alpha}_7 + 24\widetilde{\alpha}_6 - 4\alpha_5 - 8\widetilde{\alpha}_5 + 12\alpha_3 = 3, \tag{3.48}$$
$$144\alpha_8 + 144\widetilde{\alpha}_6 - 144\alpha_6 - 48\widetilde{\alpha}_5 + 48\alpha_5 - 72\widetilde{\alpha}_3 + 72\alpha_3 = 6, \tag{3.49}$$
$$144\widetilde{\alpha}_8 + 144\alpha_6 - 144\widetilde{\alpha}_6 - 48\alpha_5 + 48\widetilde{\alpha}_5 - 72\alpha_3 + 72\widetilde{\alpha}_3 = 6. \tag{3.50}$$

Further, we have simplifying assumptions D(1) and $\widetilde{D}(1)$. We can write D(1) and $\widetilde{D}(1)$ in the form of $\alpha's$ as following,

$$\begin{aligned}\sum_{j=1}^{s} d_j &= \sum_{i,j=1}^{s} \widetilde{b}_i a_{ij} + \sum_{j=1}^{s} b_j \widetilde{c}_j - \sum_{j=1}^{s} b_j \\ &= \widetilde{\alpha}_2 + \alpha_2 - \alpha_1 \\ &= 0.\end{aligned}$$

Similarly, other D and $\widetilde{D}$ conditions are,

$$\widetilde{\alpha}_2 + \alpha_2 - \alpha_1 = 0, \tag{3.51}$$
$$\alpha_2 + \widetilde{\alpha}_2 - \widetilde{\alpha}_1 = 0, \tag{3.52}$$
$$\widetilde{\alpha}_4 + \alpha_3 - \alpha_2 = 0, \tag{3.53}$$
$$\alpha_4 + \widetilde{\alpha}_3 - \widetilde{\alpha}_2 = 0, \tag{3.54}$$
$$\widetilde{\alpha}_7 + \alpha_5 - \alpha_3 = 0, \tag{3.55}$$
$$\alpha_7 + \widetilde{\alpha}_5 - \widetilde{\alpha}_3 = 0, \tag{3.56}$$
$$\widetilde{\alpha}_8 + \alpha_6 - \alpha_4 = 0, \tag{3.57}$$
$$\alpha_8 + \widetilde{\alpha}_6 - \widetilde{\alpha}_4 = 0. \tag{3.58}$$

We can get reduced form of equations eq (3.45) to eq (3.50) by using $D(\xi)$ and $\widetilde{D}(\xi)$ conditions in them. First we can simplify eq (3.49), eq (3.50) by calculating eq (3.49)- 24 $\times$ eq (3.46) and eq (3.50)-24 $\times$ eq (3.45) respectively as follows,

$$24\alpha_6 + 8\widetilde{\alpha}_5 - 8\alpha_5 = 3, \tag{3.59}$$
$$24\widetilde{\alpha}_6 + 8\alpha_5 - 8\widetilde{\alpha}_5 = 3. \tag{3.60}$$

We can again find some more suitable form of equation's eq (3.59) and eq (3.60) by calculating eq (3.59)-4$\widetilde{c}_3$eq (3.45) and eq (3.60)-4$c_3$eq (3.46). Hence, the equations eq (3.49) and eq (3.50) has been reduced in the following form,

$$24\alpha_6 + 8\widetilde{\alpha}_5 - 8\alpha_5 - 24\alpha_4 - 12\widetilde{\alpha}_3 + 12\alpha_3 = -1,$$
$$24\widetilde{\alpha}_6 + 8\alpha_5 - 8\widetilde{\alpha}_5 - 24c_3\widetilde{\alpha}_4 - 12c_3\alpha_3 + 12c_3\widetilde{\alpha}_3 = 3 - 4c_3.$$

