A new hyhbrid coefficient of conjugate gradient method

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Article Info	ABSTRACT
	Hybridization is one of the popular approaches in modifying the conjugate gradient method. In this paper, a new hybrid conjugate gradient is suggested and analyzed in which the parameter β_k is evaluated as a convex combination of β_k^{RMIL} while using exact line search. The proposed method is shown to possess both sufficient descent and global convergence properties. Numerical performances show that the proposed method is promising and has overpowered other hybrid conjugate gradient methods in its number of iterations and central processing unit per time.

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1.   INTRODUCTION

In unconstrained optimization, consider the following objective function;

$$\min\left\{f(x) : x \in R^n\right\} \tag{1}$$

where $f : R^n \rightarrow R$ is a continuously differentiable function which is bounded from below and R^n denotes as n – dimensional Euclidean space [1-3]. Generally, with any $x_0 \in R^n$ as an initial guess, a sequence $\{x_k\}$ is generated by employing the CG iterative method given by;

$$x_{k+1} = x_k + \alpha_k d_k, \qquad k = 0,1,2,... \tag{2}$$

where x_k is the kth iterative point and $\alpha_k > 0$ is a step size while the search direction d_k is defined by;

$$d_k = \begin{cases} -g_k & \text{if} \quad k = 0 \\ -g_k + \beta_k d_{k-1} & \text{if} \quad k \geq 1 \end{cases} \tag{3}$$

The scalar β_k is called the coefficient of CG and g_k is the gradient of f at point x_k. Step size $\alpha_k > 0$ is the stepsize determined by using exact line search, given as;

$$f(x_k + \alpha_k d_k) = \min_{\alpha \geq 0} f(x_k + \alpha d_k).$$

(4)

In the study of CG methods, a lot of modifications have been made but it is lacking in term of its superior. This study proposed a new method to outperform the number of iteration and CPU time compared to the previous coefficients. Hybrid CG method is known to be a combination of some classical CG methods combining the good criterion. In this paper, a new approach is suggested in order to get a new hybrid conjugate gradient algorithm. The new algorithm is a result from combining RMIL and SMR conjugate algorithms. Under exact line search, SMR has good computational properties while RMIL has strong convergence properties [1-2]. All the good criteria were combined in order to obtain a better practical algorithm. Section two will discuss the motivation of the algorithm and the new hybrid conjugate gradient algorithm. Section three presents the convergence analysis. Numerical experiments are discussed at section four and the last section concludes all the works in this paper.

2.   LITERATURE REVIEW

The exact line search is well known to provide the optimal step size [4]. Recent studies have shown that the newer technologies with faster processors and better equipment have successfully eliminated the speed problems often suffered by exact line search as demonstrated by Rivaie et al [1]. This motivates plenty of its applications for solving unconstrained optimization problems. Different conjugate gradient method yield different choices for calculating the CG coefficient β_k. Some well known formulas for β_k are;

$$\beta_k^{HS} = \frac{g_k^T (g_k - g_{k-1})}{(g_k - g_{k-1})^T d_{k-1}}$$

(7)

$$\beta_k^{FR} = \frac{g_k^T g_k}{\|g_{k-1}\|^2}$$

(8)

$$\beta_k^{PRP} = \frac{g_k^T (g_k - g_{k-1})}{\|g_{k-1}\|^2}$$

(9)

$$\beta_k^{CD} = -\frac{g_k^T g_k}{d_{k-1}^T g_{k-1}}$$

(10)

$$\beta_k^{DY} = \frac{g_k^T g_k}{(g_k - g_{k-1})^T d_{k-1}}$$

(11)

$$\beta_k^{RMIL} = \frac{g_k^T (g_k - g_{k-1})}{\|d_{k-1}\|^2}$$

(12)

$$\beta_k^{LS} = \frac{g_k^T (g_k - g_{k-1})}{-d_{k-1}^T g_{k-1}}$$

(13)

$$\beta_k^{SMR} = \max\left\{0, \frac{\|g_k\|^2 - |g_k^T g_{k-1}|}{\|d_{k-1}\|^2}\right\} \tag{14}$$

