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NATURAL BASE CONSTRUCTION FOR ABSORPTION COEFFICIENT ESTIMATION IN HETEROGENEOUS PARTICIPATING MEDIA WITH DIVERGENT BEAMS

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ABSTRACT

The domain partition for the construction of a natural base is presented in order to solve the inverse problem of absorption coefficient estimation from the available measurements (experimental noisy data) of transmitted radiation.

Within the framework of Lebesgue measure, a family of reconstruction algorithms is constructed based on Bregman distances using a q-discrepancy functional. The geometric computational aspects are briefly discussed as well as the assembly of the algebraic linear systems and the algorithms for their solution.

NOMENCLATURE

a	area
c	cone
D	Bregman distance
e	element (polygon)
E	Total number of elements (polygons)
F	ratio of measured and calculated values
h	nonlinear relation between outgoing radiation intensity (measurement) and the intensity of the radiation at the source
J	total number of sources
$m(V)$	measure of V
p	polygon
q	index of the q-discrepancy fuctional
$\underset{\rightarrow}{x}$	spatial coordinate
V	domain of analysis
η_q	q-discrepancy functional
λ	Lagrange multiplier
σ	absorption coefficient
σ_0	reference value for absorption coefficient
σ_e	absorption coefficient of element e
Φ	radiation intensity
χ	characteristic function
Ω	angular coordinate
∂V	boundary of V

INTRODUCTION

The estimation of material properties and internally distributed sources in participating media, where emission, absorption and scattering takes place, has been carried out with the solution of inverse radiative transfer problems. A few examples of the application of such inverse problems will now be given. Dobkin and Son (1991) estimated the radiative thermal conductivity of uranium hexafluoride. Li and Özisik (1992), Siewert (1993), and Holl and McCormick (1995) estimated inhomogeneous source terms. Mengüç et al. (1994) estimated the effective scattering phase function of pulverized coal particles. Silva Neto and Özisik (1995) estimated the phase function, the single scattering albedo and the optical thickness of an anisotropically scattering plane-parallel medium. McCormick (1984, 1986, 1992) has been working on very useful reviews on this subject.

Avoiding the solution of the transport equation, a diffusion approach, valid for highly scattering media, is used (Ladyzhets, 1995 , Erokhin et al., 1995).

A relatively simpler problem, but with relevant technological application in non-destructive testing in industry and diagnosis and treatment in medicine, is that in which scattering can be neglected, being absorption the dominant mode of interaction of the radiation with the medium. Computerized Tomography (CT) and Single Photon Emission Computerized Tomography (SPECT) are within this context

(Sakami and Lallemand, 1993, Lopes et al., 1997, Isakov, 1998).

Reis and Roberty (1992) built a base for the solution of the inverse problem of transmission tomography with parallel beams. In this work we present the construction of a base for divergent beams. As this represents a realistic physical situation in which divergent beams originated from sources located around the medium under investigation, are measured on the other side of it after undergoing absorption interactions, the base constructed is then called natural base. The base constructed in this manner is consistent with the data generated, becoming a convenient substrate for absorption coefficient estimation in heterogeneous participating media, or image recovery, when an incomplete set of data is available.

This reconstruction problem, in the context of Lebesgue measure, allows the introduction of special cases of Csiszer's measure (Kapur and Kesavan, 1992), here called q-discrepancy, that considers the distance from the quantity to be recovered from a reference value. Several Lebesgue type norms are then considered, from which the quadratic deviation (energy) and the entropy functional are the most commonly used.

The use of the concept of Bregman distance (Bregman, 1967) between the reconstructed quantity and a reference value yields the development of a family of algorithms that interpolates or extrapolates the algebraic reconstruction methods. As we have to deal with noisy data, the family of Bregman functions obtained using the q-discrepancy functional may be used as the norms for Tikhonov regularization.

Here we present the methodology from the computational geometry concepts up to the construction of the linear algebraic system of equations to be solved for the medium property estimation.

MATHEMATICAL FORMULATION OF THE DIRECT PROBLEM

Consider a purely absorbing heterogeneous two-dimensional medium, with no internal radiation sources subjected to externally generated divergent radiation beams.