Secondly, we can simplify eq (3.47) and eq (3.48) by calculating eq (3.47)-eq (3.59) and eq (3.48)-eq (3.60) respectively as follows which we can ignore,

$$\widetilde{\alpha}_7 + \alpha_5 - \alpha_3 = 0,$$
$$\alpha_7 + \widetilde{\alpha}_5 - \widetilde{\alpha}_3 = 0.$$

Lastly, using equation eq (3.54) in eq (3.45) and using equation eq (3.53) in eq (3.46) we can get the following equation,

$$\alpha_3 + \widetilde{\alpha}_3 = \frac{2}{3}.$$

Hence, there are 7 equations for finding 7 unknowns.

$$\alpha_1 = 1, \tag{3.61}$$
$$\widetilde{\alpha}_1 = 1, \tag{3.62}$$
$$\alpha_2 = \frac{1}{2}, \tag{3.63}$$
$$\widetilde{\alpha}_2 = \frac{1}{2}, \tag{3.64}$$
$$\alpha_3 + \widetilde{\alpha}_3 = \frac{2}{3}, \tag{3.65}$$
$$24\alpha_6 + 8\widetilde{\alpha}_5 - 8\alpha_5 - 24\alpha_4 - 12\widetilde{\alpha}_3 + 12\alpha_3 = -1, \tag{3.66}$$
$$24\widetilde{\alpha}_6 + 8\alpha_5 - 8\widetilde{\alpha}_5 - 24c_3\widetilde{\alpha}_4 - 12c_3\alpha_3 + 12c_3\widetilde{\alpha}_3 = 3 - 4c_3. \tag{3.67}$$

Writing eq (3.61) to eq (3.67) in the form of elementary weights,

$$\begin{aligned}
\sum b_i =&1,\\
\sum \widetilde{b}_i =&1,\\
\sum b_i\widetilde{c}_i =&\frac{1}{2},\\
\sum \widetilde{b}_i c_i =&\frac{1}{2},\\
\sum b_i\widetilde{c}_i^2 + \sum \widetilde{b}_i c_i^2 =&\frac{2}{3},\\
24\sum \widetilde{c}_i b_i \widetilde{a}_{ij} c_j + 8\widetilde{b}_i c_i^3 - 8 b_i \widetilde{c}_i^3 - 24\sum b_i \widetilde{a}_{ij} c_j - 12\sum \widetilde{b}_i c_i^2 + 12\sum b_i \widetilde{c}_i^2 =& -1,\\
24\sum c_i \widetilde{b}_i a_{ij}\widetilde{c}_j + 8 b_i \widetilde{c}_i^3 - 8\widetilde{b}_i c_i^3 - 24 c_3\sum \widetilde{b}_i a_{ij}\widetilde{c}_j - 12\sum b_i\widetilde{c}_i^2 + 12 c_3 \sum \widetilde{b}_i c_i^2 =&3-4c_3.
\end{aligned}$$

We can expand equations for these Butcher tableaux.

$$\begin{array}{c|ccc}
0 & 0 & 0 & 0\\
c_2 & a_{21} & 0 & 0\\
c_3 & a_{31} & a_{32} & 0\\
\hline
 & b_1 & b_2 & b_3
\end{array}
\qquad
\begin{array}{c|ccc}
\widetilde{c}_1 & \widetilde{a}_{11} & 0 & 0\\
\widetilde{c}_2 & \widetilde{a}_{21} & \widetilde{a}_{22} & 0\\
1 & \widetilde{a}_{31} & \widetilde{a}_{32} & \widetilde{a}_{33}\\
\hline
 & \widetilde{b}_1 & \widetilde{b}_2 & \widetilde{b}_3
\end{array}$$

