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Method for estimating closed-form solutions of the light diffusion equation for turbid media of any boundary shape

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Abstract

This paper reports a method of estimating an approximate closed-form solution to the light diffusion equation for any type of geometry involving Dirichlet's boundary condition with known source location. It is based on estimating the optimum locations of multiple imaginary point sources to cancel the fluence at the extrapolated boundary by constrained optimization using a genetic algorithm. The mathematical derivation of the problem to approach the optimum solution for the direct-current type of diffuse optical systems is described in detail. Our method is first applied to slab geometry and compared with a truncated series solution. After that, it is applied to hemispherical geometry and compared with Monte Carlo simulation results. The method provides a fast and sufficiently accurate fluence distribution for optical reconstruction.

1. INTRODUCTION

Diffuse optical tomography (DOT) is a medical imaging modality that aims to reconstruct the internal optical properties of biological tissues [1]. Although it has an ill-posed inversion problem and lower resolution (~5 mm) [2,3], it has received much interest from both the bio-optics research and medical communities. This is due mainly to the advantages of DOT in assisting in the diagnosis of deeply seated abnormalities related to vasculature diseases [1,4-8]. The first advantage is the correlation between optical absorption of tissue in the near-infrared (NIR) region (700–900 nm) and tissue blood content [1,3,9]. In the NIR window, water is almost transparent, and the average optical scattering coefficient of tissue is lower, which allow deeper light penetration. Because oxygenated and deoxygenated hemoglobin are the main absorbing constituents of tissue, DOT maps blood vasculature and blood oxygen saturation [9]. Identifying vascular abnormalities allows detection of vessel rupture, such as brain aneurysm and trauma, and abnormally high vascular density in epileptic foci and in tumors. Malignant tumors pose high demand for nutrition and oxygen due to their increased proliferation compared to most normal tissue. This triggers hormonal and neural system signals to increase tumor angiogenesis [8]. Furthermore, chemotherapy responses can be assessed repeatedly by monitoring how the tumor vasculature is altered

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throughout the course of treatment [10]. The second advantage of DOT is its portability, relative low cost, and easy instrumentation compared to some other imaging modalities, such as magnetic resonance imaging (MRI).

Since the inversion problem is ill-posed, accurately reconstructing the absorption coefficient of every voxel of a heterogeneous medium is not possible, because the number of unknowns is usually more than double the number of measurements. The perturbation method is usually used, where it is assumed that the scattered fluence generated by the heterogeneity is much smaller than the incident fluence. The information about the background absorption and scattering coefficients has to be known, and is usually estimated by fitting measurements acquired at a normal site. Furthermore, the measurements at the suspicious area are typically subtracted from the measurements acquired at the normal site and normalized to the background to obtain the perturbation that results from the suspicious area. Additionally, the light fluence distribution of every voxel within the tissue for every source location with respect to the geometry has to be known for reconstruction [2-5]. This is either computed by analytical closed-form formulas derived in the literature [3,11-15], estimated using finite-element methods [4,16-19], or statistically inferred using Monte Carlo modeling of light (MCML) transport in turbid media [3,20,21]. The first method is fairly quick using MATLAB. The second method is also acceptable speed-wise if COMSOL Multiphysics software is used. However, the third method is time consuming. For example, with a personal computer (PC) of a Core i5-460M 2.53 GHz CPU and 4GB DDR2 RAM on a 32-bit Windows 7 operating system, the first and second methods can generate the forward weight matrix of a semi-infinite medium using a probe of 10 sources and 14 detectors within seconds to minutes depending on the mesh size. The third one usually requires more than 12 h to generate the needed fluence distribution with adequate signal-to-noise ratio (SNR) for 10 source locations using CPU-based MCML code. Note that Alerstam *et al.* developed a GPU-based MCML code that is 600× faster than CPU-based code on Core i7 PC, which opens up the possibility of using MC simulations for solving inverse problems in biomedical optics in the future [22].

