Practical Optimization Algorithms
实用优化算法

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Dec 2, 2021

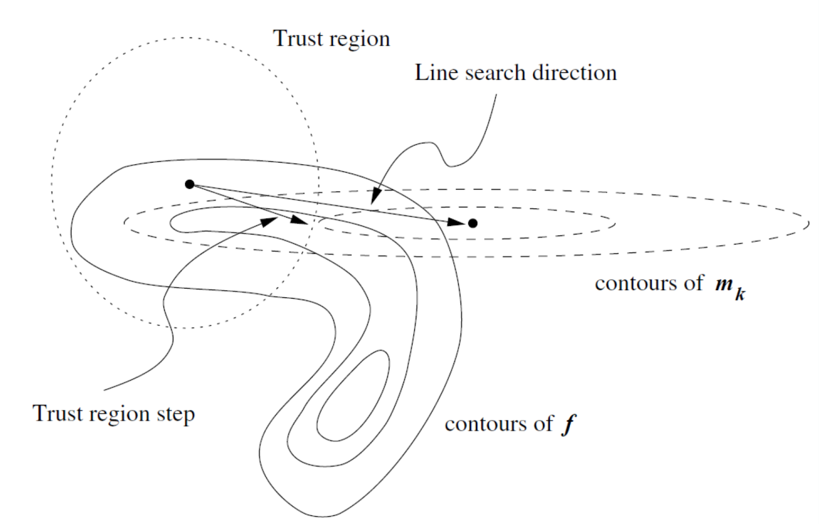
Chapter VI: Trust-Region Methods (信赖域方法)

Outline of the Trust-Region Approach

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.

- Line search methods use it to generate a search direction （主要用于产生搜索方向）, and then focus their efforts on finding a suitable step length α along this direction.
- Trust-region defines a region around the current iterate within which they trust the model to be an adequate representation of the objective function,
- 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



Outline of the Trust-Region Approach

- In this chapter, we will assume that the model function m_k that is used at each iteration x_k is quadratic. Moreover m_k is based on the Taylor-series expansion of f around x_k , which is

$$f(x_k + p) = f_k + g_k^T p + \frac{1}{2} p^T \nabla f^2 (x_k + tp) p, \tag{6.1}$$

  where $f_k = f(x_k), g_k = \nabla f(x_k)$ and $t \in (0, 1)$.

- By using an approximation B_k to the Hessian in the second-order term, m_k is defined as follows:

$$m_k(p) = f_k + g_k^T p + \frac{1}{2} p^T B_k p \tag{6.2}$$

  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.

Outline of the Trust-Region Approach

- When $B_k = \nabla^2 f(x_k)$, the approximation error in the model function m_k is $\mathcal{O}(\|p\|^2)$, so this model is especially accurate when $\|p\|$ is small. This choice $B_k = \nabla^2 f(x_k)$ leads to the trust-region Newton method.
- In the other part, we emphasis the generality of the trust-region approach by assuming little about B_k except symmetry and uniform boundedness.

Outline of the Trust-Region Approach

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

$$\min_{p\in\mathcal{R}^n} m_k(p) = f_k + g_k^T p + \frac{1}{2} p^T B_k p, \quad s.t. \;\; \|p\| \leq \Delta_k \tag{6.3}$$

where $\Delta_k > 0$ is the trust-region radius.

Outline of the Trust-Region Approach

The classification of trust-region methods are decided by the choice of B_k and norm for trust region in the model (6.3). For example,

- If $B_k = 0$ in (6.3) and define the trust region using the Euclidean norm, the trust-region method identifies with the steepest descent line search approach;
- 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.

Outline of the Trust-Region Approach

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.

Outline of the Trust-Region Approach

In practical algorithms, we choose the size of the region according to the performance of the algorithm during previous iterations

- 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.

Outline of the Trust-Region Approach

- Define the ratio

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

  the numerator is called the actual reduction, and the denominator is the predicted reduction.

- Note that since the step p_k is obtained by minimizing the model m_k over a region that includes the step $p = 0$, the predicted reduction will always be nonnegative. Thus
  - if ρ_k is negative, the new objective value $f(x_k + p_k)$ is greater than the current value $f(x_k)$, so the step must be rejected.
  - 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.

