Optical Tomography using the Boltzmann Transport Equation with a gradient descent approach

by

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to obtain the degree of Bachelor of Science at the Delft University of Technology, to be defended publicly on Tuesday August 17, 2021 at 10:00 AM.

Student number: 4617827
Project duration: April 19, 2021 – July 9, 2021
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An electronic version of this thesis is available at http://repository.tudelft.nl/.
Acknowledgements

I would like to thank dr. ir. Danny Lathouwers, for supervising and helping me during my bachelor thesis. Danny was very patient, critical and provided extremely useful feedback. He and I had a lot of meetings and valuable discussions, for which he made enough time and for which I am grateful. I would also like to thank prof. dr. ir Jan Leen Kloosterman for being part of the thesis committee. Finally, I would like to thank Mika Hoorweg, a fellow student doing his bachelor thesis with Danny, for helping me with valuable discussions about python and the theory.

E. van Lieshout
Leiden, July 2021
The goal of this project was to investigate a reconstruction method for the absorption and scatter cross sections for optical tomography. Optical tomography is an important technique to study since it uses optical photons, thus being safer than imaging methods using radiation, and it could potentially be better in imaging certain parts of the body.

The reconstruction method is based on the Boltzmann Transport Equation and makes use of gradient descent. A model to reconstruct these cross sections has been made by discretising the system, determining the gradients using the adjoint theory, speeding up the gradient descent using the stabilised Barzilai-Borwein method, creating realistic detector and transmitter placement and implementing all of this in python. We started with reconstructing simple geometries, small homogeneous systems, and extended towards more patient like systems, which are also seen in the real world, such as brain and breast tumours.

The stabilised Barzilai-Borwein gradient descent reduced computation time significantly and all simple geometries were successfully reconstructed using realistic detector and transmitter placement, after which it could be concluded that this method was able to reconstruct simple geometries. For larger and more complex realistic cases this method was, unfortunately, unable to create a valid reconstruction and when realistic detector and transmitter placement was applied, the solutions did not converge. These cases were not valid since the reconstructed cross sections were not close to the real solution. This might have been the case since the systems were simply too large and photons were unable to pass through the system. Unfortunately, it could therefore not be concluded with the obtained results whether or not this method is able to detect surface tumours in the adult brain, infant brain and the breast.

For further research different smaller systems like arthritis in finger joints and skin surface imaging can still be tried to find out whether this method is more effective in imaging smaller systems or not. Also to try and make the solutions for the realistic detector and transmitter converge in further research, different placements of the detectors and transmitters could be tried or changing their ratio.
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There are many medical imaging techniques using different aspects of physics. Some more harmful than the others. The most common techniques are SPECT, CT, X-Ray, PET, MRI and Ultrasound, which all use radiation except for the last two techniques. One lesser-known technique makes use of visible photons, which is generally safer than using radiation. This technique is called optical tomography. This technique is important to study since it is safe to use and could potentially be better in imaging certain parts of the body. In this report we will research a reconstruction method for optical tomography.

1.1. Optical Tomography
The way optical tomography works is that transmitters and detectors of near-infrared light are placed around the imaging subject. The transmitters transmit the photons into the system. These photons travel through the subject being scattered or being absorbed on their way, potentially exiting the subject and be detected by the detector. The way the outgoing photons have been scattered and absorbed after travelling through the subject gives information about the structures inside the subject. These structures, tissue, bone, et cetera in a human body, have different probabilities to scatter or absorb photons. The main advantage of optical imaging is that the optical absorption and scatter coefficients differ a lot between different structures [23]. Just like you can see red light very dispersed through your fingertips, but not through a piece of bone of comparable thickness. This is also a limitation of optical tomography. Where gamma radiation can pass through the whole body with ease, optical light does not. Optical tomography can therefore only be used for small subjects. Although the resolution might be low since optical scatter coefficients are generally high, this imaging technique is still clinically significant [2], because it can detect differences in tissue due to the variety of absorption and scatter coefficients as mentioned before. One of the main challenges, beside finding proper applications, is achieving high image quality and accuracy since it requires an effective reconstruction algorithm [7].

1.2. Goal of the Project
The goal of the project is to investigate a reconstruction method for optical tomography. The method will be based on a gradient descend approach. The aim is to reconstruct optical absorption and scatter coefficients. The physics model will be described by the Boltzmann Transport Equation. Starting from simple geometries, like a small homogeneous system, we will extend towards more patient like geometries, which are also seen in practice. At the end of the report, the method will be evaluated.

