*Bull. Nov. Comp. Center*, Num. Anal., 15 (2011), 17–24


# Trust-Region solvers: performance and applications in geosciences

Nikolay I. Gorbenko

## Introduction

The Trust-Region (TR) algorithms are relatively new iterative algorithms for solving nonlinear optimization problems. High efficiency of the TR methods was demonstrated in a number of recent publications [1]. They have the global convergence and local super-convergence, which differ them from the line search methods, commonly used for solving Inverse Problems [2]. The TR techniques are used in a number of well-known SW libraries such as IMSL, TAO, GALAHAD, LANCELOT, etc. the TR solvers were implemented in FORTRAN. Let us explain the main difference of the TR methods from the classical Newton ones. Assume we have a current guess of the solution for the optimization problem. An approximate model can be constructed near to the current point. Solution of the approximate model can be taken as the next iteration point. The classical line search algorithms also solve approximate models to obtain the search directions. However, in the TR algorithms, the approximation model is only "trusted" in the region near to the current iteration. This seems reasonable, because for general nonlinear functions, the local approximate models (such as linear and quadratic approximations) can only fit the original function locally. The region that the approximate model is trusted is called "trust region". The trust region is adjusted from iteration to iteration, i.e. if computations indicate the approximation model fit the original problem quite well, the TR can be enlarged. Otherwise when the approximation works not good enough the trust region will be reduced.

## 1. Trust-Region algorithms

Trust-Region algorithms allow to solve:

- nonlinear least squares problem (without and with bound constraints);
- system of nonlinear equations (without and with bound constraints);
- minimization of functional (without constraints).

Let us explain some details of the TR approach through the example of a nonlinear least squares problem:

$$\min_{x \in R^n} \|F(x)\| = \min_{x \in R^n} \|y - f(x)\|_2^2, \tag{1}$$
$$y \in R^m, \quad x \in R^n, \quad f : R^n \to R^m, \quad m > n,$$

where $f$ is a continuous differentiable function. It is easy to see that step for the TR method is the solution of the subproblem

$$\min_{x \in R^n} \|F(x_k) + J(x_k)^T d\|_2^2, \quad \text{where} \quad \|d\|_2^2 \le \Delta_k, \tag{2}$$

that is the approximation of the target function in the neighborhood of the current point $x_k$, and $J(x_k)$ is the Jacobi matrix of $F$.

Consider the TR pseudo-code for solving a nonlinear least squares problem:

Step 1: Choose the initial guess $x_1 \in R^n$, $\Delta_1 > 0$.

Step 2: Solution of (2) gives the value of $d_k$.

If $\|F(x_k)\|_2 = \|F(x_k) + J(x_k)^T d\|_2$ then stop.

Compute $r_k = \dfrac{\|F(x_k)\|_2 - \|F(x_k + d_k)\|_2}{\|F(x_k)\|_2 - \|F(x_k) + J(x_k)^T d_k\|_2}$.

Step 3: Choose

$$x_{k+1} = \begin{cases} x_k + d_k, & \text{if } r_k > 0, \\ x_k, & \text{otherwise.} \end{cases}$$

Define

$$\Delta_{k+1} = \begin{cases} \alpha_1 \|d_k\|_2, & \text{if } r_k < \nu_1, \\ 2\Delta_k, & \text{if } \nu_1 \le r_k < \nu_2, \\ \max\{\alpha_2 \|d_k\|_2, \Delta_k\}, & \text{if } r_k \ge \nu_2. \end{cases}$$

Step 4: $k = k + 1$, go to Step 2.

The main problem of the TR methods is to solve subproblem (2) that was studied by many authors. The following lemma is well known [1]:

**Lemma.** *A vector $d^* \in R^k$ is a solution to the problem*

$$\min_{d \in R^n} \Big(g^T d + \frac{1}{2} d^T B d\Big), \quad \|d\|_2 \le \Delta,$$

*where $g \in R^n$, $B \in R^{n \times n}$ is a symmetric matrix, and $\Delta > 0$, if and only if there exits $\lambda^* \ge 0$ such that $(B + \lambda^* I)d^* = -g$ and $(B + \lambda^* I)$ is semi-definite, $\|d^*\|_2 \le \Delta$ and $\lambda^*(\|d^*\|_2 - \Delta) = 0$.*

The case where $B + \lambda^* I$ has zero eigenvalues is called a "hard" case and $d^*$ can be written down as $d^* = -(B + \lambda^* I)^+ g + \nu$, where $\nu$ is a vector in the null space of $B + \lambda^* I$. Except for the hard case, $\lambda^*$ is the unique solution of the equation

$$\frac{1}{\|(B + \lambda^* I)^{-1}\|_2} - \frac{1}{\Delta} = 0.$$

For solving this equation we use the Newton method to calculate $\lambda^*$.

