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NEW CONJUGATE GRADIENT METHODS FOR SOLVING LARGE-SCALE UNCONSTRAINED OPTIMIZATION PROBLEMS

MOHD RIVAIE BIN MOHD ALI

Thesis Submitted in Fulfillment of the Requirement for the Degree of Doctor of Philosophy in the Faculty of Science and Technology Universiti Malaysia Terengganu

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Conjugate gradient methods hold an important role in unconstrained optimizations. Numerous recent studies and modifications have been aimed to improve these methods. In this research, four modifications of the conjugate gradient coefficient (β_k) are proposed in order to solve unconstrained optimization problems using exact line searches.

Theoretical proof is shown that these β_k fulfill sufficient descent conditions and possess global convergence properties. They also possess linear convergence rates

and fulfill the angle condition, suggesting that these coefficients always converge faster compared with steepest descent methods.

All these new β_k are tested based on 24 standard optimization test problems utilizing *Maple 14* subroutine programming and compared with six well-known conjugate gradient methods, namely Fletcher and Reeves, Polak and Ribierre, Hestenes and Steifel, Liu and Storey, Dai and Yuan and the conjugate descent method. The test functions selected consist of small and large-scale problems. For every test problem, four different initial points are used, ranging from that closest to the solution point, to that furthest away.

The numerical results based on the number of iterations and CPU time are analyzed using the performance profile presented by Dolan and More. It is found that these new formulas perform better than the original conjugate gradient methods, retain their simplicity and possess global convergence properties. It is also shown that the numerical results concur with the theoretical proof.

Abstrak tesis yang dikemukakan kapada Senat Universiti Malaysia Terengganu sebagai memenuhi keperluan untuk ijazah Doktor Falsafah.

KAEDAH KECERUNAN KONJUGAT BARU UNTUK MENYELESAIKAN MASALAH PENGOPTIMUMAN TAK BERKEKANGAN BERSKALA BESAR

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Januari 2013

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Kaedah kecerunan konjugat memainkan peranan yang penting dalam permasalahan pengoptimuman tak berkekangan. Sehingga kini, banyak pengubahsuaian dan kajian dilakukan bagi meningkatkan kecekapan kaedah ini. Dalam kajian ini, dicadangkan empat pekali baru kaedah kecerunan konjugat (β_k) bagi menyelesaikan masalah pengoptimuman tak berkekangan dengan menggunakan carian garis tepat.

Pembuktian secara teori menunjukkan kesemua rumus baru β_k telah memenuhi syarat cukup penurunan dan memiliki sifat peminimuman sejagat. Rumus baru β_k ini

juga menumpu secara linear dan memenuhi syarat sudut yang membolehkannya menumpu lebih cepat berbanding kaedah penurunan tercuram.

Rumus baru β_k ini telah diuji berdasarkan 24 masalah piawai pengoptimuman menggunakan pengaturcaraan berutin *Maple 14*. Perbandingan kesemua β_k baru ini telah dilakukan dengan enam kaedah kecerunan konjugat lain yang terkenal iaitu, kaedah Fletcher dan Reeves, Polak dan Ribierre, Hestenes dan Steifel, Liu dan Storey, Dai dan Yuan dan, kaedah Penurunan Konjugat. Masalah piawai pengoptimuman yang telah dipilih merangkumi masalah berskala kecil sehingga ke masalah berskala besar. Bagi setiap masalah piawai pengoptimuman, empat titik awal berlainan telah digunakan bermula dari titik yang hampir ke titik yang jauh dari titik minimum sebenar.

Keputusan berangka berdasarkan bilangan lelaran dan masa CPU telah dianalisis menggunakan profil prestasi oleh Dolan dan More. Keputusan berangka telah menunjukkan bahawa pencapaian rumus baru ini adalah lebih baik berbanding kaedah kecerunan konjugat asal, lebih mudah dan memenuhi sifat peminimuman sejagat. Keputusan berangka ini juga telah menyokong pembuktian secara teori.