CLASSIFICATION AND OPTIMIZATION IN X-RAY TOMOGRAPHY

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ABSTRACT

In this paper we represent our recent results in a short and simplified version. They have been obtained by mathematical modeling based on a transport equation. A formal method for estimating quality of reconstruction in X-ray tomography is established. The approach consists in using the notion "measure of visibility" which has been introduced and substantiated in the previous authors' papers (Anikonov,1999; Anikonov, Kovtanyuk, and Prokhorov, 2002). In partiqular, the defined coefficient of contrast is a suitable modification of the visibility measure and this coefficient becomes a criterion function for classification of all cases into groups with a good, intermediate and poor visibility. Also, the measure of visibility allows us to set and investigate optmization problems by control of an energy level of sounding radiation. While the results are directly applicable to tomography using soft X-ray. In the end of the paper, we point out to certain possible developments.

Keywords Classification, Optimization, X-Ray, Tomography

1 GENERAL DESCRIPTION

We consider the steady-state process of soft X-ray migration in a substance, which can be described by the following transport equation:

$$\omega \cdot \nabla_r f(r,\omega,E) + \mu(r,E) f(r,\omega,E) = \mu_s(r,E) \int_\Omega k(r,\omega \cdot \omega',E) f(r,\omega',E) d\omega', \tag{1.1}$$

where $r \in G$, G is a bounded convex domain in R^3, Ω is the unit sphere in R^3, $E \in I = [E_1, E_2],\ 0 < E_1 < E_2 < \infty.$ The function f is treated as the density of the photon flux at the point r, moving in the direction ω with energy E. The functions $\mu(r,E)$ and $\mu_s(r,E)$ are called the coefficients of attenuation and scattering, respectively. The absorption coefficient $\mu_a(r,E)$ is defined as $\mu_a = \mu - \mu_s$. Without loss of generality, we assume that the indicatrix of scattering $k(r,\omega\cdot\omega',E)$ is normalized so that the integral of $k(r,\omega\cdot\omega',E)$ with respect to $\omega' \in \Omega$ is equal to 1. For simplicity, we consider the case of absence of internal sources of radiation. Hereafter the variable E is any fixed value of energy and only in Section 3 we analyse certain quantities and their dependence on E.

To describe heterogeneity of the medium G we consider domains $G_i, i = 1,\dots,p$, such that $G_i \subset G,\ G_i \cap G_j = \varnothing,$ if $i \neq j$ and the union G_0 of all G_i is dense in $\overline{G}, (\overline{G_0} = \overline{G})$. We designate the boundary of G_0 by ∂G_0 and for simplicity suppose that each G_i is a strictly convex domain with smooth boundary of the class C^1. The surface $\partial G_0,$ being the union of all $\partial G_i,$ is smooth also. Assume that the nonnegative functions $\mu(r,E)$ and $\mu_s(r,E)$ are uniformly continuous in $G_i \times I, i = 1,\dots,p,$ and they may have nonzero jumps on ∂G_i. Hereafter, the following notations are admitted. Letter z denotes a point of the surface ∂G_0; $\mu_i(z,E),\ \mu_{si}(z,E),$ and $\mu_{ai}(z,E),$ are the limit values of the functions $\mu(r,E), \mu_s(r,E)$ and $\mu_a(r,E)$, respectively, when $r \to z$; $r \in G_i$. The jump of μ is defined by the equality: $[\mu\ (z,E)] = \mu_j(z,E) - \mu_l(z,E),\ \ z \in \partial G_j \cap \partial G_l,\ j > l.$ The jumps $[\mu_s(z,E)]$ and $[\mu_a(z,E)]$ have the same sense.

Let $d(r,\omega)$ be the length of the intersection of the ray $L_{r,\omega} = \{r + t\omega,\ t > 0\}$ and the set $\overline{G},(r,\omega) \in \overline{G} \times \Omega$, then the points $\xi = r - d(r,-\omega)\omega$ and $\eta = r + d(r,\omega)\omega$ belong to ∂G. We denote the set of such pairs (ξ,ω) as Γ^- and the set of pairs (η,ω) as Γ^+. The transport equation (1.1) is added by the following boundary conditions:

$$f(\xi,\omega,E) = h(\xi,\omega,E),(\xi,\omega) \in \Gamma^-, \qquad (1.2)$$

$$f(\eta,\omega,E) = H(\eta,\omega,E),(\eta,\omega) \in \Gamma^+, \qquad (1.3)$$

where h and H are interpreted as the density of input and output radiation at ∂G, respectively. For simplicity, we assume that the nonnegative functions $h_1(r,\omega,E) = h(r - d(r,-\omega)\omega,\omega,E)$ and $k(r,\omega\cdot\omega',E)$ are uniformly continuous everywhere.

