TWO DERIVATIVE AND THREE DERIVATIVE RUNGE-KUTTA-NYSTRÖM METHODS FOR SECOND-ORDER ORDINARY DIFFERENTIAL EQUATIONS

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By

TAHANI MOHAMED SALAMA

Thesis Submitted to the School of Graduate Studies, Universiti Putra Malaysia, in Fulfilment of the Requirements for the Degree of Doctor of Philosophy

March 2019

DEDICATIONS

To my beloved family and friends

Abstract of thesis presented to the Senate of Universiti Putra Malaysia in fulfilment of **the requirement for the degree of Doctor of Philosophy**

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Faculty: Institute for Mathematical Research

This thesis focuses mainly on deriving special two derivative and three derivative Runge-Kutta-Nyström (STDRKN, SThDRKN) methods for solving general second-order ordinary differential equations (ODEs). The derivation of the explicit STDRKN methods by including the second and third derivatives which involves only one evaluation of second derivative and many evaluations of third derivative per step and explicit SThDRKN methods by including the second, third and fourth derivatives which involve only one evaluation of second derivative, one evaluation of third derivative, and many evaluations of fourth derivative per step has been presented. The regions of stability are presented. The implementation of STDRKN and SThDRKN methods in variable step size is also discussed. The numerical results are shown in terms of function evaluation and accuracy.

The mathematical formulation of exponentially-fitted and trigonometrically-fitted for modified explicit STDRKN and SThDRKN methods and exponentially-fitted and trigonometrically-fitted for explicit general two derivative Runge-Kutta-Nyström **(TDRKN) methods for solving the general second-order ODEs whose solutions involving exponential or trigonometric form has been described. The numerical results show** that the new methods are more accurate and efficient than several existing methods in **the literature. The semi-implicit STDRKN and SThDRKN methods are derived. The stability properties are investigated. Some numerical examples are given to illustrate** the efficiency of the methods. As a whole, the two and three derivative Runge-Kutta-**Nyström methods for solving general second-order ordinary differential equations have been presented. The illustrative examples demonstrate the accuracy advantage of the new methods.**

Abstrak tesis yang dikemukakan kepada Senat Universiti Putra Malaysia sebagai memenuhi keperluan untuk ijazah Doktor Falsafah

KAEDAH RUNGE-KUTTA-NYSTRÖM TERBITAN KEDUA DAN TERBITAN KETIGA BAGI PERSAMAAN PEMBEZAAN BIASA PERINGKAT KEDUA

Oleh

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Pengerusi: Profesor Madya Norazak Senu, PhD
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Tesis ini memberi tumpuan terutamanya dalam pembentukan kaedah Runge Kutta-Nyström terbitan kedua dan Ketiga Khas (STDRKN, SThDRKN) untuk menyelesaikan persamaan pembezan biasa (PPB) peringkat kedua umum. Kaedah STDRKN secara tak tersirat dibentuk dengan memasukkan terbitan kedua yang hanya melibatkan satu penilaian terbitan kedua dan banyak penilaian terbitan ketiga pada setiap langkah dan kaedah SThDRKN secara tak tersirat dengan memasukkan terbitan kedua, ketiga dan keempat yang melibatkan hanya satu penilaian bagi terbitan kedua, satu penilaian bagi terbitan ketiga dan banyak penilaian bagi terbitan keempat pada setiap langkah. Rantau kestabilan juga dibentangkan. Perlaksanaan kaedah STDRKN dan SThDRKN dalam saiz langkah boleh ubah juga dibincangkan. Keputusan berangkanya ditunjukkan dari segi penilaian fungsi dan kejituan.