We describe how to use the TR region method for a nonlinear least square method with a simple bound constraining. Let

$$\min_{l<x<u} f(x) = \min_{l<x<u} \frac{1}{2}\|F(x)\|^2.$$

The first order necessary conditions for a vector minimizer for (1) are stated as

$$D(x)^{-2}\nabla f(x) = D(x)^{-2} F'^T(x) F(x) = 0, \tag{3}$$

where $D$ is the diagonal scaling matrix [3]:

$$D(x) = \mathrm{diag}\big(|\nu_1(x)|^{-1/2}, |\nu_2(x)|^{-1/2}, \ldots, |\nu_n(x)|^{-1/2}\big), \tag{4}$$

with

$$\nu_i = \begin{cases} x_i - u_i, & \text{if } \nabla f(x)_i < 0 \text{ and } u_i < \infty, \\ x_i - l_i, & \text{if } \nabla f(x)_i > 0 \text{ and } l_i > -\infty, \\ \min(x_i - l_i, u_i - x_i), & \text{if } \nabla f(x)_i = 0 \text{ and } u_i < \infty \text{ or } l_i > -\infty, \\ -1, & \text{if } \nabla f(x)_i < 0 \text{ and } u_i = \infty, \\ 1, & \text{if } \nabla f(x)_i > 0 \text{ and } l_i = -\infty, \\ 1, & \text{if } \nabla f(x)_i = 0 \text{ and } u_i = -l_i = \infty. \end{cases}$$

for $i = 1, 2, \ldots, n$.

Let $\Omega = \{x \in R^n;\ l \le x \le u\}$, and write $\mathrm{int}(\Omega)$ for a strict non-empty interior of $\Omega$. At each iteration, the basic structure of the method involves the solution to an elliptical trust-region subproblem and computation of a search step to update the current iteration. Let $x_i \in \mathrm{int}(\Omega)$ and trust-region size $\Delta > 0$ be given. We consider the elliptical trust-region subproblem given by:

$$\min_p \big\{ m_k(p) :\ \|D_k p\| \le \Delta_k \big\},$$

where $m_k(p)$ is quadratic model for $f$ at $x_k$, i.e.

$$m_k(p) = \frac{1}{2}\|F_k + F'_k p\|^2 = \frac{1}{2}\|F_k\|^2 + F_k^T F'_k p + \frac{1}{2} p^T F_k'^T F'_k p. \tag{5}$$

Let $p_{\mathrm{tr}}(\Delta_k)$ and $p_{\mathrm{c}}(\Delta_k)$ be a solution and the Cauchy point of trust-region subproblem (4), respectively. Namely, $p_{\mathrm{c}}(\Delta_k)$ is a minimizer of $m_k$ along the scaling steepest descent direction $d_k$ subject to the satisfaction of the trust-region bound, i.e.

$$p_{\mathrm{c}}(\Delta_k) = \tau_k d_k = -\tau_k D_k^{-2} F_k^T F_k', \tag{6}$$

where

$$\tau_k = \arg\min_{x>0} \big\{ m_k(\tau d_k) : \ \|\tau D_k d_k\| \le \Delta_k \big\}.$$

The function $m_k(\tau d_k)$ is quadratic in $\tau$, and the unconstrained minimizer has the form $\tau = -\nabla f_k^T d_k / \|F_k' d_k\|^2$ and $\tau_k$ is given by

$$\tau_k = \min\left( \frac{\|D_k^{-1} F_k'^T F_k\|^2}{\|F_k' D_k^{-2} F_k'^T F_k\|^2}, \frac{\Delta_k}{\|D_k^{-1} F_k'^T F_k\|} \right) \tag{7}$$