Although it is preferable to use the quick and simple closed-form solutions, closed-form solutions of the light diffusion equation are derived in the literature for only a few Dirichlet's boundary condition (BC) geometries, including infinite, semi-infinite [3,11], concave and convex cylindrical geometries [12,13], and slab geometry [14,15]. Thus, for the BC in breast imaging, which has an almost hemispherical boundary in many cases, researchers either use the finite-element method to estimate the light fluence distribution, or they compress the breast with the DOT probe and use the semi-infinite analytical solution. Using the finite-element method is not time-consuming but rather complex to implement, while the second method of compressing the tissue and deforming the lesions underneath, especially shallow lesions close to the surface, may also affect the accuracy of the estimated optical properties of the lesions.

In this paper, we propose a novel numerical method for quick estimation of an approximate closed-form solution of the light diffusion equation for any type of BC geometry with known source locations. We use the genetic algorithm (GA) package in MATLAB 2012a to find the optimum locations of multiple imaginary sources outside the extrapolated boundary

to cancel the light fluence at the extrapolated boundary of the turbid medium under study. In this context, the underlying mathematical theory is explained in detail, and then applied to slab geometry and to hemispherical geometry for one arbitrarily selected source location. The number of imaginary sources is increased from one to five to assess how adding more imaginary sources affects the accuracy of the generated three-dimensional (3D) fluence distribution inside the volume of interest, as compared with the fluence distribution generated using Monte Carlo simulation for the same geometry and source location. Note that, in this paper, DOT systems of the direct-current (DC) type are considered, where the phase of the fluence of each source contribution at the extrapolated boundary is considered zero. That said, the theory can also be extended to frequency-domain systems by considering the average phase of all source contributions in the optimization.

2. MATHEMATICAL BACKGROUND

For DC DOT systems, measurements are acquired from the detectors of the DC source after they have been turned on for a while. This means that a steady state can be assumed, and, therefore, time-independent fluence is used throughout this paper. For an infinite unbounded turbid medium, the time-independent solution to the light diffusion equation [3] is given as

$$\psi(\vec{r}) = \frac{A}{4\pi Dr} e^{-\mu_{\text{eff}} r}. \quad (1)$$

Here, ψ is the fluence rate (W/cm^2), $\vec{r}$ is the source-to-observation displacement vector and r its amplitude (centimeters), A is the proportionality constant (watts), μ_{eff} is the effective attenuation coefficient (cm^{-1}), and D is the diffusion coefficient (centimeters). For a bounded scattering medium, if we assume that the real source is a pencil beam incident normal to the bounding surface S toward the scattering medium, we can approximate our real anisotropic source by another isotropic one located inside the scattering medium with one transport mean-free-path distance l'_t beneath the real boundary normal to its surface, as shown in Fig. 1, [3].

This distance is defined as

$$l'_t = \frac{1}{\mu_a + \mu'_s}, \quad (2)$$

where μ_a is the absorption coefficient of the scattering medium, and the reduced scattering coefficient, μ'_s , is defined as

$$\mu'_s = (1 - g) \mu_s. \quad (3)$$

In Eq. (3), μ_s is the scattering coefficient, and g is the scattering anisotropy. Note that the diffusion approximation is assumed in context (i.e., $\mu'_s \gg \mu_a$). The general case of a

refractive-index-mismatched BC falls into the category of homogeneous Cauchy BCs. In this case, to account for the boundary effects on the fluence distribution inside the turbid medium, a linear combination of the fluence rate and its normal derivative to the real boundary has to equal zero:

$$\psi(\vec{r}) - 2C_R D \nabla \psi(\vec{r}) \cdot \vec{n} = 0. \quad (4)$$

Here, $\vec{n}$ is the bounding surface normal pointing toward the scattering medium, and C_R is defined as

$$C_R = \frac{1 + R_{\text{eff}}}{1 - R_{\text{eff}}}, \quad (5)$$

where R_{eff} is the effective reflection coefficient, and represents the probability of a photon being reflected back into the scattering medium when it is incident on the ambient medium regardless of the angle of incidence. For a refractive-index-matched boundary, R_{eff} is zero, and consequently, C_R is unity [3].