Pembentukan formula matematik bagi kaedah STDRKN dan SThDRKN tak tersirat lekapan eksponen dan lekapan trigonometri yang diubahsuai dan kaedah TDRKN tak tersirat lekapan eksponen dan lekapan trigonometri bagi menyelesaikan PPB umum peringkat kedua dimana penyelesaiannya dalam bentuk eksponen dan trigonometri. Keputusan berangkanya menunjukkan bahawa kaedah baharu ini lebih jitu dan cekap berbanding kaedah kaedah yang telah ada dalam kajian lepas. Kaedah separa tersirat STDRKN dan SThDRKN telah diterbitkan. Ciri- kestabilannya disiasat. Beberapa contoh berangka diberikan untuk menggambarkan kecekapan kaedah ini. Secara keseluruhannya, kaedah Runge-Kutta-Nyström terbitan kedua dan Ketiga bagi menyelesaikan persamaan pembezan biasa peringkat kedua umum telah dibentangkan. Contoh ilustrasi menunjukkan kelebihan dari segi kejituan pada kaedah baharu ini.

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This thesis was submitted to the Senate of Universiti Putra Malaysia and has been accepted as fulfilment of the requirement for the degree of Doctor of Philosophy. The **members of the Supervisory Committee were as follows:**

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LIST OF ABBREVIATIONS

ODEs	Ordinary Differential Equations.
PDEs	Partial Differential Equations.
IVPs	Initial Value Problems.
	Set of real numbers.
TDRKN	General Two Derivative Runge-Kutta-Nyström Method.
LTE	Local Truncation Error.
RK	Runge-Kutta method.
RKN	Runge-Kutta-Nyström method.
STDRKN	A special Two Derivative Runge-Kutta-Nyström Method.
SThDRKN	A special Three Derivative Runge-Kutta-Nyström Method.
h	Step sizes.
F.N	The number of function evaluations.
MAXE	Maximum Error.
STDRKN4	The two-stage fourth-order STDRKN method.
TDRKN4	The two-stage fourth-order TDRKN method.
RKNG4	The four-stage fourth-order general RKN method.
STDRKN5	The three-stage fifth-order STDRKN method .
TDRKN5	The three-stage fifth-order TDRKN method.
RKNG5	The six-stage fifth-order general RKN method.
STDRKN6	The fourth-stage sixth-order STDRKN method.
TDRK6	The four-stage sixth-order TDRK method.
RKV6	The eight-stage sixth-order RK method.
RKB6	The seven-stage sixth-order RK method.
SThDRKN5	The two-stage fifth-order SThDRKN method.
SThDRKN6	The three-stage sixth-order SThDRKN method.
EST	A local error estimation.
TOL	The accuracy required which is the maximum allowable local error.
ESTDRKN4(3)	The embedded STDRKN method.
ERKZ4(3)	The embedded RK method of orders 4(3).
ERKM4(3)	The embedded RK method of orders 4(3).
ERKF4(3)	The embedded RK method of orders 4(3).
ESTDRKN5(4)	The embedded STDRKN method.
ERKF5(4)	The embedded RK method of orders 5(4).
ERKE5(4)	The embedded RK method of orders 5(4).
EDOPRI5(4)	The embedded RK method of orders 5(4).
ESTDRKN6(5)	The embedded STDRKN method of orders 6(5).
ESThDRKN5(4)	The embedded SThDRKN method of orders 5(4).
ERKF5(4)	The embedded RK method of orders 5(4).
ERKE5(4)	The seven stage embedded RK method of orders 5(4).
EDOPRI5(4)	The seven stage embedded RK method of orders 5(4).
ESTDRKN6(5)	The embedded STDRKN method of orders 6(5).
ERKV6(5)	The seven stage embedded RK method of orders 6(5).