The search step $p(\Delta_k)$ used in our algorithm is defined by a linear combination of the two vectors $p_{\mathrm{tr}}(\Delta_k)$ and $\tau_k$, i.e.

$$p(\Delta_k) = t\bar{p}_{\mathrm{c}}(\Delta_k) + (1-t)\bar{p}_{\mathrm{tr}}(\Delta_k) \tag{8}$$

where $t \in [0,1]$ is a suitably chosen scalar. The vector $\bar{p}_{\mathrm{c}}(\Delta_k)$ in (8) is equal to $q$, where $q = q^1 - \alpha q^2$ is component-wise given by

$$(q^1)_i = \begin{cases} (l - x_k)_i, & \text{if } (x_k + p_{\mathrm{tr}}(\Delta_k))_i \le l_i, \\ p_{\mathrm{tr}}(\Delta_k)_i, & \text{if } l_i < (x_k + p_{\mathrm{tr}}(\Delta_k))_i < u_i, \\ (u - x_k)_i, & \text{if } (x_k + p_{\mathrm{tr}}(\Delta_k))_i \ge u_i; \end{cases} \tag{9}$$

$$(q^2)_i = \begin{cases} (l - x_k)_i, & \text{if } (x_k + p_{\mathrm{tr}}(\Delta_k))_i \le l_i, \\ 0, & \text{if } l_i < (x_k + p_{\mathrm{tr}}(\Delta_k))_i < u_i, \\ (u - x_k)_i, & \text{if } (x_k + p_{\mathrm{tr}}(\Delta_k))_i \ge u_i. \end{cases} \tag{10}$$

At the $k$th iteration we consider the second degree polynomial $r(\alpha) = m_k(q^1 - \alpha q^2)$. On the basis of the current information, $r(\alpha)$ simulates the restriction of $f$ at the points $q^1 - \alpha q^2$ for $\alpha$ varying from 0 to 1. Therefore we compute the value $\alpha^*$ that minimizes this model and choose $\alpha$ according to fixed lower and upper bounds, $0 < \alpha_1 < \alpha_2 < 1$. This means that we set

$$\alpha^* = \arg\min_{\alpha} r(\alpha) = \frac{F_k^T F_k' q^2 + (q^1)^T F_k'^T F_k' q^2}{(q^2)^T F_k'^T F_k' q^2}, \quad \alpha = \max(\alpha_1, \min(\alpha^*, \alpha_2)).$$

Now we consider the choose of the vector $\bar{p}_{\mathrm{c}}(\Delta_k)$. If the point $(x_k + p_{\mathrm{c}}(\Delta_k)) \in \mathrm{int}(\Omega)$, we simply take $\bar{p}_{\mathrm{c}}(\Delta_k) = p_{\mathrm{c}}(\Delta_k)$. Otherwise, $\bar{p}_{\mathrm{c}}(\Delta_k)$ is a simple scaling of $p_{\mathrm{c}}(\Delta_k)$ obtained by a step-back along it. In other words, letting $\lambda^k$ be the stepsize along $p_{\mathrm{c}}(\Delta_k)$ to the boundary, i.e.

$$\lambda^k = \min_{l \le x \le u} \Delta_i^k, \quad \Delta_i^k = \begin{cases} \max\Big\{ \frac{(l - x_k)_i}{(p_{\mathrm{c}}(\Delta_k))_i}, \frac{(u - x_k)_i}{(p_{\mathrm{c}}(\Delta_k))_i} \Big\}, & \text{if } (p_{\mathrm{c}}(\Delta_k))_i \ne 0, \\ \infty, & \text{if } (p_{\mathrm{c}}(\Delta_k))_i = 0. \end{cases}$$

The step $\bar{p}_{\mathrm{c}}(\Delta_k)$ is given by

$$\bar{p}_{\mathrm{c}}(\Delta_k) = \begin{cases} p_{\mathrm{c}}(\Delta_k), & \text{if } \lambda^k > 1, \\ \theta\lambda^k p_{\mathrm{c}}(\Delta_k), & \text{otherwise,} \end{cases} \tag{11}$$

for some fixed $\theta \in [0, 1]$.

