UNIVERSITI PUTRA MALAYSIA

IMPLEMENTATION OF SYMMETRIC RANK-ONE METHODS FOR UNCONSTRAINED OPTIMIZATION

FARZIN MODARRES KHIYABANI

FS 2010 41

IMPLEMENTATION OF SYMMETRIC RANK-ONE METHODS FOR UNCONSTRAINED OPTIMIZATION

By

FARZIN MODARRES KHIYABANI

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

December 2010

DEDICATION

To

My Father and My Mother

For their support, encouragement and love

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

IMPLEMENTATION OF SYMMETRIC RANK-ONE METHODS FOR UNCONSTRAINED OPTIMIZATION

By

FARZIN MODARRES KHIYABANI

December 2010

Chair: Prof. Malik Hj. Abu Hassan, Ph.D.

Faculty: Science

The focus of this thesis is on analyzing the theoretical and computational aspects of some quasi-Newton (QN) methods for locating a minimum of a real valued function f over all vectors $x \in \mathbb{R}^n$. In many practical applications, the Hessian of the objective function may be too expensive to calculate or may even be unavailable in the explicit form. QN methods endeavor to circumvent the deficiencies of Newtons method (while retaining the basic structure and thus preserving, as far as possible, its advantages) by constructing approximations for the Hessian iteratively. Among QN updates, symmetric rank-one (SR1) update has been shown to be an effective and reliable method of such algorithms. However, SR1 is an awkward method, even though its performance is in general better than well known QN updates. The problem is that the SR1 update may not retain positive definiteness and may become undefined because the denominator becomes zero. In recent years considerable attention has been directed towards preserving and ensuring the positive definiteness of SR1 update, but improving the quality of the estimates has rarely been studied in depth.

Our purpose in this thesis is to improve the Hessian approximation updates and study the computational performance and convergence property of this update.

First, we briefly give some mathematical background. A review of different minimization methods that can be used to solve unconstrained optimization problems is also given. We consider a modification of secant equation for the SR1 update. In this method, the Hessian approximation is updated based on modified secant equation, which uses both gradient and function value information in order to get a higher-order accuracy in approximating the second curvature of the objective function. We then examine a new scaled memoryless SR1 method based on modified secant equation for solving large-scale unconstrained optimization problems. We prove that the new method possesses global convergence. The rate of convergence of such algorithms are also discussed.

Due to the presence of SR1 deficiencies, we introduce a restarting procedure using eigenvalue of the SR1 update. We also introduce a variety of techniques to improve Hessian approximations of the SR1 method for small to large-sized problems, including multi-step, extra updating methods along with the structured method which uses partial information on Hessian.

Variants of SR1 update are tested numerically and compared to several other famous minimization methods. Finally, we comment on some achievement in our research. Possible extensions are also given to conclude this thesis.

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

IMPLIMENTASI BAGI KAEDAH PANGKAT-SATU BERSIMETRI UNTUK PENGOPTIMUMAN TAK BERKEKANGAN

Oleh

FARZIN MODARRES KHIYABANI

Disember 2010

Pengerusi: Profesor Malik Abu Hassan, Ph.D.

Fakulti: Sains

Tesis ini tertumpu kepada menganalisis teori dan aspek komputasi beberapa kaedah kuasi-Newton (QN) untuk melokasikan suatu minimum bagi suatu fungsi nilai nyata f ke atas semua vector $x \in \mathbb{R}^n$. Dalam kebanyakan kegunaan praktik, Hessian bagi fungsi matlamat mungkin terlalu mahal untuk dihitung atau tiada terdapat dalam bentuk tak tersirat. Kaedah QN cuba untuk menghalang kekurangan kaedah Newton (sementara menyimpan struktur asas dan dengan demikian menyimpan sejauh mungkin kebaikannya) dengan membina penghampiran untuk Hessian secara lelaran. Di kalangan kemaskinian QN, kemaskinian pangkat-satu bersimetri (SR1) telah menunjukkan kaedah berkesan dan dipercayai bagi algoritma tersebut. Bagaimanapun SR1 adalah suatu kaedah kekok, walaupun prestasinya secara am lebih baik daripada kemaskinian QN yang terkenal. Masalahnya ialah kemaskinian SR1 mungkin tidak menyimpan tentu positifnya dan boleh menjadi tak tertakrif sebab penyebutnya menjadi sifar. Kebelakang ini banyak tumpuan diberi ke arah penyimpanan dan memastikan tentu positifnya bagi kemaskinian SR1 tetapi memperbaiki kualiti anggaran kurang dikaji secara mendalam.

