UNIVERSITI PUTRA MALAYSIA

MODIFIED QUASI-NEWTON TYPE METHODS USING GRADIENT FLOW SYSTEM FOR SOLVING UNCONSTRAINED OPTIMIZATION

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By

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June 2016

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In this thesis, we are mainly concerned with finding the numerical solution of nonlinear unconstrained optimization problems via gradient flow system. First, we give some brief mathematical background and then we consider a famous class of optimization methods called the quasi-Newton methods. Specifically, we focus on a class of quasi-Newton method named Broyden-Fletcher-Goldfarb-Shanno (BFGS) method.

We investigate the possible use of control theory, particularly theory on gradient flow system to derive some modified line search and trust region methods for optimization. The implementation of these methods in line search algorithm in their original forms would generate a Newton-type matrix which require inversion of a non-sparse matrix or equivalently solving a linear system in every iteration. Thus, an approximation of the proposed methods via BFGS update is constructed. Numerical experiments are carried out to illustrate the numerical performance and efficiency of the proposed methods by comparing the number of iterations, the number of function evaluations and also the CPU time in second. Our computational results show that the proposed methods are comparable with the existing standard methods. Other than that, we also analyse the global convergence properties of the modified methods. It is shown that the modified methods converge globally and the rate of convergence is superlinear convergence.

We also implement the Newton-type methods on trust region framework by using unit step length to adjust the radius of the region to obtain desired reduction in the objective function. We make an approximation to the proposed Newton-type matrix by using BFGS updating scheme and then apply this modified Newton-type matrix to generate new quadratic approximation subproblem. Numerical results are established to demonstrate the efficiency of our modified methods. Our proposed methods outperform the standard trust region method in term of lower number of function evaluations and much reduction in computational time. It is proved under appropriate assumptions that the modified trust region methods are globally convergent.

Abstrak tesis yang dikemukakan kepada Senat Universiti Putra Malaysia sebagai memenuhi keperluan untuk ijazah Sarjana Sains

UBAHSUAIAN KAEDAH KUASI-NEWTON JENIS DENGAN SISTEM ALIRAN KECERUNAN UNTUK MENYELESAIKAN PENGOPTIMUMAN TAK BERKEKANGAN

Oleh

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Dalam tesis ini, kami bertumpu terhadap mencari penyelesaian berangka untuk masalah pengoptimuman tak linear tak berkekangan dengan menggunakan sistem aliran kecerunan. Pertamanya, kami memperkenalkan sedikit latar belakang matematik secara ringkas dan kemudian kami mempertimbangkan suatu kelas pengoptimuman yang terkenal disebut sebagai kaedah kuasi-Newton. Secara khususnya, kami memberi tumpuan kepada satu kelas kaedah kuasi-Newton bernama kaedah Broyden-Fletcher-Goldfarb-Shanno (BFGS).

Kami menyisat kemungkinan untuk penggunaan teori kawalan, terutamanya teori sistem aliran kecerunan untuk mendapatkan beberapa kaedah ubahsuaian dalam gelintaran garis dan rantau kepercayaan untuk pengoptimuman. Pelaksanaan kaedah tersebut dalam kaedah carian talian dalam bentuk asal mereka akan menjana matriks Newton -jenis yang memerlukan penyongsangan matriks yang tumpat atau penyelesaian sistem linear dalam setiap lelaran. Oleh itu, suatu anggaran terhadap kaedah yang dicadangkan melalui kemaskini BFGS telah dibina. Ujikaji-ujikaji berangka dilaksanakan untuk menggambarkan prestasi berangka dan kecekapan kaedah yang dicadangkan dengan membandingkan bilangan lelaran, bilangan penilaian fungsi dan juga masa CPU dalam unit saat. Keputusan berangka menunjukkan bahawa kaedah yang dicadangkan adalah standing dengan kaedah standard yang sedia ada. Selain daripada itu, kami juga menganalisis sifat penumpuan sejagat untuk kaedah yang telah diubah suai. Ia menunjukkan bahawa kaedah yang telah diubah suai bertumpu sejagatnya dan kadar penumpuan adalah penumpuan superlinear.