The scalar $t$ in (8) is chosen in order to satisfy the following conditions

$$\rho(p(\Delta_k)) = \frac{m_k(0) - m_k(p(\Delta_k))}{m_k(0) - m_k(\bar{p}_{\mathrm{c}}(\Delta_k))} \geq \beta_1, \tag{12}$$

for the given constant $\beta_1 \in (0, 1)$ and

$$m_k(p(\Delta_k)) \leq m_k(p_{\mathrm{tr}}(\Delta_k)). \tag{13}$$

To meet conditions (12), (13), we compute the scalar $t$ in (8) according to the following strategy. If $\rho(p_{\mathrm{tr}}(\Delta_k)) \geq \beta_1$, we simply set $t = 0$, i.e. we choose $p(\Delta_k) = \bar{p}_{\mathrm{tr}}(\Delta_k)$ as potential step. Otherwise, we fix $p(\Delta_k)$ so that $x_k + \bar{p}_{\mathrm{tr}}(\Delta_k)$ is the point which lies on the segment from $x_k + \bar{p}_{\mathrm{tr}}(\Delta_k)$ to $x_k + \bar{p}_{\mathrm{c}}(\Delta_k)$ and satisfies $\rho(p(\Delta_k)) = \beta_1$.

In fact, $p(\Delta_k)$ is given by (8) setting

$$t = \frac{z^T u - w}{\|u\|^2}, \tag{14}$$

where

$$u = F_k'(\bar{p}_{\mathrm{c}}(\Delta_k) - \bar{p}_{\mathrm{tr}}(\Delta_k)), \quad z = -(F_k + F_k'\bar{p}_{\mathrm{tr}}(\Delta_k)),$$

$$w = \Bigg((z^T u)^2 - 2\|u\|^2\Big(F_k^T F_k'(\bar{p}_{\mathrm{tr}}(\Delta_k) - \beta_1\bar{p}_{\mathrm{c}}(\Delta_k)) - \frac{1}{2}\|F_k'\bar{p}_{\mathrm{tr}}(\Delta_k)\|^2 - \frac{\beta_1}{2}\|F_k'\bar{p}_{\mathrm{c}}(\Delta_k)\|^2\Big)\Bigg)^{1/2}.$$

A good agreement between the model function $m_k$ and the target function $f$ is ensured for the following standard condition

$$\rho_f(p(\Delta_k)) = \frac{f(x_k) - f(x_k + p(\Delta_k))}{m_k(0) - m_k(p(\Delta_k))} \geq \beta_2 \tag{15}$$

with a given constant $\beta_2 \in (0, 1)$. If this condition is not met, we reject $p(\Delta_k)$ and adjust the trust-region size $\Delta_k$ with a successive reduction so that $p(\Delta_k)$ satisfies the accuracy requirement (14).

**Algorithm** (the $k$th iteration).

Let $x_k \in \mathrm{int}(\Omega)$, $\Delta_k > 0$, $\beta_1, \beta_2, \delta_1 \in (0,1)$, $\Delta_{\min} > 0$, $\alpha \in (0,1)$, be given.

Compute the matrix $D_k$ by (3).

Set $\bar{\Delta}_k = \max\{\Delta_k, \Delta_{\min}\}$, set $\Delta_k^* = \bar{\Delta}_k$.

Repeat

  Set $\Delta_k = \Delta_k^*$.

  Find the solution $p_{\mathrm{tr}}(\Delta_k)$ to problem (4).

  Compute the Cauchy step $p_{\mathrm{c}}(\Delta_k)$ by (6).

  Compute $\bar{p}_{\mathrm{tr}}(\Delta_k)$ and $\bar{p}_{\mathrm{c}}(\Delta_k)$ by (9)–(11).

  Find $t$ such that (12), (13) be satisfied.

  Set $\Delta_k^* = \delta_1 \Delta_k$.

## 2. Numerical results

We apply our TR methods to several standard test problems found for the unconstrained and constrained optimizations in collection tests from CUTEr and Minpack. The TR solvers show the excellent performance vs. VNI IMSL Fortran library v5.0 and TAO v1.8.1. On benchmark tests, the TR solvers give the following average 10 times speed-ups vs. IMSL and 5 times average speed-ups vs. TAO (Figure 1).

