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Lukšan, Ladislav
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L. Lukšan, C. Matonoha, J. Vlček

Institute of Computer Science, AS CR, Prague

1 Introduction

Basic optimization methods for minimization of function $F : \mathcal{R}^n \to \mathcal{R}$ can be realized in various ways which differ in direction determination and step-size selection. Line-search and trust-region realizations are most popular. Trust-region methods can be advantageously used when the Hessian matrix of the objective function (or its approximation) is indefinite, ill-conditioned or singular. This situation often arises in connection with the Newton method for general objective function (indefiniteness) or with the Gauss-Newton method for nonlinear least-squares (near-singularity).

2 Trust-region methods

Trust-region methods generate points $x_i \in \mathcal{R}^n$, $i \in \mathcal{N}$, in such a way that x_1 is arbitrary and

$$x_{i+1} = x_i + \alpha_i d_i, \quad i \in \mathcal{N}, \tag{1}$$

where $d_i \in \mathcal{R}^n$ are direction vectors and $\alpha_i > 0$ are step-sizes.

A crucial part is a direction determination. There are various commonly known methods for computing direction vectors satisfying certain conditions which we now mention briefly. To simplify the notation, we omit index i.

The most sophisticated method is based on a computation of the optimal locally constrained step. In this case, vector $d \in R^n$ is obtained by solving subproblem

$$\min \quad Q(d) = \frac{1}{2} d^T B d + g^T d \quad \text{subject to} \quad \|d\| \le \Delta, \tag{2}$$

where function $Q(d)$ locally approximates difference $F(x_i + d) - F(x_i)$. Necessary and sufficient conditions for this solution are

$$\|d\| \le \Delta, \quad (B + \lambda I)d = -g, \quad B + \lambda I \succeq 0, \quad \lambda \ge 0, \quad \lambda(\Delta - \|d\|) = 0, \tag{3}$$

where λ is a Lagrange multiplier. The Moré-Sorensen (MS) method [7] is based on solving nonlinear equation $1/\|d(\lambda)\| = 1/\Delta$ with $(B + \lambda I)d(\lambda) + g = 0$ by the Newton method using the sparse Choleski decomposition of $B + \lambda I$. This method is very robust but requires 2-3 Choleski decompositions per iteration.

Simpler methods are based on minimization of $Q(d)$ on the two-dimensional subspace containing Cauchy step $d_C = -(g^T g / g^T B g) g$ and Newton step $d_N = -B^{-1} g$. The most popular is the dog-leg (DL) method [8], [2], where $d = d_N$ if $\|d_N\| \le \Delta$ and $d = (\Delta / \|d_C\|) d_C$ if $\|d_C\| \ge \Delta$. In the remaining case, d is a convex combination of d_C and d_N such that $\|d\| = \Delta$. This method requires only one Choleski decomposition per iteration.

If B is not sufficiently sparse, then the sparse Choleski decomposition of B is expensive. In this case, iterative methods based on conjugate gradients are more suitable. Steihaug [10] and Toint [11] proposed a method based on the fact that $Q(d_{k+1}) < Q(d_k)$ and $\|d_{k+1}\| > \|d_k\|$ hold in the subsequent CG iterations if CG coefficients are positive. We either obtain an unconstrained solution with a sufficient precision or stop on the trust-region boundary if a negative curvature is indicated or the trust-region is left. When suitable preconditioning is used, then this method (PST) is very efficient in practice. Note that $\|d_{k+1}\|_C > \|d_k\|_C$ (where $\|d_k\|_C^2 = d_k^T C d_k$) holds instead of $\|d_{k+1}\| > \|d_k\|$ if preconditioner C (symmetric and positive definite) is used. Thus the solution on the trust-region boundary obtained by the preconditioned CG method can be farther from the optimal locally constrained step than the solution obtained without preconditioning. This insufficiency is usually compensated by the rapid convergence of the preconditioned CG method.

The solution on the trust-region boundary obtained by the Steihaug-Toint method can be rather far from the optimal solution. This insufficiency can be overcame by using the Lanczos process [3]. Initially, the conjugate gradient algorithm is used as in the Steihaug-Toint method. At the same time, the Lanczos tridiagonal matrix is constructed from the CG coefficients. If a negative curvature is indicated or the trust-region is left, we turn to the Lanczos process. In this case, $d = Z\tilde{d}$, where $\tilde{d}$ is obtained by solving subproblem

$$\min \quad \frac{1}{2}\tilde{d}^T T \tilde{d} + \|g\| e_1^T \tilde{d} \quad \text{subject to} \quad \|\tilde{d}\| \le \Delta. \tag{4}$$

Here $T = Z^T B Z$ (with $Z^T Z = I$) is the Lanczos tridiagonal matrix and e_1 is the first column of the unit matrix. This method cannot be successfully preconditioned, since preconditioning changes trust-region constraint $\|d\| \le \Delta$ to $\|d\|_C \le \Delta$, where C changes in each major iteration and can be ill-conditioned.