Kami juga melaksanakan kaedah Newton-jenis dalam rangka kerja rantau kepercayaan dengan menggunakan unit panjang langkah untuk menyesuaikan jejari rantau ini untuk mendapatkan pengurangan yang diingini dalam fungsi objektif . Kami membuat anggaran untuk matrik Newton -jenis yang dicadangkan dengan menggunakan BFGS kemaskini skim dan kemudian menggunakan matrik Newton-jenis ini yang diubahsuai untuk menjana penghampiran subproblem kuadratik baru. Keputusan berangka yang ditubuhkan untuk menunjukkan kecekapan kaedah diubahsuai oleh kami . Kaedah yang dicadangkan oleh kami mengatasi kaedah rantau kepercayaan standard dari segi jumlah yang lebih rendah dalam penilaian fungsi dan pengurangan masa pengiraan yang banyak. Ia dibuktikan di bawah andaian yang sesuai bahawa kaedah rantau kepercayaan diubahsuai bertumpu secara sejagat.

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I certify that a Thesis Examination Committee has met on 01 June 2016 to conduct the final examination of Yap Chui Ying on her thesis entitled "Modified Quasi-Newton Type Methods Using Gradient Flow System for Solving Unconstrained Optimization" in accordance with the 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 Master of Science.

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LIST OF ABBREVIATIONS

x	real-valued vectors where $x = (x_1, x_2, \cdots, x_n)^T$
x_k	the kth approximation to x^*, a minimum of $f(x)$
$f(x)$,f_k	function of x, function f at x_k
$\mathbb{R}^n$	linear n-dimensional Real space
$g(x)$	the $n \times 1$ gradient vector of $f(x)$ where $g_i = \frac{\partial f}{\partial x_i}$ for $i = 1, 2, \cdots, n$
g_k	the gradient vector $f(x)$ at x_k
$G(x)$	the $n \times n$ Hessian matrix of f(x) where $G_{ij} = \frac{\partial^2 f}{\partial x_i \partial x_j}$ for $i, j = 1, 2, \cdots, n$.
G_k	the Hessian of $f(x)$ at x_k
A^T	transpose of A
B_k	an $n \times n$ matrix that is a kth approximation of the Hessian
H_k	an $n \times n$ matrix that is a kth approximation of the inverse Hessian
$\|\cdot\|$	an arbitrary norm of $(\cdot)$
min	minimum
$\det(A)$	determinant of A
$\mathrm{Tr}(A)$	trace of A
I	identity matrix
BFGS	Broyden-Fletcher-Goldfarb-Shanno

CHAPTER 1

INTRODUCTION

1.1 Preliminaries

In these recent years, the area of optimization has received extensive attention primarily due to the rapid growth and development progress in computer technology. Many application problems can be formulated as optimization problems and hence optimization has been a basic tool in diverse areas no matter in applied mathematics, medicines, engineering or in economics. New optimization algorithms and theoretical techniques have been generated aiming to deal with choosing the best alternative to certain mathematical defined problems. In short, optimization is the central to any problem especially those involving decision making. The purpose of all such decision making is either to minimize cost or to maximize profit.

1.2 Optimization Problem

Optimization problem is dealing with the methods for selecting the least value (the *minimum*) or the greatest value (the *maximum*) of a function of any number of independent variables called the *objective function*. Note that any maximization problem can be represented equivalently in the minimization form by multiplying a factor of -1 to the objective function. Thus, optimization can be considered as minimization without loss of generality.

The general form of optimization problem is

$$\begin{aligned} &\min f(x) \\ &\text{s.t. } x \in \Omega, \end{aligned} \tag{1.1}$$

where $f(x)$ is an objective function, $x \in \mathbb{R}^n$ is a n-vector of independent variables and $\Omega \subset \mathbb{R}^n$ is a constraint set or feasible region.