We use the common 1D basin modeling equation (16) derived from Darcy's law and the assumption of mass conservation:

$$R(t,z)\frac{\partial P(t,z)}{\partial t} = \frac{\partial}{\partial z}\Big(D(t,z)\frac{\partial P(t,z)}{\partial z}\Big) + f(t,z), \tag{16}$$

where $P$ is the excess pore pressure, $R$ is the effective compressibility of porous media, $D$ is the fluid conductivity matrix with allowance for the permeability anisotropy and $f$ is a sources term that includes external and

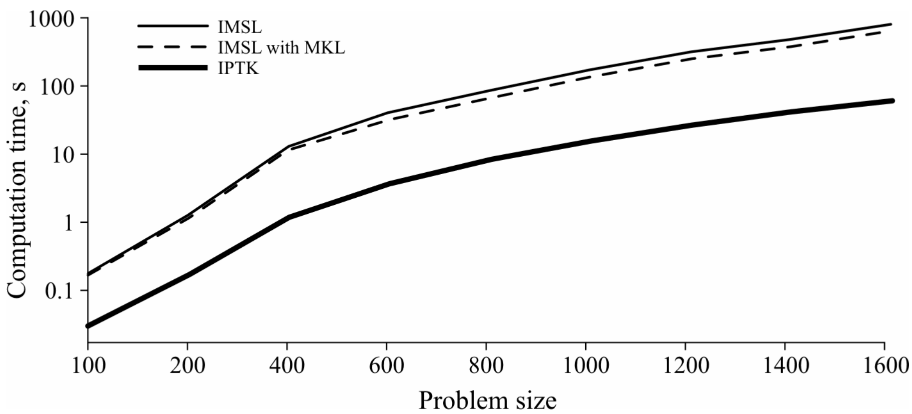


**Figure 1.** Comparison with IMSL

internal overpressuring factors: sedimentation and hidrocarbon generation [5]. It is needed to solve equation (16) for $P$ as a function of depth $z$ and time $t$ with some imposed boundary and initial conditions.

The forward model operator $C[x]$ corresponding to the numerical solution of (1) is determined for a limited set of parameters $X$ controlling the current values of the coefficients of (16). Some of the control parameters such as isobaric extensibility and isothermal compressibility of the pore water are treated as fixed physical properties. Parameters such as a temperature gradient, compaction and conduction constants are considered to be regionally fixed parameters. The sedimentation rate and the lateral conduction are specified at each particular location. A data transformation operator $T[a]$ is introduced, which transforms data from the space $A$ of observations to a space with common scaling that is the modeling output. The inverse problem with respect to the present-day excess pore pressure profile can be formulated as minimization of an object function, describing the norm of the vector of misfit between the real data and the modeling results, i.e., nonlinear least squares.

The modeling-inversion scheme is a common tool in both the prediction from seismic data and the estimation from well logs. The model can be