From (7)-(13), g_k and g_{k-1} are the abbreviations of $g(x_k)$ and $g(x_{k-1})$ which are the gradients of $f(x)$ at points x_k and x_{k-1} respectively. Euclidean norm of the vectors is denoted by $\|\ \|$. The above corresponding methods are known as HS (Hestenes and Steifel [5]), FR (Fletcher and Reeves [6]), PRP (Polak and Ribierre [7]), CD (Conjugate Descent by Fletcher [8]), DY (Dai and Yuan [9]), RMIL (Rivaie, Mustafa, Ismail and Leong [1]), SMR (Syarafina, Mustafa and Rivaie [2]) and LS (Liu-Storey [10]) respectively. All of these methods have finite convergence properties under exact line search due to strictly convex quadratic function $f(x)$. From all the methods mentioned above, some of these such as (8), (10) and (11) have strong convergence properties but not excellent in practical performance due to jamming problem. Meanwhile, methods in (7), (9) and (13) have better performance though lacking in convergence properties [11]. Conjugate gradient method can be classified into three different groups; classical, scaled and hybrid CG method [12]. Due to their simple approach, CG methods in (7) - (14) are said to be classical. Detailed discussions are available in [13-24].

In this paper, the main objective is to focus on hybrid conjugate gradient method. The idea is to combine different conjugate algorithms to use the projections to form a new hybrid convex-combination algorithm in order to avoid jamming [11]. Early hybrid conjugate gradient algorithm was first proposed by Touati-Ahmed and Storey [25]. Some well known hybrid conjugate algorithms are;

$$\beta_k^{HDY} = \max\{0, \min\{\beta_k^{HS}, \beta_k^{DY}\}\} \tag{15}$$

$$\beta_k^{HHUS} = \max\{0, \min\{\beta_k^{PRP}, \beta_k^{FR}\}\} \tag{16}$$

$$\beta_k^{HLSCD} = \max\{0, \min\{\beta_k^{LS}, \beta_k^{CD}\}\} \tag{17}$$

$$\beta_k^{HJHJ} = \frac{\|g_k\|^2 - \max\{0, \frac{\|g_k\|}{\|g_{k-1}\|} g_k^T g_{k-1}\}}{\max\{\|g_{k-1}\|^2, d_{k-1}^T(g_k - g_{k-1})\}} \tag{18}$$

From (15)-(18) HDY is a modification effort from Dai and Yuan [9] combining its algorithm with Hestenes and Steifel [5], HHUS was introduced by Hu and Storey [26], HLSCD is the combination of LS [10] and CD [8] and HJHJ is a hybrid CG from Jinbao-Han-Jiang [27]. From (18), it is easy to know the algorithm is a combination of various classical CG methods [28-30].

3. NEW HYBRID CG METHOD

Motivated by the idea of combining various CG algorithm from (15)-(18), a new hybrid coefficient is proposed between RMIL [1] and SMR [2] where the methods are respectively known by (12) and (14). The new coefficient introduced is as follows;

$$\beta_k^{HSMR} = \max\{0, \min\{\beta_k^{SMR}, \beta_k^{RMIL}\}\} \tag{19}$$

where HSMR stands for Hybrid-Syarafina-Mustafa-Rivaie method. This new method is suggested due to the restart strategy proposed in [31]. It is suitable to set $\beta_k = 0$, which implies a restart along g_k. If $\beta_k < 0$, the search direction d_k from (3) tend to almost opposite to d_{k-1}. By restricting the CG coefficient to $\beta_k \geq 0$ the two consecutive search directions are prevented from tending to be almost opposite [32]. The new algorithm of β_k^{HSMR} is given as follows;
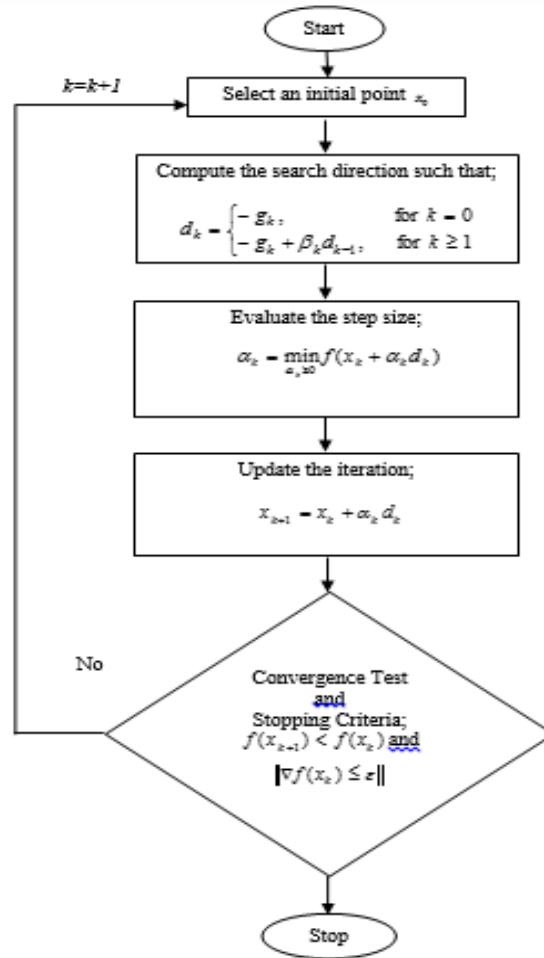
Figure 1. Conjugate Gradient Algorithm