Without going into unnecessary detail, if we use the Taylor expansion to the first order with Eq. (4), it can be shown that there exists an extrapolated boundary surface (S_{ext}) constructed point-by-point by projecting each point in the real bounding surface (S) to a corresponding point at distance normal to the real boundary tangent plane toward the ambient medium, as shown in Fig. 1. For the closed-form solution to satisfy the BC, the fluence rate must vanish at the extrapolated boundary. For this to happen, provided that we have a real (positive) isotropic source inside, there must be one or multiple imaginary (negative) isotropic sources in the ambient medium outside the extrapolated surface representing the reduction in fluence rate inside the scattering medium due to photons going toward the boundary and not coming back. Ideally, the number of needed imaginary sources for a general boundary surface is infinity. However, if the surface is regular and deterministic in shape, the number of balancing sources can be finite for an approximate closed-form solution.

3. OPTIMIZATION PROBLEM

For semi-infinite geometries of a single boundary plane, one negative imaginary source placed symmetrically to the original isotropic source around the extrapolated plane will be sufficient to force the fluence around the extrapolated surface to be exactly zero. However, for curved and/or complex geometries, using one negative source is certainly not sufficient to make the fluence zero at every point on the extrapolated surface no matter where the imaginary source is placed with respect to the real one. The novel idea here is to use a constrained optimization technique to find the optimum locations of multiple imaginary sources, outside the extrapolated boundary, that minimize the sum of squared fluence on the extrapolated surface. The resulting linear combination of space-shifted versions of Eq. (1) accounting for the fluence contribution of the real source and the imaginary sources at the

optimized locations will result in an approximately closed-form solution to the diffusion equation for that particular boundary for the given real source location.

A. Slab Geometry

To formulate the problem, we start by defining the boundary surface S (see Fig. 1), which consists of two planes sandwiching the scattering medium of a d_{th} thick slab. Next, we define the extrapolated surface, which consists of two planes shifted away from the scattering medium surface by $2C_R D$ distance. On the surface, we choose a finite number of points for which the optimization algorithm shall try to minimize the sum of fluence contributions from the real and imaginary sources by adjusting the locations of the imaginary sources only. Of course, because it is impossible to optimize by taking into account every point on the extrapolated surface, we have to choose a finite number of points to be taken into account while performing optimization. The minimum distance between these points, such that the resulting solution is sufficiently valid for all points on the extrapolated surface, is problem dependent, but it should be dependent on l'_t and how fast the shape is curving.

If a pencil beam is incident on the medium surface at the origin $(0, 0, 0)$ and if diffusion approximation is assumed, this beam can be approximated by a real isotropic source at $(0, 0, -l'_t)$. The contribution of the real isotropic source on the fluence at the extrapolated boundary can be calculated as follows for every x and y :

$$\psi_{s,ext}(x, y) = \frac{e^{-\mu_{eff}|\vec{r}_{s,ext}(x, y, 2C_R D)|}}{4\pi D|\vec{r}_{s,ext}(x, y, 2C_R D)|} + \frac{e^{-\mu_{eff}|\vec{r}_{s,ext}(x, y, -d_{th} - 2C_R D)|}}{4\pi D|\vec{r}_{s,ext}(x, y, -d_{th} - 2C_R D)|}. \quad (6)$$

In Eq. (6), $\vec{r}_{s,ext}(x, y, z_b)$ is the spatial displacement vector from $(0, 0, -l'_t)$ to the point (x, y, z_b) at the extrapolated surface, and it can be calculated as follows:

$$|\vec{r}_{s,ext}(x, y, z_b)| = \left[x^2 + y^2 + (-l'_t - z_b)^2 \right]^{1/2}, \quad (7)$$

where $z_b = 2C_R D$ for the upper extrapolated plane, and $z_b = -d_{th} - 2C_R D$ for the lower extrapolated plane. Similarly, for an imaginary source at an optimum point (x_{is}, y_{is}, z_{is}) , we can write its normalized infinite-geometry solution contribution for every x and y on the two extrapolated planes as