Writing these seven equations in their expanding forms as follows,

$$b_1 + b_2 + b_3 = 1, \tag{3.68}$$

$$\widetilde{b}_1 + \widetilde{b}_2 + \widetilde{b}_3 = 1, \tag{3.69}$$

$$b_1\widetilde{c}_1 + b_2\widetilde{c}_2 + b_3 = \frac{1}{2}, \tag{3.70}$$

$$\widetilde{b}_2 c_2 + \widetilde{b}_3 c_3 = \frac{1}{2}, \tag{3.71}$$

$$b_1\widetilde{c}_1^2 + b_2\widetilde{c}_2^2 + b_3 + \widetilde{b}_2 c_2^2 + \widetilde{b}_3 c_3^2 = \frac{2}{3}, \tag{3.72}$$

$$\begin{aligned}24b_2(\widetilde{c}_2\widetilde{a}_{22}c_2 - \widetilde{a}_{22}c_2) + \widetilde{b}_2 c_2^2(8c_2 - 12) + \widetilde{b}_3 c_3^2(8c_3 - 12)&\\ +b_1\widetilde{c}_1^2(12 - 8\widetilde{c}_1) + b_2\widetilde{c}_2^2(12 - 8\widetilde{c}_2) + 4b_3 = -1,&\end{aligned} \tag{3.73}$$

$$\begin{aligned}24\widetilde{b}_2(c_2^2\widetilde{c}_1 - c_3 c_2\widetilde{c}_1) + b_1\widetilde{c}_1^2(8\widetilde{c}_1 - 12c_3) + b_2\widetilde{c}_2^2(8\widetilde{c}_2 - 12c_3)&\\ +b_3(8 - 12c_3) + \widetilde{b}_2 c_2^2(12c_3 - 8c_2) + 4\widetilde{b}_3 c_3^3 = 3 - 4c_3.&\end{aligned} \tag{3.74}$$

Take $c_2, c_3, \widetilde{c}_1, \widetilde{c}_2$ as parameters. Solving 7 equations numbered from eq (3.68) to eq (3.74), we can find 7 unknowns which includes b's, $\widetilde{b}'s$ and $\widetilde{a}_{22}$. Also using consistency condition, we can have the value of $\widetilde{a}_{21}$,

$$\widetilde{c}_2 = \widetilde{a}_{21} + \widetilde{a}_{22}. \tag{3.75}$$

Writing equation eq (3.57) in the form of elementary weights and its expanded form in terms of coefficients, we can find a_{32},

$$\begin{aligned}\sum \widetilde{b}_i a_{ij} \widetilde{a}_{jk} c_k + \sum \widetilde{c}_i b_i \widetilde{a}_{ij} c_j - \sum b_i \widetilde{a}_{ij} c_j = 0,\\ \widetilde{b}_3(a_{32}\widetilde{a}_{22}c_2) + b_2(\widetilde{c}_2\widetilde{a}_{22}c_2 - \widetilde{a}_{22}c_2) = 0.\end{aligned} \tag{3.76}$$

Using consistency conditions, a_{21} and a_{31} can be calculated,

$$c_2 = a_{21}, \tag{3.77}$$

$$c_3 = a_{31} + a_{32}. \tag{3.78}$$

Finally, writing eq (3.54) and eq (3.58) in the form of elementary weights and their expanded form of coefficients, we can find $\widetilde{a}_{32}$ and $\widetilde{a}_{33}$ by solving their expanded form.