Optimization problem can be further categorized into constrained optimization problem and unconstrained optimization problem. Constrained optimization is involved with minimizing an objection function with the presence of constraints on some variables where the constraints can be equality constraints or inequality constraints. The general constrained optimization problem can be presented as below:

$$\begin{aligned} & \min f(x) \\ \text{s.t. } & c_i(x) = 0, i = 1, 2, \cdots, n, \\ & d_j(x) \geq 0, j = 1, 2, \cdots, m. \end{aligned} \tag{1.2}$$

When there is no constraint being imposed to the objective function or the constraint set $x = \mathbb{R}^n$, then the optimization problem (1.1) is known as an unconstrained optimization problem:

$$\min_{x \in \mathbb{R}} f(x). \tag{1.3}$$

The problem is known as linear programming if both the objective functions and constraint functions consist of linear functions. Otherwise, the problem is called nonlinear programming.

The scope of this thesis is limited to nonlinear unconstrained optimization problems, in which f is assumed to be continuous and differentiable. Before we go further, we shall state some mathematical background of unconstraind optimization.

1.3 Basic Definitions and Theorems

In this section, we recall some essential theorems and definitions on linear algebra and calculus which are very helpful for discussion on our main topic. Hence, this chapter also serves as base and background for the studies of the subsequent chapters. The proof of the theorems, properties and lemmas can be referred to any book of numerical optimization, for example Nocedal and Wright (1999), and Sun and Yuan (2006).

1.3.1 Function and Derivatives

This section present some background of set theory and multivariable calculus.

Definition 1.1 : *A δ-neighborhood of a point $x \in \mathbb{R}^n$ is the set*

$$N_\delta(x) = \{y \in \mathbb{R}^n : \|y - x\| < \delta\},$$

where δ is some positive number.

We can also called the neighborhood as a *ball* with radius δ and center x.

Definition 1.2 : *Let $D \subset \mathbb{R}^n$ and $x \in D$. The point x is said to be*
(i) an interior point of D if the set D contains some neighborhood of x. The set of all such points of D is called the interior of D and is denoted by int(D).
(ii) a boundary point of D if every neighborhood of x contains a point in D and a point not in D. The set of all boundary points of D is called the boundary of D.

Definition 1.3 : *A set D is said to be open if it contains a neighborhood of each of its points which is also meant that each of its points is an interior point, or equivalently, if D contains no boundary points.*

Definition 1.4 : *A set D is said to be closed if it contains its boundary.*

It can be shown that a set is closed if and only if its complement is open. (see for example Fridy (2000)).

Definition 1.5 : *A set that is contained in a ball of finite radius is said to be bounded.*

Definition 1.6 : *A set is compact if it is both closed and bounded.*

There exists a convergent subsequence with a limit in D for every sequence $\{x_k\}$ in a compact set D. Thus, compact sets are important in optimization problems.

Theorem 1.1 (Weierstrass Theorem): *Let $f : \Omega \to \mathbb{R}$ be a continuous function, where $\Omega \subset \mathbb{R}^n$ is a compact set. Then, there exists a point $x_0 \in \Omega$ such that $f(x_0) \leq f(x)$ for all $x \in \Omega$. In other words, f achieves its minimum on Ω.*

It is crucial to discuss about continuity, Lipschitz continuity and differentiability because they contribute in obtaining minimizer of problem (1.3).

Definition 1.7 : *A function $f : \mathbb{R}^n \to \mathbb{R}$ is said to be continuous at $\bar{x} \in \mathbb{R}^n$ if, for any given $\epsilon > 0$, there exists $\delta > 0$ such that $\|x - \bar{x}\| < \delta$ implies $|f(x) - f(\bar{x})| < \epsilon$. A function f is said to be continuous on D if it is continuous at every point in an open set $D \subset \mathbb{R}^n$.*

There is another stronger form of continuity which able to guarantee the existence and uniqueness of the solution to the objective function which is Lipschitz continuity.