For the steady- state situation, and no spectral dependency, the following mathematical formulation is obtained from the Boltzmann equation,

$$\underrightarrow{\Omega}.\ \Phi(\underrightarrow{x},\underrightarrow{\Omega}) + \sigma(\underrightarrow{x})\Phi(\underrightarrow{x},\underrightarrow{\Omega}) = 0 \qquad in \ \left\{V \subset \Re^2, \underrightarrow{\Omega} \quad 4\pi\right\} \tag{1a}$$

$$\Phi(\underrightarrow{x},\underrightarrow{\Omega}) = \Phi_{in}(\underrightarrow{x},\underrightarrow{\Omega}) \quad for \ \underrightarrow{\Omega}.\underrightarrow{n} < 0 \qquad in \ \underrightarrow{x} \quad \partial V_1 \tag{1b}$$

where $\Phi(\underrightarrow{x},\underrightarrow{\Omega})$ is the radiation intensity, $\sigma(\underrightarrow{x})$ is the absorption coefficient, $\underrightarrow{x}$ represents the spatial coordinates and $\underrightarrow{\Omega}$ the angular coordinates, and $\underrightarrow{n}$ is the outward normal. As can be seen in Eq. (1b), the incoming radiation is given somewhere at the boundary of the medium, ∂V_1. If the geometry, the intensity of the radiation coming from the external sources, Φ_{in}, and the absorption coefficients, $\sigma(\underrightarrow{x})$, are known, the outgoing radiation intensity can be calculated at the same or different locations at the boundary, i.e. ∂V_2 ,

$$\Phi(\underrightarrow{x},\underrightarrow{\Omega}) = \Phi_{out}(\underrightarrow{x},\underrightarrow{\Omega}) \qquad for \ \underrightarrow{\Omega}.\underrightarrow{n} > 0 \qquad in \ \underrightarrow{x} \quad \partial V_2 \tag{2}$$

In such a case problem (1) is called direct problem. If any of these quantities are unknown we have an inverse problem.

As described in the following section, we consider in this work the estimation of the absorption coefficient $\sigma(\underrightarrow{x})$.

MATHEMATICAL FORMULATION OF THE INVERSE PROBLEM

Consider now the situation shown in Fig.1. Radiation emanated by source j is attenuated by the medium, and the transmitted radiation is measured. From physical reasoning (detectors are of finite size), and for computational purposes, the radiation beams are grouped in cones c_{jn_j} with $n_j = 1,2...,\ N_j$.

From Eqs. (1-2), we write

$$\int_{c_{jn_j}} \sigma(\underrightarrow{x})d\underrightarrow{x} = h_{jn_j} \quad , j = 1,2,...,J,\ \mathrm{n_j} = 1,2,...,N_j \tag{3}$$

Where J is the total number of sources and h_{jn_j} relates nonlinearly the outgoing radiation intensity measured at ∂V_2, Φ_{meas}, to the incoming radiation intensity at ∂V_1, Φ_{in}, with

$$\Phi_{meas}(\underrightarrow{x},\underrightarrow{\Omega}) = \Phi_{out}(\underrightarrow{x},\underrightarrow{\Omega}) + noise \tag{4}$$

Considering the domain partition from the intersection of all cones $n_j = 1,2,...,\ N_j$, for all sources, $j = 1,2,...,\ J$, the original domain V is divided in a set of polygons, p_e, here called natural elements, whose characteristic functions are χ_e, such that $V = \bigcup_{e=1}^{E} p_e$, where E is the total number of elements. Using the natural base $\{\chi_e, \mathrm{e} = 1, 2,..., \mathrm{E}\}$ related to the polygons p_e, the unknown function $\sigma(\underrightarrow{x})$ can be represented as a Lebesgue simple function

$$\sigma(\underrightarrow{x}) = \sum_{\mathrm{e}=1}^{\mathrm{E}} \sigma_e \chi_e \tag{5}$$

