Newton Trust Region method for numerical unconstrained optimisation

Main theory and examples

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Overview of the Problem

Problem Definition

It is possible to formally define the problem of unconstrained optimisation as follows:

Unconstrained optimisation (global minimiser)

Given a smooth function $f : \mathbb{R}^n \to \mathbb{R}$, we seek $\mathrm{x}^* \in \mathbb{R}^n$ such that
$f(\mathrm{x}^*) \leq f(\mathrm{x}) \ \forall \mathrm{x} \in \mathbb{R}^n$
The element x^* is said to be a *global minimiser* of f

Usually, the information available on f is only *local* (e.g. ∇f), and hence all we are able to get are local minima:

Local minimiser

The element x^* is said to be a *local minimiser* of f if $\exists B(\mathrm{x}^*, \delta)$ such that
$f(\mathrm{x}^*) \leq f(\mathrm{x}) \ \forall \mathrm{x} \in B(\mathrm{x}^*, \delta)$

Newton's Method

Let's define $g(x) = \nabla f(x)$ and $B(x)$ the hessian of f (or a suitable approximation). Follows that $B(x)$ is also symmetric.

Local minimum characterisation

Let $x^* \in \mathbb{R}^n$ satisfy $g(x^*) = 0$, and $B(x^*) \geq 0$. Then x^* is a local minimiser of f.

So, a possible way of solving the problem is to use Newton's Method to find roots of the gradient g.

At each iteration k, the Newton step p_k can be found by *unconstrained* minimisation of the model function $m_k(p)$:

$$m_k(p) = f(x_k) + g(x_k)^T p + \frac{1}{2} p^T B(x_k) p \approx f(x_k + p)$$

If $B(x_k)$ is SPD, the Newton step $p_k = -B(x_k)^{-1} g(x_k)$ is also a global minimiser of $m_k(p)$.

Some Issues

However, there are some issues in characterising the Newton step this way:

- If B_k is not positive definite, then the unconstrained minimum of $m_k(p)$ does NOT exist.

  In fact, if $p \in Aut(\lambda)$, where λ is a negative eigenvalue of B_k, then $m_k(p) \approx -\lambda ||p||_2^2$, so the newton step cannot be interpreted as the model function minimum

- Even if the minimum exists, $m_k(p)$ is just a *local* approximation of f in a certain point x_k, ad as such is accurate only for small values of $||p||$. If the newton step is too large, the behavior of f and m can disagree importantly.

  In these cases the decrease of function f and the convergence properties to a root of g can be lost.

Local Convergence

The plain Newton Method is extremely fast (quadratic convergence), convergence results apply only locally, that is, if the initial guess x_0 is close enough to the solution x^*.

There are some way to extend this result to Global Convergence:

- **Line Search Approach**

  Here the Newton direction is left unchanged, and the effort is directed to finding the optimal scaling factor α_k in order to achieve a sufficient reduction $f(x_k) - f(x_k + \alpha_k p_k)$ (E.g. the Armijo rule)

- **Trust Region**

  Here instead, the effort is directed to finding both the direction and the length together, by only considering steps that lie in a region where the approximation $f(x_k + p) \approx m_k(p)$ holds

Trust Region Approach

Trust Region approach

The trust region method introduces the parameter Δ_k to define a neighborhood $T(\Delta_k)$ in which $m_k(p)$ is trusted, i.e. sufficiently close to $f(x_k + p)$:

$$T(\Delta_k) = \{p \in \mathbb{R}^n \text{ s.t. } ||p||_2 \leq \Delta_k\}$$

At each iteration, the step is chosen by solving the *constrained* minimisation

$$p_k = \arg\min_{p \in T(\Delta_k)} m_k(p) \tag{1}$$

Finding a numerical solution of (1) will be denoted as "TR subproblem"

To evaluate whether $T(\Delta_k)$ is appropriate, we define the factor ρ_k:

$$\rho_k = \frac{f(x_k) - f(x_k + p_k)}{m_k(0) - m_k(p_k)} = \frac{actual(p_k)}{pred(p_k)} \tag{2}$$

For accurate models, $\rho_k \approx 1$, while if $\rho_k << 1$ then the predicted reduction was too optimistic.