It is known (Anikonov, Kovtanyuk, and Prokhorov, 2002). that the classical direct problem of determination of f from (1.1) and (1.2) with given μ,μ_s,k,h has the unique solution, if $\mu(r,E) \ge \mu_s(r,E)\ (\mu_a(r,E) \ge 0), r \in G_0.$ The function $f(r,\omega,E)$ appears to be nonnegative and continuous everywhere.

Here, we are interested in the problem of determination of the surface ∂G_0 from (1.1), (1.2) and (1.3), when $H(\eta,\omega,E)$ is given. As far as other functions are concerned, we only assume that they belong to certain classes of functions.

It is easy to see that this problem (1.1), (1.2) and (1.3) is a tomography problem, because the surface ∂G_0 describes the internal structure of the medium G.

Under rather general assumptions this problem had been researched in (Anikonov,1999; Anikonov, Kovtanyuk, and Prokhorov, 2002), where the theorems of uniqueness had been proved. Also, the corresponding algorithms were constructed and tested. A variant of solving this problem is based on the following 2-D modification of the heterogeneity indicator (Anikonov, Nazarov, and Prokhorov, 2002):

$$Ind^*(r,E) = \left| \nabla_r \int_{\Omega_1} f(r + d(r,\omega)\omega,\omega,E)d\omega \right|,\ (r,\omega) \in (G \cap P) \times \Omega_1, \qquad (1.4)$$

where P is a plane in R^3 such that $G \cap P \ne \varnothing$, the operator ∇_r acts with respect to the space variables in P, $\Omega_1 = \Omega \cap P^*$ and P^* is the plane in R^3, passing through the origin and parallel to the plane P.

Consider the following functions:

$$\tau(z,\omega,E) = \int_0^{d(r,\omega)} \mu(r + t\omega,E)dt,\ (r,\omega) \in \overline{G} \times \Omega, \qquad (1.5)$$

$$m(z,\omega,E) = [\mu(z,E)] f(z,\omega,E) - [\mu_s(z,E] \int_\Omega k(z,\omega\cdot\omega',E) f(z,\omega',E)d\omega', \qquad (1.6)$$

$$mv(z,\omega,E) = m(z,\omega,E)\exp(-\tau(z,\omega,E)), \qquad (1.7)$$

$$M(z,E) = mv(z,s,E) + mv(z,-s,E), \qquad (1.8)$$

where $s \in \Omega_1$ and s is a tangent vector to the line $\partial G_0 \cap P$ at the point $z \in \partial G_0 \cap P$. The function $\tau(z,\omega,E)$ is often called the optical depth of the point z in the direction ω for energy E, and $|mv(z,\omega,E)|$ was called in (Anikonov, Nazarov, and Prokhorov, 2002) the measure of visibility of the medium G in the point z in the direction ω for energy E.

We proved the equality:

$$Ind^*(r,E) = |M(z,E)| |Ln|r - z|| + O(1),\ r \in G_0 \cap P,\ z \in \partial G_0 \cap P, \qquad (1.9)$$

where $O(1)$ means a bounded function. It is easy to see that if $M(z,E) \ne 0,$ then $Ind^*(r,E) \to \infty,$ as $r \to z$. Just this property allows us to determine $\partial G_0 \cap P$ and even the surface $\partial G_0,$ if number of planes P is sufficiently large.

2 CLASSIFICATION AND ESTIMATION

We designate the greatest value of $f(z,\omega,E)$ with respect to $\omega\in\Omega$ by $f^*(z,E),$ and the value $\max\left(\mu_l(z,E),\mu_j(z,E)\right)$ by $\mu^*(z,E),\ z\in\partial G_l\cap\partial G_j,\ l<j$. Suppose that $f^*(z,E)>0$ and $\mu^*(z,E)>0,$ that takes place in many cases.

