PRACTICAL OPTIMIZATION ALGORITHMS 实用优化算法

徐翔

数学科学学院 浙江大学

Dec 2, 2021

Chapter VI: Trust-Region Methods (信赖域方 |

法)

Line search methods and trust-region methods both generate steps with the help of a quadratic model (二次函数模型) of the objective function, but they use this model in different ways.

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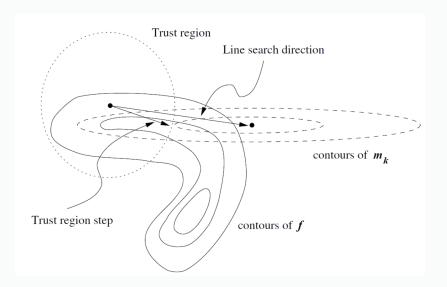
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- then choose the step to be the approximate minimizer of the model in this region.
- In effect, they choose the direction and length of the step simultaneously.
- If a step is not acceptable, they reduce the size of the region and find a new minimizer.
- In general, the direction of the step changes whenever the size of the trust region is altered.

TRUST-REGION AND LINE SEARCH STEPS



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$$f(x_k + p) = f_k + g_k^T p + \frac{1}{2} p^T \nabla f^2(x_k + tp) p,$$
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Outline of the Trust-Region Approach

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where B_k is some symmetric matrix. The difference between $m_k(p)$ and $f(x_k+p)$ is $\mathcal{O}(\|p\|^2)$, which is small when p is small.

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- In the other part, we emphasis the generality of the trust-region approach by assuming little about B_k except symmetry and uniform boundedness.

To obtain each step, we seek a solution of the subproblem

$$\min_{p \in \mathcal{R}^n} m_k(p) = f_k + g_k^T p + \frac{1}{2} p^T B_k p, \quad s.t. \quad ||p|| \le \Delta_k$$
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where $\Delta_k > 0$ is the trust-region radius.

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- If B_k is chosen to be the exact Hessian $\nabla^2 f(x_k)$, the resulting approach is called the trust-region Newton method;
- If B_k is defined by means of a quasi-Newton approximation, we obtain a trust-region quasi-Newton method.

The size of the trust region is critical to the effectiveness of each step.

- If the region is too small, the algorithm misses an opportunity to take a substantial step that will move it much closer to the minimizer of the objective function.
- If too large, the minimizer of the model may be far from the minimizer of the objective function in the region, so we may have to reduce the size of the region and try again.

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- If the model is consistently reliable, producing good steps and accurately
 predicting the behavior of the objective function along these steps, the size
 of the trust region may be increased to allow longer, more ambitious, steps
 to be taken.
- A failed step is an indication that our model is an inadequate representation of the objective function over the current trust region. After such a step, we reduce the size of the region and try again.

Define the ratio

$$\rho_k = \frac{f(x_k) - f(x_k + p_k)}{m_k(0) - m_k(p_k)} \tag{6.4}$$

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 - if ρ_k is close to 1, there is good agreement between the model m_k and the function f over this step, so it is safe to expand the trust region for the next iteration.
 - If ρ_k is positive but not close to 1, we do not alter the trust region, but if it is close to zero or negative, we shrink the trust region.

Algorithm 1 (Trust Region)

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Theorem

The vector p^* is a global solution of the trust-region problem

$$\min_{p \in \mathbb{R}^n} m(p) = f + g^T p + \frac{1}{2} p^T B p, \quad s.t. \quad ||p|| \le \Delta$$
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 p^* is feasible and there is a scalar $\lambda \geq 0$ such that the following conditions are satisfied:

$$(B + \lambda I)p^* = -g, (6.6a)$$

$$\lambda(\Delta - \|p^*\|) = 0,\tag{6.6b}$$

$$(B + \lambda I)$$
 is positive semi-definite. (6.6c)

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- When B_k is positive definite and $\|B_k^{-1}g_k\| \leq \Delta_k$, the solution of (6.3) is easy to identify it is simply the unconstrained minimum $p_k^B = -B_k^{-1}g_k$ of the quadratic $m_k(p)$.