$$\psi_{is,ext}(x, y) = -\frac{e^{-\mu_{eff}|\vec{r}_{is,ext}(x, y, 2C_R D)|}}{4\pi D|\vec{r}_{is,ext}(x, y, 2C_R D)|} - \frac{e^{-\mu_{eff}|\vec{r}_{is,ext}(x, y, -d_{th} - 2C_R D)|}}{4\pi D|\vec{r}_{is,ext}(x, y, -d_{th} - 2C_R D)|}, \quad (8)$$

where $\vec{r}_{is,ext}(x, y, z_b)$ is the spatial displacement vector from (x_{is}, y_{is}, z_{is}) to the point at the extrapolated surface (x, y, z_b) . This, in turn, can be calculated as follows:

$$|\vec{r}_{is,ext}(x, y, z_b)| = \left[(x_{is} - x)^2 + (y_{is} - y)^2 + (z_{is} - z_b)^2 \right]^{1/2}. \quad (9)$$

Let us now consider $\Psi_{s,ext}$ and $\Psi_{is,ext}$, with the vectors having values of $\psi_{s,ext}$ and $\psi_{is,ext}$, respectively, for every discretized x and y value at the extrapolated boundary. For one imaginary source solution, the idea is to find x_{is} , y_{is} , and z_{is} to minimize the following squared l_2 -norm:

$$J \left(X_{is} = \begin{bmatrix} x_{is} \\ y_{is} \\ z_{is} \end{bmatrix} \right) = \left\| \Psi_{s,ext} + \Psi_{is,ext}(X_{is}) \right\|^2. \quad (10)$$

In Eq. (10), J is the nonlinear cost function of the parameters to be optimized [23,24] and represents the summation of squares of the fluence (SSF) at every point on the extrapolated boundary surface. Similarly, for n number of imaginary sources, the function to be minimized would be

$$J \left(X_{is} = \begin{bmatrix} X_{is1} \\ X_{is2} \\ \vdots \\ X_{isn} \end{bmatrix} \right) = \left\| \Psi_{s,ext} + \Psi_{is,ext}(X_{is1}, X_{is2}, \dots, X_{isn}) \right\|^2, \quad (11)$$

where

$$\Psi_{is,ext}(X_{is}) = \Psi_{is1,ext}(X_{is1}) + \Psi_{is2,ext}(X_{is2}) + \dots + \Psi_{isn,ext}(X_{isn}). \quad (12)$$

B. Hemispherical Geometry

For hemispherical geometries (e.g., good approximation for breast surface geometry), the boundary surface is defined by its radius, R_{hsp} , where its extrapolated boundary is another hemispherical surface with a radius of $R_{ext} = R_{hsp} + 2C_R D$ (see Fig. 2). In spherical coordinates, the pencil beam, incident normal to the tangent of the hemispherical boundary surface at $(R_{hsp}, \theta_s, \phi_s)$, is approximated by another real isotropic source beneath the real surface at (R_s, θ_s, ϕ_s) , where $R_s = R_{hsp} - l'_t$. Then, for every point on the extrapolated surface (R_{ext}, θ, ϕ) , we can define the fluence contribution of the real source using its normalized infinite-geometry solution form as follows:

$$\psi_{s,\text{ext}}(\theta, \varphi) = \frac{e^{-\mu_{\text{eff}}|\vec{r}_{s,\text{ext}}(\theta, \varphi)|}}{4\pi D|\vec{r}_{s,\text{ext}}(\theta, \varphi)|}. \quad (13)$$

In Eq. (13), $\vec{r}_{s,\text{ext}}(\theta, \varphi)$ is the spatial displacement vector from $(R_s, \theta_s, \varphi_s)$ to the point at the extrapolated surface $(R_{\text{ext}}, \theta, \varphi)$, and it can be calculated as follows:

$$|\vec{r}_{s,\text{ext}}(\theta, \varphi)| = \left[(R_{\text{ext}} \sin \theta \cos \varphi - R_s \sin \theta_s \cos \varphi_s)^2 + (R_{\text{ext}} \sin \theta \sin \varphi - R_s \sin \theta_s \sin \varphi_s)^2 + (R_{\text{ext}} \cos \theta - R_s \cos \theta_s)^2 \right]^{1/2}. \quad (14)$$