Algorithm 2.1: Conjugate Gradient Algorithm

A complete algorithm of CG method could be generated as follows:

Step 1:   Initialization. Set $k = 0$ and select $x_0 \in \Re^n$, $d_0 = -g_0$, if $g_0 = 0$, stop.

Step 2:   Compute β_k^{HSMR} based on (19).

Step 3:   Compute search directions d_k based on (3). If $\|g_k\| \le \varepsilon$, then stop. Otherwise, go to the next step.

Step 4:   Compute for α_k based on exact line search (4) .

Step 5:   Updating new initial point using (2).

Step 6:   Convergence test and stopping criteria. If $f(x_{k+1}) < f(x_k)$ and $\|g_k\| \le \varepsilon$ then, stop. Otherwise go to Step 2 with $k = k+1$.

4.   CONVERGENCE ANALYSIS

In this section, the convergence analysis based on exact line search in (4) is analysed. An algorithm has to possess both sufficient descent condition and global convergence properties for a method to be converged.

4.1.   Sufficient Descent Condition

Sufficient descent condition holds when

$$g_k^T d_k \le -C\|g_k\|^2 \text{ for } k \ge 0 \text{ and } C > 0 \tag{20}$$

Theorem 1: Consider a CG method with search direction (3) and β_k^{HSMR} defined as (19), then, condition (20) will hold for all $k \geq 0$. **Proof:** From (3), know that $g_0^T d_0 = -C\|g_0\|^2$. Hence, condition (20) holds. In order to show condition (20) also hold for $k \geq 1$, multiply (3) by g_k^T. Then,

$$g_k^T d_k = -g_k^T g_k + \beta_k^{HSMR} g_k^T d_{k-1} = -\|g_k\|^2 + \beta_k^{HSMR} g_k^T d_{k-1} \tag{21}$$

For $k = 1$, it is easy to know that $g_1^T d_1 = -\|g_k\|^2 < 0$. Assume that $g_{k-1}^T d_{k-1} < 0$ holds for $k-1$ and $k \geq 2$. To prove that $g_k^T d_k < 0$ for all k, consider these two cases:

CASE I: If $\beta_k^{RMIL} = \dfrac{g_k^T(g_k - g_{k-1})}{\|d_{k-1}\|^2} < 0$, automatically β_k^{HSMR} return to 0 such that $\beta_k^{SMR} \geq 0$. When $\beta_k^{HSMR} = 0$, it is known that $g_k^T d_k = -\|g_k\|^2 < 0$.

CASE II: If $\beta_k^{RMIL} = \dfrac{g_k^T(g_k - g_{k-1})}{\|d_{k-1}\|^2} \geq 0$, then, $\beta_k^{HSMR} \neq 0$ and can either be β_k^{SMR} or β_k^{RMIL}.

Since the line search is exact, it is known that $g_k^T d_{k-1} = 0$. Thus, $g_k^T d_k = -\|g_k\|^2$ implying d_k is a sufficient descent direction. Hence, the descent condition holds i.e., $g_k^T d_k \leq -C\|g_k\|^2$. The proof is completed.

