Numerical Optimisation: Trust region methods

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Lecture 4

Trust region: idea

- Choose a region around the current iterate $f(x_k)$ in which we trust a model.
- Choose a relatively easy solvable model which we trust is an adequate representation of f in this region.
- Compute the direction and step length which minimise the model in the trust region.
- The size of the trust region is critical to effectiveness. If the region is too small, the algorithm will make little progress. If the region is too large, the minimiser of the model can be far away from the minimiser of f.
- If the model is consistently reliable, the trust region may be increased.
- If the step length is not acceptable, reduce the size of the trust region and find a new minimiser. In general both the direction and step length change when the trust region changes.

Trustregion: model

Here we assume a quadratic model based on Taylor expansion of f at x_k

$$m_k(p) = f(x_k) + g_k^T p + \frac{1}{2} p^T B_k p,$$

where $g = \nabla f(x_k)$, and B_k is a symmetric approximation to the Hessian $\nabla^2 f(x_k)$.
In general we only assume symmetry and uniform boundedness for B_k. The difference between $\nabla^2 f(x_k + tp)$, $t \in (0, 1)$ and $m_k(p)$ is $\mathcal{O}(\|p\|^2)$.

The choice of $B_k = \nabla^2 f(x_k)$ leads to **trust region Newton methods** and the model accuracy is $\mathcal{O}(\|p\|^3)$.

In each step we solve

$$\min_{p\in\mathbb{R}^n} m_k(p) = f(x_k) + g_k^{\mathrm{T}} p + \frac{1}{2} p^{\mathrm{T}} B_k p, \quad \text{s.t. } \|p\| \le \Delta_k, \quad \text{(CM)}$$

and $\Delta_k > 0$ is the radius of the trust region. The constraint can be equivalently written $p^{\mathrm{T}} p \le \Delta_k^2$.

If B_k is positive definite the minimum of the unconstrained quadratic model problem m_k is $p^B = -B_k^{-1} g_k$. If $\|p^B\| = \|B_k^{-1} g_k\| \le \Delta_k$ this is also the solution to the constrained problem and we call p^B a full step.

Solution in other cases is less straight forward but can usually be obtained at moderate computational cost. In particular, only approximate solution is necessary to obtain convergence and good practical behaviour.

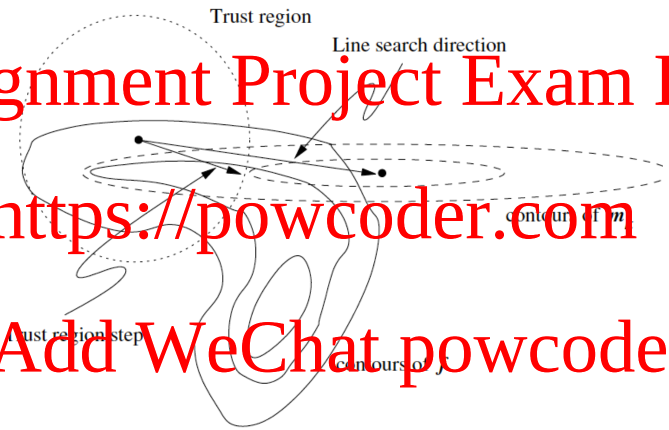

Figure: Nocedal Wright Fig 4.1

Choice of trust region radius Δ_k

Compare the actual reduction in objective function to the predicted reduction i.e. reduction in the model m_k.

$$\rho_k = \frac{f(x_k) - f(x_k + p)}{m_k(0) - m_k(p)}$$

- $\rho_k < 0$: $f(x_k) < f(x_k + p)$ – reject step, shrink trust region and try again

- $\rho_k > 0$, small – accept step, shrink trust region for next iteration
- $\rho_k > 0$, but significantly smaller than 1 – accept the step and do not alter trust region

- $\rho \approx 1$: good agreement between f and m_k – accept step and expand trust region for next iteration.

Algorithm: Trust region

Given $\hat{\Delta} > 0, \Delta_0 \in (0, \hat{\Delta})$ and $\eta \in [0, \frac{1}{4})$
for $k = 1, 2, 3, \ldots$ **do**
  Obtain p_k by (approximatively) solving (CM)
  Evaluate $\rho_k = \frac{f(x_k) - f(x_k + p)}{m_k(0) - m_k(p)}$
  if $\rho_k < \frac{1}{4}$ **then**
    $\Delta_{k+1} = \frac{1}{4}\Delta_k$
  else
    if $\rho_k > \frac{3}{4}$ **and** $\|p_k\| = \Delta_k$ **then**
      $\Delta_{k+1} = \min(2\Delta_k, \hat{\Delta})$
    else
      $\Delta_{k+1} = \Delta_k$
    end if
  end if
  if $\rho_k > \eta$ **then**
    $x_{k+1} = x_k + p_k$
  else
    $x_{k+1} = x_k$
  end if
end for