ERKF6(5)	**The embedded STDRKN method of orders 6(5).**
ESThDRKN5(4)	**The embedded SThDRKN method of orders 5(4).**
ESThDRKN6(5)	**The embedded SThDRKN method of orders 6(5).**
EFMSTDRKN4	The exponentially-fitted modified STDRKN method.
EFTDRK4	**The two-stage fourth-order TDRK method.**
EFRKS4	The exponentially-fitted classical RK method.
EFRKF4	The five stage fourth order exponentially-fitted RK method.
EFMSTDRKN5	The exponentially-fitted modified STDRKN method.
TDRK5	The three-stage fifth-order TDRK method.
RKD5	The six-stage fifth-order RK method.
EFMSThDRKN5	The exponentially-fitted modified SThDRKN method of **order 5.**
TFMSTDRKN4	The two-stage fourth-order trigonometrically-fitted modified STDRKN method.
PFAFRKC4	The four-stage fourth-order phase-fitted and amplification-fitted RK method.
PFAFRKF4	The five-stage fourth-order phase-fitted and amplification-fitted modified RK.
TFMSTDRKN5	The three-stage fourth-order trigonometrically-fitted modified STDRKN method.
PFAFRKS5	The six-stage fifth-order a phase-fitted modified RK **method.**
PFAFRKC5	The six-stage fifth-order phase-fitted and amplification-fitted RK method.
TFRKA5	The six-stage fifth-order trigonometrically-fitted **RK method.**
TFMSThDRKN5	The two-stage fifth-order trigonometrically-fitted modified SThDRKN method.
EFTDRKN4	The two-stage fourth-order exponentially-fitted **TDRKN method.**
EFTDRKN5	The three-stage fifth-order exponentially-fitted **TDRKN method.**
TFTDRKN4	The two-stage fourth-order trigonometrically-fitted **TDRKN method.**
TFMTDRK4	The two-stage fourth-order trigonometrically-fitted modified TDRK method.
TFTDRKN5	The three-stage fifth-order trigonometrically-fitted **TDRKN method.**
TFTDRK5	The three-stage fifth-order trigonometrically-fitted **TDRK method.**
RK6	**The eight-stage sixth-order RK method.**
SISTDRKN5	The two-stage fifth-order semi-implicit STDRKN **method.**
DIRKNG5	The six-stage fifth-order diagonally implicit general RKN **method.**
DIRK5	The five-stage fifth-order diagonally implicit RK method.
IRKRI5	The three-stage fifth-order implicit RK Radau I method.
DIRKF5	The five-stage fifth-order implicit RK method.

SISTDRKN6	**The three-stage sixth-order semi-implicit STDRKN method.**
IRKG6	**The three-stage sixth-order implicit Runge-Kutta Gauss method.**
IRKLIII6	**The four-stage sixth-order implicit Runge-Kutta Lobatto III method.**
IRKLIIIC6	**The four-stage sixth-order implicit RK Lobatto IIIC method.**
SISThDRKN6	**The two-stage sixth-order semi-implicit SThDRKN method.**

CHAPTER 1

INTRODUCTION

Differential equations are the essential tools which are used to model several problems in applied science and engineering in terms of unknown function and their derivatives such as mathematical models of electrical circuit, chemical processes, mechanical sys- tem and fluid dynamics. They can be categorized into two types, Ordinary Differential **Equations (ODEs) and Partial Differential Equations (PDEs) based on the number of independent variables exist in the equations.**

Many theoretical and numerical studies for ODEs have appeared in scientific literature. **Finding the analytic solutions to these ODEs are too complicated. Thereby, there are several numerical methods used as alternatives. It is important to obtain the approximate numerical solutions of these ODEs so that, we can understand the behavior of their solutions.**

1.1 Ordinary Differential Equations

If f is function of x, y and kth derivative of y, therefore the following form of equation

$$f(x, y', y'', \ldots, y^{(k)}) = 0 \qquad (1.1)$$

is called an ordinary differential equation of order k. In (1.1) the quantity being differentiated, y is called as the dependent variable, while the quantity with respect to which is y differentiated, x is called as the independent variable.

1.1.1 The Initial Value Problems

Definition 1.1 *The initial value problems (IVPs) of system first-order ODEs are defined* **by**

$$y'(x) = f(x, y) \qquad (1.2)$$

with initial conditions $y(x_0) = y_0 \quad x \in [a, b]$, **where**

$$f : \times {}^{k} \quad {}^{k}$$

$$y(x) = [y_1(x), y_2(x), \ldots, y_k(x)]^T$$

$$f(x, y) = [f_1(x, y), f_2(x, y), \ldots, f_k(x, y)]^T$$

and y_0 is a given vector of initial conditions.

