

A Trust Region-cg Regularization Method for the Reconstruction of High Energy Spectrum Function

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Abstract: In this paper, we consider the reconstruction of high energy spectrum function. High energy spectrum function, such as the spectrum of synchrotron radiation, has been well understood, whereas reconstruction of the spectrum function is still not mature because of the ill-posed inverse process. The spectrum function of the synchrotron radiation satisfies the Laplace transform, while solving the Laplace transform is a typically ill-posed problem. This paper develops a trust region-cg regularization method, a kind of iterative method to solve the reconstruction problem for the high energy spectrum. Numerical experiments are given to illustrate the efficiency of the method.

Keywords: regularization; reconstruction; trust region method; high energy spectrum function.

1. INTRODUCTION

High energy spectrum, such as the synchrotron radiation (SR) is emitted by electrons orbiting in a storage ring. It provides X-rays which are used for a wide range of analytical techniques. Due to its good characteristics, it has been applied to many fields since it has been observed. Since the spectrum of SR source can be accurately calculated, we often get the SR spectrum by theoretical calculation instead of experimental measurement. But in reality, the validity of calculation is affected by many factors and we are interested in the spectral distribution at the samples [1],[11].

The reconstruction of the real spectrum is a difficult task because it requires an ill-posed inverse problem to be dealt with. When SR with spectrum distribution traverse the filtration, the intensity is attenuated. The signal obtained satisfies ([1],[11])

$$I(d) = a \int_{E_0}^{E_1} f(E) e^{-\mu(E)d} E [1 - e^{-\mu_g(E)D}] dE \quad (1)$$

where E is the energy of the light, $\mu(E)$ is the absorption coefficient of the filtration, $\mu_g(E)$ is the

absorption coefficient of the gas filled in the chamber, d is the thickness of the filtration, D is the length of the ion chamber, E_0 and E_1 are respectively, the minimum and maximum photon energy of the incident light. Here, $a = Gq / \varepsilon_{ion}$ is the gain of the amplifier, q is the electron charge, ε_{ion} is the ionization energy of the gas filled in the chamber.

Considering the wedged filtration and the width of the beam, Equation (1) has to be corrected, i.e.

$$I(d) = a \int_{E_0}^{E_1} \frac{f(E) [1 - e^{-\mu(E)\omega \tan \theta}]}{\mu(E)\omega \tan \theta} E [1 - e^{-\mu_g(E)D}] e^{-\mu(E)d} dE \quad (2)$$

where ω is the width of the light, θ is the apex angle of the filtration.

By variable replacement, Equation (2) can be rewritten as

$$I(d) = a \int_{\mu_0}^{\mu_1} g(\mu) e^{-\mu d} d\mu, \quad (3)$$

where

$$g(\mu) = \frac{f[E(\mu)] E(\mu) e^{-\mu_g E(\mu) D} [1 - e^{-\mu \omega \tan \theta}]}{\mu \omega \tan \theta} \frac{dE}{d\mu} \quad (4)$$

It is clear that (3) is a Laplace integral equation, which is a special operator equation of the first kind, hence the ill-posed nature it inherits. This means that even if a least squares solution with minimal norm in space exists, it may oscillate severely with the perturbation of the observation. So, direct solution of (3) or finding its least square errors (LSE) solution should be avoided. To see this, first we formulate the problem in the Hilbert space:

$$K : F \rightarrow R, (Kf)(d) = I(d)$$

where F and R are two Hilbert spaces, whose norm is induced by inner product and $f \in F, I \in R$.

In the following discussion, we will present how to solve the above operator equation with the trust region method.