3.2. Global Convergence Properties

From [1] and [2], it is known that β_k^{SMR} and β_k^{RMIL} can be simplified to:

$$0 \leq \beta_{k+1} \leq \frac{\|g_{k+1}\|^2}{\|d_k\|^2} \tag{22}$$

Case II stated that β_k^{HSMR} and can either be β_k^{SMR} or β_k^{RMIL} if $\beta_k^{RMIL} = \dfrac{g_k^T(g_k - g_{k-1})}{\|d_{k-1}\|^2} \geq 0$. Then, from [1, 2] and [18], in the analysis of global convergence properties, the following assumption is needed.

Assumption 1

1. f is bounded below on the level set R^n and is continuous and differentiable in a neighbourhood N of the level set $\ell = \{x \in R^n \mid f(x) \leq f(x_0)\}$ at the initial point x_0.
2. The gradient $g(x)$ is Lipschitz continuous in N, so, there exists a constant $L > 0$ such that; $\|g(x) - g(y)\| \leq L\|x - y\|$ for any $x, y \in N$.

Under this assumption, the following lemma is obtained, which was proved by Zoutendijk [33].

Lemma 1: Suppose that Assumption 1 holds. Consider any CG methods of the form (3) where d_k is a descent search direction and α_k satisfies the exact minimization rules. Then the following conditions known as Zoutendijk conditions hold;

$$\sum_{k=0}^{\infty} \frac{(g_k^T d_k)^2}{\|d_k\|^2} < \infty.$$

The proof of this lemma can be seen from [25]. By using this lemma; the following convergence theorem of the conjugate gradient method can be obtained by using (22).

Theorem 1: Suppose that Assumption 1 holds. Consider any CG methods in the form of (3) and (2) where α_k is obtained by the exact minimization rules. Also, suppose that Assumption 1 and the descent condition hold. Then either:

$$\lim_{k \to \infty} \|g_k\| = 0 \quad \text{or} \quad \sum_{k=0}^{\infty} \frac{\left(g_k^T d_k\right)^2}{\|d_k\|^2} < \infty .$$

Proof: By induction, if Theorem 1 is not true then, there exists a constant $c > 0$ such that:

$$\|g_k\| \geq c \tag{23}$$

Rewriting (3) and squaring both sides, we get:

$$\|d_{k+1}\|^2 = (\beta_{k+1})^2 \|d_k\|^2 - 2g_{k+1}^T d_{k+1} - \|g_{k+1}\|^2 \tag{24}$$

Using $\left(g_{k+1}^T d_{k+1}\right)^2$ and dividing both sides,

$$\frac{\|d_{k+1}\|^2}{\left(g_{k+1}^T d_{k+1}\right)^2} = \frac{(\beta_{k+1})^2 \|d_k\|^2}{\left(g_{k+1}^T d_{k+1}\right)^2} - \frac{2}{g_{k+1}^T d_{k+1}} - \frac{\|g_{k+1}\|^2}{g_{k+1}^T d_{k+1}}$$

By completing the square, the equation becomes:

$$= \frac{(\beta_{k+1})^2 \|d_k\|^2}{\left(g_{k+1}^T d_{k+1}\right)^2} - \left(\frac{1}{\|g_{k+1}\|} + \frac{\|g_{k+1}\|}{g_{k+1}^T d_{k+1}}\right)^2 + \frac{1}{\|g_{k+1}\|^2} \leq \frac{(\beta_{k+1})^2 \|d_k\|^2}{\left(g_{k+1}^T d_{k+1}\right)^2} + \frac{1}{\|g_{k+1}\|^2}$$

Applying (22), yields

$$= \left(\frac{\|g_{k+1}\|^2}{\|d_k\|^2}\right)^2 \frac{\|d_k\|^2}{\left(g_{k+1}^T d_{k+1}\right)^2} + \frac{1}{\|g_{k+1}\|^2} = \frac{\|g_{k+1}\|^2}{\|d_k\|^2 \|d_{k+1}\|^2} + \frac{1}{\|g_{k+1}\|^2} \leq \frac{1}{\|d_k\|^2} + \frac{1}{\|g_{k+1}\|^2} \tag{25}$$

From (25), noting that:

$$\frac{1}{\|d_0\|^2} = \frac{1}{\|g_0\|^2} ,$$

then,

$$\frac{\|d_k\|^2}{\left(g_k d_k\right)^2} = \frac{1}{\|g_0\|^2} + \frac{1}{\|g_k\|^2}$$

Hence,

$$\frac{\|d_k\|^2}{\left(g_k d_k\right)^2} \leq \sum_{i=0}^{k} \frac{1}{\|g_i\|^2} \text{ and } \frac{\left(g_k d_k\right)^2}{\|d_k\|^2} \geq \frac{c^2}{k}$$

Then, from (23) and (25), it follows; $\sum_{k=0}^{\infty} \frac{\left(g_k^T d_k\right)^2}{\|d_k\|^2} = \infty$. This contradicts the Zoutendijk condition in Lemma 1.