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- In this case, we call p_k^B the *full step*.
- The solution of (6.3) is not so obvious in other cases, but it usually be found without too much computational expense.
- In any case, as described above, we need only an approximate solution to obtain convergence and good practical behavior.

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- Although in principle we are seeking the optimal solution of the subproblem (6.3), it is enough for global convergence purposes to find an approximate solution p_k that lies within the trust region and gives a sufficient reduction in the model.
- The sufficient reduction can be quantified in terms of the Cauchy point, which we denote by p_k^C .

Algorithm 2 (Cauchy Point Calculation)

Find the vector p_k^s that solves a linear version of (6.3), that is,

$$p_k^s = \arg\min_{p \in \mathcal{R}^n} f_k + g_k^T p, \quad s.t. \quad ||p|| \le \Delta_k;$$
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Calculate the scalar $\tau_k > 0$ that minimizes $m_k(\tau p_k^s)$ subject to satisfying the trust-region bound, that is

$$\tau_k = \arg\min_{\tau \ge 0} m_k(\tau p_k^s), \quad s.t. \quad \|\tau p_k^s\| \le \Delta_k \tag{6.8}$$

Algorithm 2 (Cauchy Point Calculation)

Find the vector p_k^s that solves a linear version of (6.3), that is,

$$p_k^s = \arg\min_{p \in \mathcal{R}^n} f_k + g_k^T p, \quad s.t. \quad ||p|| \le \Delta_k;$$
(6.7)

Calculate the scalar $\tau_k > 0$ that minimizes $m_k(\tau p_k^s)$ subject to satisfying the trust-region bound, that is

$$\tau_k = \arg\min_{\tau \ge 0} m_k(\tau p_k^s), \quad s.t. \quad \|\tau p_k^s\| \le \Delta_k \tag{6.8}$$

Set

$$p_k^C = \tau_k p_k^s$$

• The solution of (6.7) is simply

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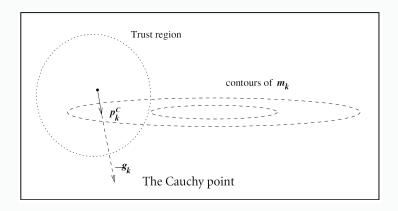
 Furthermore, a closed-form definition of the Cauchy point can be written in the following

$$p_k^C = -\tau_k \frac{\Delta_k}{\|\nabla f(x_k)\|} \nabla f(x_k), \tag{6.9}$$

where

$$\tau_k = \begin{cases} 1, & \text{if } \nabla f(x_k)^T B_k \nabla f(x_k) \le 0\\ \min\left\{ \|\nabla f(x_k)\|^3 / (\nabla f(x_k)^T B_k \nabla f(x_k)), \mathbf{1} \right\} & \text{otherwise.} \end{cases}$$
(6.10)

CAUCHY POINT FOR A SUBPROBLEM



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- Specifically, a trust-region method will be globally convergent if its steps p_k attain a sufficient reduction in m_k ; that is, they give a reduction in the model m_k that is at least some fixed multiple of the decrease attained by the Cauchy step at each iteration.
- The model reduction obtained by the Cauchy point is

$$m_k(0) - m_k(p_k^C) \le \frac{1}{2} \|\nabla f(x_k)\| \min \left\{ \Delta_k, \frac{\|\nabla f(x_k)\|}{\|B_k\|} \right\}$$

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- The reason is that by always taking the Cauchy point as our step, we are simply implementing the steepest descent method with a particular choice of step length.
- Since steepest descent performs poorly even if an optimal step length is used at each iteration, to make the Trust Region algorithm efficient in practice, we have to improve on the Cauchy point.