Definition. *The coefficient of contrast* æ(z,ω,E) *at the contact point* z *, in the direction* ω *and for energy* E *is defined by the equality:*

$$\text{æ}(z,\omega,E)=(\mu^*(z,E)\cdot f^*(z,E))^{-1}\left|m(z,\omega,E)\right|,\ (z,\omega)\in\partial G_0\times\Omega \tag{2.1}$$

We proved the following statement.

Theorem 2.1. *For any functions* μ,μ_s,k,h *and the corresponding solution of the direct problem* f *the following assertions are valid:*

a) $0\le\text{æ}(z,\omega,E)\le 1;$

b) if æ$(z,\omega,E)>0$ *for all* $(z,\omega)\in\partial G_0\times\Omega,$ *then the tomography problem* (1.1), (1.2), *and* (1.3) *has no more than one solution;*

c) if æ$(z,\omega,E)=0$ *for* $(z,\omega)\in\partial G_j\times\Omega$ *(j is a fixed index), then there are infinitely much different functions* $\tilde{\mu},\tilde{\mu}_s$ *and domains* $\tilde{G}_j$ *that stand for* μ,μ_s *and* G_j*, respectively, so that the corresponding solutions* $\tilde{f}(r,\omega,E)$ *to the direct problems are the same everywhere, coinciding* with $f(r,\omega,E).$

Roughly speaking, Theorem 2.1. means that successful solving the tomography problem is possible only in the case: æ$(z,\omega,E)>0.$ Moreover, consideration of the formulae (1.7), (1.8) and (1.9) leads us to the idea: the more is the value æ$(z,\omega,E),$ the better is the quality of the reconstruction, at least, by means of $Ind^*(r,E).$ This theoretical conclusion has been confirmed by numerical experiments such as follows.

Let G be the unit ball centred at the origin; $P=\left\{r:\ r=(r_1,\ r_2,\ r_3),\ r_3=0\right\};$ $G_i=\left\{r:r\in R^3,\left|r-a_i\right|<0.2\right\},\ i=2,3,4,$ $a_2=\left(0,\ 0.5,\ 0\right),$ $a_3=\left(0.25\sqrt{3},\ -0.25,\ 0\right),$ $a_4=\left(-0.25\sqrt{3},\ -0.25,\ 0\right),$ $G_1=G\setminus\left(\overline{G_2\cup G_3\cup G_4}\right);$ $k(r,\omega\cdot\omega',E)=3(1+(\omega\cdot\omega')^2)/16\pi;$ $h_1(r,\omega,E)\equiv 1;$ $\mu(r,E)=1,\ \mu_s(r,E)=1$ for $r\in G_1;$ $\mu(r,E)=1,\ \mu_s(r,E)=0$ for $r\in G_2;$ $\mu(r,E)=0.8,\ \mu_s(r,E)=0.3$ for $r\in G_3;$ $\mu(r,E)=0,\ \mu_s(r,E)=0$ for $r\in G_4.$ We see that $\left[\mu(z,E)\right]=0,\left[\mu_s(z,E)\right]=-1$ for $z\in\partial G_1\cap\partial G_2,$ $\left[\mu(z,E)\right]=-0.2,\left[\mu_s(z,E)\right]=-0.7$ for $z\in\partial G_1\cap\partial G_3,$ and $\left[\mu(z,E)\right]=-1,$ $\left[\mu_s(z,E)\right]=-1$ for $z\in\partial G_1\cap\partial G_4.$ The domain G_1 is treated as the purely scattering envelope for the inclusions G_2,G_3 and $G_4.$ The domains G_2 and G_4 are interpreted as a pure absorbing body and vacuum, respectively. The body G_3 is a scattering and absorbing medium and absorption predominates over scattering.