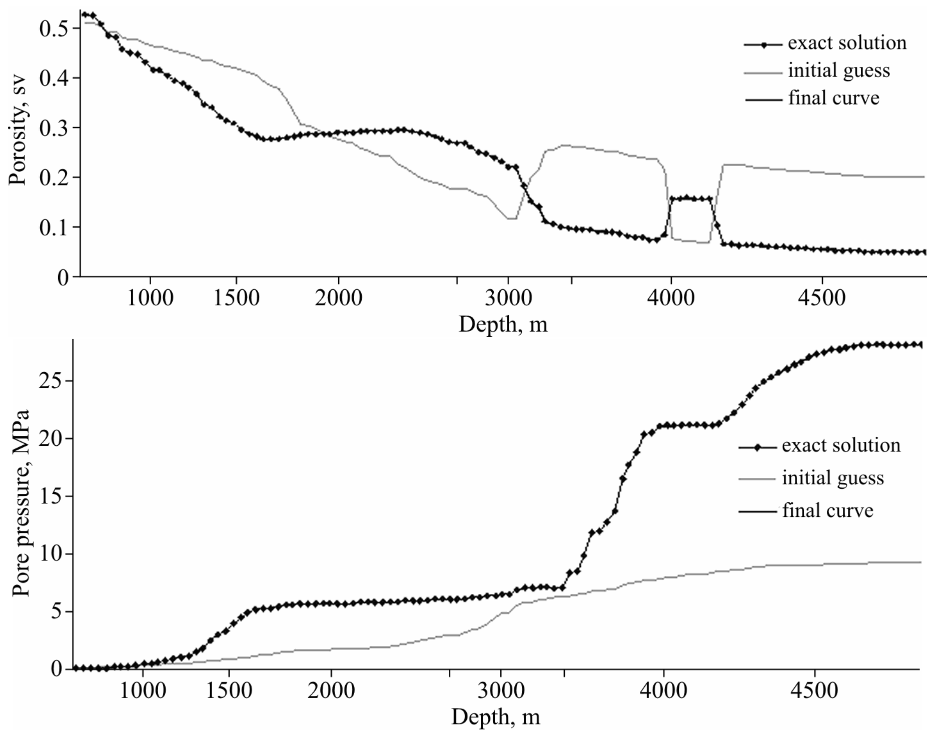


**Figure 2.** Porosity (top) and pressure (bottom) comparison on synthetic data

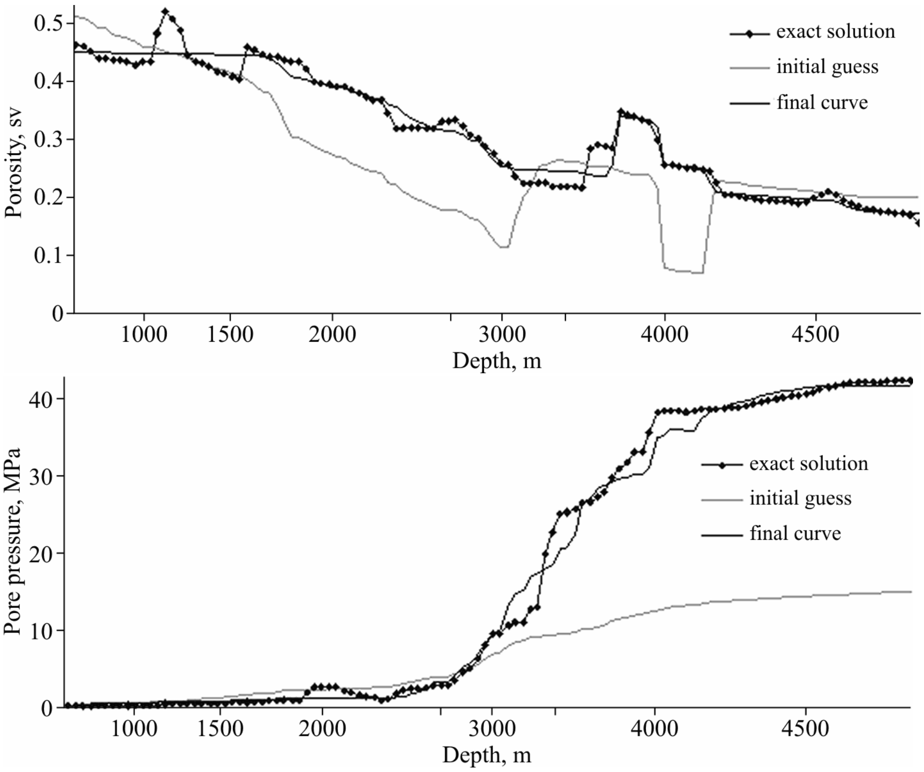


**Figure 3.** Application of the modeling-inversion technique to data derived from the sonic log: results of porosity (top) and pressure (bottom) comparison

calibrated by the same scheme when sufficient data are available. This scheme was verified on synthetic data (Figure 2). Practical examples from the North Sea reveal that our method is fully applicable to real data (Figure 3).

## References


[1] Conn A.R., Gould N.I.M., Toint P.L. Trust-Region Methods. — Englwood Clffs, New Jersey: Society for Industrial and Applied Mathematics, 2000.

[2] Lavrentiev M.M., Avdeev A.V., Lavrentiev Jr. M.M., Priimenko V.I. Inverse Problems of Mathematical Physics. — The Netherlands: VSP Publ., 2003.

[3] Coleman T.F., Li Y. An interior trust-region approach for minimization subject to bounds // SIAM J. Optim. — 1996. — Vol. 6, No. 3. — P. 418–445.

[4] Cuter. — http://hsl.rl.ac.uk/cuter.

[5] Madatov A.G., Helle H.B., Sereda V.-A.I. A modeling and inversion technique applied to pore pressure evaluation // 57th EAEG Conference, Glasgow, May 29, June 2, 1955.