Trust Region approach - Algorithm

Data: $\Delta_{max} > 0$, $\Delta_0 \in (0, \Delta_{max})$, ϵ, $\eta \in (0, \epsilon)$, x_0, tol, $\alpha < 1$, $\omega > 1$

while $||g(x_k)|| > tol\ ||g(x_0)||$ **do**

$p_k \leftarrow$ Solve (1)

$\rho_k \leftarrow$ Evaluate (2)

if $\rho_k < \epsilon$ **then**

$\Delta_{k+1} \leftarrow \alpha \Delta_k$ `// Poor agreement, shrink Trust Region`

else if $\rho_k > 1 - \epsilon$ **then**

$\Delta_{k+1} \leftarrow \omega \Delta_k$ `// Good agreement, widen Trust Region`

else

$\Delta_{k+1} \leftarrow \Delta_k$ `// Ok agreement, keep Trust Region`

if $\rho_k > \eta$ **then**

$x_{k+1} = x_k + p_k$

else

$x_{k+1} = x_k$ // Decrease in f is not enough

end

TR subproblem

Cauchy step

The Cauchy step obtained by solving a very rough approximation of (1) based on the gradient direction, very similar to a Line Search approach: $p_k^C = -\tau_k g_k$, where

$$\tau_k = \arg\min_{t \geq 0} m(-t g_k) \;\; \text{s.t.} \;\; p_k^C \in T(\Delta_k)$$

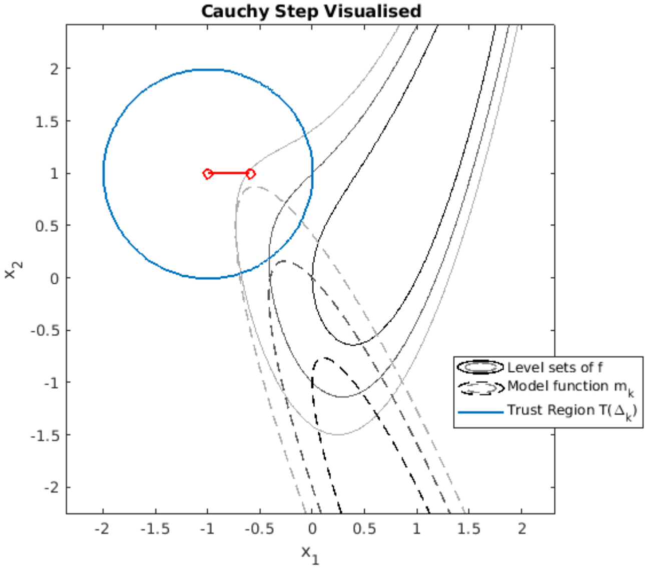
By direct substitution, it is possible to find an easy formula for τ_k:

$$\tau_k = \begin{cases} \frac{\Delta_k}{||g_k||} & \text{if } g_k^T B_k g_k \leq 0 \\ \min\left(\frac{\Delta_k}{||g_k||}, \frac{||g_k||^2}{g_k^T B_k g_k}\right) & \text{otherwise} \end{cases}$$

This method has strong similarities with the steepest descent

- **PROS**: it is very cheap and is enough to get global convergence
- **CONS**: it is a very rough estimate, and can slow down the overall procedure

Cauchy step - Example (Rosenbrock function)



Dogleg Method

When $B(x)$ is always SPD, we can find an improvement of the Cauchy point with the following observations:

- We already noted that the unconstrained minimiser of $m_k(p)$ is $p_k^B = -B_k^{-1}g$, and for $\Delta_k \geq ||p_k^B||$ this is also the solution of (1). This will always hold in the limit of large Δ_k
- On the other hand, in the limit of small Δ_k, the linear part of the quadratic model is dominant, so the solution can be effectively approximated by the "unconstrained Cauchy step" $p_k^U = -\frac{||g_k||^2}{g_k^T B_k g_k} g_k$

The approximate solution while Δ_k varies can then be approximated by combining the two limits in a piecewise linear path, whose length is governed by the parameter τ:

$$p_k^D(\tau) = \begin{cases} \tau p_k^U & \text{if } \tau \in (0,1] \\ p_k^U + (\tau - 1)(p_k^B - p_k^U) & \text{if } \tau \in (1,2] \end{cases} \tag{3}$$

Dogleg Method

For $\Delta_k < ||p_k^B||$ choice of τ in (3) must be done to enforce $p_k^D(\tau) \in T(\Delta_k)$, and this is made easy by the following lemma

Dogleg monotonicity lemma

If B_k is SPD, then

1. $||p_k^D(\tau)||$ is a monotonically increasing function of τ
2. $m_k(p_k^D(\tau))$ is a monotonically decreasing function of τ

This implies that the equation $||p_k^D(\tau)|| = \Delta_k$ has unique solution, and that the minimum value of m_k along this path is obtained exactly there. Finding such intersection reveals to be trivial, as it is a quadratic equation.