Tujuan tesis ini ialah untuk memperbaiki kemaskinian penghampiran Hessian dan mengkaji prestasi komputasi dan sifat penumpuan bagi kemaskinian ini. Pertama, kita beri beberapa latarbelakang matematik. Suatu sorotan bagi kaedah peminimuman yang berbeza yang digunakan untuk menyelesaikan masalah pengoptimuman tak berkekangan juga diberi. Kita pertimbangkan suatu pengubahsuaian bagi persamaan sekan untuk kemaskinian SR1. Dalam kaedah ini penghampiran Hessian dikemaskinikan berdasarkan ke atas persamaan sekan terubahsuai yang menggunakan kedua-dua maklumat nilai fungsi dan kecerunan supaya suatu kejituan peringkat lebih tinggi dalam menghampirkan kelengkungan kedua bagi fungsi matlamat diperolehi. Kemudian kita memeriksa suatu kaedah SR1 baru yang berskala tak beringatan berdasarkan ke atas persamaan sekan terubahsuai untuk menyelesaikan masalah pengoptimuman tak berkekangan berskala besar. Kita buktikan bahawa kaedah baru tersebut mempunyai penumpuan sejagat. Kadar penumpuan bagi algoritma kaedah tersebut juga dibincangkan.

Oleh sebab wujudnya kekurangan SR1, kita memperkenalkan suatu prosidur mula semula menggunakan nilaeigen bagi kemaskinian SR1. Juga kita perkenalkan berbagai teknik untuk memperbaiki penghampiran Hessian bagi kaedah SR1 untuk masalah dari bersaiz kecil kepada besar, termasuk multi-langkah, kaedah kemaskini lebihan bersama sama kaedah berstruktur yang menggunakan maklumat separa ke atas Hessian.

Berbagai kemaskinian SR1 diuji secara berangka dan dibandingkan dengan beberapa kaedah peminimuman terkenal yang lain. Akhir sekali kita komen ke atas beberapa kejayaan dalam penyelidikan kita. Perlanjutan penyelidikan yang mungkin juga diberi untuk menyimpul tesis ini.

ACKNOWLEDGEMENTS

These three years of research on my PhD thesis have been a thoroughly enjoyable experience, which I have already begun to look back at with nostalgia. I would like to take this opportunity to thank all of those who have made this journey worthwhile.

First and foremost, thanks to *God Almighty* for his grace, wisdom and comfort throughout my thesis. There were times where things were very tough and God was there to protect and give strength to overcome heavy storms and strong waves. This was indeed a very long journey and I praise you God always.

I am particulary grateful to Prof. Dr. Malik B Hj Abu Hassan, chairman of the supervisory committee, whose his excellent supervision, helpful guidance and continuous encouragement from the initial to the final stage enabled me to develop a deeper understanding of mathematics. I am grateful for having the opportunity to work under his supervision. His invaluable assistance and comment in the preparation and completion of this thesis are also highly appreciated. I would like to thank my co-supervisor, Assoc. Prof. Dr. Wah June Leong, for being a good listener, his invaluable discussion and carefully proof-read my numerous drafts. Thanks for your negative and positive comments, they have made me grow from strength to strength and realize that if I want to be a good scientist, I really need to work harder. He has patiently helped me in my quest for becoming a mathematician, and I have learnt a lot from his work ethic which I deeply admire. I would also like to thank the other member of my supervisory committee, Dr. Mansor Monsi, for his involvement and the fresh perspective that he brought to our discussion. I would also like to thank Prof. Dr. Toomanian, who provided me

with my first experience in graduate research. Thanks too to Prof. Dr. Mirnia who convinced me to pursue a PhD in Optimization.

