UNIVERSITI PUTRA MALAYSIA

IMPLEMENTATION OF SYMMETRIC RANK-ONE METHODS FOR UNCONSTRAINED OPTIMIZATION

FARZIN MODARRES KHIYABANI

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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

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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.

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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:

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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 Supervisory Committee were as follows:

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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

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