Similarly, for an imaginary source at an optimum point $(R_{is}, \theta_{is}, \varphi_{is})$, we can write its normalized infinite-geometry solution contribution for every point $(R_{\text{ext}}, \theta, \varphi)$ on the extrapolated boundary surface as

$$\psi_{is,\text{ext}}(\theta, \varphi, R_{is}, \theta_{is}, \varphi_{is}) = -\frac{e^{-\mu_{\text{eff}}|\vec{r}_{is,\text{ext}}(\theta, \varphi, R_{is}, \theta_{is}, \varphi_{is})|}}{4\pi D|\vec{r}_{is,\text{ext}}(\theta, \varphi, R_{is}, \theta_{is}, \varphi_{is})|}, \quad (15)$$

where $\vec{r}_{is,\text{ext}}$ is the spatial displacement vector from $(R_{is}, \theta_{is}, \varphi_{is})$ to the point at the extrapolated surface $(R_{\text{ext}}, \theta, \varphi)$. This in turn can be calculated as follows:

$$|\vec{r}_{is,\text{ext}}(\theta, \varphi, R_{is}, \theta_{is}, \varphi_{is})| = \left[(R_{\text{ext}} \sin \theta \cos \varphi - R_{is} \sin \theta_{is} \cos \varphi_{is})^2 + (R_{\text{ext}} \sin \theta \sin \varphi - R_{is} \sin \theta_{is} \sin \varphi_{is})^2 + (R_{\text{ext}} \cos \theta - R_{is} \cos \theta_{is})^2 \right]^{1/2}. \quad (16)$$

Let us now consider $\Psi_{s,\text{ext}}$ and $\Psi_{is,\text{ext}}$, with the vectors having values of $\Psi_{s,\text{ext}}$ and $\Psi_{is,\text{ext}}$, respectively, for every discretized θ and φ value at the extrapolated boundary. For one imaginary point source, the idea is to find R_{is} , θ_{is} , and φ_{is} to minimize the following squared l_2 -norm:

$$J \left(X_{is} = \begin{bmatrix} R_{is} \\ \theta_{is} \\ \varphi_{is} \end{bmatrix} \right) = \|\Psi_{s,\text{ext}} + \Psi_{is,\text{ext}}(X_{is})\|^2. \quad (17)$$

In Eq. (17), J is the nonlinear cost function of the parameters to be optimized [23,24], and represents the SSF at every point on the extrapolated boundary surface. Similarly, for n number of imaginary sources, the function to be minimized would be

$$J \left(X_{is} = \begin{bmatrix} X_{is1} \\ X_{is2} \\ \vdots \\ X_{isn} \end{bmatrix} \right) = \left\| \Psi_{s,\text{ext}} + \Psi_{is,\text{ext}}(X_{is1}, X_{is2}, \dots, X_{isn}) \right\|^2, \quad (18)$$

where

$$\Psi_{is,\text{ext}}(X_{is}) = \Psi_{is1,\text{ext}}(X_{is1}) + \Psi_{is2,\text{ext}}(X_{is2}) + \dots + \Psi_{isn,\text{ext}}(X_{isn}). \quad (19)$$

C. Optimization Algorithm

It is possible to use a gradient descent minimization technique in which the gradient of the cost function is calculated and used in an iterative approach to progress toward its minimum value. The gradient in that case can be computed as follows:

$$\nabla J(X_{is}) = 2[\nabla \Psi_{is,\text{ext}}(X_{is})]^T \begin{bmatrix} \Psi_{s,\text{ext}} \\ + \Psi_{is,\text{ext}}(X_{is}) \end{bmatrix}, \quad (20)$$

where T is the matrix transpose operation, and $\nabla \Psi_{is,\text{ext}}$ is the Jacobian matrix of the imaginary source contribution to the fluence at the extrapolated boundary. It can be computed as

$$\nabla \Psi_{is,\text{ext}}(X_{is}) = \nabla \Psi_{is1,\text{ext}}(X_{is1}) + \nabla \Psi_{is2,\text{ext}}(X_{is2}) + \dots + \nabla \Psi_{isn,\text{ext}}(X_{isn}). \quad (21)$$