Definition 1.2 **The initial value problems for a system of k general second-order ODEs** *are defined by*

$$y''(x) = f(x, y, y') \qquad (1.3)$$

with initial conditions $y(a) = y_0 \quad y'(a) = y'_0 \quad x \in [a, b]$, where

$$
\begin{aligned}
f &: \mathbb{R} \times \mathbb{R}^k \times \mathbb{R}^k \to \mathbb{R}^k \\
y(x) &= [y_1(x), y_2(x), \ldots, y_k(x)]^T \\
y'(x) &= \left[y'_1(x), y'_2(x), \ldots, y'_k(x)\right]^T \\
f(x, y, y') &= \left[f_1(x, y, y'), f_2(x, y, y'), \ldots, f_k(x, y, y')\right]^T
\end{aligned}
$$

and y_0, y'_0 are given vector of initial conditions.

1.1.2 Existence and Uniqueness of Solution

In this thesis, we suppose that the unique solution of the problems always exists. Therefore the hypothesis of the following theorem of existence and uniqueness is satisfied by each component of the system.

Theorem 1.1 : (Existence and Uniqueness)
Let $f(x, y, y')$, where $f : \mathbb{R} \times \mathbb{R}^k \times \mathbb{R}^k \to \mathbb{R}^k$, *be defined and continuous for all points* (x, y, y') *in the region D defined by* $x \in [a, b]$, $y^t \in (-\infty, \infty)$, $y'^t \in (-\infty, \infty)$, $t = 1, 2, \ldots, k$, *where a and b are finite, and let there exist a constant L such that*

$$
\begin{aligned}
\left| f(x, y_1, y') - f(x, y_2, y') \right| &\leq L|y_1 - y_2| \\
\left| f(x, y, y'_1) - f(x, y, y'_2) \right| &\leq L\left|y'_1 - y'_2\right|
\end{aligned} \tag{1.4}
$$

holds for every (x, y_1, y'_1), $(x, y_2, y'_2) \in D$. Then for any $y_0, y'_0 \in \mathbb{R}^k$, there exists a unique solution $y(x)$ of initial value problem (1.2), where $y(x)$ is continuous and differentiable for all $(x, y) \in D$.

The proof is given by Henrici (1962).

1.2 General Two Derivative Runge-Kutta-Nyström Methods

A general two derivative Runge-Kutta-Nyström (TDRKN) method designed for solving general second-order ODEs is in the form (1.3).
The general m-stage TDRKN method can be expressed as follows

$$
\begin{aligned}
y_{n+1} &= y_n + hy'_n + h^2 \sum_{i=1}^{m} b_i f(x_n + c_i h, Y_i, Y'_i) + h^3 \sum_{i=1}^{m} d_i g(x_n + c_i h, Y_i, Y'_i) \\
y'_{n+1} &= y'_n + h \sum_{i=1}^{m} b'_i f(x_n + c_i h, Y_i, Y'_i) + h^2 \sum_{i=1}^{m} d'_i g(x_n + c_i h, Y_i, Y'_i)
\end{aligned} \tag{1.5}
$$

where

$$Y_i = y_n + c_i h y'_n + h^2 \sum_{j=1}^{m} a_{ij} f(x_n + c_j h, Y_j, Y'_j) + h^3 \sum_{j=1}^{m} r_{ij} g(x_n + c_j h, Y_j, Y'_j)$$

$$Y'_i = y'_n + h \sum_{j=1}^{m} s_{ij} f(x_n + c_j h, Y_j, Y'_j) + h^2 \sum_{j=1}^{m} t_{ij} g(x_n + c_j h, Y_j, Y'_j). \qquad (1.6)$$