Theorem [More, Sorensen]

$p^\star$ is a global solution of the trust region problem (CM)

$$\min_{p \in \mathbb{R}^n} m_k(p) = f(x_k) + g_k^{\mathrm{T}} p + \frac{1}{2} p^{\mathrm{T}} B_k p, \quad \text{s.t. } \|p\| \le \Delta_k$$

if and only if $p^\star$ is feasible and there is a scalar $\lambda \ge 0$ such that the following conditions are satisfied:

$$(B + \lambda I) p^\star = -g_k, \tag{1a}$$

$$\lambda(\Delta - \|p^\star\|) = 0, \tag{1b}$$

$$B + \lambda I \ \text{ is positive semidefinite.} \tag{1c}$$

Solution of (CM) for different radii

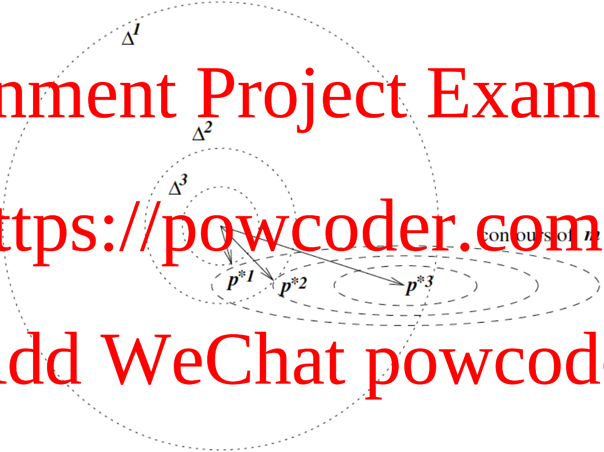

Figure: Nocedal Wright Fig 4.2 (note that $p_3^\star$ and $p_1^\star$ should be swapped)

Solution of (CM) for different radii

For Δ_1, $\|p^\star\| < \Delta$ hence $\lambda = 0$ and so

$$Bp^\star = -g_k$$

with B positive semidefinite from (1)(a,c).

For Δ_2, Δ_3 the solution lies on the boundary of the respective trust region, hence $\|p^\star\| = \Delta$ and $\lambda \geq 0$. From (1)(a) we have

$$\lambda p^\star = -Bp^\star - g_k = -\nabla m_k(p^\star)$$

Thus if $\lambda > 0$, $p^\star$ is collinear with the negative gradient of m_k and normal to its contours.

Cauchy point

Cauchy point p^C is the minimiser of m_k along the steepest descent direction $-g_k$ subject to the trust region bound.

Find p^s:

$$p^s = \arg\min_{p \in \mathbb{R}^n} f(x_k) + g_k^{\mathrm{T}} p, \quad \text{s.t. } \|p\| \leq \Delta_k$$

Calculate the scalar $\tau_k > 0$:

$$\tau_k = \arg\min_{\tau \geq 0} m_k(\tau p^s) \quad \text{s.t. } \|\tau p^s\| \leq \Delta_k.$$

Set $p^C = \tau_k p^s$.

The solution to the first problem can be written down explicitly, simply by going as far as allowed in the steepest descent direction

$$p^s = -\frac{\Delta_k}{\|g\|} g.$$

To obtain τ_k we substitute $p^s = -\frac{\Delta_k}{\|g_k\|} g_k$ into the second problem we obtain

$$\arg\min_{\tau} m_k(\tau p^s) = f(x_k) - \tau \underbrace{\frac{\Delta_k}{\|g_k\|} g_k^{\mathrm{T}} g_k}_{\geq 0} + \frac{1}{2}\tau^2 \frac{\Delta_k^2}{\|g_k\|^2} g_k^{\mathrm{T}} B_k g_k$$

subject to $\|\tau g_k \frac{\Delta_k}{\|g_k\|}\| \leq \Delta_k \Leftrightarrow \tau \in [-1, 1]$.

We consider two cases:

- $g_k^{\mathrm{T}} B_k g_k \leq 0$: $m_k(\tau p^s)$ decreases monotonically whenever $g_k \neq 0$. Hence, the minimum is attained for largest $\tau \in [-1, 1]$ i.e. $\tau = 1$.