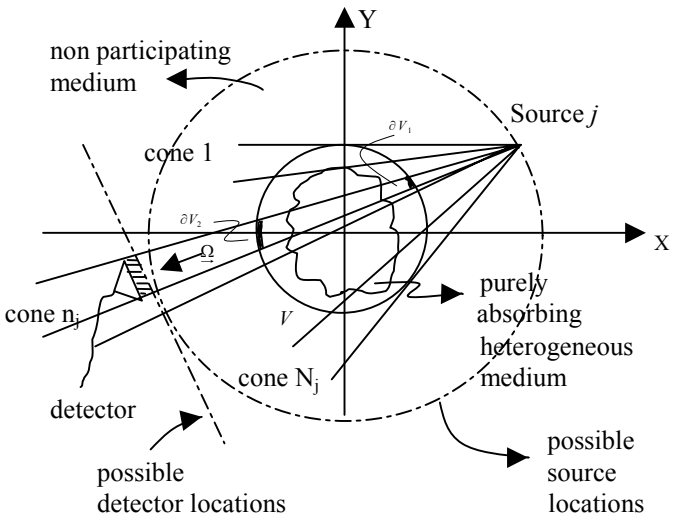

Figure 1 – Basic geometry and coordinate system.

Our inverse problem is then reduced to the estimation of the coefficients σ_e, $e = 1,2,...,E$.

Eq.(5) implies on the assumption that an average value σ_e can be used instead of taking into account the variation with the spatial coordinate $\sigma(\underset{\rightarrow}{x})$ within the element *e*.

In many applications of interest, a heterogeneous media is actually composed of a number of regions with different properties, but within each region the material properties may be considered fairly uniform. Therefore, the use of a constant value σ_e for each element *e* may be as a matter of fact a reasonably good approximation.

As in the solution of the inverse problem the interfaces of the regions that compose the domain *V* under analysis may not be known a priori, the natural base (or even any other base) may not perfectly represent these interfaces.

As an element *e* located near one of such interfaces may cover parts of two or more regions, in addition to the noise inherent to the experimental data acquisition there will be an error due to the imperfect interface representation by the computational mesh (natural base) generated.

Introducing Eq.(5) into Eq.(3) we get a discretized version of the latter

$$\sigma_{e_{c_{jn_j}}} \int_{c_{jn_j}} \chi_e d\underset{\rightarrow}{x} = \sigma_{e_{c_{jn_j}}} a_e = h_{jn_j}, \quad j = 1,2,...,J, \quad n_j = 1,2,...,N_j \tag{6}$$

where a_e is the area of the polygon (element) e.

The characteristic function, χ_e, related to a particular polygon, p_e, constructed from the intersection of specific cones, n_j^*, originated one at each source $j = 1, 2,..., J$, is obtained by

$$\chi_e(n_1^*, n_2^*,..., n_J^*) = \prod_{j=1}^{J} \chi_{c_{jn_j^*}} \tag{7}$$

where $\chi_{c_{jn_j^*}}$ is the characteristic function of the cone $c_{jn_j^*}$.

NATURAL BASE CONSTRUCTION

A computer code for the automatic mesh generation was written in the MATLAB environment. Besides the intersection of the cones, the boundary of the circular domain V as well as a regular square mesh, here called pixel mesh, are taken into account for the domain partition in the polygons $p_e, e = 1, 2,..., E$. In Fig. 2 we present such domain partition considering 8 sources with 16 cones for each source, and a 10x10 regular pixel mesh.

First the intersections of all lines within the circular domain V are calculated (observe that each cone has two limiting lines). The points where the intersections take place, are the vertices of the polygons p_e.

Now a major task has to be performed, that is, from a set of vertices $(x_1, y_1), (x_1, y_2),..., (x_L, y_L)$, where L is the total number of intersection points, we have to identify those that form a polygon. An algorithm has been developed, in which for each pixel, we sequentially investigate for all intersection points contained in the interior or at the boundary of the pixel, all possible elements that can be created around each intersection point. Obviously each intersection point has to be a vertice of all polygons created around it. The polygons constructed in this way are characterized by the indices that relate the intersection points with the indices of all lines (cones, circular domain and pixel mesh) that gave origin to them. Afterwards, in the polygons numbering step, if a polygon is created identical to the polygon created by another of its vertices, the element counter is not increased by one. In this way multiplicity is avoided in the process of polygons numbering, and at the same time the vertices that belong to each polygon are determined.

