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A Switching Algorithm Based on Modified Quasi-Newton Equation[†]

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Abstract. In this paper, a switching method for unconstrained minimization is proposed. The method is based on the modified BFGS method and the modified SR1 method. The eigenvalues and condition numbers of both the modified updates are evaluated and used in the switching rule. When the condition number of the modified SR1 update is superior to the modified BFGS update, the step in the proposed quasi-Newton method is the modified SR1 step. Otherwise the step is the modified BFGS step. The efficiency of the proposed method is tested by numerical experiments on small, medium and large scale optimization. The numerical results are reported and analyzed to show the superiority of the proposed method.

Key words: Quasi-Newton equation; SR1 method; BFGS method; Large scale optimization.

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1 Introduction

In this paper, we concern with the Quasi-Newton(QN) methods for unconstrained optimization

$$\min f(x), \tag{1}$$

where $x \in R^n$ and $f(x)$ is a twice continuously differentiable function. Denote $g = \nabla f(x)$ the gradient of f, H an approximation to the inverse Hessian matrix of f. Starting from an initial point x_0 and initial matrix H_0, a QN method generates sequences $\{x_k\}$ and $\{H_k\}$ using the iteration

$$x_{k+1} = x_k + \alpha_k d_k$$

where d_k is a search direction, generally descent and generated from either $B_k d_k = -g_k$ (B_k is an approximation to the Hessian of f) or $d_k = -H_k g_k$, and α_k is a step-length along the direction d_k and is determined using any inexact line searches. When $d_k = -H_k g_k$ is used to generate the search direction, the matrix H_k is required to satisfy the Quasi-Newton equation

$$H_k y_{k-1} = s_{k-1}, \tag{2}$$

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where $s_{k-1} = x_k - x_{k-1}$, $y_{k-1} = g_k - g_{k-1}$.

Different methods arise from the large variety of matrices H satisfying (2) and from varying schemes to determine step length α_k at each iteration. The famous SR1 method employs the symmetric rank-one update

$$H_{k+1} = H_k + \frac{(s_k - H_k y_k)(s_k - H_k y_k)^T}{(s_k - H_k y_k)^T y_k} \tag{3}$$

and has quadratic termination property without requiring exact line searches (see [1,2]). However, the SR1 method is numerical instable due to the fact that its denominator may be zero or nearly zero. Also the updates may not preserve the positive definiteness even when the previous H_k is positive definite. The rank-two update, BFGS update

$$H_{k+1} = H_k + \left(1 + \frac{y_k^T H_k y_k}{s_k^T y_k}\right) \frac{s_k s_k^T}{s_k^T y_k} - \frac{H_k y_k s_k^T + s_k y_k^T H_k}{s_k^T y_k} \tag{4}$$

is used most widely in quasi-Newton methods and has some useful properties (see [3]).

Some recent results on SR1 update show, comparing with other Quasi-Newton updates such as BFGS and DFP updates, that whenever SR1 update is available, it is more efficient. It is proved in [4] that the sequence of approximate Hessian matrices of $f(x)$ generated by the SR1 update converges to the actual Hessian at the solution, provided that the search directions $\{d_k\}$ are uniformly linearly independent, and that the iterates $\{x_k\}$ converges to x^*. Whereupon SR1 update is paid more attention by many researchers (See [4-7]). Some studies show that the main reason of instable numerical behavior of the SR1 method is the unsuitable eigenvalue's ratio. To overcome the setback of the SR1 update, various variants to the SR1 method are proposed, for example, self-adjusting variable metric algorithm, switching algorithm, multi-direction parallel algorithm (see [8-11]).

In order to improve the efficiency of quasi-Newton methods, Xu and Zhang in [12] proposed a modified Quasi-Newton equation

$$H_{k+1}\hat{y}_k = s_k, \tag{5}$$

where

$$\hat{y}_k = \left(1 + \frac{\theta_k}{s_k^T y_k}\right) y_k, \quad \theta_k = 6(f_k - f_{k+1}) + 3(g_k + g_{k+1})^T s_k.$$

With the equation (5), the symmetric rank-one update(HSR1) has the form

$$H_{k+1} = H_k + \frac{(s_k - H_k \hat{y}_k)(s_k - H_k \hat{y}_k)^T}{(s_k - H_k \hat{y}_k)^T \hat{y}_k}, \tag{6}$$

and the BFGS update has the form

$$H_{k+1} = H_k + \left(1 + \frac{\hat{y}_k^T H_k \hat{y}_k}{s_k^T \hat{y}_k}\right) \frac{s_k s_k^T}{s_k^T \hat{y}_k} - \frac{H_k \hat{y}_k s_k^T + s_k \hat{y}_k^T H_k}{s_k^T \hat{y}_k}. \tag{7}$$

The above method is called modified BFGS (MBFGS) update in this paper. These modified QN-updates efficiently exploit both gradient and function information. Numerical results reported in [13] show that both of the HSR1 and MBFGS updates are more competitive to the general SR1 and BFGS updates respectively. We also notice that if the HSR1 update solves a practical problem, its efficiency is usually better than the other QN updates (SR1, BFGS and MBFGS, for instance). Meanwhile this modified update has the same setback as the SR1 update.