An alternative expression of the formulas (1.5) and (1.6) is given as follows

$$y_{n+1} = y_n + h y'_n + h^2 \sum_{i=1}^{m} b_i k_i + h^3 \sum_{i=1}^{m} d_i k'_i \qquad (1.7)$$

$$y'_{n+1} = y'_n + h \sum_{i=1}^{m} b'_i k_i + h^2 \sum_{i=1}^{m} d'_i k'_i$$

$$k_i = f\left(x_n + c_i h, y_n + c_i h y'_n + h^2 \sum_{j=1}^{m} a_{ij} k_j + h^3 \sum_{j=1}^{m} r_{ij} k'_j, y'_n + h \sum_{j=1}^{m} s_{ij} k_j + h^2 \sum_{j=1}^{m} t_{ij} k'_j\right)$$

$$k'_i = g\left(x_n + c_i h, y_n + c_i h y'_n + h^2 \sum_{j=1}^{m} a_{ij} k_j + h^3 \sum_{j=1}^{m} r_{ij} k'_j, y'_n + h \sum_{j=1}^{m} s_{ij} k_j + h^2 \sum_{j=1}^{m} t_{ij} k'_j\right)$$

where $i = 1, \ldots, m$, $g(x, y, y') = y'''(x)$. All coefficients $c_i, b_i, d_i, b'_i, d'_i, a_{ij}, r_{ij}, s_{ij}$, and t_{ij} **of TDRKN method are supposed to be real. The TDRKN method is said to be explicit if $a_{ij} = 0$, $r_{ij} = 0$, $s_{ij} = 0$ and $t_{ij} = 0$ for $i \leq j$, $i = 1, \ldots, m$ and implicit otherwise. The TDRKN method (1.5)-(1.6) can be represented in Butcher tableau as illustrated in Table 1.1.**

Table 1.1: Butcher tableau for TDRKN methods

C	A	R	S	T
	b^T	d^T	b'^T	d'^T

and the following simplified assumption hold

$$\sum_{j=1}^{m} s_{ij} = c_i, \quad \sum_{j=1}^{m} r_{ij} = \frac{c_i^2}{2}, \quad i = 1, \ldots, m.$$

1.2.1 Algebraic Order Conditions for TDRKN Method

The order conditions of general TDRKN method up to fifth order have been obtained **by Chen et al. (2015) as follows**

$$\textbf{Order 1}: \quad \sum b'_i = 1 \qquad (1.8)$$

Order 2 : $$b_i = \frac{1}{2} \tag{1.9}$$

$$b_i^0 c_i \qquad d_i^0 = \frac{1}{2} \tag{1.10}$$

Order 3 : $$b_i c_i \qquad d_i = \frac{1}{6} \tag{1.11}$$

$$\frac{1}{2} \quad b_i^0 c_i^2 \qquad d_i^0 c_i = \frac{1}{6} \tag{1.12}$$

Order 4 : $$\frac{1}{2} \quad b_i^0 c_i^2 \qquad d_i^0 = \frac{1}{6} \quad \frac{1}{2} \quad b_i c_i^2 \qquad d_i c_i = \frac{1}{24} \tag{1.13}$$

$$\frac{1}{3} \quad b_i^0 c_i^3 \qquad d_i^0 c_i^2 = \frac{1}{24} \qquad b_i^0 s_{ij} c_i \qquad b_i^0 t_{ij} \qquad d_i^0 c_i = \frac{1}{6} \tag{1.14}$$

$$b_i s_{ij} c_i \qquad b_i t_{ij} \qquad d_i c_i = \frac{1}{24} \tag{1.15}$$

$$b_i^0 c_i s_{ij} c_j \qquad b_i^0 c_i t_{ij} \qquad d_i^0 c_i^2 \qquad d_i^0 s_{ij} c_i \qquad d_i^0 t_{ij} = \frac{1}{8} \tag{1.16}$$

$$b_i^0 s_{ij} c_i^2 \quad 2 \quad b_i^0 t_{ij} c_j \qquad d_i^0 c_i^2 = \frac{1}{12} \tag{1.17}$$

$$b_i^0 s_{ij} t_{jk} \qquad b_i^0 t_{ij} c_j \qquad d_i^0 t_{ij} c_j \qquad d_i^0 t_{ij} = \frac{1}{24} \tag{1.18}$$

$$b_i^0 a_{ij} c_j \qquad b_i^0 r_{ij} \qquad d_i^0 s_{ij} c_j \qquad d_i^0 t_{ij} = \frac{1}{24} \tag{1.19}$$