$$\begin{aligned}\sum b_i \widetilde{a}_{ij} c_j + \sum \widetilde{b}_i c_i^2 - \sum \widetilde{b}_i c_i &= 0,\\ \sum b_i \widetilde{a}_{ij} a_{jk} \widetilde{c}_k + \sum c_i \widetilde{b}_i a_{ij} \widetilde{c}_j - \sum \widetilde{b}_i a_{ij} \widetilde{c}_j &= 0,\\ b_2\widetilde{a}_{22}c_2 + b_3(\widetilde{a}_{32}c_2 + \widetilde{a}_{33}c_3) + \widetilde{b}_2(c_2^2 - c_2) + \widetilde{b}_3(c_3^2 - c_3) &= 0, \qquad (3.79)\\ b_2(\widetilde{a}_{22}c_2\widetilde{c}_1) + b_3(\widetilde{a}_{32}c_2\widetilde{c}_1 + \widetilde{a}_{33}a_{31}\widetilde{c}_1 + \widetilde{a}_{33}a_{32}\widetilde{c}_2) + \widetilde{b}_2(c_2^2\widetilde{c}_1 - c_2\widetilde{c}_1) & \qquad (3.80)\\ + c_3\widetilde{b}_3(a_{31}\widetilde{c}_1 + a_{32}\widetilde{c}_2) + \widetilde{b}_3(a_{31}\widetilde{c}_1 + a_{32}\widetilde{c}_2) &= 0.\end{aligned}$$

$\widetilde{a}_{11}, \widetilde{a}_{31}$ can be found using consistency conditions,

$$\widetilde{c}_1 = \widetilde{a}_{11}, \tag{3.81}$$

$$1 = \widetilde{a}_{31} + \widetilde{a}_{32} + \widetilde{a}_{33}. \tag{3.82}$$

Lastly, choosing the values of parameters $c_2 = \frac{1}{4}, c_3 = \frac{1}{2}, \widetilde{c}_1 = \frac{1}{3}, \widetilde{c}_2 = \frac{2}{3}$ and finding unknown values of Butcher tableaux by solving eq (3.68) to eq (3.82), we get the following α and $\widetilde{\alpha}$ method.

$$\begin{array}{c|ccc} 0 & 0 & 0 & 0\\ \frac{1}{4} & \frac{1}{4} & 0 & 0\\ \frac{1}{2} & \frac{37}{116} & \frac{21}{116} & 0\\ \hline & -\frac{1}{8} & \frac{7}{4} & -\frac{5}{8} \end{array} \qquad \begin{array}{c|ccc} \frac{1}{3} & \frac{1}{3} & 0 & 0\\ \frac{2}{3} & \frac{44}{63} & -\frac{2}{63} & 0\\ 1 & -\frac{5}{3} & \frac{236}{45} & -\frac{116}{45}\\ \hline & \frac{20}{9} & -\frac{40}{9} & \frac{29}{9} \end{array}$$

Further moving towards finding the starting methods β and $\widetilde{\beta}$, we need to find the values of $\alpha_3, \widetilde{\alpha}_3, \alpha_5, \widetilde{\alpha}_5, \alpha_7, \widetilde{\alpha}_7$. Firstly,

$$\begin{aligned}\alpha_3 &= \sum b_i \widetilde{c}_i^2 = b_1 \widetilde{c}_1^2 + b_2 \widetilde{c}_2^2 + b_3 \\ &= -\frac{1}{8}\left(\frac{1}{3}\right)^3 + \frac{7}{4}\left(\frac{2}{3}\right)^2 - \frac{5}{8} \\ &= \frac{5}{36}\end{aligned}$$

Similarly, we have $\widetilde{\alpha}_3 = \frac{19}{36}$, $\alpha_7 = -\frac{1}{9}$, $\widetilde{\alpha}_7 = \frac{1}{3}$, $\alpha_7 = \frac{7}{36}$, $\widetilde{\alpha}_7 = \frac{1}{4}$. Moreover, we have

$$\beta_1 = 0, \tag{3.83}$$
$$\widetilde{\beta}_1 = 0. \tag{3.84}$$

Since,

$$\alpha_3 = \frac{1}{3} + 2\beta_2.$$

Therefore,

$$\beta_2 = -\frac{7}{72}. \tag{3.85}$$

Similarly, we have

$$\widetilde{\beta}_2 = \frac{7}{72}, \tag{3.86}$$
$$\beta_3 = -\frac{5}{216}, \tag{3.87}$$
$$\widetilde{\beta}_3 = -\frac{5}{72}, \tag{3.88}$$
$$\beta_4 = \frac{5}{72}, \tag{3.89}$$
$$\widetilde{\beta}_4 = \frac{5}{216}. \tag{3.90}$$