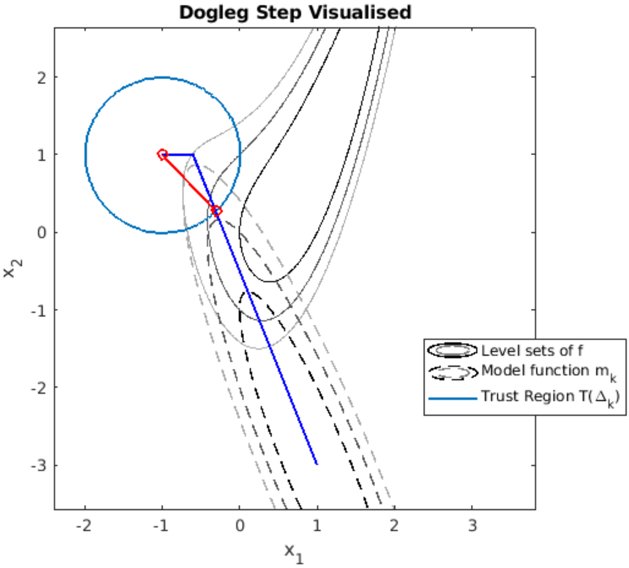
PROS

- it is cheap, requiring only one factorisation
- when $\Delta_k \geq ||p_k^B||$ it gives the exact solution

CONS

- It only works when B(x) is SPD

Dogleg step - Example (Rosenbrock function)



Exact solution - characterisation

The exact solution of the constrained minimisation (1) can be characterised by the following theorem:

Theroem

The vector $p^* \in T(\Delta)$ is a solution to

$$\arg\min_{p \in T(\Delta)} f + g^T p + \frac{1}{2} p^T B p$$

if and only if $\exists \lambda > 0$ such that

$$(B + \lambda I)p^* = -g$$
$$\lambda(||p^*|| - \Delta) = 0$$
$$(B + \lambda I) \geq 0$$

To approximate p^*, it's possible to numerically solve the above system of equations (exact solution approximation)

Exact solution - approximation

Some observations on this result:

- If B is SPD and the Newton step $p^N = -B^{-1}g \in T(\Delta)$, then $\lambda = 0$ and p^N is the solution to (1).
- When B is not SPD, this theorem implies that $\lambda \neq 0$, and therefore $||p^*|| = \Delta$, i.e. the minimum lies on the border of $T(\Delta)$.

When either $B \not\geq 0$ or p^N is not feasible, follows from $-(B + \lambda I)p^* = g$ that

$$\exists \lambda > 0 \quad \text{s.t} \quad p(\lambda) = -(B + \lambda I)^{-1} g \quad \text{and} \quad ||p(\lambda)|| = \Delta \tag{4}$$

is the solution of (1).

Considering the factorisation $B = Q\Lambda Q^T$, where $\Lambda = diag(\lambda_1, ...\lambda_n)$, with $\lambda_1 \leq \lambda_2 ... \leq \lambda_n$, the last condition $(B + \lambda I) \geq 0$ implies $\lambda \geq -\lambda_1$.

Exact solution - approximation

Under the simplifying hypothesis that $q_i^T g \neq 0 \ \forall i$, the scalar function

$$||p(\lambda)||^2 = ||Q(\Lambda + \lambda I)^{-1} Q^T g||^2 = \sum_{i=1}^{n} \frac{(q_i^T g)^2}{(\lambda_i + \lambda)^2}$$

is monotonically decreasing function in $(-\lambda_1, +\infty)$ and since

$$\lim_{\lambda \to -\lambda_1} ||p(\lambda)||^2 = +\infty \ \text{ and } \lim_{\lambda \to +\infty} ||p(\lambda)||^2 = 0$$

there is a unique value λ^* consistent with (4), which can be computed using Newton's Method as the root of $\phi(\lambda) = \frac{1}{||p(\lambda)||} - \frac{1}{\Delta}$.

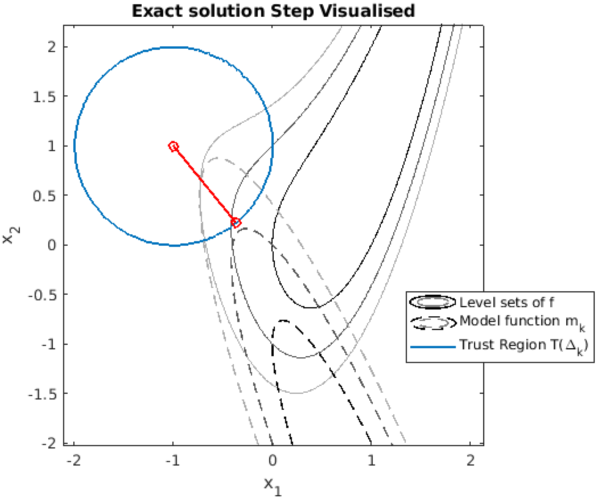
PROS

- Very accurate approximation of p^*

CONS

- Evaluation of ϕ is very costly (requires the factorisation of B)
- An estimate of λ_1 is required