In Fig. 3 we present a sketch of the algorithm. In Fig. 4 are shown the results obtained with the algorithm for the pixel $(6,6)$ of Fig. 2, and the vertices numbers are given within parenthesis. In Table 1 are given the number of the vertices and the areas of the polygons shown in Fig. 4. In Table 2 are given the coordinates of the vertices. In Fig. 4 a symmetry line here called sector line is also shown. The base has to be constructed

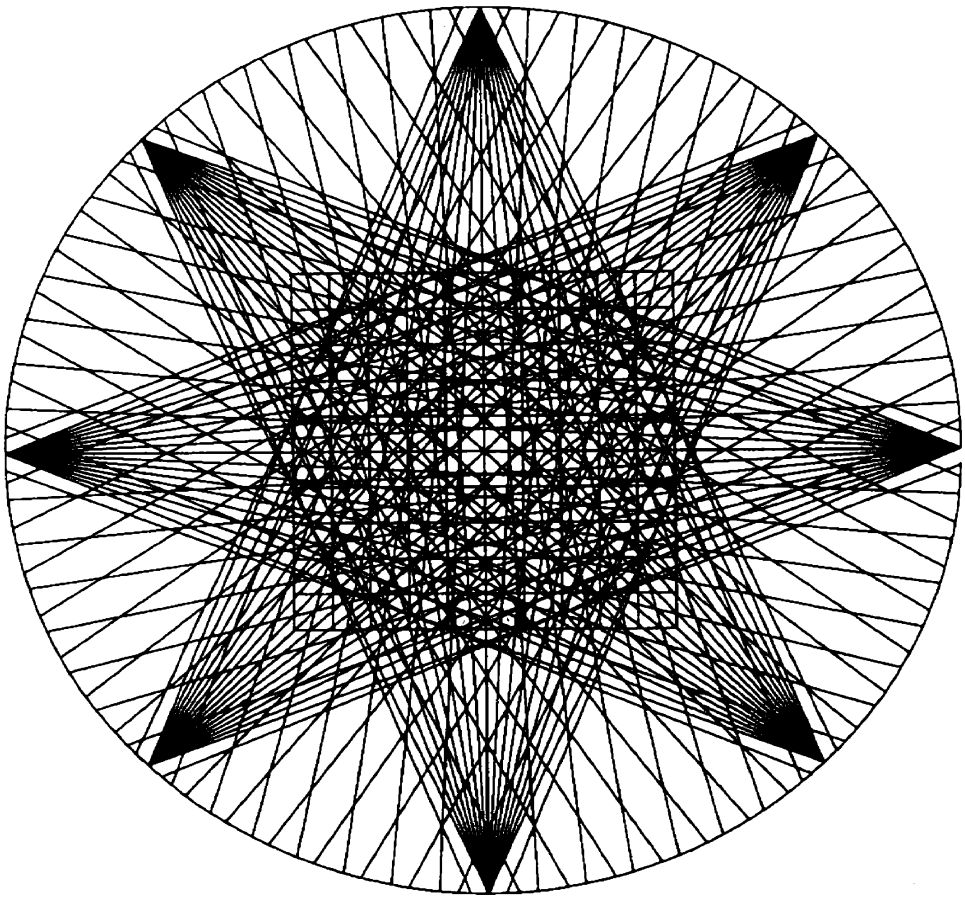

Figure 2 – Domain partition with divergent beams and a regular pixel mesh. 8 sources, 16 cones per source and a 10x10 regular pixel mesh.

only within one sector. If a full base for the whole domain is needed , it is obtained by replication.

The output of the computer code written for the construction of the natural base of simple Lebesgue functions consists on the ordered listing of all polygons, their areas and optionally their vertices.