Definition 1.8 : *A function $f : \mathbb{R}^n \to \mathbb{R}$ is said to be globally Lipschitz-continuous on $\mathbb{R}^n$ if there exists a real number $L > 0$ (called the Lipschitz constant), such that*

$$\|f(y) - f(x)\| \leq L \|y - x\|, \textit{for } \forall y, x \in \mathbb{R}^n. \tag{1.4}$$

The function f is called locally Lipschitz-continuous, if for each $x \in \mathbb{R}^n$ there exists a real number $L > 0$ such that f is Lipschitz-continuous on the open ball of center x and radius L

$$\|f(y) - f(x)\| \leq L \|y - x\|, \text{for } \forall y, x \in N_L(x) \cap \mathbb{R}^n. \tag{1.5}$$

Definition 1.9 : *A continuous function $f : \mathbb{R}^n \to \mathbb{R}$ is said to be continuously differentiable at $x \in \mathbb{R}^n$ if $\left(\frac{\partial f}{\partial x_i}\right)(x)$ exists and is continuous, for $i = 1, \cdots, n$.*

The gradient of f at x is defined as

$$\nabla f(x) = \left[\frac{\partial f}{\partial x_1}(x), \cdots, \frac{\partial f}{\partial x_n}(x)\right]^T. \tag{1.6}$$

A function f is said to be continuously differentiable on D if it is continuously differentiable at every point of an open set $D \subset \mathbb{R}^n$.

Definition 1.10 : *A continuous function $f : \mathbb{R}^n \to \mathbb{R}$ is said to be twice continuously differentiable at $x \in \mathbb{R}^n$ if $\left(\frac{\partial^2 f}{\partial x_i \partial x_j}\right)(x)$ exists and is continuous, for $i, j = 1, \cdots, n$.*

The Hessian of f at x is defined as the $n \times n$ symmetric matrix with elements

$$[\nabla^2 f(x)]_{ij} = \frac{\partial^2 f}{\partial x_i \partial x_j}(x), \tag{1.7}$$

for $1 \leq i, j \leq n$. A function is said to be twice continuously differentiable on D if it is twice continuously differentiable at every point of an open set $D \subset \mathbb{R}^n$. Thus, the relationships between Lipschitz continuity, continuity and differentiability can be expressed in the theorems below where the proof can be found in Sideris (2013).

Theorem 1.2 : *Every locally Lipschitz-continuous function is continuous.*

1.3.2 Optimality Conditions for Unconstrained Optimization

Generally, there are two kinds of minimizers which are local minimizer and global minimizer. Here we present the conditions for a point x^* to be a minimizer.

Definition 1.11 : *A point x^* is called*
(i) a local minimizer if there exists $\delta > 0$ such that $f(x^*) \leq f(x)$ for all $x \in \mathbb{R}^n$ satisfying $\|x - x^*\| < \delta$.
(ii) a strict local minimizer if there exists $\delta > 0$ such that $f(x^*) < f(x)$ for all $x \in \mathbb{R}^n$ with $x \neq x^*$ and satisfying $\|x - x^*\| < \delta$.
(iii) a global minimizer if $f(x^*) \leq f(x)$ for all $x \in \mathbb{R}^n$.
(iv) a strict global minimizer if $f(x^*) < f(x)$ for all $x \in \mathbb{R}^n$ with $x \neq x^*$.

In practice, due to obtaining a global minimizer is a difficult task, most algorithms are only capable to find a local minimizer, which is a point that achieves the smallest value of f in its neighborhood. Thus, we usually have to be satisfied with finding local minimizers. Taylor's theorem is the common mathematical tool used to study minimizers of smooth functions. Thus, here we present the Taylor's theorem before we discuss the necessary conditions for optimality. Its proof is easily available in most calculus textbook.

Theorem 1.3 :(Taylor's Theorem) *Let $f : \mathbb{R}^n \to \mathbb{R}$ be a continuosly differentiable function and $p \in \mathbb{R}^n$. Thus we have that*

$$f(x+p) = f(x) + \nabla f(x+tp)^T p, \tag{1.8}$$

for some $t \in (0,1)$. Futhermore, if f is twice differentiable, we obtain

$$\nabla f(x+p) = \nabla f(x) + \int_0^1 \nabla^2 f(x+tp)p \, dt, \tag{1.9}$$

and that

$$f(x+p) = f(x) + \nabla f(x)^T p + \frac{1}{2} p^T \nabla^2 f(x+tp)p, \tag{1.10}$$

for some $t \in (0,1)$.