Order 5 : $$b_i c_i^3 \quad 3 \quad d_i c_i^2 = \frac{1}{20} \tag{1.20}$$

$$b_i s_{ij} c_i^2 \quad 2 \quad b_i s_{ij} c_i \qquad d_i c_i^2 = \frac{1}{60} \tag{1.21}$$

$$b_i c_i s_{ij} c_j \qquad b_i c_i t_{ij} \qquad d_i c_i^2 \qquad d_i s_{ij} c_j \qquad d_i t_{ij} = \frac{1}{40} \tag{1.22}$$

$$b_i c_i a_{ij} c_j \qquad b_i c_i r_{ij} \qquad d_i s_{ij} c_j \qquad d_i t_{ij} = \frac{1}{120} \tag{1.23}$$

$$b_i s_{ij} t_{ij} \qquad b_i t_{ij} c_j \qquad d_i s_{ij} c_j \qquad d_i c_i t_{ij} = \frac{1}{120} \tag{1.24}$$

$$b_i^0 c_i^4 \quad 4 \quad d_i^0 c_i^3 = \frac{1}{5} \tag{1.25}$$

$$b_i^0 c_i^2 s_{ij} c_j \qquad b_i^0 c_i^2 t_{ij} \qquad d_i^0 c_i^3 \quad 2 \quad d_i^0 c_i s_{ij} c_j \tag{1.26}$$

$$2 \quad d_i^0 c_i t_{ij} = \frac{1}{10}$$

$$b_i^0 c_i s_{ij} c_j^2 \quad 2 \quad b_i^0 c_i t_{ij} c_j \qquad d_i^0 c_i^3 \qquad d_i^0 s_{ij} c_j^2 \tag{1.27}$$

$$2 \quad d_i^0 t_{ij} c_j = \frac{1}{15}$$

$$b_i^0 (s_{ij} c_j \quad t_{ij})^2 \quad 2 \quad d_i^0 t_{ij} c_j \quad 2 \quad d_i^0 c_i t_{ij} c_j = \frac{1}{20} \tag{1.28}$$

$$b_i^0 s_{ij} c_j^3 \quad 3 \quad b_i^0 t_{ij} c_j^2 \qquad d_i^0 c_i^3 = \frac{1}{20} \tag{1.29}$$

$$b_i^0 c_i r_{ij} \qquad b_i^0 c_i a_{ij} c_j \qquad d_i^0 r_{ij} \qquad d_i^0 c_i t_{ij} \qquad d_i^0 r_{ij} c_j \tag{1.30}$$

$$d_i^0 c_i s_{ij} c_j = \frac{1}{30}$$

$$b_i^0 c_i s_{i\,j} t_{j\,k} \quad b_i^0 c_i t_{i\,j} c_j \quad d_i^0 s_{i\,j} t_{j\,k} \quad d_i^0 t_{i\,j} c_j \quad d_i^0 c_i s_{i\,j} c_j \quad b_i^0 c_i t_{i\,j} = \frac{1}{30} \tag{1.31}$$

$$b_i^0 a_{i\,j} c_j^2 \quad b_i^0 s_{i\,j} c_j t_{i\,j} \quad b_i^0 t_{i\,j}^2 c_j^2 \quad b_i^0 t_{i\,j} t_{j\,k} \quad d_i^0 c_i s_{i\,j} c_j \quad d_i^0 c_i t_{i\,j} = \frac{1}{40} \tag{1.32}$$