Outline of the Trust-Region Approach

Algorithm 1 (Trust Region)

Given $\hat{\Delta} > 0$, $\Delta_0 \in (0, \hat{\Delta})$, and $\eta \in [0, \frac{1}{4})$
for $k = 0, 1, 2, \cdots;$
  Obtain p_k by (approximately) solving (6.3);
  Evaluate ρ_k from (6.4);
  if $\rho_k < \frac{1}{4}$;
    $\Delta_{k+1} = \frac{1}{4}\Delta_k$
  else if $\rho_k > \frac{3}{4}$ and $\|p_k\| = \Delta_k$
      $\Delta_{k+1} = \min(2\Delta_k, \hat{\Delta})$
    else
      $\Delta_{k+1} = \Delta_k;$
  if $\rho_k > \eta$
    $x_{k+1} = x_k + p_k$
  else
    $x_{k+1} = x_k;$
end(for).

Outline of the Trust-Region Approach

Theorem

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

$$\min_{p\in\mathcal{R}^n} m(p) = f + g^T p + \frac{1}{2}p^T Bp, \quad s.t. \quad \|p\| \leq \Delta \tag{6.5}$$

if and only if

p^* is feasible and there is a scalar $\lambda \geq 0$ such that the following conditions are satisfied:

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

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

$$(B + \lambda I) \quad \text{is positive semi-definite.} \tag{6.6c}$$

Outline of the Trust-Region Approach

- In most of our discussions, we define $\|\cdot\|$ to be the Euclidean norm, so that the solution p_k^* of (6.3) is the minimizer of m_k in the ball of radius Δ_k.
- Thus, the trust-region approach requires us to solve a sequence of subproblems (6.3) in which the objective function and constraint (which can be written as $p^T p \leq \Delta_k^2$) are both quadratic.
- 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 $m_k(p)$.
- 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.

The Cauchy Point

- Intuition: line search methods do not require optimal step lengths to be globally convergent. In fact, only a crude approximation to the optimal step length that satisfies certain loose criteria is needed.
- A similar situation applies in trust-region methods.
- 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 .

The Cauchy Point

Algorithm 2 (Cauchy Point Calculation)

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

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

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

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

Set

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

.

The Cauchy Point

- The solution of (6.7) is simply

$$p_k^s = -\frac{\Delta_k}{\|\nabla f(x_k)\|}\nabla f(x_k)$$

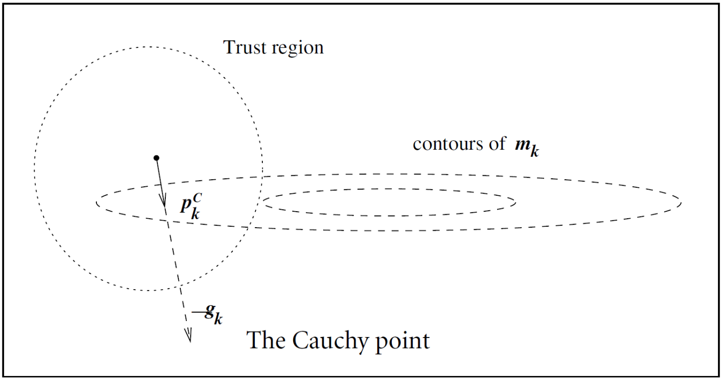
- Furthermore, a closed-form definition of the Cauchy point can be written in the following

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

where

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

Cauchy Point For A Subproblem



The Cauchy Point

- The Cauchy step p_k^C is inexpensive to calculate - no matrix factorizations are required - and is of crucial importance in deciding if an approximate solution of the trust-region subproblem is acceptable.
- 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

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

THE CAUCHY POINT

Algorithm 3 (Trust Region)

Given $\hat{\Delta} > 0$, $\Delta_0 \in (0, \hat{\Delta})$, and $\eta = 0$
for $k = 0, 1, 2, \cdots;$
  Calculate $p_k = p_k^C$;
  Evaluate ρ_k from (6.4);
  if $\rho_k < \frac{1}{4}$;
    $\Delta_{k+1} = \frac{1}{4}\Delta_k$
  else if $\rho_k > \frac{3}{4}$ and $\|p_k\| = \Delta_k$
    $\Delta_{k+1} = \min\left\{2\Delta_k, \hat{\Delta}\right\}$
  else
    $\Delta_{k+1} = \Delta_k;$
  if $\rho_k > \eta = 0$
    $x_{k+1} = x_k + p_k$
  else
    $x_{k+1} = x_k;$
end(for).