SOLUTION OF THE INVERSE PROBLEM

Due to the large number of degrees of freedom generated by the many intersections of all N_j cones originated at the J sources, the problem at hand usually becomes underdetermined with less experimental data available, h_{jn_j}, than the number of unknowns to recover , σ_e. As this problem has more than one solution, it is solved as an optimization problem in which an objective function is satisfied according to a criterion established a priori. To construct the objective function we start with special cases of Csiszer's measure (Kapur and Kesavan, 1992) defined by the q-discrepancy

$$\eta_q(\sigma) = \frac{1}{1+q} \int_V \sigma \frac{\sigma^q - \left(\frac{1}{m(V)}\right)^q}{q} d\underline{x} \tag{8}$$

which represents the deviation of the expected value for σ from a prior $1/m(V)$, with $m(V)$ being a measure such as $m(V) = Ea_e$, and index q can be varied yielding different discrepancy functionals.

Using the Bregman distance (Bregman, 1967) between the quantity to be reconstructed, σ, and a reference value, σ_0, produced by the q-discrepancy functional

$$\begin{aligned} D_q(\sigma, \sigma_0) &= D\left[\eta_q(\sigma), \eta_q(\sigma_0)\right] \\ &= \eta_q(\sigma) - \eta_q(\sigma_0) - \left\langle \eta_q(\sigma_0), \sigma - \sigma_0 \right\rangle \end{aligned} \tag{9}$$

a family of objective functions can be constructed.

From Eqs.(8) and (9) we get

$$D_q(\sigma,\sigma_0) = \frac{1}{1+q}\int_V \left[\sigma\frac{\sigma^q - \sigma_0^q}{q} + \sigma_0^q(\sigma_0 - \sigma)\right]dx \quad (10)$$

For $q \to 0$ we obtain a negative entropy (cross entropy) functional

$$D_0(\sigma,\sigma_0) = \lim_{q\to 0} D_q(\sigma,\sigma_0) = \int_V \left[\sigma \ln\left(\frac{\sigma}{\sigma_0}\right) + \sigma_0 - \sigma\right]dx \quad (11)$$

and for $q = 1$ the usual energy functional is obtained

$$D_1(\sigma,\sigma_0) = \frac{1}{2}\int_V (\sigma - \sigma_0)^2 dx \quad (12)$$

To recover σ we want to find a minimum of the Bregman distance, D_q, given by Eq. (10), produced by the q-discrepancy, given by Eq.(8), with the original problem given by Eq.(3), as a constraint.

Using the Lagrangian based on the Bregman distance,

$$L_q(\sigma,\sigma_0,\lambda) = \frac{1}{1+q}\int_V \left[\sigma\frac{\sigma^q - \sigma_0^q}{q} + \sigma_0^q(\sigma_0 - \sigma)\right]dx + \sum_{j=1}^{J}\sum_{n_j=1}^{N_j} \lambda_{jn_j}\left[h_{jn_j} - \int_{c_{jn_j}} \sigma(\underline{x})dx\right] \quad (13)$$

where λ_{jn_j} is the Lagrange multiplier, a family of action by line or action by blocks algorithms is constructed.

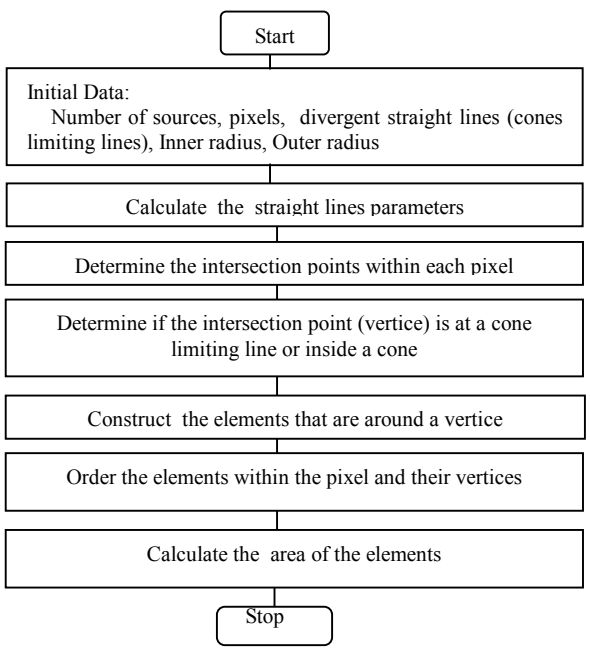

Figure 3 –Sketch of the algorithm for automatic natural base mesh generator for divergent beams.