The report is outlined as follows: The report is divided into chapters, which are theory, the model and its implementation, results, discussion and finally the conclusion. The theory chapter is about the Boltzmann transport equation, absorption and scatter coefficients, discretisation, determining the gradients and applying gradient descent with optimisation. The model chapter explains the geometry of the model, how detectors and transmitters are placed, defines the objective function, explains how it all has been implemented into python and outlines all the cases we have studied. The results of the cases studied are then shown in the successive chapter with the discussion following that chapter. Our conclusions are then based on that in the conclusion chapter.
2.1. Boltzmann Equation

In this work we make use of the 2D Boltzmann Transport Equation (BTE). This equation describes the properties of transport in arbitrary media. In our case the transport of photons. The BTE is formulated as follows [5]:

\[
\Omega \cdot \nabla \phi(r, \Omega) + \Sigma^t \phi(r, \Omega) - \frac{1}{4\pi} \int_{4\pi} d\Omega' \Sigma^s(\Omega' \rightarrow \Omega)\phi(r, \Omega') = 0, \tag{2.1}
\]

where \( \Omega \) is the direction [rad] in which the photons travel, \( \phi \) is the flux of photons \([\text{m}^{-2}\text{s}^{-1}]\), which is the amount of photons passing through a unit area per second, \( r \) is the position \([\text{m}]\) in the system, \( \Sigma^t \) is the total cross section \([\text{cm}^{-1}]\) and \( \Sigma^s \) is the scatter cross section \([\text{cm}^{-1}]\). In 2.1.1 we will explain more about the cross sections. The BTE has 3 terms, the first term describes the streaming of photons through the surface, the second term describes the total loss of photons due to scattering and absorption by the system and the third term describes the photons from all directions \( \Omega' \) scattering into the direction \( \Omega \). Since \( \Sigma^t \) is assumed to be isotropic, which means independent of the angle, equation 2.1 can be rewritten as:

\[
\Omega \cdot \nabla \phi(r, \Omega) + \Sigma^t \phi(r, \Omega) - \frac{\Sigma^s}{4\pi} \int_{4\pi} d\Omega' \phi(r, \Omega') = 0. \tag{2.2}
\]

2.1.1. Absorption and Scatter coefficients

Macroscopic cross sections are the main focus on in this report. There are three cross sections [10]: Total \( \Sigma^t \), Absorption \( \Sigma^a \) and Scatter \( \Sigma^s \). Note that the total cross section is the sum of the absorption and scatter cross sections. From now on we will mainly focus on the absorption and scatter cross sections and refer to them as the absorption and scatter coefficients or just the coefficients. The coefficients describe the probability that a photon will interact per unit length travelled and be absorbed or scattered by the system in the following way:

\[
\Sigma_e^{-\Sigma^a} \Delta x \equiv \text{The probability that a photon has its first interaction in } \Delta x, \quad \tag{2.3}
\]

and thus has a mean path until first interaction:

\[
\bar{x} = \frac{1}{\Sigma}. \quad \tag{2.4}
\]

The absorption and scatter coefficients are what mainly determines the properties of the used system. They are the coefficients that drive the BTE and determine the photon flux in our system. These coefficients are interesting since the human body is made up out of multiple components all having different coefficients. This difference in the coefficients affects the flux of photons differently in the system. The coefficients can be retrieved by measurement of the outward photon flux, which is unique
2.2. Discretisation

To run the simulations in python space, direction and angles in the BTE need to discretised. The discretisation is outlined in the following subsections.

2.2.1. Discretisation of Space and Direction

The discretisation of space is done by taking an \((L_x \times L_y)\) square, which is turned into a grid of \((N_x \times N_y)\) blocks, with \(\Delta x = L_x/N_x\) and \(\Delta y = L_y/N_y\). The angles \(\Omega\) are discretised by using the discrete ordinate method. The discrete ordinate method is used to split the BTE in different partial differential equations, by discretising the angle [20]. The BTE is then solved for the set of discrete angles over \(4\pi\).

The discretisation in \(n\) directions is done as follows:

\[
\int_{4\pi} f(\Omega) d\Omega \approx \sum_{k=1}^{n} w_k f(\Omega_k). \tag{2.5}
\]

In the 2D case the total number of ordinates is [19]:

\[
n = (4 \times N \times (N + 2)/8). \tag{2.6}
\]

Their weights and directions for \(N=(2,4,6)\) are given in table 2.1. Directions in 3D are given in the table, in our report just the values for \(\mathbf{i}\) and \(\mathbf{j}\) should be taken, since we are working in a 2D space. It should be noted that only directions for the first quadrant are given, the directions are first flipped in the x-direction, then the 2 quadrants are flipped in the y-direction. This way the same directions and weights span over \(4\pi\). In the table the weights are given such that they sum up to be equal to 1, however, in this report, it has been used that they sum up to be equal to \(4\pi\) since they span \(4\pi\). A visual representation of \(S_8\) in 3D is given in Figure 2.1.