Convergence to Stationary Points

Theorem

- Suppose that $B_k \leq \beta$ for some constant β,
- f is continuously differentiable and bounded below on the level set

$$\left\{x \middle| f(x) \leq f(x_0)\right\},$$

- Then, if above algorithm is not terminate in finite steps, we have

$$\liminf_{k\to\infty} \|\nabla f(x_k)\| = 0.$$

The Cauchy Point

Algorithm 4 (Trust Region)

Given $\hat{\Delta} > 0$, $\Delta_0 \in (0, \hat{\Delta})$, and $\eta \in (0, \frac{1}{4})$
for $k = 0, 1, 2, \cdots$;
  Calculate $p_k = p_k^C$;
  Evaluate ρ_k from (6.4);
  if $\rho_k < \frac{1}{4}$;
    $\Delta_{k+1} = \frac{1}{4}\Delta_k$
  else if $\rho_k > \frac{3}{4}$ and $\|p_k\| = \Delta_k$
      $\Delta_{k+1} = \min\left\{2\Delta_k, \hat{\Delta}\right\}$
    else
      $\Delta_{k+1} = \Delta_k$;
  if $\rho_k > \eta$
    $x_{k+1} = x_k + p_k$
  else
    $x_{k+1} = x_k$;
end(for).

Convergence to Stationary Points

Theorem

- Suppose that $B_k \leq \beta$ for some constant β,
- f is continuously differentiable and bounded below on the level set

$$\left\{ x \middle| f(x) \leq f(x_0) \right\},$$

- Then, if above algorithm is not terminate in finite steps, we have

$$\liminf_{k \to \infty} \|\nabla f(x_k)\| = 0.$$

Improve the Cauchy Point

- Since the Cauchy point p_k^C provides sufficient reduction in the model function m_k to yield global convergence, and since the cost of calculating it is so small, why should we look any further for a better approximate solution of (6.3)?
- 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.

Improve the Cauchy Point

- Since we will be focusing on the internal workings of a single iteration, so we drop the subscript k from the quantities to simplify the notation
- With this simplification, we restate the trust-region subproblem as follows:

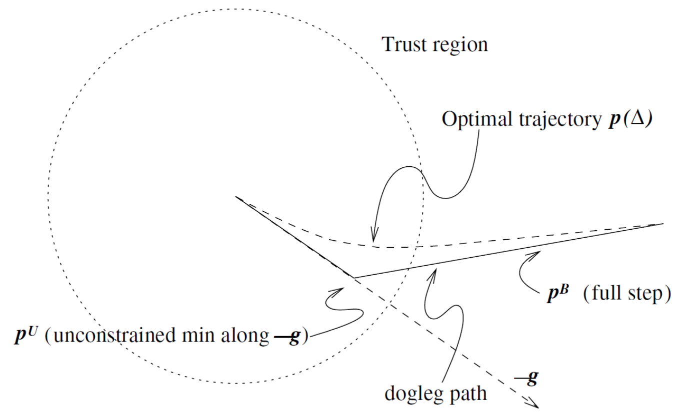
$$\min_{p \in \mathcal{R}^n} m(p) = f + g^T p + \frac{1}{2} p^T B p, \quad s.t. \quad \|p\| \leq \Delta \tag{6.11}$$

- We denote the solution of above problem by $p^*(\Delta)$, to emphasize the dependence on Δ.

Improve the Cauchy Point

- A number of algorithms for generating approximate solutions p_k to the trust-region problem (6.11) start by computing the Cauchy point and then try to improve on it.
- 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



Exact trajectory and dogleg approximation

The Dogleg Method

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

where

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

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

The Dogleg Method

- The dogleg method chooses p to minimize the model m along this path, subject to the trust-region bound.
- In fact, it is not even necessary to carry out a search, because the dogleg path intersects the trust-region boundary at most once and the intersection point can be computed analytically. The following theorem proves these claims.