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$$\min_{p \in \mathbb{R}^n} m(p) = f + g^T p + \frac{1}{2} p^T B p, \quad s.t. \quad ||p|| \le \Delta$$
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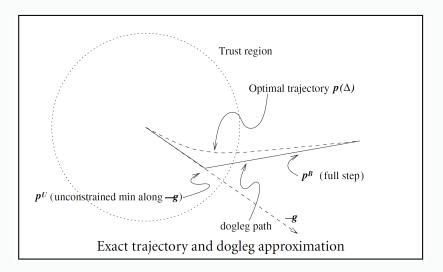
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• We denote the solution of above problem by $p^*(\Delta)$, to emphasize the dependence on Δ .

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- The improvement strategy is often designed so that the full step $p_B = -B^{-1}g$ is chosen whenever B is positive definite and $\|p_B\| \leq \Delta$.
- When B_k is the exact Hessian or a quasi-Newton approximation, this strategy can be expected to yield superlinear convergence.



The Dogleg Method

$$\tau_k = \begin{cases} \tau p^U, & 0 \le \tau \le 1, \\ p^U + (\tau - 1)(p^B - p^U), & 1 \le \tau \le 2 \end{cases}$$
 (6.12)

where

$$p^U = -\frac{g^T g}{g^T B g} g$$

is the unconstrained minimizer of $m(\cdot)$ along the steepest descent direction.

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Let B be positive definite. Then

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- $m(\tilde{p}(\tau))$ is a decreasing function of τ .

• It follows from above theorem that the path $\tilde{p}(\tau)$ intersects the trust-region boundary $\|p\|=\Delta$ at exactly one point if $\|p^B\|\geq \Delta$, and nowhere otherwise.

The Dogleg Method

- It follows from above theorem that the path $\tilde{p}(\tau)$ intersects the trust-region boundary $\|p\|=\Delta$ at exactly one point if $\|p^B\|\geq \Delta$, and nowhere otherwise.
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- Since m is decreasing along the path, the chosen value of p will be at p^B if $\|p^B\| \leq \Delta$, otherwise at the point of intersection of the dogleg and the trust-region boundary.
- ullet In the latter case, we compute the appropriate value of au by solving the following scalar quadratic equation:

$$||p^U + (\tau - 1)(p^B - p^U)||^2 = \Delta^2.$$

TWO-DIMENSIONAL SUBSPACE MINIMIZATION

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- This is a problem in two variables that is computationally inexpensive to solve.
- After some algebraic manipulation it can be reduced to finding the roots of a fourth degree polynomial.

Algorithm 5 (CG-Steihaug)

Given $\epsilon > 0$; **Set** $p_0 = 0$, $r_0 = g$, $d_0 = -r_0$;

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Given \epsilon > 0; Set p_0 = 0, r_0 = g, d_0 = -r_0; if \|r_0\| \le \epsilon; return p = p_0; for j = 0, 1, 2, \cdots
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```

Find $\tau \geq 0$ such that $p = p_i + \tau d_i$ satisfies $||p|| = \Delta$ return p;

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Given \epsilon>0; Set p_0=0, r_0=g, d_0=-r_0; if \|r_0\|\leq \epsilon; return p=p_0; for j=0,1,2,\cdots if d_j^TBd_j\leq 0; Find \tau such that p=p_j+\tau d_j minimizes m(p) and satisfies \|p\|=\Delta; return p; else  \text{Set } \alpha_j=r_j^Tr_j/(d_j^TBd_j); \text{Set } p_{j+1}=p_j+\alpha_jd_j; \\ \text{if } \|p_{j+1}\|\geq \Delta \\ \text{Find } \tau\geq 0 \text{ such that } p=p_j+\tau d_j \text{ satisfies } \|p\|=\Delta \text{ return } p;
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Algorithm 5 (CG-Steihaug) Given $\epsilon > 0$; Set $p_0 = 0$, $r_0 = q$, $d_0 = -r_0$; if $||r_0|| < \epsilon$; return $p = p_0$; for $j = 0, 1, 2, \cdots$ if $d_i^T B d_i \leq 0$; Find τ such that $p = p_j + \tau d_j$ minimizes m(p) and satisfies $||p|| = \Delta$; return p; else Set $\alpha_i = r_i^T r_i / (d_i^T B d_i)$; Set $p_{i+1} = p_i + \alpha_i d_i$; if $||p_{i+1}|| \geq \Delta$ Find $\tau \geq 0$ such that $p = p_j + \tau d_j$ satisfies $||p|| = \Delta$ return p; else Set $r_{i+1} = r_i + \alpha_i B d_i$; if $||r_{i+1}|| \le \epsilon ||r_0||$ return $p = p_{i+1}$