In Eq. (21), $\nabla \Psi_{isn,\text{ext}}(X_{isn})$ is the Jacobian matrix of the fluence contribution vector of the imaginary source n . However, the gradient descent method lacks the ability to constrain the imaginary source positions from falling inside the scattering medium on top of the real source (i.e., undesired global minimum for such a general optimization problem), and not to reach infinity away from the extrapolated boundary (i.e., undesired local minima for such optimization problems). We tried gradient descent even with certain routines that check if the solution falls inside the medium. If not, it reinitializes its location, but this makes the algorithm slower, and the results are not reproducible for a fixed number of iterations. Hence, we implemented a constrained optimization technique using the GA toolbox in MATLAB R2012a.

The GA is an algorithm inspired from biological evolution that well suits problems that require searching through a huge number of possibilities for solutions. The GA algorithm starts with a randomly generated population of chromosomes (i.e., candidate solutions vectors; different X_{is} in our case) within the constrained range specified. Next, it calculates the fitness $f(X_{is}) = J(X_{is})$ of each chromosome X_{is} . After that, it applies “natural selection”

together with genetics-inspired operators (we chose two operators in our code: mutation, and crossover) to create a new population of offspring (new children solutions for X_{is}). Next, it replaces the current population with the new population and repeats the previous steps (with the exception of the first step, of course) [25]. Each new population is called a generation, and the algorithm repeats for N number of generations (see Table 1). Note that the selection operator chooses those chromosomes in the population that will be allowed to reproduce, and, on average, the fitter chromosomes produce more offspring than the less fit ones.

It should be noted that we tried $f(X_{is}) = J(X_{is})$, $f(X_{is}) = [J(X_{is})]^2$, $f(X_{is}) = [J(X_{is})]^3$, $f(X_{is}) = [J(X_{is})]^4$, and $f(X_{is}) = [J(X_{is})]^5$ as the fitness function for the GA algorithm. Note that we achieved the best results with $f(X_{is}) = [J(X_{is})]^5$, as reported here in the following section.

4. SIMULATION RESULTS AND COMPARISON

In the following, we assumed a homogeneous scattering medium of $\mu_a = 0.05 \text{ cm}^{-1}$, $\mu'_s = 6 \text{ cm}^{-1}$, and a refractive index of 1.33. All the boundaries are assumed to be of matched refractive index (i.e., $C_R = 1$), while the ambient medium is assumed to be nonscattering (i.e., $\mu'_s = 0 \text{ cm}^{-1}$).

First, in Table 2 we compare the truncated-series solution of the slab geometry for different slab thicknesses with the GA optimized solution for two imaginary sources in terms of the sum of squared fluence at the extrapolated boundary to the power of 5 (i.e., $[J(X_{is})]^5$). In this GA optimization, the x and y axes are discretized nonlinearly from -12 to 12 cm with 19-by-19 pixels.

Second, a hemispherical boundary surface is assumed to be interfacing with the ambient medium, while the second circular face is considered to have the same tissue properties. Hence, the only boundary considered here is the hemispherical boundary, where the radius of the hemisphere R_{hsp} is set to 3 cm , and the origin is set to the sphere center. The C++ code for MCML [20] is used as the standard for comparison, where the BCs are adjusted for our specifications. The number of photons used in the simulation is 50 million, to achieve adequate SNR for the fluence distribution inside the hemisphere.