Definition 1.12 : *Let $f : \mathbb{R}^n \to \mathbb{R}$. A vector $d \in \mathbb{R}^n$ is known as a descent direction for f at x if there exists $\delta > 0$ such that*

$$f(x + \lambda d) < f(x), \tag{1.11}$$

for all $\lambda \in (0, \delta)$.

Theorem 1.4 : *Let $f : \mathbb{R}^n \to \mathbb{R}$ be differentiable at $x \in \mathbb{R}^n$. A vector $d \in \mathbb{R}^n$ is a descent direction of f at x if*

$$\langle \nabla f(x), d \rangle < 0. \tag{1.12}$$

By using the Taylor's second order expansion,

$$f(x_k + \lambda d) = f(x_k) + \lambda \nabla f(x_k)^T d + o(\lambda),$$

then it is clearly to see that

$$\exists \delta > 0 \text{ such that } f(x_k + \lambda d) < f(x_k), \forall \lambda \in (0, \delta)$$

if and only if d is a descent direction of f at x_k.

Most line search algorithms demand d_k to be a descent direction because this property guarantees to lower the function f along this search direction.

Clearly, definiteness or semidefiniteness of the Hessian plays a crucial role in the necessary and sufficient conditions in optimization. To check the positive definiteness of the Hessian matrix of f at x, we have the following definition:

Definition 1.13 : *Let $A \in \mathbb{R}^{n \times n}$ be symmetric. A is said to be*
(i) positive definite if $v^T Av > 0, \forall v \in \mathbb{R}^n, v \neq 0$.
(ii) positive semidefinite if $v^T Av \geq 0, \forall v \in \mathbb{R}^n$.
(iii) negative definite if $v^T Av < 0, \forall v \in \mathbb{R}^n, v \neq 0$.
(iv) negative semidefinite if $v^T Av \leq 0, \forall v \in \mathbb{R}^n$.
(v) indefinite if it is neither positive semidefinite nor negative semidefinite.

The following part presents the discussion about the first-order optimality condition. The proofs of these results are available in most text books (for example Nocedal and Wright (1999)). For the purpose of clarification, we duplicate some of the proofs to this thesis.

Theorem 1.5 (First-Order Necessary Condition): *If x^* is a local minimizer and f is continuously differentiable in an open neighborhood of x^*, then*

$$\nabla f(x^*) = 0. \tag{1.13}$$

Proof:
Suppose there is a contradiction that $\nabla f(x^*) \neq 0$. Taking the vector $d = -\nabla f(x^*)$ yields

$$d^T \nabla f(x^*) = -\|\nabla f(x^*)\|^2 < 0.$$

Due to ∇f is continuous near x^*, there exists a scalar $T > 0$ such that

$$d^T \nabla f(x^* + td) < 0,$$

for all $t \in [0, T]$. For any $\bar{t} \in [0, T]$,

$$f(x^* + \bar{t}d) = f(x^*) + \bar{t}d^T \nabla f(x^* + td),$$

can be obtained for some $t \in [0, \bar{t}]$ by Taylor's theorem. Hence,

$$f(x^* + \bar{t}d) < f(x^*),$$

for all $\bar{t} \in [0, T]$. This contradicts the assumption that x^* is a local minimizer as we have obtained a direction leading away from x^* along which f decreases. □

Remark 1.1 : *A point x^* is called a stationary point if $\nabla f(x^*) = 0$.*

Thus, according to Theorem 1.5, any local minimizer must be a stationary point. In the following, we will discuss about the second-order conditions for a local minimum.