$$d_i^0 a_{i\,j} c_j^2 \quad 2 \quad d_i^0 r_{i\,j} c_j \quad d_i^0 s_{i\,j} c_j^2 \quad 2 \quad d_i^0 t_{i\,j} c_j = \frac{1}{60} \tag{1.33}$$

$$b_i^0 t_{i\,j} c_j^2 \quad d_i^0 s_{i\,j} c_j^2 \quad 2 \quad d_i^0 t_{i\,j} c_j = \frac{1}{60} \tag{1.34}$$

$$b_i^0 a_{i\,j} t_{i\,j} \quad b_i^0 r_{i\,j} c_j \quad d_i^0 s_{i\,j} t_{i\,j} \quad b_i^0 t_{i\,j} c_j = \frac{1}{120} \tag{1.35}$$

$$b_i^0 t_{i\,j} t_{j\,k} \quad d_i^0 s_{i\,j} t_{j\,k} \quad d_i^0 t_{i\,j} c_j = \frac{1}{120} \tag{1.36}$$

$$b_i^0 s_{i\,j} r_{j\,k} \quad b_i^0 t_{i\,j} t_{j\,k} \quad d_i^0 a_{i\,j} c_j \quad d_i^0 r_{i\,j} = \frac{1}{120}: \tag{1.37}$$

1.3 Taylor Series Expansion

If the function $y(x)$ is sufficiently differentiable, then $y(x \quad h)$ can be expanded in Taylor series form as follows

$$y(x \quad h) = y(x) \quad hy^0(x) \quad \frac{h^2}{2} y^{00}(x) \quad ::: \quad \frac{h^p}{p} y^p(x) \quad ::: \tag{1.38}$$

where $y^p = \frac{d^p y}{dx^p}$ $p = 1 \; 2 \; :::$

Similarly, we can write the Taylor series expansion of $y(x_n \quad h)$ as follows

$$y(x_n \quad h) = y(x_n) \quad hy^0(x_n) \quad \frac{h^2}{2} y^{00}(x_n) \quad ::: \quad \frac{h^p}{p} y^p(x_n) \quad ::: \tag{1.39}$$

In practice all terms up to h^p are included, that is

$$y(x_{n \quad 1}) = y(x_n \quad h) = y(x_n) \quad hy^0(x_n) \quad \frac{h^2}{2} y^{00}(x_n) \quad ::: \quad \frac{h^p}{p} y^p(x_n) \quad h^{p \quad 1} E_{p \quad 1}(e_n): \tag{1.40}$$

where $E_{p \quad 1}(e_n)$, $x_n \leq e_n \leq x_n \quad h$, is the residual term. By removing the residual term from (1.40), we obtain the Taylor series expansion of order p as follows

$$y(x_{n \quad 1}) = y(x_n) \quad hy^0(x_n) \quad \frac{h^2}{2} y^{00}(x_n) \quad ::: \quad \frac{h^p}{p} y^p(x_n): \tag{1.41}$$

From (1.41) the general form of one step method can be defined as

$$y_{n \quad 1} = y_n \quad hF(x_n \; y_n \; h) \tag{1.42}$$

where the function $F(x_n \ y_n \ h)$ is called the increment function and y_n is the estimation of the exact solution $y(x_n)$.

Definition 1.3 (see Dormand (1996))
The exact solution $y(x_n)$ will satisfy

$$y(x_{n \ 1}) = y(x_n) \quad hF(x_n \ y(x_n) \ h) \quad LTE_{n \ 1} \tag{1.43}$$

where $LTE_{n \ 1}$ is called the local truncation error.

Definition 1.4 (see Dormand (1996))
The one step method (1.42) is said to have order p if p is the largest positive integer such that

$$y(x \quad h) - y(x) - hF(x \ y \ h) = O(h^{p \ 1}) \tag{1.44}$$

1.4 Problem Statement

When we solve differential equations, we can sometimes use the available extra information that comes with the problems or information that is cheap to compute. In that case, it may be worthwhile include the extra information in the formulation of the numerical method. For many fields of applied sciences defined by (1.3), it is possible to construct higher derivatives of the solution in order to develop the variation of Runge-Kutta type (RK) methods. The theory of numerical methods for general second-order ordinary differential equations has been developed in large and excellent general purpose algorithms mainly based on Runge-Kutta-Nyström methods (RKN).