We use a version of the Monte-Carlo method which is called the method of conjugated trajectories for calculation of æ(z,ω,E) and $Ind^*(r,E).$ For each point $(z,\omega,E),$ up to 500 trajectories were taken into account. The results obtained are as follows: æ$(z,\omega,E)=0.9121$ for $z\in\partial G_2,\ \ z=(0,0.7,0),$ $\omega=(1,0,0);$ æ$(z,\omega,E)=0.4681$ for $z\in\partial G_3,\ \ z=\left(0.35\sqrt{3},-0.35.0)\right),\ \omega=\left(-0.5,-0.5\sqrt{3},0\right);$ æ$(z,\omega,E)=0.0001$ for $z\in\partial G_4,\ \ z=\left(-0.35\sqrt{3},-0.35,0)\right),\ \omega=\left(-0.5\sqrt{3},0.5,0\right).$ These values allow us to classify the proposed reconstruction of $\partial G_2\cap P,\partial G_3\cap P$ and $\partial G_4\cap P$ as good, intermediate and poor cases, respectively. The reconstructions implemented by $Ind^*(r,E)$ are shown at the figure 1. They appear to be well consistent with the previous conclusions obtained by means of æ(z,ω,E).

Remark 2.1. Another version of a criterion function for classification can be the function æ$_1(z,\omega,E) =$ æ$(z,\omega,E)\exp(-\tau(z,\omega,E))$ taking into account the optical depth of the point z.

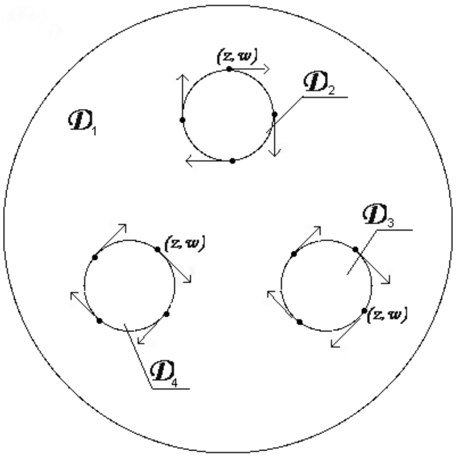

Figure 1a

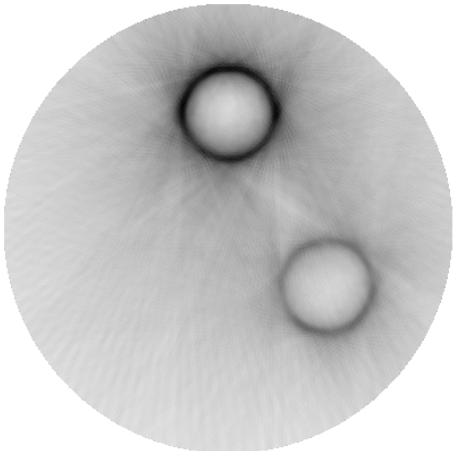

Figure 1b

Figure 1a: The original internal structure of a plane section of a medium G. The boundary inhomogeneities to be reconstructed are the circles $\mathcal{D}_1, \mathcal{D}_2$ and $\mathcal{D}_4$ ($\mathcal{D}_i = \partial G_i \cap P,\ i = 1,\ldots,4$). At the marked points z, at which the contrast coefficient æ(z,ω) in the directions ω tangent to the circles at these points is evaluated.

Figure 1b: The reconstruction of the internal structure of the plane section of the medium G by use of the heterogeneity indicator whose values are proportional to the gray scale. One circle is reconstructed distinctly, the second is reconstructed worse, and the third cannot be discerned at all; this corresponds to the formal estimation of reconstruction quality.

3 OPTIMIZATION AND QUASIOPTIMIZATION

Following the pointed idea: the greater is $M(z,E)$, the better is the quality of reconstruction, we consider a problem of maximization of $M(z,E)$. Let us fix a point $z \in \partial G_0$ and define the goal function $\Phi(z,E) = (h^*)^{-1}|M(z,E)|$, where h^* is the greatest value of $h(\xi,\omega,E)$.

Optimization problem. *Determine the value* $E^*, E^* \in [E_1, E_2]$ *providing the greatest value to the goal function* $\Phi(z,E)$, $(\Phi(z,E^*) \geq \Phi(z,E))$.

We have used real data (Hubbell, Seltzer, 1995) and calculated some functions $\Phi(z,E)$ concerned with various substances. Not rarely such functions oscillate rather strongly with respect to E. In these cases determination of the optimal energy level E^* is not a light problem.