Theorem 1.6 (Second-Order Necessary Conditions): *If x^* is a local minimizer of f and $\nabla^2 f$ exists and is continuous in an open neighborhood of x^*, then $\nabla f(x^*) = 0$ and $\nabla^2 f(x^*)$ is positive semidefinite.*

Proof:
We have known from Theorem 1.3 that $\nabla f(x^*) = 0$, hence only thing left is to show that $\nabla^2 f(x^*)$ is positive semidefinite. Suppose for the sake of contradiction that $\nabla^2 f(x^*)$ is not positive semidefinite. A vector d is being picked such that $d^T \nabla^2 f(x^*) p < 0$, and due to $\nabla^2 f$ is continuous near x^*, there exists a scalar $T > 0$ such that

$$d^T \nabla^2 f(x^* + td)d < 0,$$

for all $t \in [0, T]$. Hence,

$$f(x^* + \bar{t}d) = f(x^*) + \bar{t}d^T \nabla f(x^*) + \tfrac{1}{2}\bar{t}^2 d^T \nabla^2 f(x^* + td)d < f(x^*).$$

is obtained by performing a Taylor series expansion around x^* for all $\bar{t} \in [0, T]$ and some $t \in [0, \bar{t}]$. This again contradicts the assumption that x^* is a local minimizer as we have found a direction leading away from x^* along which f decreases as in Theorem 1.3. □

Next, we describe the second-order sufficient conditions on the derivatives of f at the point z^* that guarantee that x^* is a local minimizer.

Theorem 1.7 :(Second-Order Sufficient Conditions) *Suppose that $\nabla^2 f$ is continuous in an open neighborhood of x^*, and that $\nabla f(x^*) = 0$ and $\nabla^2 f(x^*)$ is positive definite. Then x^* is a strict local minimizer of f.*

Proof:
Since the Hessian is continuous and positive definite at x^*, a radius $r > 0$ is chosen so that $\nabla^2 f(x)$ remains positive definite for all x in the open ball $D = \{z | \, \|z - x^*\| < r\}$. Taking any nonzero d with $\|d\| < r$, $x^* + d \in D$ will be obtained and so

$$f(x^* + d) = f(x^*) + d^T \nabla f(x^*) + \tfrac{1}{2} d^T \nabla^2 f(z) d = f(x^*) + \tfrac{1}{2} d^T \nabla^2 f(z) d,$$

where $z = x^* + td$ for some $t \in (0, 1)$. Since $z \in D$, we have $d^T \nabla^2 f(z) d > 0$, and therefore

$$f(x^* + d) > f(x^*),$$

which shows the result. □

1.3.3 Convexity

The concept of *convexity* plays an essential role in the study of optimization. Many practicals problems possess this property, which generally makes them easier to be solved in both theory and practise. The term "convex" is applicable to both sets and functions. In this subsection, we present the elementary concepts of convex sets and convex functions.

Definition 1.14 : *Let the set $S \in \mathbb{R}^n$. If, for any $x_1, x_2 \in S$, we have*

$$\alpha x_1 + (1 - \alpha) x_2 \in S, \tag{1.14}$$

for all $\alpha \in [0, 1]$, then S is said to be a convex set.

This above definition indicates that the straight line segment connecting any two points in S lies entirely inside S. In other words, it also states that S is path-connected which is two arbitrary points in S can be joined by a continous path.

Definition 1.15 : *Suppose that $S \subset \mathbb{R}^n$ is a nonempty convex set and let $f : S \subset \mathbb{R}^n \to \mathbb{R}$. Then f is said to be convex on S if we have*

$$f(\alpha x_1 + (1 - \alpha) x_2) \le \alpha f(x_1) + (1 - \alpha) f(x_2), \tag{1.15}$$

for any $x_1, x_2 \in S$ and all $\alpha \in [0, 1]$.

We say that f is *strictly convex* if the above inequality in (1.15) is strict whenever $x_1 \neq x_2$ and α is in the open interval (0,1). A function f is said to be *uniformly* (or *strongly*) *convex* on S if there is a constant $c > 0$ such that for any $x_1, x_2 \in S$,

$$f(\alpha x_1 + (1 - \alpha) x_2) \le \alpha f(x_1) + (1 - \alpha) f(x_2) - \frac{1}{2} c \alpha (1 - \alpha) \|x_1 - x_2\|^2. \tag{1.16}$$

A function f is called a *concave* (strictly concave, uniformly concave) function if $-f$ is a convex (strictly convex, uniformly convex) function on S.

