A REGULARIZED GMRES METHOD FOR INVERSE BLACKBODY RADIATION PROBLEM

by

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The inverse blackbody radiation problem is focused on determining temperature distribution of a blackbody from measured total radiated power spectrum. This problem consists of solving a first kind of Fredholm integral equation and many numerical methods have been proposed. In this paper, a regularized generalized minimal residual method is presented to solve the linear ill-posed problem caused by the discretization of such an integral equation. This method projects the original problem onto a lower dimensional subspaces by the Arnoldi process. Tikhonov regularization combined with the generalized cros validation criterion is applied to stabilize the numerical iteration process. Three numerical examples indicate the effectiveness of the regularized generalized minimal residual method.

Key words: *blackbody radiation, inverse problem, generalized minimal residual method, regularization*

Introduction

During theoretical study of blackbody radiation problems, we often use a set of inaccurate experimental data to calculate other physical data. The inverse blackbody radiation (BRI) problem is one of the examples. According to Planck's law, the mathematical model of the blackbody radiation can be expressed as [1]:

$$w(\nu) = \frac{2h\nu^3}{c^2}\int_0^\infty \frac{a(T)}{\mathrm{e}^{h\nu/kT}-1}\mathrm{d}T \tag{1}$$

where frequency $\nu \in [V_1, V_2]$, $w(\nu)$ is the total radiated power spectrum, T – the absolute temperature and the range of T usually goes from 100 to 1000 K, $a(T)$ – the area temperature distribution, c – the speed of light, k – the Boltzmann's constant, and h – the Planck's constant. The direct problem of blackbody radiation is to calculate $w(\nu)$ by $a(T)$ while the BRI problem is to obtain $a(T)$ by solving in integral eq. (1). The BRI problem is important in remote sensing applications.

For convenience letting $G(\nu) = c^2 w(\nu)/2h\nu^3$ and then expression (1) is equivalent to:

$$G(\nu) = \int_0^\infty \frac{a(T)}{\mathrm{e}^{\mathrm{h}\nu/\mathrm{kT}}-1}\mathrm{d}T = \int_0^\infty K(\nu, T)a(T)\,\mathrm{d}T \tag{2}$$

where integral kernel $K(\nu, T) = (\mathrm{e}^{h\nu/kT} - 1)^{-1}$. Equation (2) is a first kind of Fredholm integral equation and is an inherently ill-posed problem [1]. Since 1982, this problem has attracted many

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scholars' attention. The first formulation for this problem was proposed by Bojarski [2] in 1982. The Laplace transform together with an iterative process was presented. Chen and Li [3], Dai and Dai [4] proved the existence and uniqueness of the solution of BRI. Sun and Jaggard [5], Dou and Hodgson [6], and Li and Xiao [7] discussed Tikhonov regularization methods. Li [8] proposed conjugate gradient method. Dou and Hodgson [9] employed maximum entropy method. Ye *et al*. [10] developed universal function set method. Wu and Dai [11] presented a regularizing Lanczos method.

Generalized minimal residual (GMRES) algorithm method [12] is a common tool for solving linear systems. Until recently GMRES method has been applied to discrete ill-posed problems. For instance Jensen and Hansen [13] systematically studied the characteristics of the regularization GMRES method. Calvettiet *et al*. [14, 15] discussed regularization GMRES method and applied the *L* curve condition number to solve linear ill-posed problems and image restoration processing. In this paper, we discrete the integral eq. (2) and introduce the GMRES method to solve the obtained linear discrete ill-posed system. This method is based on the Arnoldi process, which yields a sequence of small least squares problems by approximating the original discrete ill-posed problem. Tikhonov regularization [1] combined with generalized cross validation (GCV) criterion [16] are used to stabilize the iteration process. Numerical results illustrate the potential of the proposed method.