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STEIHAUG'S APPROACH

Algorithm 5 (CG-Steihaug)

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for j = 0, 1, 2, \cdots
      if d_i^T B d_i \leq 0;
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             return p;
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                   Find \tau \geq 0 such that p = p_j + \tau d_j satisfies ||p|| = \Delta return p;
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                   if ||r_{i+1}|| \le \epsilon ||r_0|| return p = p_{i+1}
                   else
                   Set \beta_{i+1} = r_{i+1}^T r_{i+1} / (r_i^T r_i), d_{i+1} = r_{i+1} + \beta_{i+1} d_i;
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                   Find \tau \geq 0 such that p = p_j + \tau d_j satisfies ||p|| = \Delta return p;
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end(for).
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Lemma

The dogleg and two dimensional subspace minimization algorithms produce approximate solution p_k of the subproblem (3) that satisfy the following estimate of decrease in the model function:

$$m_k(0) - m_k(p_k) \ge c_1 \|g_k\| \min\left\{\Delta_k, \frac{\|g_k\|}{\|B_k\|}\right\}$$
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Theorem

• Let p_k be any vector such that $||p_k|| \le \Delta_k$ and $m_k(0) - m_k(p) \ge c_2(m_k(0) - m_k(p_k^C))$.

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Theorem

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- Then p_k satisfies (6.13) with $c_1 = \frac{c_2}{2}$. In practice, if p_k is the exact solution p^* of (6.3), then it satisfies (6.13) with $c_1 = \frac{1}{2}$.

• Global convergence results for trust-region methods come in two varieties, depending on whether we set the parameter η in Algorithm 4 to zero or to some small positive value.

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- Global convergence results for trust-region methods come in two varieties, depending on whether we set the parameter η in Algorithm 4 to zero or to some small positive value.
- when $\eta=0$ (that is, the step is taken whenever it products a lower value of f), we can show that the sequence of gradients $\{g_k\}$ has a limit point at zero.
- For the more stringent acceptance test with $\eta>0$, which requires the actual decrease in f to be at least some small fraction of the predicted decrease, we have the stronger result that $g_k\to 0$.

We provide the global convergence results for both case.

We assume throughout that the approximate Hessians B_k are bounded in norm, and that f is bounded below on the level set

$$S \equiv \left\{ x | f(x) \le f(x_0) \right\}. \tag{6.14}$$

For later reference, we define an open neighborhood of this set by

$$S(R_0) \equiv \{x | ||x - y|| < R_0 \text{ for some } y \in S\}.$$

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To allow our results to be applied more generally, we also allow the length of the approximate solution p_k of (6.3) to exceed the trust-region bound, provided that it stays within some fixed multiple of the bound; that is,

$$||p_k|| \le \gamma \Delta_k$$
, for some constant $\gamma \le 1$. (6.15)

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- Let $\eta = 0$ in Algorithm 4.
- Suppose that $\|B_k\| \leq \beta$ for some constant β , that f is bounded below on the level set S defined by (6.14) and Lipschitz continuously differentiable in the neighborhood $S(R_0)$ for some $R_0 > 0$, and that all approximate solution of (6.3) satisfy the inequalities (6.13) and (6.15), for some positive constant c_1 and γ .