Theorem

Let B be positive definite. Then

- $\|\tilde{p}(\tau)\|$ is an increasing function of τ, and
- $m(\tilde{p}(\tau))$ is a decreasing function of τ.

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.
- 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.
- In the latter case, we compute the appropriate value of τ by solving the following scalar quadratic equation:

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

Two-Dimensional Subspace Minimization

- When B is positive definite, the dogleg method strategy can be made slightly more sophisticated by widening the search for p to the entire two-dimensional subspace spanned by p^U and p^B(equivalently, g and $-B^{-1}g$).
- The subproblem could be replaced by

$$\min_{p} m(p) = f + g^T p + \frac{1}{2} p^T B p, \quad s.t. \quad \|p\| \leq \Delta, p \in [g, B^{-1}g].$$

- 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.

Steihaug's Approach

Algorithm 5 (CG-Steihaug)

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 $d_j^T B d_j \leq 0$;
        Find τ such that $p = p_j + \tau d_j$ minimizes $m(p)$ and satisfies $\|p\| = \Delta$;
        return p;
    else
        Set $\alpha_j = r_j^T r_j / (d_j^T B d_j)$; Set $p_{j+1} = p_j + \alpha_j d_j$;
        if $\|p_{j+1}\| \geq \Delta$
            Find $\tau \geq 0$ such that $p = p_j + \tau d_j$ satisfies $\|p\| = \Delta$ **return** p;
            else Set $r_{j+1} = r_j + \alpha_j B d_j$;
            if $\|r_{j+1}\| \leq \epsilon \|r_0\|$ **return** $p = p_{j+1}$
            else
            Set $\beta_{j+1} = r_{j+1}^T r_{j+1} / (r_j^T r_j)$, $d_{j+1} = r_{j+1} + \beta_{j+1} d_j$;
end(for).

Reduction Obtained by The Cauchy Point

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:

$$m_k(0) - m_k(p_k) \geq c_1 \|g_k\| \min\left\{\Delta_k, \frac{\|g_k\|}{\|B_k\|}\right\} \tag{6.13}$$

Theorem

- Let p_k be any vector such that $\|p_k\| \leq \Delta_k$ and $m_k(0) - m_k(p) \geq c_2\big(m_k(0) - m_k(p_k^C)\big)$.
- 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 $c_1 = \frac{1}{2}$.

Convergence to Stationary Points

- 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.

Convergence to Stationary Points

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

$$S \equiv \{x | f(x) \leq f(x_0)\}. \tag{6.14}$$

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

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

where R_0 is a positive constant.
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,

$$\|p_k\| \leq \gamma \Delta_k, \text{ for some constant } \gamma \leq 1. \tag{6.15}$$

Convergence to Stationary Points

The first result deals with the case $\eta = 0$.

Theorem

- 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.
- We then have

$$\lim_{k\to\infty} \inf \|g_k\| = 0. \tag{6.16}$$

Convergence to Stationary Points

Theorem (Schultz, Schnabel and Byrd)

- Let $\eta \in (0, \frac{1}{4})$ 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.
- We then have

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

Convergence to Stationary Points

- Suppose that the assumptions of above theorem are satisfied and in addition that f is twice continuously differentiable in the level set S.
- 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

$$m(0) - m(p) \geq c_1 \big(m(0) - m(p^*)\big), \tag{6.18a}$$

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

  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

Theorem

- 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,

$$\|p_k - p_k^N\| = o(\|p_k^N\|) \tag{6.19}$$

- 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^*.

Scaling

- Recalling our definition of a trust region - a region around the current the current iterate within which the model $m_k(\cdot)$ is an adequate representation of the true objective $f(\cdot)$ - it is easy to see that a *spherical* trust region may not be approximated when f is poorly scaled.
- 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.
- 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.

Scaling

- Elliptical trust regions can be defined by

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

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

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

- 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.
- For instance, we may have

$$\|p\|_1 \leq \Delta_k, \text{ or } \|p\|_\infty \leq \Delta_k,$$

- or their scaled counterparts

$$\|Dp\|_1 \leq \Delta_k, \text{ or } \|Dp\|_\infty \leq \Delta_k.$$

Thanks For Your Attention