Therefore, we apply the Steihaug-Toint method to subproblem

$$\min \quad \tilde{Q}(d) = Q_{\tilde{\lambda}}(d) = \frac{1}{2} d^T (B + \tilde{\lambda} I) d + g^T d \quad \text{subject to} \quad \|d\| \le \Delta. \tag{5}$$

Number $\tilde{\lambda} \ge 0$, which approximates λ in (3), is found by solving a small-size subproblem (4) with tridiagonal matrix T obtained by using a small number of the Lanczos steps. This method [6], like method [3], combines good properties of the Moré-Sorensen and the Steihaug-Toint methods. Moreover, it can be successfully preconditioned. The point on the trust-region boundary obtained by this method is usually closer to the optimal solution in comparison with the point obtained by the original Steihaug-Toint method.

3 A shifted Steihaug-Toint method

A (preconditioned) shifted Steihaug-Toint method (PSST) differs from the standard one by using shifted subproblem (5), where number $\tilde{\lambda}$ approximates λ in (3). Number $\tilde{\lambda}$ has to be chosen in such a way that $\tilde{\lambda} = 0$ if $\|d\| < \Delta$, where d is a solution of (2), which is true if $0 \le \tilde{\lambda} \le \lambda$.

If we denote $\mathcal{K}_k = \operatorname{span}\{g, Bg, \ldots, B^{k-1} g\}$ the Krylov subspace of dimension k, then (under some assumptions) we can prove the following assertions. Let

$$d_k(\lambda_i) = \arg\min_{d \in \mathcal{K}_k} Q_{\lambda_i}(d), \quad \text{where} \quad Q_\lambda(d) = \frac{1}{2} d^T (B + \lambda I) d + g^T d.$$

Then

$$\lambda_i \le \lambda_j \quad \Leftrightarrow \quad \|d_k(\lambda_i)\| \ge \|d_k(\lambda_j)\|.$$

Moreover, if

$$d_j = \arg\min_{d \in \mathcal{K}_j} Q(d) \quad \text{subject to} \quad \|d\| \le \Delta, \quad \text{where} \quad Q(d) = \frac{1}{2}\, d^T B d + g^T d$$

with corresponding Lagrange multipliers $\lambda_j,\ j \in \{1, \dots, n\}$, then for $1 \le k \le l \le n$ we have

$$\lambda_k \le \lambda_l.$$

Let's return to subproblem (5). If we set $\tilde{\lambda} = \lambda_k$ for some $k \le n$, then $0 \le \tilde{\lambda} = \lambda_k \le \lambda_n = \lambda$. As a consequence of this inequality, one has that $\lambda = 0$ implies $\tilde{\lambda} = 0$, so that $\|d\| < \Delta$ implies $\tilde{\lambda} = 0$. Thus the shifted Steihaug-Toint method reduces to the standard one in this case. At the same time, if B is positive definite and $\tilde{\lambda} > 0$, then one has $\Delta \le \|(B + \tilde{\lambda} I)^{-1} g\| < \|B^{-1} g\|$. Thus the unconstrained minimizer of (5) is closer to the trust-region boundary than the unconstrained minimizer of (2) and we can expect that $d(\tilde{\lambda})$ is closer to the optimal locally constrained step than d. Finally, if $\tilde{\lambda} > 0$, then matrix $B + \tilde{\lambda} I$ is better conditioned than B and we can expect that the shifted Steihaug-Toint method will converge more rapidly than the original one.

The shifted Steihaug-Toint method consists of the three major steps. First, we carry out $k \ll n$ steps of the unpreconditioned Lanczos method [3] to obtain tridiagonal matrix $T \equiv T_k = Z_k^T B Z_k$, where $Z_k \in \mathcal{R}^{n \times k}$ is the matrix whose columns form an orthonormal basis in $\mathcal{K}_k$. Then we solve subproblem (4) using the Moré-Sorensen method [7] to obtain Lagrange multiplier $\tilde{\lambda}$. Finally, we apply the (preconditioned) Steihaug-Toint method [10],[11] to subproblem (5) to obtain direction vector $d = d(\tilde{\lambda})$.

4 Conclusion

A numerical comparison of methods for computing direction vectors mentioned in section 2 implies several conclusions [6]. If problems do not have sparse Hessian matrices, then direct methods MS and DL can be much worse than iterative methods PST and PSST. On the other hand, direct methods can be more efficient for ill-conditioned but reasonably sparse problems. Comparing PST and PSST, we can see that PSST is usually slightly worse than PST, measured by the computational time, since it uses additional operations for determining the Lanczos matrix T and computing parameter $\tilde{\lambda}$. Nevertheless, if the problems are difficult, then PSST is much better than PST. Thus the total computational time can be lower for PSST.

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