- $g_k^{\mathrm{T}} B_k g_k > 0$: $m_k(\tau p^s)$ is strictly convex quadratic function in τ, thus the minimum is either the unconstraint minimiser whenever in $[-1, 1]$ or otherwise 1 ($\arg\min_{\tau=\{-1,1\}} m_k(\tau p^s)$)

$$\tau_k = \begin{cases} 1 & g_k^{\mathrm{T}} B_k g_k \leq 0 \\ \min\left(\|g_k\|^3 / (\Delta_k g_k^{\mathrm{T}} B_k g_k), 1\right) & g_k^{\mathrm{T}} B_k g_k > 0. \end{cases}$$

Cauchy point for positive definite B_k

Sufficient reduction in the model is reduction of at least a positive fraction of that achieved by the Cauchy point p^C.

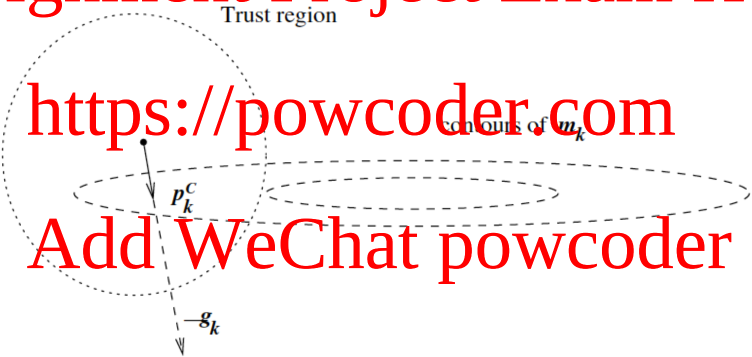

Figure: Nocedal Wright Fig 4.3

Improvement on Cauchy point

- Cauchy points p^C provides sufficient reduction to yield global convergence.
- Cauchy points is cheap to compute.
- Cauchy point essentially corresponds to the steepest descent method with a particular choice of step length. Steepest descent performance can be very poor even with optimal step length.
- In Cauchy point the information in B is only used to compute the step length. Superlinear convergence can only be expected when B is used to compute both the descend direction and the step length.
- A number of trust region methods compute the Cauchy points and then attempt to improve on it. Often, the full step i.e. $p^B = -B^{-1}g_k$ is chosen whenever B is positive definite and $\|p^B\| \leq \Delta_k$. When $B = \nabla^2 f(x_k)$ or a quasi-Newton approximation, this strategy can be expected to yield superlinear convergence.

The dogleg method

Assumption: B positive definite.

If $p^B = -B^{-1} g_k$ with $\|p^B\| \leq \Delta_k$ it is just the unconstrained minimum

$$p^\star = p^B, \quad \|p^B\| \leq \Delta_k$$

On the other hand if Δ is small w.r.t. $\|p^B\|$ the restriction to $\|p^B\| \leq \Delta$ ensures that the quadratic term in m_k has little effect on the solution of (CM) and it could be omitted i.e.

$$p^\star \approx -\frac{\Delta_k}{\|g_k\|} g_k, \quad \Delta_k \ll \|p^B\|.$$

For intermediate values of Δ_k, the solution $p^\star(\Delta_k)$ typically follows a curved trajectory (Fig. 4.4 Nocedal, Wright).

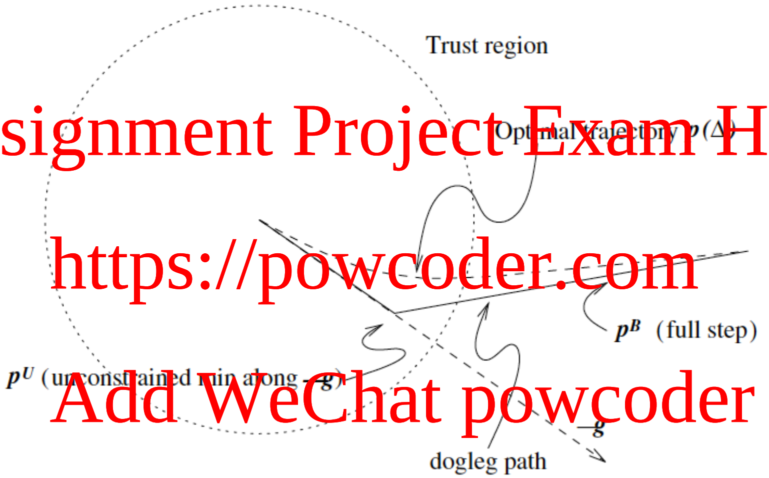

Figure: Nocedal Wright Fig 4.4

The dogleg method replaces the curved trajectory with path consisting of two line segments.