In practice, all parameters of radiation are given for a finite number of their variables. Therefore, principally, the optimization problem can be solved by computer exertion. At the same time, it is desirable to replace too complex function $\Phi(z,E)$ by a more simple approximation depending on less number of parameters. To this end, we consider the following function:

$$A(z,\omega,E) = [\mu_a(z,E)]\, f_0(z,\omega,E)\exp(-\tau(z,\omega,E)),\ (z,\omega,E) \in \partial G_0 \times \Omega \times I, \qquad (3.1)$$

where $f_0(z,\omega,E) = h_1(z,\omega,E)\cdot\exp(-\tau(z,-\omega,E))$.

Introduce the function $\lambda(r,E)$ which equals to $\mu_s(r,E)/\mu(r,E)$ if $\mu(r,E) > 0$ and equals to zero if $\mu(r,E) = 0$. Hereafter, this and other functions are considered as elements from the space L_∞ with corresponding norms. We have proved the following statement.

Theorem 3.1. *If* $\|\lambda(r,E)\|<1,$ *then the following estimation is valid:*

$$|mv(z,\omega,E)-A(z,\omega,E)| \le \|h_1(r,\omega,E)\| \frac{\|\lambda(r,E)\| \|[\mu_a(z,E)]\|}{1-\|\lambda(r,E)\|} \exp(-\tau(z,\omega,E)) +$$

$$\|[\mu_s(z,E)]\| \|W(z,\omega,\omega',E)\| \exp(-\tau(z,\omega,E)), \quad (3.2)$$

where $W(z,\omega,\omega',E)=f(z,\omega,E)-f(z,\omega',E),\ (z,\omega,E)\in \partial G_0 \times \Omega \times I.$

Note, that the estimation (3.2) is essentially useful when absorption predominates over scattering. In particular, absence of scattering yields the coincidence of $A(z,\omega,E)$ and $mv(z,\omega,E)$. Perhaps, another relation between absorption and scattering requires another approximation.

The approximation $A(z,\omega,E)$ allows us to define the new goal function

$\Phi_A(z,E)=(h^*)^{-1}|A(z,s,E)+A(z,-s,E)|,$ and to set the problem:

Quasioptimization problem. *Determine the value* $E^{**}, E^{**}\in[E_1,E_2]$ *providing the greatest value to the goal function* $\Phi_A(z,E),$ *when the point* z *is fixed.*

It is clear that use of $\Phi_A(z,E)$ is more suitable in tomography than $\Phi(z,E),$ and the main question concerns with closeness of E^* and $E^{**}.$ For the time being, we only represent the results of one numerical experiment. Let G be the unit ball centred in the origin; $P=\{r:\ r=(r_1,r_2,0)\};$ $G_2=\{r:\ r\in R^3, |r-a|<0.2\},\ a=(0,0.2,0);\ G_1=G\setminus \bar{G}_2;$ $k(r,\omega\cdot\omega',E)=3(1+(\omega\cdot\omega')^2)/16\pi,\ z=(0,0,0);\ \mu(r,E)=0.5E^{-7/2}+0.3,\ \mu_s(r,E)=0.05$ for $r\in G_1$ and $\mu(r,E)=1.5E^{-7/2}+0.3,\ \mu_s(r,E)=0.03$ for $r\in G_2$. Note, that all parameters are expressed in scaled numbers and a choice of μ,μ_s corresponds to soft x-ray (Hubbell, Seltzer, 1995). Just as in the experiments in Section 2, the values of $\Phi(z,\alpha_i)$ and $\Phi_A(z,\alpha_i),$ $E_1=\alpha_1<\alpha_2<\ldots<\alpha_n=E_n,\ \alpha_1=0.5,\ \alpha_{i+1}=\alpha_i+0.1,\ n=20,$ have been calculated by the Monte-Carlo method with the same level of accuracy. The results seem to be successful: $E^*=1,\ E^{**}=0.997,\ \varepsilon=100\%\,|\,\Phi(z,E^*)-\Phi_A(z,E^{**})\,|\,/\,\Phi(z,E^*)=4\%$. Importance of a choice of the optimal energy level E^* is illustrated in the figure 2, where the various reconstructions obtained by the heterogeneity indicator are shown. We don't present the case $E=E^{**}$, because images obtained by $Ind^*(r,E)$ for $E=E^*$ and for $E=E^{**}$ appear to be identical to our eyes. Thus, we can recommend the quasioptimal energy level E^{**} for sounding radiation to provide almost the best reconstruction.