Thanks also go to the School of Graduate Studies (SGS) of Universiti Putra Malaysia for the full Doctoral scholarship (GRF) that supported me throughout three years of this degree. I am also thankful to the staff of Universiti Putra Malaysia for their full co-operation given to me right from the beginning of the application process until my graduation day. Their continuous help, encouragement and support are highly appreciated. Not forgetting my colleagues and friends who have always been looking forward to my graduation day. You have encouraged me without pressuring me! Additional thanks to Dr. Farid, whom I have the privilege of working with on many occasions and on many different topics which have been key to my PhD research. My most sincere gratitude to Mr. Gholipour, as one of the best teachers I have ever had.

I would like to thank my friends from beyond the research world, who were always enthusiastic and supportive of my work. Thank you all my friends from Tabriz university, Dr. Faghfouri, Dr. Pourmahmood, Dr. Haji badali, Dr. Ilmakchi and so many more. Extra special thanks must go to my most dear friend Dr. Mehdi Salimi for his help and support.

My deepest gratitude and love to my parents, *Masoud and Mahnaz*, for their love, support, guidance and mostly believing in me throughout my study life and making sure that my dream becomes a reality. I would like to thank God for blessing me with such a wonderful parents.

Lastly, I offer my regards and blessings to all of those who supported me in any

respect during the completion of this thesis.

I certify that a Thesis Examination Committee has met on 10 December 2010 to conduct the final examination of Farzin Modarres Khiyabani on his thesis entitled "Implementation of symmetric rank-one methods for unconstrained optimization" in accordance with Universities and University Colleges Act 1971 and the Constitution of the Universiti Putra Malaysia [P.U.(A) 106] 15 March 1998. The Committee recommends that the student be awarded the Doctor of Philosophy.

Member of the Thesis Examination Committee were as follows:

Fudziah binti Ismail, PhD
Associate Professor
Faculty of Science
Universiti Putra Malaysia
(Chairman)

Mohamed b Suleiman, PhD
Professor
Faculty of Science
Universiti Putra Malaysia
(Internal Examiner)

Norihan bt Md Arifin, PhD
Associate Professor
Faculty of Science
Universiti Putra Malaysia
(Internal Examiner)

Diptesh Ghosh, PhD
Associate Professor
Indian Institute of Management Ahmedabad
India
(External Examiner)

SHAMSUDDIN SULAIMAN, PhD
Professor and Deputy Dean
School of Graduate Studies
Universiti Putra Malaysia

Date: 18 January 2011

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 Supervisory Committee were as follows:

Malik b Hj Abu Hassan, PhD
Professor
Faculty of Science
Universiti Putra Malaysia
(Chairman)

Leong Wah June, PhD
Associate Professor
Faculty of Science
Universiti Putra Malaysia
(Member)

Mansor b Monsi, PhD
Senior Lecturer
Faculty of Science
Universiti Putra Malaysia
(Member)

HASANAH MOHD GHAZALI, PhD
Professor and Dean
School of Graduate Studies
Universiti Putra Malaysia

Date:

DECLARATION

I declare that the thesis is my original work except for quotations and citations which have been duly acknowledged. I also declare that it has not been previously, and is not concurrently, submitted for any other degree at Universiti Putra Malaysia or at any other institution.