2. TRUST REGION-CG REGULARIZATION METHOD

Trust region methods are a kind of relatively new methods in nonlinear programming. Many scholars have devoted to this area (see refs. [5], [6], [12], [13] and the reference therein). However, most of their work is focused on the well-posed problems. Recent works have introduced the optimization method to deal with ill-posed problems ([7]-[9]). Trust region-cg method is an useful method, which not only guarantees the global convergence, but also assures the velocity of convergence in the local part. Let us consider the minimization problem

$$\min_{x \in R^n} f(x) \quad (5)$$

when we try to solve the above problem by using the trust region method, we should give the trust region radius at first. After that, we could solve the quadratic sub problem of the approximation problem about (5)

$$\min_{\xi} \psi(x_c + \xi) = f(x_c) + (g(x_c), \xi) + \frac{1}{2} (H_c \xi, \xi) \quad (6)$$

$$s.t. \|\xi\| \leq \Delta_c \quad (7)$$

the trust region radius demonstrate how well we could trust this quadratic approximation model. At the same time, we call this algorithm as trust region method.

Now let us consider how to solve the discrete operator equation

$$Kf = i \quad (8)$$

with the trust region method. In the above equation,

$K \in R^m \times R^n$ is a discrete operator, $f \in R^n$

is the input value we need, i is the observation.

Firstly, we form the unconstrained optimization problem as follows

$$M[f, i_\delta] := \|Kf - i_\delta\|^2 \rightarrow \min \quad (9)$$

where $K : F \subset D(K) \rightarrow I$ is a bounded linear operator, F and I are both Hilbert spaces. We always assume that the equation

$$Kf = i_\delta \quad (10)$$

has at least one solution. But the solution may not depend continuous on the r.h.s. i_δ .

According to the idea of Tikhonov regularization, we should add a penalty to the functional $M[f, i_\delta]$ i.e., we determine the following functional

$$M^\alpha[f, i_\delta] := \|Kf - i_\delta\|^2 + \alpha \Omega[f], \quad (11)$$

where $\Omega[f]$ serves as the stabilizer, α is the so-called regularization parameter, which can be determined by a priori or a posteriori technique. We will not discuss this but refer to refs. [2],[4],[8].

In order to numerically solve the abstract problem, we have to transfer the infinite dimensional problem to the finite dimensional problem by projection. This is a trivial task. Hence, without loss of generality, we assume that Equation (10) has been in the discrete case, and we still denote it by (10).

Based on the idea of trust region method [14], we should construct an approximate model to the original problem given the current iterate. We only trust the model in the neighborhood of the iterate f_k . Note that is a twice differentiable functional about f , hence we can construct the trust regionsubproblem (TRS) in the following way:

$$\min_{s \in F_n} g_k^T s + \frac{1}{2} (Hess_k s, s) := \phi_k(s), \quad (12)$$

$$s.t. \|s\| \leq \Delta_k, \quad (13)$$

where $g_k = M'[f_k, i_\delta] = K^*(Kf_k - i_\delta)$, K^* is the adjoint of K , $Hess_k = K^*K$ for $\Omega[f]$ as $\|f\|^2$, $\Delta_k > 0$ is the trust region radius, F_n is the projection of F . In practice, we often take $F_n = R^n$.

In each iteration of the trust region method, we need to solve the operator problem (12)-(13) accurately and inaccurately to obtain the trial step about the next iteration. This trial step is generally called the trust region step. Whether we should trust this step is depend on certain standard. The standard is determined on the ratio between the predicted reduction and the actual reduction. For any trial step, the predicted reduction is defined by the reduction in the approximate model,

$$Pred_k = \phi_k(0) - \phi_k(s_k). \quad (14)$$

The actual reduction is the reduction in the objective function, defined by

$$Ared_k = M[f_k, i_\delta] - M[f_{k+1}, i_\delta]. \quad (15)$$

And we define the ratio between the actual and the predicted reduction by

$$r_k = \frac{Ared_k}{Pred_k}, \quad (16)$$

which is used to decide whether the trial step is acceptable and to adjust the new trust region radius.

According to [8], this choice of r_k is equivalent to a truncated conjugate gradient method with safeguard of step size within the trust region.

Let s_k be the solution of sub problem (12)-(13). It is shown by [3] that trust region sub problem satisfies the following condition

$$Pred_k \geq c \min \left\{ \Delta_k, \frac{\|g_k\|}{\|Hess_k\|} \right\} \quad (17)$$

where $c > 0$ is a constant. The iterate satisfying the above expression is called the sufficiently decreasing step.