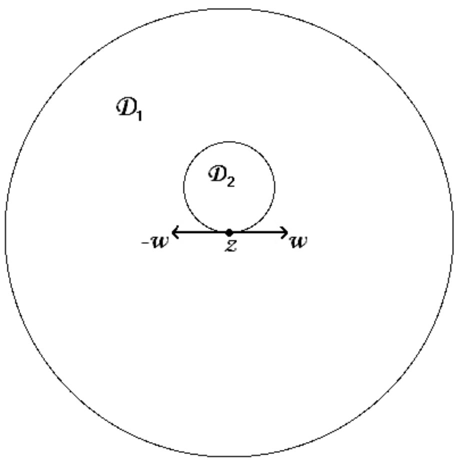

Figure 2a

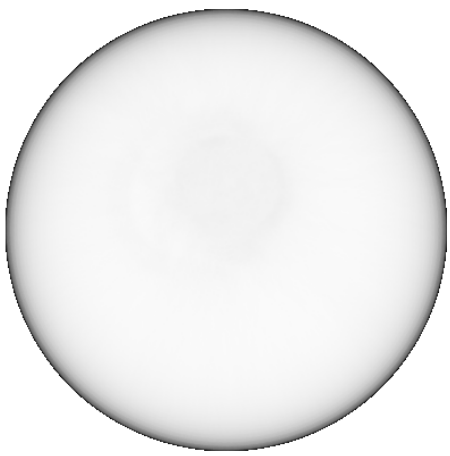

Figure 2b

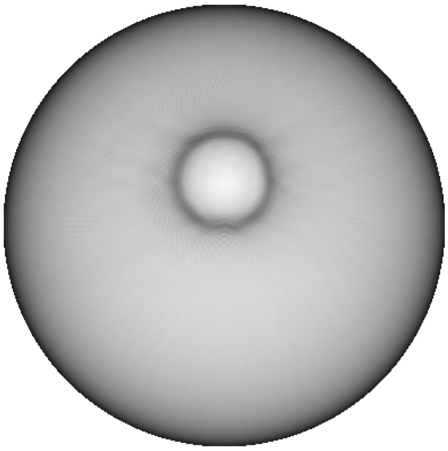

Figure 2c

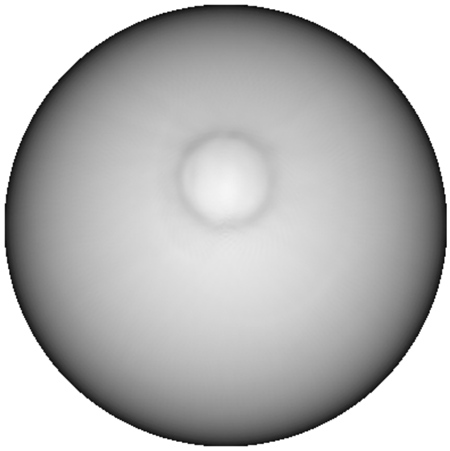

Figure 2d

Figure 2a: The original internal structure of the plane section of the medium G. The circle $\mathcal{D}_2 = \partial G_2 \cap P$ is to be reconstructed. The value $\Phi(z, E)$ has been calculated at the marked point z, (ω is a tangent vector).

Figure 2b: Reconstruction obtained in the case $E = 0.6$ cannot be discerned by eyes, because the corresponding value $\Phi(z, E)$ is too small.

Figure 2c: The best reconstruction corresponding to the optimal energy $E = 1$.

Figure 2d: Reconstruction in the case $E = 2$ seems to be an image of low quality.

In conclusion, we give some comments. Here we have considered the monochromatic case which is adequate to soft X-ray. Mainly, our further investigations are directed to research of similar problems for more general mathematical models taking into account such processes as Compton scattering and pair production. Certain steps on this way have been implemented by this time. Particularly, we established the methods of determination of the attenuation coefficient for a rather general case (see § 1.4 and § 1.7 in (Anikonov, Kovtanyuk, and Prokhorov, 2002)). Also, we studied certain mathematical aspects (Anikonov, Konovalova, 2004) and applied computer methods for the case of Compton scattering. On the whole, we try to obtain the results which can be widely applied to X-ray tomography.

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