Discretization and regularization

In practice, the range of T usually goes from 100 K to 1000 K, and ν goes from 0 Hz to $2\cdot10^{14}$ Hz. Assuming the range of T is $[T_1, T_2]$, then eq. (2) can be expressed approximately as:

$$G(\nu) = \int_{T_1}^{T_2} \frac{a(T)}{\mathrm{e}^{h\nu/kT} - 1}\mathrm{d}T \tag{3}$$

Let $\nu \in [V_1, V_2]$, we choose n collocation points: $\nu_1 = V_1 + l(V_2 - V_1)/(n-1), l = 0, 1, \ldots n-1$ on the $[V_1, V_2]$, then eq. (3) becomes:

$$G(\nu_l) = \int_{j=0}^{n-1} \frac{a(T)}{\mathrm{e}^{h\nu_l/kT} - 1}\mathrm{d}T, \quad l = 0, 1, \ldots, n-1 \tag{4}$$

The numerical quadrature ruler $\int_a^b f(x)\mathrm{d}x \approx (b-a)f(a)$ with n intervals of equal length on $[T_1, T_2]$ is discreted as:

$$G(\nu_l) = \sum_{j=0}^{n-1}\int_{t_j}^{t_{j+1}} \frac{a(T)}{\mathrm{e}^{h\nu_l/kT} - 1}\mathrm{d}T = \sum_{j=0}^{n-1}\frac{T_2 - T_1}{n}\frac{a(t_j)}{\mathrm{e}^{h\nu_l/kt_j} - 1} \tag{5}$$

If the vectors $\boldsymbol{x}$ and $\boldsymbol{b}$ are defined by $\boldsymbol{x} = [a(t_0), \ldots, a(t_{n-1})]^T$, $\boldsymbol{b} = [G(\nu_0), \ldots, G(\nu_{n-1})]^T$, and if the $n\times n$ square matrix $[\boldsymbol{A}]$ is defined by $\boldsymbol{A} = (d/\mathrm{e}^{h\nu_l/kt_j - 1})_{n\cdot n}$ where $d = (T_2 - T_1)/n$ then eq. (5) can be written as:

$$\boldsymbol{Ax} = \boldsymbol{b} \tag{6}$$

It is well known that the discretization of integral in eq. (3) gives rise to an discrete linear ill-posed system, which means that: (1) the system (6) might not have a solution, (2) the solution might not be unique, and (3) the solution – if it exists and is unique – does not depend continuously on the right-hand side. In addition the matrix $\boldsymbol{A}$ is ill-conditioned. Straightforward solution of the system (6) is typically not meaningful. In order to avoid this difficulty, the linear system (6) can be replaced by a nearby system which is well-conditioned and the computed solution is a good approximation. This replacement is known as regularization.

One of the most common methods of regularization is Tikhonov regularization [1], which replaces the system (6) by the minimization problem $\min_x \left\|\boldsymbol{Ax}-\boldsymbol{b}\right\|^2 + \lambda^2\left\|\boldsymbol{x}\right\|^2$ or equivalently:

$$(\boldsymbol{A}^T\boldsymbol{A} + \lambda^2\boldsymbol{I})\,\boldsymbol{x} = \boldsymbol{A}^T\boldsymbol{b} \tag{7}$$

where λ^2 is a regularization parameter and $\|\cdot\|$ denotes the 2-matrix norm. Combining the GMRES method with Tikhonov regularization [1], system (6) is projected onto a Krylov subspace. The projected problem is also ill-posed. Since the dimension of the projected problem is usually small relative to n, regularization of the projected problem is much less expensive.

Regularized GMRES method

The GMRES method which based on the Arnoldi process is a popular iterative method for solving large linear system with a non-symmetrical non-singular matrix. In exact arithmetic, for a given starting vector r_0, the GMRES method projects system (6) to Krylov subspace: $K_\mathrm{m}(\boldsymbol{A}, \boldsymbol{r}_0) = \mathrm{span}\{\boldsymbol{r}_0, \boldsymbol{Ar}_0, \ldots \boldsymbol{A}^{m-1}\boldsymbol{r}_0\}$ and determines iterates $x_m \in x_0 + K_m(\boldsymbol{A}, \boldsymbol{r}_0)$, $m = 1, 2, \ldots$, which satisfy: $\left\|b - Ax_m\right\| = \min_{x\in K_m(A,b)}\left\|b - Ax\right\|$.

We use notation $(\boldsymbol{x}, \boldsymbol{y}) = \boldsymbol{x}^T\boldsymbol{y}$, $\boldsymbol{x}, \boldsymbol{y} \in R^\mathrm{N}$ in the following Arnoldi process.

Algorithm 1. (The Arnoldi process)

(1) let $\boldsymbol{x}_0$ be a starting vector. Compute $\boldsymbol{r}_0 = \boldsymbol{b} - \boldsymbol{Ax}_0$ and $v_1 = \boldsymbol{r}_0/\|\boldsymbol{r}_0\|$; (2) for $j = 1, \ldots, m$; (2.1) compute $\eta = \boldsymbol{Av}_j$; (2.2) for $i = 1, \ldots, j$ compute $h_{ij} = (\eta, \mathrm{v}_i)$ and $\eta = \eta - h_{ij}v_i$, (2.3) compute $h_{j+1,j} = \|\eta\|$, and (2.4) compute $v_{j+1} = \eta/h_{j+1,j}$.