Writing eq (3.83) to eq (3.90) in the form of elementary weights,

$$\begin{aligned}
\sum b_i &= 0,\\
\sum \widetilde{b}_i &= 0,\\
\sum b_i\widetilde{c}_i &= -\frac{7}{72},\\
\sum \widetilde{b}_i c_i &= \frac{7}{72},\\
\sum b_i\widetilde{c}_i^2 &= -\frac{5}{216},\\
\sum \widetilde{b}_i c_i^2 &= -\frac{5}{72},\\
\sum b_i\widetilde{a}_{ij}c_i &= \frac{5}{72},\\
\sum \widetilde{b}_i a_{ij}\widetilde{c}_i &= \frac{5}{216}.
\end{aligned} \tag{3.91}$$

Writing the set of equations (3.91) in expanded form for the Butcher tableaux

$$\begin{array}{c|ccc}
0 & 0 & 0 & 0\\
C_2 & A_{21} & 0 & 0\\
C_3 & A_{31} & A_{32} & 0\\
\hline
 & B_1 & B_2 & B_3
\end{array}
\qquad
\begin{array}{c|ccc}
0 & 0 & 0 & 0\\
\widetilde{C}_2 & \widetilde{A}_{21} & 0 & 0\\
\widetilde{C}_3 & \widetilde{A}_{31} & \widetilde{A}_{32} & 0\\
\hline
 & \widetilde{B}_1 & \widetilde{B}_2 & \widetilde{B}_3
\end{array}$$

as follows,

$$B_1 + B_2 + B_3 = 0, \tag{3.92}$$

$$\widetilde{B}_1 + \widetilde{B}_2 + \widetilde{B}_3 = 0, \tag{3.93}$$

$$B_2\widetilde{C}_2 + B_3\widetilde{C}_3 = -\frac{7}{72}, \tag{3.94}$$

$$\widetilde{B}_2 C_2 + \widetilde{B}_3 C_3 = \frac{7}{72}, \tag{3.95}$$

$$B_2\widetilde{C}_2^2 + B_3\widetilde{C}_3^2 = -\frac{5}{216}, \tag{3.96}$$

$$\widetilde{B}_2 C_2^2 + \widetilde{B}_3 C_3^2 = -\frac{5}{72}, \tag{3.97}$$

$$B_3\widetilde{A}_{32}C_3 = \frac{5}{72}, \tag{3.98}$$

$$\widetilde{B}A_{32}\widetilde{C}_3 = \frac{5}{216}. \tag{3.99}$$

Solving eq (3.92) to eq (3.99), we will have the following β and $\widetilde{\beta}$ method.

$$
\begin{array}{c|ccc}
0 & 0 & 0 & 0 \\
\frac{1}{4} & \frac{1}{4} & 0 & 0 \\
\frac{1}{2} & \frac{16}{27} & -\frac{5}{54} & 0 \\
\hline
 & \frac{1}{3} & -\frac{3}{8} & \frac{1}{24}
\end{array}
\qquad
\begin{array}{c|ccc}
0 & 0 & 0 & 0 \\
\frac{1}{3} & \frac{1}{3} & 0 & 0 \\
\frac{2}{3} & -6 & \frac{20}{3} & 0 \\
\hline
 & -\frac{41}{36} & \frac{17}{9} & -\frac{3}{4}
\end{array}
$$

