Chapter 3

Research scope in conjugate gradient method and objective of the work

Although the Conjugate Gradient method have been experienced an intensive theoretical and computational research for last few decades, there is a huge research scope in this area. There are some very important open problems, which requires further investigations. Some of the problems are listed below and out of these we have investigated three of the open problems and found some new and better result.

These problems are

- Why is the initial search direction critical ?
- What is the best Conjugacy condition ?
- Why does the sequence of step length tend to vary in a totally unpredictable manner ?
- What is the influence of accuracy of the line search procedure on the performances of Conjugate Gradient algorithms ?
- How can we use the function values in to generate new Conjugate Gradient algorithms ?
- Can we take advantage of problem structure to design more effective nonlinear Conjugate Gradient algorithms ?
- How can we consider the second order information in Conjugate Gradient algorithms?
- What is the best scaled Conjugate Gradient algorithm ?
- What is the best hybrid Conjugate Gradient algorithm ?
- What is the most convenient restart procedure of Conjugate Gradient algorithms ?
- What is the most suitable criterion for stopping the Conjugate Gradient iterations ?
- What is the interrelationship between Conjugate Gradient and quasi-Newton algorithms, including here the limited memory quasi-Newton algorithms ?
- Can the nonlinear Conjugate Gradient be extended to solve simple bounded constrained optimization?

The popularity of these method is remarkable partially due to their simplicity both in the algebraic expression and their implementation in computer codes and partially due their efficiency in solving large scale unconstrained optimization problem.

Objectives of the work

In this thesis we have considered some open problems associated to the nonlinear conjugate gradient algorithms for unconstrained optimization and we have solved some of the problems associated to the nonlinear conjugate gradient algorithms for unconstrained optimization. These problems mainly refer to the initial direction, the conjugacy condition and the step length computation etc. The general nonlinear method always considers a critical search direction to find a convergent solution. In the present thesis our aim is to establish the fact that the convergent solution can also be obtained for nonlinear function,even if the search direction is different from the initial search direction taken in most of the algorithms of the nonlinear conjugate gradient method to get a convergent solution and with the help of this new initial search direction we have got a new modified form of conjugacy condition and using this the step length can also be determined.

In this thesis we have used various test functions which are as follows

Extended Powell function :

$$f(x)=\sum_{i=1}^{n/4}(x_{4i-3}+10x_{4i-2})^2+5(x_{4i-1}-x_{4i})^2+(x_{4i-2}-2x_{4i-1})^4+10(x_{4i-3}-x_{4i})^4 \tag{3.1}$$

Broyden Tridiagonal function :

$$f(x)=(3x_1-2x_1^2)^2+\sum_{i=2}^{n-1}(3x_i-2x_i^2-x_{i-1}-2x_{i+1}+1)^2+(3x_n-2x_n^2-x_{n-1}+1)^2$$
$$x_0=[-1,-1,..........,-1] \tag{3.2}$$

Extended Rosenbrock function :

$$f(x)=\sum_{i=1}^{\frac{n}{2}}c(x_{2i}-x_{2i-1}^2)^2+(1-x_{2i-1})^2$$
$$x_0=[-1.2,1,......,-1.2,1],c=100 \tag{3.3}$$

Generalized Rosenbrock function :

$$f(x)=\sum_{i=1}^{n-1} c(x_{i+1}-x_i^2)^2+(1-x_i)^2$$
$$x_0=[-1.2,1,......,-1.2,1], c=100 \quad (3.4)$$

Extended Trigonometric function:

$$f(x)=\sum_{i=1}^{n}\left(\left(n-\sum_{j=1}^{n}\cos x_j\right)+i(1-\cos x_i)-\sin x_i\right)^2$$
$$x_0=[0.2, 0.2, ..., 0.2] \quad (3.5)$$

Sphere function :

$$f(x)=\sum_{i=1}^{n} x_i^2, \quad x_i \in \mathbb{R}^n$$
$$-5.12 \le x_i \le 5.12 \quad (3.6)$$

Hyper Ellipsoid function :

$$f(x)=\sum_{i=1}^{n}\sum_{j=1}^{i} x_i^2, \quad x_i \in \mathbb{R}^n$$
$$-65.53 \le x_i \le 65.53 \quad (3.7)$$

Zakharov Function :

$$f(x)=\sum_{i=1}^{n} x_i^2+(\sum_{i=1}^{n} 0.5ix_i)^2+(\sum_{i=1}^{n} 0.5ix_i)^4, \quad (3.8)$$
$$x_i \in \mathbb{R}^n, -5 \le x_i \le 10$$