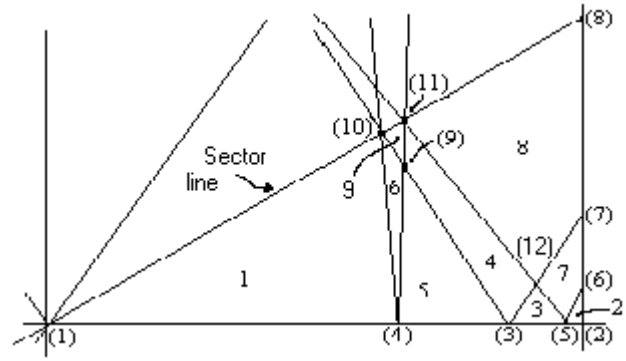

Figure 4 – Polygons and vertices in pixel (6,6).

Table 1 – Polygons and vertices numbering in pixel (6,6).

ELEMT.	NORMAL AREA	TNV[1]	ELEMENT VERTICES			
1	5.37E-02	3	(1)	(4)	(10)	
2	4.72E-04	3	(2)	(6)	(5)	
3	1.40E-03	3	(3)	(5)	(12)	
4	9.59E-03	4	(3)	(12)	(11)	(9)
5	1.65E-02	3	(3)	(9)	(4)	
6	2.83E-03	3	(4)	(9)	(10)	
7	1.53E-03	4	(5)	(6)	(7)	(12)
8	4.39E-02	4	7	8	11	12
9	3.40E-04	3	9	11	10	

[1]TNV= Total number of vertices

Table 2- Coordinates of the vertices shown in Fig.4 and listed in Table 1.

vertice	1	2	3	4	5	6	7	8	9	10	11	12
x	0	0.8	0.7	0.5	0.78	0.8	0.8	0.8	0.53	0.5	0.52	0.7
y	0	0	0	0	0	0.03	0.1	0.33	0.18	0.18	0.2	0.4

Looking for the stationary point, we make $\frac{\partial L_q(\sigma,\sigma_0,\lambda)}{\partial\sigma} = 0$. Using the discretized version of Eq.(3), given by Eq.(6), we get

$$\sigma = \sigma_0\left[1 + q\frac{\sum_{j=1}^{J}\sum_{n_j=1}^{N_j}\lambda_{jn_j}\chi_{jn_j}}{\sigma_0^q}\right]^{1/q} \quad (14)$$

Lets look at the two particular cases for $q \to 0$ (entropy) and $q = 1$ (energy).

Entropy. Taking the limit of Eq.(14) as q goes to zero,

$$\sigma = \sigma_0 \exp\left[\sum_{j=1}^{J} \sum_{n_j=1}^{N_j} \lambda_{jn_j} \chi_{jn_j} \right] \tag{15}$$

Plugging Eq. (15) into Eq. (6), where we consider each cone separately,

$$\sum_{e \in c_{jn_j}} \sigma_{e_0} \exp\left[\lambda_{jn_j}(e)\right] a_e = h_{jn_j} \tag{16}$$

Considering $\lambda_{jn_j}(e)$ constant for every element in cone c_{jn_j}, Eq. (16) can be written as

$$F_{jn_j} = \exp\left[\lambda_{jn_j}(e)\right] = \frac{h_{jn_j}}{\sum_{e \in c_{jn_j}} \sigma_{e_0} a_e} \tag{17}$$

We are now in a position to write an iterative procedure for the reconstruction of σ_e, one cone at a time :

for k=1, 2,... until convergence is achieved
for source $j = 1$ up to J
for cone $n_j = 1$ up to N_j

$$F_{jn_j}^{k+1} = \frac{h_{jn_j}}{\sum_{e \in c_{jnj}} \sigma_e^k a_e}$$

$$for \quad all \quad e \in c_{jn_j}$$

$$\sigma_e^{k+1} = \sigma_e^k F_{jn_j}^{k+1}$$

Here becomes evident that the reconstruction problem at hand relies on the measured data, on an initial guess for the unknowns and on an adequate bookkeeping of the sources, cones, elements and their areas. Therefore, the partition of the domain on a natural base as presented before becomes very convenient for computational purposes.