The Arnoldi process generates an orthonormal matrix $\boldsymbol{V}_{m+1} = [\boldsymbol{v}_1, \boldsymbol{v}_2, \ldots, \boldsymbol{v}_{m+1}]$ whose columns are orthonormal bases of $K_\mathrm{m}(\boldsymbol{A}, \boldsymbol{r}_0)$, and an upper Hessenberg matrix $\boldsymbol{H}_\mathrm{m} = (h_{ij}) \in \in R^{\mathrm{m},\mathrm{m}-1}$. In matrix form we have:

$$\boldsymbol{AV}_m = \boldsymbol{V}_m\boldsymbol{H}_m + h_{m+1,m}\boldsymbol{v}_{m+1}\boldsymbol{e}_1^T \tag{8}$$

where $\boldsymbol{e}_1$ is the first canonical vector.

Let $$\widetilde{\boldsymbol{H}}_m = \begin{pmatrix} \boldsymbol{H}_m \\ h_{m+1,m}\boldsymbol{v}_{m+1}\boldsymbol{e}_1^T \end{pmatrix},$$

the GMRES method computes the approximation $\boldsymbol{x}_m = \boldsymbol{x}_0 + \boldsymbol{V}_\mathrm{m}\boldsymbol{y}$, where $\boldsymbol{y}$ solves the least squares problem:

$$\left\|\boldsymbol{b} - \boldsymbol{Ax}_m\right\| = \min_{y\in R^m}\left\|\boldsymbol{b} - \boldsymbol{A}(\boldsymbol{x}_0 + \boldsymbol{V}_m\boldsymbol{y}\right\| = \min_{y\in R^m}\left\|\left\|\boldsymbol{r}_0\right\|\boldsymbol{e}_1 - \widetilde{\boldsymbol{H}}_m\boldsymbol{y}\right\| \tag{9}$$

Generally with the increasing iteration, the largest and the smallest singular value of matrix $\widetilde{\boldsymbol{H}}_m$ will approximate those of matrix $\boldsymbol{A}$, respectively. This means that the problem (9) inherits properties of the system (6) and is also a small ill-posed problem. Therefore we use Tikhonov regularization method to regularize (9) and solve:

$$(\widetilde{\boldsymbol{H}}_m^T\widetilde{\boldsymbol{H}}_{\boldsymbol{m}} + \lambda^2\boldsymbol{I})\,\boldsymbol{y} = \left\|r_0\right\|\widetilde{\boldsymbol{H}}_m^T\boldsymbol{e}_1 \tag{10}$$

Suppose that the singular value decomposition (SVD) of $\widetilde{\boldsymbol{H}}_m$ is given by:

$$\widetilde{\boldsymbol{H}}_m = \boldsymbol{P}\begin{pmatrix} \Omega \\ \boldsymbol{0} \end{pmatrix}\boldsymbol{Q}^T \tag{11}$$

where $\boldsymbol{P} = [\boldsymbol{p}_1, \ldots, \boldsymbol{p}_{m+1}]$ and $\boldsymbol{Q} = [\boldsymbol{q}_1, \ldots, \boldsymbol{q}_m]$ are matrices with orthonormal columns, and the diagonal matrix $\Omega = \mathrm{diag}(\omega_1, \ldots, \omega_m)$. In terms of the decomposition of (11) the solution of (10) can be expressed as:

$$\boldsymbol{y} = \|\boldsymbol{r}_0\| \sum_{i=1}^{m} \frac{\omega_i^2}{\omega_i^2 + \lambda^2} \frac{\boldsymbol{P}_{1i}}{\omega_i} \boldsymbol{q}_i \tag{12}$$

There exists different ways of choosing the regularization parameter. Here the GCV criterion is employed. This method is to find the parameter λ that minimizes the GCV function:

$$G(\lambda) = \frac{\left\|(\boldsymbol{I} - \boldsymbol{H}\boldsymbol{H}_\lambda^{\#})\|\boldsymbol{r}_0\|\boldsymbol{e}_1\right\|^2}{[\mathrm{tr}(\boldsymbol{I} - \boldsymbol{H}\boldsymbol{H}_\lambda^{\#})]^2}$$

where $\boldsymbol{H}_\lambda^{\#} = (\boldsymbol{H}\boldsymbol{H}_\lambda^{\#} + \lambda^2 \boldsymbol{I})^{-1} \boldsymbol{H}^T$. Here the symbol $\boldsymbol{H}$ is $\widetilde{\boldsymbol{H}}_m$ in eq. (8) and tr($\boldsymbol{A}$) denotes the trace of $\boldsymbol{A}$.