FARZIN MODARRES KHIYABANI

Date: 10 December 2010

TABLE OF CONTENTS

		Page
ABSTRACT		iii
ABSTRAK		v
ACKNOWLEDGEMENTS		vii
APPROVAL		x
DECLARATION		xii
LIST OF TABLES		xvii
LIST OF FIGURES		xix
LIST OF ABBREVIATIONS		xx
CHAPTER		
1	**INTRODUCTION**	1
	1.1 Preliminaries	1
	1.2 General Form of Optimization Problems	2
	1.3 Basic Definitions	3
	1.4 Optimality Conditions for Unconstrained Minimization	9
	1.5 Convexity	10
	1.6 Rates of Convergence	13
	1.7 Objective of the Research	16
	1.8 Outline of Thesis	17
2	**LITERATURE REVIEW**	20
	2.1 Overview of Techniques in Solving Nonlinear Unconstrained Problems	20
	2.2 Line-search Method	21
	2.3 Steepest Descent Method	23
	2.4 Conjugate Gradient Methods	26
	2.5 Newton Method	27
	2.6 Quasi-Newton Methods	29
	2.6.1 Broyden-Fletcher-Goldfarb-Shanno (BFGS) Update	35
	2.6.2 Davidon–Fletcher–Powell (DFP) Update	37
	2.6.3 Symmetric Rank-one (SR1) Update	38
	2.7 Convergence of the Quasi-Newton Methods	42
	2.8 Limited Memory Quasi-Newton Methods	44
	2.9 Conclusion	48
3	**IMPROVED HESSIAN APPROXIMATION WITH MODIFIED SECANT EQUATIONS FOR SYMMETRIC RANK-ONE METHOD**	49
	3.1 Introduction	49
	3.2 Modified Secant Equation	51
	3.3 The Symmetric Rank-one Update with Modified Secant Equation	55
	3.4 Positive Definiteness of the Modified Symmetric Rank-one Update	56
	3.4.1 Scaling the Identity	57
	3.4.2 The σ-optimal Update	58
	3.5 Description of Modified Symmetric Rank-one Methods	61
	3.6 Convergence Analysis	63

3.7 Numerical Results 71
3.8 Conclusion 86

4 **MEMORYLESS MODIFIED SYMMETRIC RANK-ONE METHOD FOR SOLVING LARGE-SCALE UNCONSTRAINED OPTIMIZATION PROBLEMS** 87
4.1 Introduction 87
4.2 Optimal Scaling Factor 88
4.3 Memoryless Modified Symmetric Rank-one Method 89
4.4 Convergence Results 90
4.5 Numerical Results 93
4.6 Conclusion 102

5 **NEW SYMMETRIC RANK-ONE METHOD WITH RESTART FOR SOLVING UNCONSTRAINED OPTIMIZATION PROBLEMS** 103
5.1 Introduction 103
5.2 Eigenvalues of Symmetric Rank-one Update 104
5.3 Optimal Scaling under the σ-Measure 109
5.4 Switching Symmetric Rank-one Method 110
5.5 Numerical Experiments 113
5.6 Conclusion 121

6 **SYMMETRIC RANK-ONE METHOD VIA MULTI-STEP AND EXTRA-UPDATE METHODS** 122
6.1 Introduction 122
6.2 Updating Techniques via Multi-step and Extra-update Schemes 125
6.2.1 Symmetric Rank-one Update via Multi-step Updating Scheme 125
6.2.2 Symmetric Rank-one Update via Extra Updating Scheme 131
6.3 Implementation and Numerical Experiments 137
6.3.1 Numerical Results for MSSR1 Algorithm 137
6.3.2 Numerical Results for EXSR1 Algorithm 143
6.4 Conclusion 153

7 **STRUCTURED SYMMETRIC RANK-ONE ALGORITHM USING PARTIAL INFORMATION ON HESSIAN FOR UNCONSTRAINED OPTIMIZATION** 155
7.1 Introduction 155
7.2 Structured Quasi-Newton Method 157
7.3 Some Applications of Structure QN Method 159
7.4 Possible Instability of Structured Symmetric Rank-one Update 161
7.5 Structured Symmetric Rank-one Method 162
7.6 Computational Results 164
7.7 Conclusion 175

8 **GENERAL CONCLUSION AND FUTURE DIRECTIONS** 176
8.1 Summary and General Conclusion 176
8.2 Future Directions 179

REFERENCES 183
APPENDIX 192
BIODATA OF STUDENT 201
LIST OF PUBLICATIONS 202