The algorithm above described consists on the Multiplicative Algebraic Reconstruction Technique (MART).

Energy. Imposing $q = 1$ in Eq. (14) yields

$$\sigma = \sigma_0 + \sum_{j=1}^{J} \sum_{n_j=1}^{N_j} \lambda_{jn_j} \chi_{jn_j} \tag{18}$$

Plugging Eq. (18) into Eq. (6), and considering each cone separately,

$$\sum_{e \in c_{jn_j}} \left[\sigma_{e_0} + \lambda_{jn_j}(e)\right] a_e = h_{jn_j} \tag{19}$$

Considering $\lambda_{jn_j}(e)$ constant for every element in cone c_{jn_j}, Eq. (19) can be written as

$$\lambda_{jn_j} = \frac{h_{jn_j} - \sum_{e \in c_{jn_j}} \sigma_{e_0} a_e}{\sum_{e \in c_{jn_j}} a_e} \tag{20}$$

Another iterative procedure, known as Algebraic Reconstruction Technique (ART), is then written for the reconstruction of σ_e, one cone at a time:

for $k = 1, 2,...$ until convergence is achieved
for source $j = 1$ up to J
for cone $n_j = 1$ up to N_j

$$\lambda_{jn_j} = \frac{h_{jn_j} - \sum_{e \in c_{jn_j}} \sigma_e^k a_e}{\sum_{e \in c_{jn_j}} a_e}$$

For all $e \in c_{jn_j}$

$$\sigma_e^{k+1} = \sigma_e^k + \lambda_{jn_j}$$

The importance of the natural base use that yields the straightforward computation of the polygons and their areas becomes evident once more.

TIKHONOV FUNCTIONAL

The Radon-Nikodyn theorem ensures the existence of the reconstruction solution as presented in the previous sections (Munroe, 1953).

As noise is present in all real applications, instead of minimizing the Lagrangian based on the Bregman distance, Eq.(13), we may use the Tikhonov functional with the regularization terms given by the Bregman distances obtained using the q-discrepancy functional,

$$T_q(\sigma, \alpha) = \left\| \sum_{e \in c_{jn_j}} \sigma_e a_e - h_{jn_j} \right\|_{\sum_{j=1}^{J} \sum_{n_j=1}^{N_j}}^2 + \alpha D_q(\sigma, \sigma_0) \tag{21}$$

where α is the regularization parameter. The second term on the right hand side of Eq. (21) gives more stability to the reconstruction problem at the expense of less accuracy, as the functional that is actually minimized is different from the original one. To find the adequate value for the regularization parameter becomes, then, an important part of the problem.

The determination of an optimal value for this parameter is possible, and has already been done for the squared residues norm (Kress, 1989), but is computationally involved. Therefore, this is usually done through comprehensive numerical experimentation.

For the solution of the inverse problem with the minimization of Tikhonov's functional minor changes on the algorithm presented in the previous section are necessary, and we refer to the algorithms proposed by Elfving (1989).

CONCLUSIONS AND FUTURE WORK

With a base that is not constructed in a natural way, the reconstruction algorithm has to deal with two kind of imperfections, one that is physical (unavoidable) due to the existence of measurement errors, and a mathematical one that comes from the partition of the domain.

The procedure here proposed for the natural base construction is straightforward and adequate in regard to computational performance (memory allocation and CPU time). Results have already been presented for the reconstruction problem using parallel beams (Reis and Roberty, 1992).

Next step of our research is the implementation of the algorithms for the solution of the inverse problem of absorption coefficient estimation using divergent beams and considering the Lagrangian based on the Bregman distance with the q-discrepancy functional.

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