Exact solution step - Example (Rosenbrock function)



Convergence Properties

Global Convergence

Assume that $\forall k$ the step p_k complies to

$$m_k(0) - m_k(p_k) \geq c_1 ||g_k|| \min\left(\Delta_k, \frac{||g_k||}{||B_k||}\right) \text{ and } ||p_k|| < \gamma\Delta_k \qquad (5)$$

for some $c_1 \in (0, 1]$, and $\gamma \geq 1$. Then

Convergence to stationary points

Assume (5) holds. If B_k is bounded below $\forall k$, f is bounded below on S and continuously Lipschitz differentiable on $S(R_0)$ for some constant R_0, then

$$\lim_k g(x_k) = 0$$

Where $S = \{x \in \mathbb{R}^n \ s.t. \ f(x) \leq f(x_0)\}$ be the level set of f in x_0 and let $S(R) = \{x \in \mathbb{R}^n \ s.t. \ ||x - y|| < R \text{ for some } y \in S\}$

Global Convergence

If an exact solution approximation of (1) is used to detemine p_k, then

Convergence to local minimiser

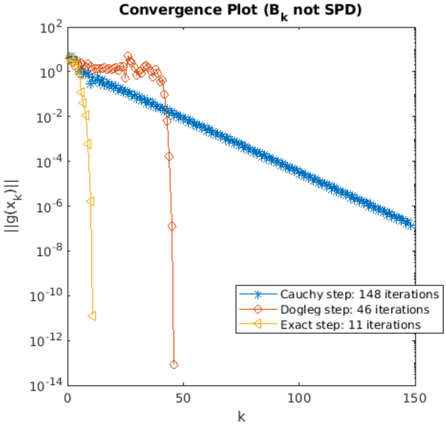
Let the assumptions of the previous theorem hold, $B(x)$ be the Hessian of $f(x)$ and $m(0) - m(p_k) \geq c_1(m(0) - m(p^*)) \; \forall k$. Then $\lim_k g(x_k) = 0$.

Moreover if S is compact, then either x_k converge to a local minimiser x^* or $\{x_k\}$ has a limit point to x^*

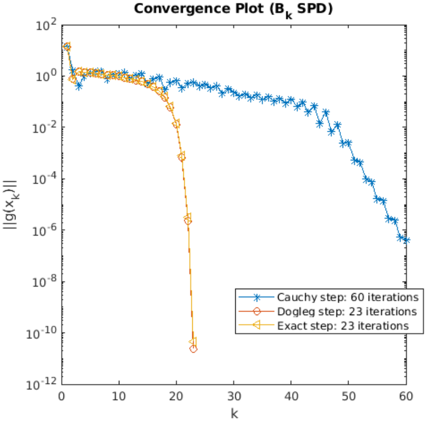
In the case of $x_k \to x^*$, some comments on local convergence:

- While being near the local minimum x^*, $p_k \approx p_k^N$ which suggests fast local convergence is kept.
- It can be proved that for large k, if $||p_k - p_k^N|| \in O(||p_k^N||)$ the Trust Region constraint becomes inactive and the convergence of$\{x_k\}$ superlinear.

Examle - Convergence profiles

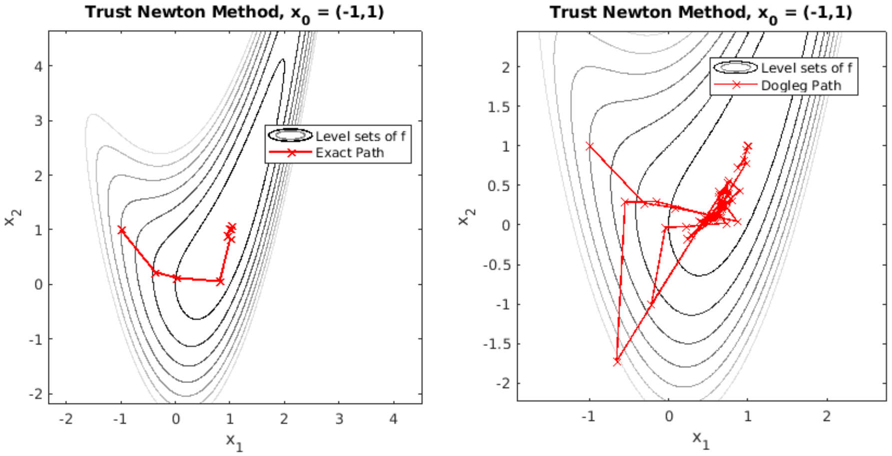


(a) If B_k is not SPD, Dogleg may fail



(b) If B_k is SPD, all methods work

Example (Rosenbrock function)



Thank You for your attention