Therefore it is quite common that in practice the trial step at each iteration of a trust region method is computed by solving the TRS (12) and (13) inexactly. One way to compute an inexact solution of (12) and (13) is the truncated conjugate gradient method [5], [6], [12]. But all of these results are about well-posed problems. Recently, for ill-posed problems with application to geophysical inverse problems and image restoration problems, the convergency and regularity of the trust region method were studied in [7], [9]. We will give an analysis of this kind of method when applying it to ill-posed problems in high energy physics.

With regard to quadratic problems, we find that the ratio $r_k \equiv 1$ except the objective functional adds a nonlinear and non-quadratic terms.

Actually, according to the minimization process of the objective functional, the functional value $M[f_k + s_k]$ will be better than $M[f_k]$ at least. Thus, generally speaking, whether the trail step s_k will be better or not, in other words, the decline of the objective functional is more or less, the trust region radius will be increase. If we use equation (16) as the principle standard, we should always accept the trail step s_k . Of course, with regard to the standard trust region method, it also accord with the above discussion.

In this paper, we define r_k by the new ratio as follows

$$r_k = \frac{M[f_k + s_k]}{M[f_k]} \text{.we use this ratio to measure}$$

whether the trial step should be accept or not and whether trust region radius should adjust or not. From this new definition, we could find that this ratio not only make full use of the deviation of the problem, but

also take advantage of the quality of the problem. Thus, it describe the essence of the problem in the whole.

Now we generate the trust region algorithm for solving ill-posed problems as follows.

Algorithm 2.1(Trust region algorithm for linear ill-posedproblems).

STEP 1. Given the initial possible values $f_0 \in R^n$,

$$\Delta_0 > 0, 0 < \tau_3 < \tau_4 < 1 < \tau_1, 0 \leq \tau_0 \leq \tau_2 < 1,$$

$\tau_2 > 0$, set $k := 1$;

STEP 2. Ifthe stopping rule is satisfied, then STOP;else, solve (12)-(13)giving s_k ;

STEP 3. Compute r_k ;

$$f_{k+1} = \begin{cases} f_k & , \text{if } r_k \leq \tau_0; \\ f_k + s_k & , \text{otherwise;} \end{cases} \quad (18)$$

Choose δ_{k+1} that satisfies

$$\Delta_{k+1} = \begin{cases} \frac{\tau_3 \|s_k\| + \tau_4 \Delta_k}{2} & , \text{if } r_k \leq \tau_2 \\ \frac{\Delta_k + \tau_1 \Delta_k}{2} & , \text{otherwise;} \end{cases} \quad (19)$$

STEP 4. Compute g_k ; $k := k + 1$;GOTO STEP 2.

In STEP2,the stopping rule is based on the discrepancy principle, i.e., at the first occurrence of the iteration index

$$k = k_D$$

such that the following inequality

$$\|Kf_k - i_\delta\| \leq \omega \delta, \omega > 1 \quad (20)$$

holds, we terminate the iteration.

The constants τ_i ($i = 0, \dots, 4$) can be chosen by users. Typical values are

$$\tau_0 = 0, \tau_1 = 2, \tau_2 = \tau_3 = 0.25, \tau_4 = 0.5.$$

The conjugate gradient method for

$$\min_{s \in R^n} \psi(s) = g_k^T s + \frac{1}{2} s^T Hess_k s \quad (21)$$

generates a sequence as follows:

$$s_{l+1} = s_l + \alpha_l \xi_l, \quad (22)$$

$$\xi_{l+1} = -g_{l+1}^{\psi} + \beta_l \xi_l, \quad (23)$$

where

$$g_l^{\psi} = \nabla \psi(s_l) = K^* K s_l + g_k, g_k = K^* (K f_k - i_{\delta}), Hess_k = K^* K.$$

α_l and β_l are determined by

$$\alpha_l = \frac{-g_l^{\psi T} \xi_l}{\xi_l^T Hess_k \xi_l}, \beta_l = \frac{\|g_{l+1}^{\psi}\|^2}{\|g_l^{\psi}\|^2}, \quad (24)$$

with the initial values $s_0 = 0, \xi_0 = -g_0^{\psi} = -g_k$.