For the GA optimization purpose, the hemispherical surface was discretized from $\theta = 0$ to $\pi/2$ rad in 15 steps, and from $\phi = 0$ to 2π rad in another 15 steps. Our pencil beam source was arbitrarily placed at $R = R_{\text{hsp}}$, $\theta = \pi/6$ rad, and $\phi = \pi/3$ rad, and it has an infinite geometry solution corresponding to one isotropic source with the same angles at

$$R_s = R_{\text{hsp}} - l'_t$$

If we apply the semi-infinite plane boundary solution, such that we place one imaginary source at $R_{is} = R_{\text{hsp}} + l'_t + 4D$, and the same source angles [i.e., in spherical coordinates with angles in degrees, $X_{is} = (3.39 \text{ cm}, 30^\circ, 60^\circ)$], the resulting fitness value $\bar{f} = 2.79 \times 10^{-08}$ at the extrapolated boundary. However, when using the GA algorithm to find the optimum location of one imaginary source results in $X_{is} = (3.23 \text{ cm}, 29.9^\circ, 60.8^\circ)$, the resulting fitness value $\bar{f} = 4.15 \times 10^{-13}$, which is at least 4 orders better than what we got from the semi-

infinite solution. Figure 3 shows comparisons among the semi-infinite planar boundary solution, the GA solution for this scenario, and the MCML solution.

If two imaginary sources are used, the resulting optimum locations using the same method are $X_{js1} = (3.39 \text{ cm}, 30.0^\circ, 59.8^\circ)$ and $X_{js2} = (4.82 \text{ cm}, 30.0^\circ, 61.4^\circ)$, while the fitness value $\hat{J} = 2.4632 \times 10^{-22}$. Figure 4 shows comparisons among the semi-infinite solution, the GA solution with two imaginary sources, and the Monte Carlo solution.

It is worth noting that increasing the number of imaginary sources will increase the average computational requirements, since the fitness calculation requires three more variables for every additional source. While this does not necessarily mean that the average resulting accuracy in terms of the fitness value is better, it depends on the geometry and the number of imaginary sources whether it is odd or even. Table 3 shows comparisons among different numbers of imaginary sources tried for the hemispherical boundary problem in terms of the fitness function value and the time latency obtained by using MATLAB on a PC of Core i5–460M 2.53 GHz CPU and 4GB DDR2 RAM on a 32-bit Windows 7 operating system.

Figures 5 and 6 show comparisons among the semi-infinite solution, the GA solutions for three and five imaginary sources, respectively, and the MCML solution.

5. DISCUSSION

Since we define the optimization goal to minimize the fifth power of the summation of squared fluence at every discretized point on the extrapolated boundary surface, this usually performs well to reduce the error in the fluence distribution in areas of high fluence, since areas of lower fluence result in smaller contributions to that summation, particularly after taking the power operator. This makes the inversion weight matrix more accurately distributed at areas of larger weight, and is acceptable for diffuse optical tomography, since areas of low weights do not contribute much in the reconstruction. Our GA method will ensure better accuracy of fluence distribution in areas of significant fluence strength for constructing the inversion weight matrix.

Note that, if we compare Figs. 3–6, we can see that the distribution of optical fluence at different y intercepts are getting closer to the MCML solution. However, in Table 3, we can see that, as we increase the number of imaginary sources, the value of the fitness gets worse on average, and the computation time also gets worse; this might be the case for this particular problem. Nonetheless, it is expected that the optimum number of imaginary sources needed to generate a sufficiently accurate solution would vary depending on the complexity of the boundary shape, the extrapolated boundary mesh size and resolution, and GAOPTIMSET parameters. Obviously, mathematically describable shapes (sphere, cylinder, parabola, etc.) will require a lower number of imaginary sources than other irregular shapes.

6. CONCLUSIONS

We report what is, to the best of our knowledge, a unique computation method that helps in estimating a closed-form solution of the light diffusion equation for any type of boundary geometry with sufficient accuracy for constructing the inversion weight matrix of diffuse

optical tomography. The mathematical basis was derived for DC types of light sources, but it can be easily extended to modulated light sources by considering the phases of the sources in the optimization. The method was applied to the hemispherical geometry suitable for breast imaging. The theory and computation procedure are general, and can also be applied to different geometries, such as transvaginal probes, which have a concave cylindrical boundary geometry. Further efforts will be devoted to implementing this method in breast imaging without any soft or hard compression of the tissue.