Now moving towards finding β^{-1} of β method and $\widetilde{\beta}^{-1}$ of $\widetilde{\beta}$ method, we will use the procedure defined in Chapter 3 to find the inverse of PRK method. Hence the final β^{-1} and $\widetilde{\beta}^{-1}$ methods are given below,

$$
\begin{array}{c|ccc}
0 & -\frac{1}{3} & \frac{3}{8} & -\frac{1}{24} \\
\frac{1}{4} & -\frac{1}{12} & \frac{3}{8} & -\frac{1}{24} \\
\frac{1}{2} & \frac{7}{27} & \frac{61}{216} & -\frac{1}{24} \\
\hline
 & -\frac{1}{3} & \frac{3}{8} & -\frac{1}{24}
\end{array}
\qquad
\begin{array}{c|ccc}
0 & \frac{41}{36} & -\frac{17}{9} & \frac{3}{4} \\
\frac{1}{3} & \frac{53}{36} & -\frac{17}{9} & \frac{3}{4} \\
\frac{2}{3} & -\frac{175}{36} & \frac{43}{9} & \frac{3}{4} \\
\hline
 & \frac{41}{36} & -\frac{17}{9} & \frac{3}{4}
\end{array}
$$

3.3 Order verification

The Harmonic Oscillator problem is,

$$y' = z, \qquad y(0) = 1, \tag{3.100}$$
$$z' = -y, \qquad z(0) = 0. \tag{3.101}$$

The exact solution for Harmonic Oscillator is $y = cos(x)$ and $z = sin(x)$. For verifying the effective order 4 behaviour, we follow the given steps:

1. Use the first starting method β to perturb y_0 to get $\bar{y}_0$. Use the second starting method $\widetilde{\beta}$ to perturb z_0 to get $\bar{z}_0$.

2. Determine the numerical solutions at $x_n = x_0 + h$ for n number of iteration using the method α on $\bar{y}_0$ to get $\bar{y}_n$ and using the method $\widetilde{\alpha}$ on $\bar{z}_0$ to get $\bar{z}_n$.

3. Determine exact solutions to obtain $y(x_n)$ and $z(x_n)$ at x_n. Use the method β to perturb $y(x_n)$ to obtain $\bar{y}(x_n)$ and use the method $\widetilde{\beta}$ to perturb $z(x_n)$ to obtain $\bar{z}(x_n)$.

4. Take the difference between numerical and exact solution to get global error, i.e $\| \bar{y}_n - \bar{y}(x_n) \|$.

Calculations for effective order 4 behaviour is given in Table 3.7.

c	h	global error	ratio
5	0.628318530717959	-0.033218943708652	
			0.0548
10	0.314159265358979	-0.001819699406986	
			0.0552
20	0.157079632679490	-1.004698861695186e-04	
			0.0577
40	0.078539816339745	-5.799977310427806e-06	
			0.0598
80	0.039269908169872	-3.466542881636059e-07	
			0.0610
160	0.019634954084936	-2.115858066531473e-08	
			0.0617
320	0.009817477042468	-1.306377228615929e-09	

Table 3.7: Global errors

True global error can be calculated for the numerical solution with step-sizes $h = 0.009817477042468$ and $h = 0.019634954084936$ as

$$ratio = \frac{yerror_{320}}{yerror_{160}} = 0.0617.$$

Solving $(1/2)^p = 0.0619$ for p (order of the method), we get p = 4 (assuming p must be integer).

Chapter 4

Conclusion

In Chapter 1, we gave a brief review of RK methods and discussed about the algebraic properties of rooted trees associated with RK methods i.e, groups of RK methods, Hopf algebra of rooted trees and effective order of RK methods.

In Chapter 2, we discussed about PRK methods to solve the system of ODE's . We extended the idea of Hopf algebra of rooted trees to the bi-color rooted trees and pointed out a connection between Hopf algebra of bi-color rooted trees and the group of PRK methods.

In Chapter 3, we have constructed an effective order three of PRK method by taking 2-stage PRK method and an effective order four of PRK method by taking 3-stage PRK.

The advantage of constructing effective order PRK methods with fewer stages is the low computational cost which is the major concern in finding the approximated solution of a large system of ODE's.

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