The following necessary and sufficient conditions for a differential convex function is established if a convex function is differentiable.

Theorem 1.8 : *Suppose that $S \subset \mathbb{R}^n$ is a nonempty open convex set and let $f : S \subset \mathbb{R}^n \to \mathbb{R}$ be a differentiable function. Then*
(a) f is convex if and only if

$$f(y) \geq f(x) + \nabla f(x)^T (y - x), \forall x, y \in S. \tag{1.17}$$

(b) f is strictly convex on S if and only if

$$f(y) > f(x) + \nabla f(x)^T (y - x), \forall x, y \in S, y \neq x. \tag{1.18}$$

(c) f is uniformly convex on S if and only if

$$f(y) \geq f(x) + \nabla f(x)^T (y - x) + \frac{1}{2} c \left\| y - x \right\|^2, \forall x, y \in S, \tag{1.19}$$

where $c > 0$ is a constant.

Proof:
Necessity: Suppose that f is a convex function, then

$$f(\alpha y + (1 - \alpha)x) \leq \alpha f(y) + (1 - \alpha) f(x),$$

is valid for all $\alpha \in (0, 1)$. Therefore,

$$\tfrac{f(x+\alpha(y-x))-f(x)}{\alpha} \leq f(y) - f(x).$$

By setting $\alpha \to 0$ gives us

$$\nabla f(x)^T (y - x) \leq f(y) - f(x).$$

Sufficiency: Assume that (1.17) holds. By choosing any $x_1, x_2 \in S$ and set $x = \alpha x_1 + (1 - \alpha)x_2$ where $\alpha \in (0, 1)$, the following inequities can be obtained:

$$\begin{array}{c} f(x_1) \geq f(x) + \nabla f(x)^T (x_1 - x), \\ f(x_2) \geq f(x) + \nabla f(x)^T (x_2 - x). \end{array}$$

Hence,

$$\begin{array}{c} \alpha f(x_1) + (1 - \alpha) f(x_2) \geq f(x) + \nabla f(x)^T (\alpha x_1 + (1 - \alpha)x_2 - x), \\ = f(\alpha x_1 + (1 - \alpha)x_2), \end{array}$$

which indicates that f is a convex function.

The other two cases (b) and (c) can be proved in similar approach. The only extra step to obtain (1.19) is to apply (1.17) to the function $f - \frac{1}{2} c \left\| \cdot \right\|^2$. $\square$

Next, the second order characteristic of a twice continuously differentiable convex function will be considered.

Theorem 1.9 : *Let $S \subset \mathbb{R}^n$ be a nonempty open convex set and suppose $f : S \subset \mathbb{R}^n \to \mathbb{R}$ be a twice continuously differentiable function. Then*
(a) f is convex if and only if its Hessian matrix is positive semidefinite at each point in S.
(b) f is strictly convex on S if its Hessian matrix is positive definite at each point in S.
(c) f is uniformly convex on S if and only if its Hessian matrix is uniformly positive definite at each point in S.

Proof:
Only the prooving for the first case is shown as the other two cases are analogous. Sufficiency: Let the Hessian matrix $\nabla^2 f(x)$ be positive semidefinite at each point $x \in S$ and take $x, \bar{x} \in S$. Then

$$f(x) = f(\bar{x}) + \nabla f(\bar{x})^T (x - \bar{x}) + \tfrac{1}{2}(x - \bar{x})^T \nabla^2 f(\hat{x})(x - \bar{x}),$$

where $\hat{x} = \bar{x} + \theta(x - \bar{x}), \theta \in (0, 1)$ by using the Mean-value Theorem. Noting that $\hat{x} \in S$, it follows from the assumption that

$$f(x) \geq f(\bar{x}) + \nabla f(\bar{x})^T (x - \bar{x}).$$

Therefore, Theorem 1.8 implies that f is a convex function.