Proposition 1. Denote $K_i = \lambda^2/(\omega_i^2 + \lambda^2)$, $\imath = 1, 2, ..., m$, then:

$$G(\lambda) = \frac{\|\boldsymbol{r}_0\|^2 \left[\sum_{i=1}^{m} (K_i \boldsymbol{P}_{1i})^2 + \boldsymbol{P}_{1m+1}^2\right]}{m + 1 - \sum_{i=1}^{m} K_1} \tag{13}$$

Proof. Following eq. (11) it is immediate to see that:

$$\boldsymbol{I} - \boldsymbol{H}\boldsymbol{H}_\lambda^{\#} = \boldsymbol{P} \begin{bmatrix} \boldsymbol{I}_m - \Omega^2(\Omega^2 + \lambda^2 \boldsymbol{I})^{-1} & \boldsymbol{0} \\ \boldsymbol{0} & 1 \end{bmatrix} \boldsymbol{P}^T$$

Since tr($\boldsymbol{AB}$) = tr($\boldsymbol{BA}$), we have:

$$\mathrm{tr}(\boldsymbol{I} - \boldsymbol{H}\boldsymbol{H}_\lambda^{\#}) = \mathrm{tr} \begin{bmatrix} \boldsymbol{I}_m - \Omega^2(\Omega^2 + \lambda^2 \boldsymbol{I})^{-1} & \boldsymbol{0} \\ \boldsymbol{0} & 1 \end{bmatrix} = m + 1 - \sum_{i=1}^{m} K_i$$

Moreover, the numerator is:

$$\left\|(\boldsymbol{I} - \boldsymbol{H}\boldsymbol{H}_\lambda^{\#}\|\boldsymbol{r}_0\|\boldsymbol{e}_1\right\| = \|\boldsymbol{r}_0\| \left\| \begin{bmatrix} \boldsymbol{I}_m - \Omega^2(\Omega^2 + \lambda^2 \boldsymbol{I})^{-1} & \boldsymbol{0} \\ \boldsymbol{0} & 1 \end{bmatrix} \boldsymbol{P}^T \boldsymbol{e}_1 \right\|^2 = \|\boldsymbol{r}_0\| \left[\sum_{i=1}^{m} (K_i \boldsymbol{P}_{1i})^2 + \boldsymbol{P}_{1m+1}^2\right]$$

thus eq. (13) holds generally.

The proposition 1 suggests that one can estimate parameter λ by finding the minimum value of eq. (13). If λ is known, then the approximate solution $\boldsymbol{x}_m = \boldsymbol{x}_0 + \boldsymbol{V}_m \boldsymbol{y}$ can be found by eq. (12). The algorithm 2 summarizes how the computations for the regularized GMRES can be organized.

Algorithm 2. (Regularized GMRES method)

(1) compute the linear system (6) by discretizing eq. (3), (2) choose a starting vector $\boldsymbol{x}_0$ and carry out m steps of the Arnoldi process, (3) compute the SVD of $\widetilde{\boldsymbol{H}}_m$, (4) solve eq. (10) using GCV criterion, (5) set $\boldsymbol{x}_m = \boldsymbol{x}_0 + \boldsymbol{V}_m \boldsymbol{y}_k$, and (6) check convergence. If not converged let $m = m + 1$ and continue iterating.

In the algorithm, the iteration number m should not be too large. Usually we can set an upper limit for the number of iteration m. If the Krylov subspace dimension increases up to the maximum iteration number and the residual norm $\|\boldsymbol{b} - \boldsymbol{A}\boldsymbol{x}_\mathrm{m}\|$ is not small enough, we can apply the restarted GMRES method to get the iterate $\boldsymbol{x}_m$.

Numerical results

The regularized GMRES method is applied to three examples. These examples are selected from [9]. The numerical results obtained by the regularized GMRES method and the exact solution are given in different figures. All computations were done in MathCAD2001.