Even without assuming the positive definite of the Hessian, we can continue the conjugate gradient method provided that $\xi_l^T Hess_k \xi_l$ is positive. If the iterate $s_l + \alpha_l \xi_l$ computed is in the trust region ball, it can be accepted, and the conjugate gradient iterates can be continued to the next iteration. Whatever $\xi_l^T Hess_k \xi_l$ is not positive or $s_l + \alpha_l \xi_l$ is outside the trust region, we can take the longest step along s_l within the trust region and terminate the calculation. The truncated conjugate gradient method for well-posed and ill-posed problems is given in [6],[9],[12], here we re-outline the algorithm for ill-posed high energy spectrum reconstruction problem.

Algorithm 2.2 (Truncated conjugate gradient method for TRS).

STEP 1. Given $s_0 = 0, \delta > 0, 0 < \tau < 1$, compute

$$g_0^{\psi} = \nabla \psi(s_0) \text{ and set}$$

$$l := 0, \xi_0 = -g_0^{\psi} = -g_k;$$

STEP 2. If $\|i_{\delta} - K f_k - K s_l\| \leq \tau \|i_{\delta} - K f_k\|$, stop,

output $s^* = s_l$; Compute $\xi_l^T Hess_k \xi_l$; If $\xi_l^T Hess_k \xi_l = 0$ GOTO STEP 4;

Calculate α_l by (25).

STEP 3. If $\|s_l + \alpha_l \xi_l\| \geq \Delta_k$, GOTO STEP 4;

Set s_l by (23) and

$$g_{l+1}^{\psi} = g_l^{\psi} + \alpha_l Hess_k \xi_l$$

Compute β_l by (25) and set ξ_{l+1} by (24);

Set $l := l + 1$ GOTO STEP 2.

STEP4. Compute $\alpha_l^* \geq 0$ satisfying $\|s_l + \alpha_l \xi_l\| = \Delta_k$;

Set $s^* := s_l + \alpha_l^* \xi_l$, and STOP.

Note that α_l^* can be computed by choosing the positive root of the quadratic equation in α :

$$\|\xi_l\|^2 \alpha^2 + 2(s_l, \xi_l) \alpha + \|s_l\|^2 - \Delta_k^2 = 0. \quad (25)$$

Combining Algorithm 2.1 and 2.2, we find the trust region-cg algorithms consist of two stage iterations: the inner loop and the outer loop. The inner loop is the truncated conjugate gradient method, the outer loop is the trust region method. Since we only want to get an approximate solution of the TRS, it does not need to be solved so exactly. Noticing this fact, in practical applications, we add in Algorithm 2.2 another stopping rule, i.e., the maximal iteration number: *itermax*. Once *itermax* is violated, we stop the inner loop and turn to the outer loop.

Let s^* be the inexact solution of (12)-(13) obtained by the truncated CG method and \hat{s} be the exact solution of (12)-(13), with the assumption that $Hess_k$ is positive

definite. It is proved that $\phi(s^*) \leq \frac{1}{2} \phi(\hat{s})$ [4], i.e., the

reduction in the approximate model is at least half of the maximum reduction at each iteration if we use truncated conjugate gradient method for solving the subproblem (12)-(13). Noticing this fact, we must safeguard that *Pred* is not too small. Therefore we add another stopping rule in the outer iteration, i.e., the value of *Pred* cannot be smaller than ϵ . Once this is satisfied, the inner iteration should be terminated.