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Fig. 1.

Pencil beam incident on an infinite d_{th} thick slab of scattering medium. The figure shows a projection of the slab on the x - z plane at $y = 0$. It also shows the infinite geometry approximation of the beam as an isotropic source 1 mean-free-path distance beneath the surface of the medium straight ahead of the beam propagation.

Fig. 2.

Pencil beam incident on a hemispherical scattering medium that is assumed to be bound only on the spherical surface with a nonscattering medium (breast-like geometry). The figure shows a projection of the hemisphere on the x - z plane at $y = 0$.

Fig. 3.
 z - x 2D fluence distribution inside the hemisphere at different y intercepts from the semi-infinite solution (top row), the GA optimized solution with one imaginary source (middle row), and the MCML solution (bottom row).

Fig. 4.
 z - x 2D fluence distribution inside the hemisphere at different y intercepts from the semi-infinite solution (top row), the GA optimized solution with two imaginary sources (middle row), and the MCML solution (bottom row).

Fig. 5. z - x 2D fluence distribution inside the hemisphere at different y intercepts from the semi-infinite solution (top row), the GD estimator solution with three imaginary sources (middle row), and the MCML solution (bottom row).

Fig. 6.
 z - x 2D fluence distribution inside the hemisphere at different y intercepts from the semi-infinite solution (top row), the GD estimator solution with five imaginary sources (middle row), and the MCML solution (bottom row).

Table 1
GA Optimization Parameters We Chose for Faster Convergence Results

GAOPTIMSET Parameter Name	Value
Generations	1×10^4
Termination tolerance on fitness function value	1×10^{-30}
Termination tolerance on constraints	1×10^{-20}
Function used in selecting parents for next generation	@selectionroulette
Function used in mutating genes	@mutationadaptfeasible
Function used to do crossover	@crossoverheuristic

Table 2
Comparison of Slab Geometry between the Truncated-Series Solution (Two Imaginary Sources Approximation) and the GA-Optimized Solution Using Two Imaginary Sources

Slab Thickness (cm)		Truncated-Series Solution		GA-Optimized Solution	
		Coordinates	J^5	Coordinates	J^5
0.5	IS1	(0.00,0.00,0.39)	$6.1911 \times 10^{+03}$	(0.00,0.00,0.41)	1.6400×10^{-06}
	IS2	(0.00,0.00,-0.89)		(0.00,0.00,-1.20)	
1.0	IS1	(0.00,0.00,0.39)	8.4027×10^{-04}	(0.00,0.00,0.39)	1.7453×10^{-12}
	IS2	(0.00,0.00,-1.89)		(0.00,0.00,-2.39)	
1.2	IS1	(0.00,0.00,0.39)	1.3481×10^{-05}	(0.00,0.00,0.39)	1.7984×10^{-14}
	IS2	(0.00,0.00,-2.29)		(0.00,0.00,-2.84)	
1.5	IS1	(0.00,0.00,0.39)	6.3510×10^{-08}	(0.00,0.00,0.39)	4.4459×10^{-17}
	IS2	(0.00,0.00,-2.89)		(0.00,0.00,-3.51)	
2.0	IS1	(0.00,0.00,0.39)	2.9520×10^{-11}	(0.00,0.00,0.39)	6.5276×10^{-21}
	IS2	(0.00,0.00,-3.89)		(-0.01,-0.02,-4.6)	

Table 3
Fitness Function Value and Time Latency Versus the Number of Imaginary Sources
Optimized Using the GA Algorithm

Number of IS	J^5	<u>Time Latency (Approx.)</u>	
		Minutes	Seconds
1	4.1500×10^{-13}	0	5
2	2.4600×10^{-22}	0	30
3	7.0792×10^{-21}	1	36
4	6.6556×10^{-16}	1	49
5	4.4276×10^{-16}	2	22
6	3.3447×10^{-15}	2	22
7	6.3438×10^{-15}	2	41
8	2.3305×10^{-14}	3	52
9	9.0311×10^{-14}	4	16
10	6.9967×10^{-15}	4	41