For numerical error estimation, we define the relative error as: $\gamma = \|a(T) - x_m\|_2 / \|a(T)\|_2$, where $a(T)$ is the exact temperature distribution and x_m – the approximate solution calculated by the regularized GMRES method.

Example 1 is a Gaussian temperature distribution given by: $a(T) = \exp[-(T-\delta)^2/25000]$, $T \in [100, 800]$, where δ is a parameter. For a given $n = 50$, we discrete (3) and obtain the linear system (6). It is easy to know that the coefficient matrix $\boldsymbol{A}$ with $\delta = 450$ is ill-conditioned because the largest singular value of matrix $\boldsymbol{A}$ is $5.153 \cdot 10^4$ and the smallest singular value is 0. Let $\delta = 200$, 450, and 600. Application of the regularized GMRES method to these distributions results the temperature distribution $a(T)$ as shown in fig. 1-3. These figures display the comparisons of the approximate solution determined by the regularized GMRES method indicated by the dotted curve and the exact solution (solid curve). Obviously the overall agreement between calculated and exact values displayed in fig. 1 and fig. 2 is excellent. For the case of $\delta = 600$ the resulted distribution shown in fig. 3 has some disagreement and the corresponding relative error $\gamma = = 0.048$. This result is good and can be acceptable.

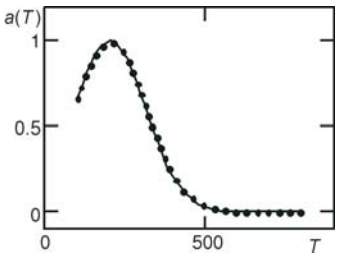

Figure 1. Comparison of exact and computed temperature distributions for δ = 200 and γ = 0.000113216

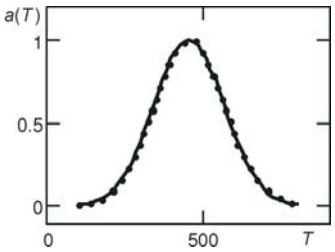

Figure 2. Comparison of exact and computed temperature distributions for δ= 450 and γ = 0.002122711

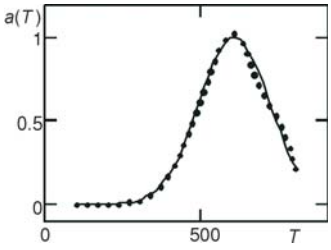

Figure 3. Comparison of exact and computed temperature distributions for δ = 600, γ = 0,048

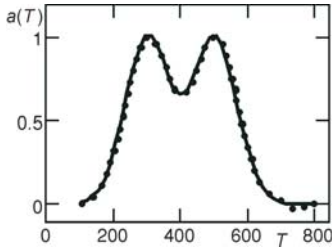

Figure 4. Comparison of exact and computed temperature distributions for δ = 450, γ = 0.009

Example 2 is the double Gaussian temperature distribution given by: $a(T) = \exp(T - - 300)^2/9000 + \exp(T - 600)^2/9000$, $T \in [100, 800]$.

The computed results in fig. 4 shows good, but the calculated distributions $a(T)$ indicated by the dotted curve have some disagreement at the right part.

Example 3 is that of a rectangular temperature case:

$$a(T) = \begin{cases} 0.5 & 100 \le T < 300 \\ 1 - \dfrac{|T - 450|}{300}, & 300 \le T < 600 \\ 0.5 & 600 \le T << 00 \end{cases}$$

In this example the distributions $a(T)$ is continuous, but not differential at some collocation points. Figure 5 shows the

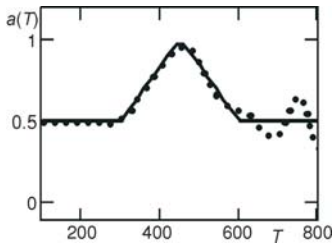

Figure 5. Comparison of exact and computed temperature distributions, γ = 0.086

calculated result (dotted curve) for this example. The agreement in the part of lower temperature is satisfactory but the oscillations appear in the right region. This phenomenon indicates that the discontinuity and the intrinsic instability of the physical problem effect the reconstructed result.

Conclusions

In this paper the regularized GMRES method is introduced to recover the $a(T)$ from the total power spectral measurements of its radiation. From the limited numerical results we find that the proposed algorithm is numerically stable and can recover the $a(T)$ which is continually differential.

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