Therefore the proof is completed.

Corollary 1: If $\sum_{k=0}^{\infty} \|d_k\|^2 = 0$, then $\sum_{k=0}^{\infty} \frac{\left(g_k^T d_k\right)^2}{\|d_k\|^2} < \infty$ holds.

Proof: By using contradiction, assume that $\|g_k\| \geq c$ and $\sum_{k=0}^{\infty} \|d_k\|^2 = \infty$. For $\|g_k\| \to \infty$, then, $\frac{1}{\|g_k\|} \to 0$.

From (25),

$$\frac{\|d_k\|^2}{\left(g_k^T d_k\right)^2} \leq \frac{1}{\|d_k\|^2}$$

then,

$$\|d_k\|^2 \leq \frac{\left(g_k^T d_k\right)^2}{\|d_k\|^2}.$$

Which leads to, $\sum_{k=0}^{\infty} \|d_k\|^2 \leq \sum_{k=0}^{\infty} \frac{\left(g_k^T d_k\right)^2}{\|d_k\|^2}$ and $\infty \leq \sum_{k=0}^{\infty} \frac{\left(g_k^T d_k\right)^2}{\|d_k\|^2}$.

This contradicts the Zoutendijk conditions. Hence the corollary holds.

5. NUMERICAL RESULTS AND DISCUSSION

This section presents the numerical performance of the new coefficient β_k^{HSMR} compared with other coefficients mentioned in (15)-(18). A list of fifteen small to large-scale unconstrained optimization test functions considered in Andrei [34] was selected as shown in Table 1. A large-scaled problem is chosen in order to detect a cynical observer preventing the algorithm being tuned in particular functions [35]. In this paper, four random initial starting points are chosen for each of test functions used to add to the complexity of the computer programming [36]. Points chosen can also be used to test the global convergence properties and the robustness of the methods. Results analyses are based on MATLAB subroutine programme on workstation Intel Core i7, 2.2 GHz tested on number of iterations and central processing time per unit. The stopping criterion is set to $\|g_k\| \leq 10^{-6}$, where $\varepsilon = 10^{-6}$. Performance profiles based on Dolan and More [37] are shown graphically in Figures 1-2 [38-39]

Table 1. List of test functions

No	Function	n	Initial Points
1	3-Hump	2	(-1,1),(1,-1),(-2,2),(2,-2)
2	6-Hump	2	(8,8),(-8,-8),(10,10),(-10,-10)
3	Booth	2	(10,10),(25,25),(50,50),(100,100)
4	Treccani	2	(5,5),(10,10),(50,50),(100,100)
5	Goldstein-Price	2	(2,-2),(5,-5),(10,-10),(13,-13)
6	Extended Himmelblau	2,4,10,100,500,1000	(10,10,..,10),(50,50,,50),(100,100,,100),(200,200,,200)
7	Extended Denschnb	2,4,10,100,500,1000	(5,5,…,5),(8,8,…,8),(13,13,…,13),(25,25,…,25)
8	Generalized Quartic	2,4,10,100,500,1000	(10,10,,10),(50,50,,50),(100,100,,100),(200,200,,200)
9	Diagonal 4	2,4,10,100,500,1000	(10,10,,10),(50,50,,50),(100,100,…100),(200,200,…200)
10	Extended Freundestein and Roth	2,4,10,100,500,1000	(1,1,…,1),(3,3,…,3),(5,5,…,5),(7,7,…,7)
11	Extended Rosenbrock	2,4,10,100,500,1000	(13,13,…,13),(16,16,…,16),(20,20,…,20),(30,30,…,30)
12	Extended Tridiagonal 1	2,4,10,100,500,1000	(10,10,...,10),(12,12,...,12),(17,17,...,17),(20,20,...,20)
13	Shalow	2,4,10,100,500,1000	(10,10,…,10),(25,25,...,25)(50,50,…,50),(100,100,…,100)
14	Extended Beale	2,4,10,100,500,1000	(1,1,…,1),(-1,-1,…,-1),(3,3,…,3),(2,2,…,2)
15	Fletchr	2,4,10,100,500,1000	(2,2,…,2),(3,3,…,3),(5,5,…,5),(7,7,…,7) (9,9,...,9)