The higher derivative terms can be used to enhance the performance of multistage methods. If these higher derivatives are available, then the most popular option is to use them to evaluate a number of terms in Taylors theorem. Therefore, a significant increase in efficiency may be achieved by the numerical integration methods which employ the higher derivative terms. Although the existence and computation of higher derivatives may put a restriction on these methods, the advantage gained may still make their use beneficial.

Herein, we will derive the special class of two derivative Runge-Kutta-Nyström methods (STDRKN) of higher orders for solving general second-order ODEs by including the second and third derivatives. In addition, we are going to cover the formulation and consider the implementation in details.

When this research study began, no study had been carried on the three derivative Runge-Kutta-Nyström method (SThDRKN) for solving general second-order ODEs by including the second, third and fourth derivatives with least function evaluations. Therefore, the aim of this research is to develop algebraic order conditions for STh-

DRKN methods to solve general second-order ODEs. The construction of numerical SThDRKN methods of different orders, the derivation of different orders of embedded SThDRKN pairs, the derivation of exponentially-fitted and trigonometrically-fitted modified explicit SThDRKN methods and the derivation of semi-implicit SThDRKN methods for solving general second-order ODEs are derived.

1.5 Scope of the Study

This study concentrate on the derivation of new coefficient and efficient codes that are based on two derivative and three derivative Runge-Kutta-Nyström methods for numerical solution of IVP. These methods will then be used for solving linear and nonlinear problems of non stiff general second order ODEs directly for both constant and variable step size mode. The properties of this method will be analyzed in terms of accuracy and computational cost. Our main motivation is to reduce the number of function evaluations where it will ensure cost efficiency.

1.6 Objectives of the Study

The objectives of this thesis are

To derive the order conditions of special class of two derivative Runge-Kutta-Nyström methods for solving general second-order ODEs. Based on the order conditions developed, STDRKN methods of orders four, five and six will be constructed.

To derive the order conditions of special class of three derivative Runge-Kutta-Nyström methods for solving general second-order ODEs. Based on the order conditions obtained, SThDRKN methods of orders five and six will be derived.

To construct the embedded STDRKN and SThDRKN methods of orders 4(3), 5(4), and 6(5) for solving general second-order ODEs using variable step size codes.

To construct exponentially-fitted and trigonometrically-fitted modified explicit STDRKN and SThDRKN methods for solving general second-order ODEs.

To construct exponentially-fitted and trigonometrically-fitted explicit TDRKN methods for solving general second-order ODEs.

To derive semi-implicit STDRKN and SThDRKN methods of orders five and six for solving general second-order ODEs.

1.7 Outline of the Study

The brief description for organization of the thesis will be provided here.
In Chapter 1, the brief of numerical integration of second-order ODEs are presented. In Chapter 2, some of the previous works on the numerical solutions of second-order ODEs are reviewed.

In Chapter 3, the formulations of explicit special two derivative and three derivative Runge-Kutta-Nyström methods are provided. The linear stability of the newly proposed methods is analyzed.

In Chapter 4, the derivation of the three pairs of embedded STDRKN methods and two pairs of embedded SThDRKN methods are presented. Based on the newly proposed methods a variable step size code is developed for solving general second-order ODEs.

In Chapter 5, the derivation of exponentially-fitted and trigonometrically-fitted modified explicit STDRKN and SThDRKN methods for solving general second-order ODEs are provided. Meanwhile, in Chapter 6, the derivation of exponentially-fitted and trigonometrically-fitted explicit TDRKN methods for solving general second-order **ODEs are derived.**

In Chapter 7, the implementation of semi-implicit STDRKN and SThDRKN methods using constant step size are presented. Finally, the conclusions of thesis and recommendations for future work are given in Chapter 8.

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