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- We then have

$$\lim \inf_{k \to \infty} \|g_k\| = 0. \tag{6.16}$$

Theorem (Schultz, Schnabel and Byrd)

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$$\lim_{k \to \infty} g_k = 0. \tag{6.17}$$

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- Suppose that $B_k = \nabla^2 f(x_k)$ for all k, and that the approximate solution p_k of (6.3) at each iteration satisfies

$$m(0) - m(p) \ge c_1 (m(0) - m(p^*)),$$
 (6.18a)

$$||p|| \le \gamma \Delta,\tag{6.18b}$$

for some fixed $\gamma > 0$. Then

$$\lim_{k \to \infty} \|g_k\| = 0.$$

Convergence to Stationary Points

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- Suppose that $B_k = \nabla^2 f(x_k)$ for all k, and that the approximate solution p_k of (6.3) at each iteration satisfies

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$$||p|| \le \gamma \Delta,\tag{6.18b}$$

for some fixed $\gamma > 0$. Then

$$\lim_{k \to \infty} \|g_k\| = 0.$$

• In addition, if the level set S of (6.14) is compact, then either the algorithm terminates at a point x_k at which the second-order necessary conditions for a local solution hold, or else $\{x_k\}$ has a limit point x^* in S at which the second-order necessary conditions hold.

LOCAL CONVERGENCE OF TR NEWTON METHODS

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- Let f be twice Lipschitz continuously differentiable in a neighborhood of a point x^* at which second-order sufficient conditions are satisfied.
- Suppose the sequence $\{x_k\}$ converges to x^* and that for all k sufficiently large, the trust-region algorithm based on (6.3) with $B_k = \nabla^2 f(x_k)$ chooses steps p_k that satisfy the Cauchy-point-based model reduction criterion (6.13) and are asymptotically similar to Newton steps p_k^N whenever $\|p_k^N\| \leq \frac{1}{2}\Delta_k$, that is,

$$||p_k - p_k^N|| = o(||p_k^N||)$$
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Local Convergence of TR Newton Methods

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• Then the trust-region bound Δ becomes inactive for all k sufficiently large and the sequence $\{x_k\}$ converges superlinearly to x^* .

It is immediate from the above theorem that if $p_k = p_k^N$ for all k sufficiently large, we have quadratic convergence of $\{x_k\}$ to x^* .

• Recalling our definition of a trust region

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- Even if the model Hessian B_k is exact, the rapid changes in f along certain directions probably will cause m_k to be a poor approximation to f along these directions.
- ullet On the other hand, m_k may be a more reliable approximation to f along these directions in which f is changing more slowly.

Since the shape of the trust region should be such that the confidence in the model is more or less the same at all points on the boundary of the region, we are led naturally to consider *elliptical* trust regions in which the axes are short in the sensitive directions and longer in the less sensitive directions.

• Elliptical trust regions can be defined by

$$||Dp|| \le \Delta, \tag{6.20}$$

where D is a diagonal matrix with positive diagonal elements, yielding the following scaled trust-region subproblem:

$$\lim_{p \in \mathbb{R}^n} m_k(p) \equiv f(x_k) + \nabla f(x_k)^T p + \frac{1}{2} p^T B_k p, \quad s.t. \quad ||Dp|| \le \Delta_k.$$
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 (6.21)

• When f(x) is highly sensitive to the value of the ith component x_i , we set the corresponding diagonal element d_{ii} of D to be large, while d_{ii} is smaller for less-sensitive components.

Trust Region in Other Norms

 Trust regions may also be defined in terms of norms other than the Euclidean norm.

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$$||p||_1 \le \Delta_k$$
, or $||p||_\infty \le \Delta_k$,

or their scaled counterparts

$$||Dp||_1 \le \Delta_k$$
, or $||Dp||_\infty \le \Delta_k$.

Chapter VI: Trust-Region Methods (信赖域方法)

THANKS FOR YOUR ATTENTION