The $P_s(t)$ from the performance profile is the fraction of problem with a ratio performance t. A solver has higher efficiency when its value of $P_s(t)$ is higher. In a set of problem P and a set of optimization solve

S, a performance comparison of problem $p \in P$ by a particular algorithm $s \in S$ is measured. Let, $t_{p,s}$ be the number of iterations or CPU time required when solving a problem $p \in P$ with solver $s \in S$. The performance ratio is defined by $r_{p,s} = \dfrac{t_{p,s}}{\min\{t_{p,s} : s \in S\}}$. From this expression, it is assumed that $r_{p,s} \in [1, r_M]$, where $r_M \geq r_{p,s}$ and $r_{p,s} = r_M$ only when problem p is not solved by solver s. Then, graphically, a graph of $P_s(t)$ versus $t \in [1, r_M]$ is plotted. In a graph of performance profile, the smallest performance ratio is 1 and it will be located at the most left of t - axis, hence, the top curve represents the most efficient method.
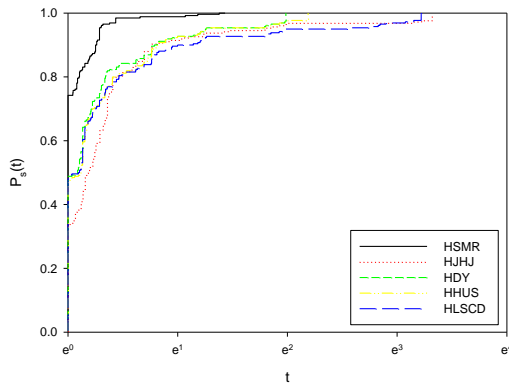

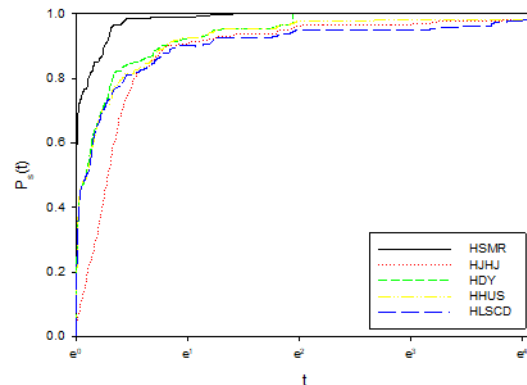Figure 1. Performance profile based on number of iterations

Figure 2. Performance profile based on CPU time

Figure 1 and Figure 2 show the performance of the CG coefficients based on number of iterations and central processing time per unit respectively for exact line search. The top left curved indicated how fast the coefficient converge while the top right determine how many test functions can be tested on given coefficient. From both figures, it is clearly indicate that the new hybrid β_k^{HSMR} outperformed the other hybrid CG coefficients.

6. CONCLUSION

In this paper, a new hybrid of CG algorithm β_k^{HSMR} is proposed and examined for solving unconstrained optimization problem. Proofs showed that the algorithm satisfies the convergence properties globally under descent conditions by using exact line search. Numerical results have shown that the new algorithm proposed is competitive and performs better than HJHJ, HDY, HHUS and HLSCD. In the future, the new algorithm is going to be tested under different search rules.

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She is a senior lecturer at the Department of Mathematics, Faculty of Science and Mathematics, Universiti Pendidikan Sultan Idris (UPSI). She graduated with a bachelor science degree in Industrial Mathematics from Universiti Teknologi Malaysia, in 2010. Upon graduation, she began her career as an Executive in banking institution. In the following year, she received an offer to continue her study as a fast-track PhD student at the same university. During her PhD journey, she developed an interest in multivariate analysis, specifically in finding patterns which deals with big data. Her research focuses on the area of dimension reduction methods specifically in climate informatics which involves analysis on huge climate-related datasets based on techniques in Data Mining. She had published her research in Scopus indexed journal and presented her work in various local and international conferences. She completed her PhD thesis at the end of 2016 and was conferred a doctorate degree in 2017.