3. NUMERICAL EXPERIMENT

Laplace transform is an important application for solving the decreasing of the optical energy in high energy physics. The conjugate gradient method was studied in [10]. However, the conjugate gradient method is not robust enough as it may still does not converge to a global minimizer. We use the truncated conjugate gradient method in the trust region framework for solving this problem. As mentioned before, the spectrum function of the synchrotron radiation satisfies the operator equation

$$(Kf)(d) = \int_{E_0}^{E_1} g(E, d) f(E) dE = I(d), d \in [d_0, d_1], \quad (26)$$

where the integral kernel is $g(E, d) = \exp(-dE)$,

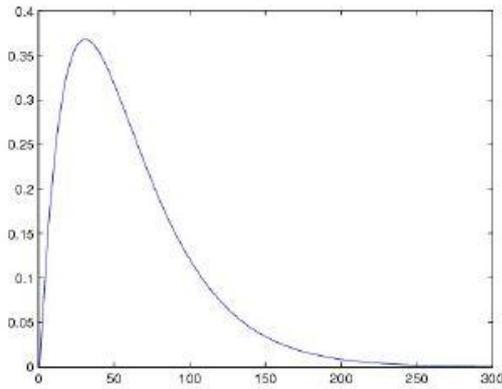


Fig.1: the exact spectrum function

In our simulation, we choose the right-hand side as

$$I(d) = \frac{1}{(d+1)^2} \quad \text{to simulate the data,}$$

$[E_0, E_1] = [0, \infty], (d_0, d_1) = (-1, \infty)$. Through simple manipulation, we compute that the exact spectrum solution is given by $f(E) = E \exp(-d)$. We generate $i_\delta(d)$ as the observation with the noise. Our purpose is to numerically reconstruct the exact solution f from i_δ .

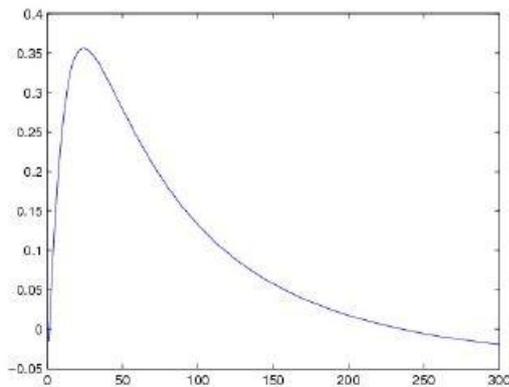


Fig.2: the reconstruction function with $\delta = 0.01$

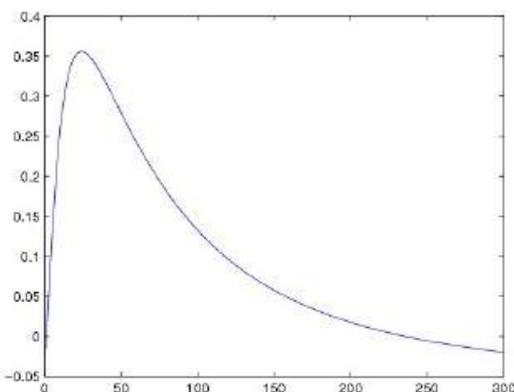


Fig.3: the reconstruction function with $\delta = 0.05$

In our simulations, we restrict $[E_0, E_1] = [0, 10], [d_0, d_1] = [0, 300]$. We choose the noise level $\delta = 0.01$ and $\delta = 0.05$, use *mid-point* rule to get a discrete equation. Let us give some notations: f_δ is defined as the approximate solutions, iter. stands for iteration steps; $k_{max} = 30, \omega = 1.2$, the initial guess value $f_0 = (0.1, 0.1, \dots, 0.1)^T$. We choose $\tau_0 = 0, \tau_1 = 2, \tau_2 = \tau_3 = 0.25, \tau_4 = 0.5$. We perform the numerical test by Matlab. The results are shown in Figs.1-3 for the exact spectrum function, the reconstruction spectrum function with $\delta = 0.01$ and the reconstruction spectrum function with $\delta = 0.05$, respectively. It can be seen that our method is valid.

4. CONCLUSIONS

We have presented the trust region method to solve ill-posed spectrum distribution function reconstruction problem. Through the numerical experiment, we can see easily that the trust region method is a relatively stable method for solving ill-posed reconstruction problems in high energy physics.

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