The first line segment runs from the origin to the minimiser of m_k along the steepest descent direction

$$p^U = -\frac{g_k^{\mathrm{T}} g_k}{g_k^{\mathrm{T}} B g_k} g_k.$$

The second line segment runs from p^U to p^B (the unconstraint minimum or full step).

Formally, the trajectory can be written as

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

The dogleg method chooses p to minimise the model m_k along this path subject the trust region bound.

The minimum along the dogleg can be found easily because
(i) $\|\tilde{p}(\tau)\|$ is an increasing function function of τ
(ii) $m(\tilde{p}(\tau))$ is a decreasing function of τ

Proof: For $\tau \in [0, 1]$ it follows from definition of p^U. For $\tau \in [1, 2]$ can be shown computing the derivative and showing that it is nonnegative (i), nonpositive (ii).
Intuition:
(i) The length of $\tilde{p}$ could only decrease with τ if $\tilde{p}(\tau)$ turns back at $\tau = 1$ i.e. the vector $p^B - p^U$ makes an angle larger than $\pi/2$ with p^U which is not possible for the steepest descent solution.
(ii) $m(\tilde{p}(2))$ is the minimum of a strictly convex function, hence $m(\tilde{p}(1)) > m(\tilde{p}(2))$ and the function decreases for $\tau \in [1, 2]$.

As a consequence the path $\tilde{p}(\tau)$ intersects the trust region boundary at exactly one point if $\|p^B\| \geq \Delta$ and the intersection point can be computed solving the quadratic equation

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

In case the exact Hessian $\nabla^2 f(x_k)$ is available, if it is positive definite, we set $B = \nabla^2 f(x_k)$ and the resulting procedure is a Newton dogleg method. If $\nabla^2 f(x_k)$ is not positive definite, we could use one of the modified Hessians and close to the solution we will recover the Newton step. However, the somewhat arbitrary perturbation introduced by the modification can interfere with the benefits of the trust region methods. In fact, the trust region introduces its own modification (1)(a,c) thus the dogleg method is most appropriate when B is positive definite.

An extension of the dogleg method

$$\min_p m_k(p) = f(x_k) + g_k^{\mathrm{T}} p + \frac{1}{2} p^{\mathrm{T}} B p \quad \text{s.t. } p \in \operatorname{span}[g, B^{-1} g].$$

The obtained minimiser is an improvement on the dogleg solution as $\tilde{p} \in \operatorname{span}[g, B^{-1}g]$. Furthermore, the reduction in the model m_k is ofter close to that achieved solving the full problem (CM) (not on the subspace). The subspace $\operatorname{span}[g, B^{-1}g]$ is a good one for looking for a minimiser for a quadratic model (Taylor theorem).

This subspace minimisation strategy can be modified for indefinite B.

Cauchy point reduction of the model m_k

The Cauchy point p^C satisfies the sufficient reduction condition

$$m_k(0) - m_k(p) \geq c_1 \|g_k\| \min\left(\Delta_k, \frac{\|g_k\|}{\|B_k\|}\right) \qquad \text{(SR)}$$

with $c_1 = \frac{1}{2}$.

Proof: Use the definition of the Cauchy point p^C and check the inequality case by case.

If a vector p with $\|p\| \leq \Delta_k$ satisfies

$$m_k(0) - m_k(p) \geq c_2(m_k(0) - m_k(p^C))$$

then it satisfies (SR) with $c_1 = c_2/2$

$$m_k(0) - m_k(p) \geq c_2(m_k(0) - m_k(p^C)) \geq \frac{1}{2} c_2 \|g_k\| \min\left(\Delta_k, \frac{\|g_k\|}{\|B_k\|}\right).$$

In particular, if p is the exact solution $p^\star$ of (CM), then it satisfies (SR) with $c_1 = \frac{1}{2}$. Note that both the dogleg and 2d-subspace minimisation algorithms satisfy (SR) with $c_1 = \frac{1}{2}$ because the both produce approximate solutions p for which $m_k(p) \leq m_k(p^C)$.

Let $\|B_k\| \leq \beta$ for some constant $\beta > 0$ and f be bounded below on the level set $S = \{x : f(x) \leq f(x_0)\}$ and Lipschitz continuously differentiable in the neighbourhood of S, $\mathcal{N}(S, R_0)$, $R_0 > 0$ and all the approximate solutions p_k of (CM) satisfy the inequalities (SR) for some $c_1 > 0$ and $\|p_k\| \leq \gamma\Delta_k, \gamma \geq 1$ (slight relaxation of trust region). We then have for

- $\eta = 0$ in Algorithm: Trust region

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

- $\eta \in (0, \frac{1}{4})$ in Algorithm: Trust region

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

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

$$\|p_k - p_k^N\| = o(\|p_k^N\|).$$

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