Necessity: Suppose that f is a convex function and let $\bar{x} \in S$. It is necessary to show that $d^T \nabla^2 f(\bar{x}) d \geq 0, \forall d \in \mathbb{R}^n$. Since S is open, then there exists $\delta > 0$ such that when $|\lambda| < \delta, \bar{x} + \lambda d \in S$. By Theorem 1.8,

$$f(\bar{x} + \lambda d) \geq f(\bar{x}) + \nabla f(\bar{x})^T d. \tag{1.20}$$

Since f is also twice differentiable at $\bar{x}$, then

$$f(\bar{x} + \lambda d) = f(\bar{x}) + \lambda \nabla f(\bar{x})^T d + \frac{\lambda^2}{2} d^T \nabla^2 f(\bar{x}) d + o(\|\lambda d\|^2). \tag{1.21}$$

Substituting (1.21) into (1.20) will give us

$$\tfrac{1}{2}\lambda^2 d^T \nabla^2 f(\bar{x}) d + o(\|\lambda d\|^2) \geq 0.$$

Dividing by λ^2 and letting $\lambda \to 0$, it follows that

$$d^T \nabla^2 f(\bar{x}) d \geq 0.$$

□

1.4 Objectives

For solving unconstrained optimization problems, iterative algorithms play an important role. In an iterative algorithm, an initial point x_0 must be given in order to get a new iterate point in the following form

$$x_{k+1} = x_k + s_k. \tag{1.22}$$

On the other hand, a dynamical system is a concept in mathematics that describe time-based systems with particular properties. Consider the system

$$\dot{x} = f(x(t), t), \tag{1.23}$$

where $f : \mathbb{R}^n \to \mathbb{R}^n$ and $x(0) = x_0$ is given. This system can be discretized to

$$x(k+1) = x(k) + \alpha f(x(k), k), \tag{1.24}$$

where $\alpha > 0$ is the step length. Clearly we can see that there are some correlationship between these optimization and discretization of dynamical system.

Gradient flow system is a classical issue in dynamical systems. The idea behind this method of gradient arose in the study of variational partial differential equations. By starting with a given initial point $x_0 \in \mathbb{R}$, a minimizer of f, denoted by x^* is to be obtained by following a curve defined by the ordinary differential equation

$$\begin{aligned} \dot{x}(t) &= -\nabla f(x(t)), \\ x(0) &= x_0, \end{aligned} \tag{1.25}$$

where ∇f is the gradient of f.

One of the advantages of the gradient method is no modification is required to be applied to nonlinear problems. Since the scope of this thesis is limited to solving nonlinear unconstrained optimization problems, hence it is very logical to think of using the gradient flow system for nonlinear unconstrained optimization.

The main objective of this thesis is to investigate the possible use of control theory, particularly theory on gradient flow system to derive some numerical methods for optimization.

The specific objectives are:
1. To derive some quasi-Newton-type methods using gradient flow system.
2. To establish the convergence properties of the proposed methods.
3. To develop optimization algorithm based on the modified methods and to perform numerical experiments for showing the efficiency of the methods.

1.5 An Overview of the Thesis

In this thesis, we are mainly concerned with solving the nonlinear unconstrained optimization problems. Firstly, a brief introduction about optimization problems and its related mathematical background is presented in this Chapter 1.

In the next chapter, we will discuss on line search methods especially the quasi-Newton methods as this thesis is mainly about modifications on quasi-Newton type methods. This chapter also reviews some literature on topics such as line search methods, quasi-Newton methods and trust region methods.

In the following four chapters, we will present our modified methods and establish their global convergence properties under some suitable conditions. In precise, Chapter 3 is mainly about implemendation of modified quasi-Newton-type methods on line search methods whereas Chapter 5 is concerned with implemendation of modified quasi-Newton-type methods on trust region methods. All the algorithms and numerical results are included in this two chapters. We presented the global convergence properties of modified quasi-Newton-type methods in Chapter 4 and Chapter 6 respectively.

Finally , Chapter 7 consists of a summary of the achivements of the previous chapter as the conclusion of this thesis. Possible future works will also be considered in this chapter.

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