Large-Scale Unconstrained Optimization

Saurav Samantaray

Department of Mathematics

Indian Institute of Technology Madras

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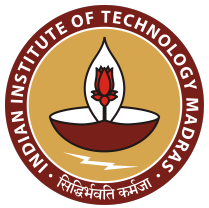

Introduction

- Many applications give rise to unconstrained optimization problems with thousands or millions of variables.
- Problems of this size can be solved efficiently only if the storage and computational costs of the optimization algorithm can be kept at a tolerable level.
- A diverse collection of large-scale optimization methods has been developed to achieve this goal, each being particularly effective for certain problem types.
- Some of these methods are straightforward adaptations of the methods described until now.
- Other approaches are modifications of these basic methods that allow approximate steps to be calculated at lower cost in computation and storage.

Introduction

- The non-linear conjugate gradient methods of can be applied to large problems without modification, owing to its minimal storage demands and its reliance on only first-order derivative information.
- The Newton method in both line search and trust-region algorithms require matrix factorizations of the Hessian matrices.
- High quality software implementations are available, which are based on factorizations that can be carried out using sparse elimination techniques.
- Newton methods are plagued with issues related to computational cost and memory requirements of these sparse factorization methods.
- If the Hessian matrix can be formed explicitly, with the above problems sorted they constitute an effective approach for solving such problems.

Introduction

- Often, however, the cost of factoring the Hessian is prohibitive, and it is preferable to compute approximations to the Newton step using iterative linear algebra techniques.
- Inexact Newton methods that use these techniques, in both line search and trust-region frameworks have attractive global convergence properties and may be super-linearly convergent for suitable choices of parameters.
- There are variants of the quasi-Newton approach, which use Hessian approximations that can be stored compactly by using just a few vectors of length n.
- These methods are fairly robust, inexpensive, and easy to implement, but they do not converge rapidly.

Inexact Newton Methods

- The basic Newton step p_k^N is obtained by solving the symmetric $n \times n$ linear system

$$\nabla^2 f_k p_k^N = -\nabla f_k. \tag{1}$$

- p_k^N can be obtained by solving the above equation (1) approximately, via inexpensive iterative solvers.
- For example the conjugate gradient (CG) method can be employed to get p_k^N.
- Both line search and trust region approaches can be derived based on this approximation, which falls in the general family of inexact Newton methods.
- In addition, we can implement these methods in a Hessian-free manner, so that the Hessian $\nabla^2 f_k$ need not be calculated or stored explicitly at all.

LOCAL CONVERGENCE OF INEXACT NEWTON METHODS

- Consider the residual for the equation (1) as:

$$r_k = \nabla^2 f_k p_k + \nabla f_k \tag{2}$$

where p_k is the inexact Newton step.

- The CG iterations are terminated when

$$||r_k|| \leq \eta_k ||\nabla f_k||, \tag{3}$$

where the sequence $\{\eta_k\}$ (with $0 < \eta_k < 1$ for all k) is called the forcing sequence.

LOCAL CONVERGENCE OF INEXACT NEWTON METHODS

Theorem

Suppose that $\nabla^2 f(x)$ exists and is continuous in a neighbourhood of a minimizer x^*, with $\nabla^2 f(x^*)$ is positive definite. Consider the iteration $x_{k+1} = x_k + p_k$ where p_k satisfies (3), and assume that $\eta_k \leq \eta$ for some constant $\eta \in [0, 1)$. Then, if the starting point x_0 is sufficiently near x^*, the sequence $\{x_k\}$ converges to x^* and satisfies

$$||\nabla^2 f(x^*)(x_{k+1} - x^*)|| \leq \hat{\eta}||\nabla^2 f(x*)(x_k - x^*)||, \qquad (4)$$

for some constant $\hat{\eta}$ with $\eta < \hat{\eta} < 1$.

LINE SEARCH NEWTON–CG METHOD

- In the line search Newton–CG method, also known as the truncated Newton method, the search direction is computed by applying the CG method to the Newton equations:

$$\nabla^2 f_k p_k^N = -\nabla f_k;$$

- and attempt to satisfy a termination test of the form

$$||r_k|| \leq \eta_k ||\nabla f_k||,$$

- The CG method is designed to solve positive definite systems.
- However, the Hessian $\nabla^2 f_k$ may have negative eigenvalues when x_k is not close to a solution.
- The CG iteration is terminated as soon as a direction of negative curvature is generated.

LINE SEARCH NEWTON–CG METHOD

- This adaptation of the CG method produces a search direction p_k that is a descent direction.
- Moreover, the adaptation guarantees that the fast convergence rate of the pure Newton method is preserved, provided that the step length $\alpha_k = 1$ is used whenever it satisfies the acceptance criteria.
- For purposes of this algorithm rewrite the linear system (1) in the form

$$B_k p = -\nabla f_k \tag{5}$$

  where B_k represents $\nabla^2 f_k$.
- For the inner CG iteration, denote the search direction by d_j and the sequence of iterates that it generates by z_j.

LINE SEARCH NEWTON–CG METHOD

- When B_k is positive definite, the inner iteration sequence $\{z_j\}$ will converge to the Newton step p_k^N that solves (5).
- At each major iteration, a tolerance ε_k that specifies the required accuracy of the computed solution.
- For concreteness the forcing sequence is chosen to be $\eta_k = \min(0.5, \sqrt{||\nabla f_k||})$ to obtain a super-linear convergence rate (one may choose differently as well).

Line Search Newton–CG

Algorithm

Given initial point x_0;
for $k = 0, 1, 2, \ldots$
    Define tolerance $\varepsilon = \min(0.5, \sqrt{||\nabla f_k||})||\nabla f_k||$;
    Set $z_0 = 0$, $r_0 = \nabla f_k$, $d_0 = -r_0 = -\nabla f_k$;
    for $j = 0, 1, 2, \ldots$
        if $d_j^T B_k d_j \leq 0$
            if $j = 0$
                return $p_k = -\nabla f_k$;
            else
                return $p_k = z_j$;
        set $\alpha_j = r_j^T r_j / d_j^T B_k d_j$;
        Set $z_{j+1} = z_j + \alpha_j d_j$;
        Set $r_{j+1} = r_j + \alpha_j B_k d_j$;
        if $||r_{j+1}|| < \varepsilon_k$
            return $p_k = z_{j+1}$;
        Set $\beta_{j+1} = r_{j+1}^T r_{j+1} / r_j^T r_j$;
        Set $d_{j+1} = -r_{j+1} + \beta_{j+1} d_j$;
    end (for)
    Set $x_{k+1} = x_k + \alpha_k p_k$, where α_k satisfies the Wolfe, Goldstein, or
        Armijo backtracking conditions (using $\alpha_k = 1$ if possible);
end

LINE SEARCH NEWTON–CG METHOD

- The main differences between the inner loop of the above algorithm and the original CG are that the specific starting point $z_0 = 0$ is used;
- and the use of a positive tolerance ε_k allows the CG iterations to terminate at an inexact solution;
- and the negative curvature test $d_j^T B_k d_j \leq 0$ ensures that p_k is a descent direction for f at x_k.
- If negative curvature is detected on the first inner iteration $j = 0$, the returned direction $p_k = -\nabla f_k$ is both a descent direction and a direction of non-positive curvature for f at x_k.