Table 2.1: In this table directions and weights are given for discrete ordinates in 3D space for the first octant. These values can also be used for 2D space, just reading values for \(\mathbf{i}\) and \(\mathbf{j}\) and taking the same weight [19].

<table>
<thead>
<tr>
<th>Approximation Order</th>
<th>(\mathbf{i})</th>
<th>(\mathbf{j})</th>
<th>(\mathbf{k})</th>
<th>Weight</th>
</tr>
</thead>
<tbody>
<tr>
<td>(S_2)</td>
<td>0.57735027</td>
<td>0.57735027</td>
<td>0.57735027</td>
<td>1</td>
</tr>
<tr>
<td>(S_4)</td>
<td>0.86889028</td>
<td>0.3500212</td>
<td>0.3500212</td>
<td>1/3</td>
</tr>
<tr>
<td></td>
<td>0.3500212</td>
<td>0.86889028</td>
<td>0.3500212</td>
<td>1/3</td>
</tr>
<tr>
<td></td>
<td>0.3500212</td>
<td>0.3500212</td>
<td>0.86889028</td>
<td>1/3</td>
</tr>
<tr>
<td>(S_6)</td>
<td>0.92618088</td>
<td>0.2666355</td>
<td>0.2666355</td>
<td>0.1761263</td>
</tr>
<tr>
<td></td>
<td>0.2666355</td>
<td>0.92618088</td>
<td>0.2666355</td>
<td>0.1761263</td>
</tr>
<tr>
<td></td>
<td>0.2666355</td>
<td>0.2666355</td>
<td>0.92618088</td>
<td>0.1761263</td>
</tr>
<tr>
<td></td>
<td>0.2666355</td>
<td>0.68150771</td>
<td>0.68150771</td>
<td>0.1572071</td>
</tr>
<tr>
<td></td>
<td>0.68150771</td>
<td>0.2666355</td>
<td>0.68150771</td>
<td>0.1572071</td>
</tr>
<tr>
<td></td>
<td>0.68150771</td>
<td>0.68150771</td>
<td>0.2666355</td>
<td>0.1572071</td>
</tr>
</tbody>
</table>
2.2. Discretisation

2.2.2. Discretisation of the Boltzmann Transport Equation

With the knowledge of the discretisation of space and direction, the BTE can be discretised. After the BTE has been multiplied with a test function $v(r, \Omega)$ and integrated over space $S$ and direction $\Omega$, it is in its weak form and yields the following discretisation [1]:

$$L \phi = (L^{(1)} + L^{(2)} + L^{(3)}) \phi,$$

with:

$$L^{(1)} \phi = \int_{4\pi} d\Omega \int_S dr v(r, \Omega) \phi(r, \Omega) \hat{n} \cdot \Omega,$$

$$L^{(2)} \phi = \int_{4\pi} d\Omega \int_S dr \Sigma_t \phi(r, \Omega) v(r, \Omega),$$

$$L^{(3)} \phi = -\int_{4\pi} d\Omega \int_S dr v(r, \Omega) \frac{\Sigma_s}{4\pi} \int_{4\pi} d\Omega' \phi(r, \Omega').$$

After the test function $v_{ik}(r, \Omega)$ is defined to be $w_k$ when it is in cell $i$ and direction $\Omega_k$ and 0 else, then for a variable $y(r, \Omega)$ the following holds:

$$\int_{4\pi} d\Omega \int_S dr y(r, \Omega) v(r, \Omega) \approx \Delta x \cdot \Delta y \cdot w_k y_i(r, \Omega).$$

Using this the three parts of the BTE can be rewritten as:

$$L^{(1)} \phi \approx \Delta \cdot w_k \sum_{face} (\Omega_k \cdot \hat{n}) \phi_{i,face},$$

$$L^{(2)} \phi \approx \Delta x \cdot \Delta y \cdot w_k \Sigma_t \phi_{i,k},$$

$$L^{(3)} \phi \approx \Delta x \cdot \Delta y \cdot w_k \frac{\Sigma_f}{4\pi} \sum_{k'=1}^n w_{k'} \phi_{i,k'},$$
with \( \phi_{\text{face}} \) in \( L^{(1)} \) being the flux of block upwind of the block \( i \), which means the block in the opposite direction that the direction \( \Omega_k \) is pointing, this is an approximation of the face value of the block. \( \Delta \) in \( L^{(1)} \) is \( \Delta x \) or \( \Delta y \) when \( \Omega_k \) points in the y-direction or x-direction respectively. Finally note that the adjoint of the Boltzmann operator \( L \) is its transpose:

\[
L^T = L^T.
\]  
(2.15)

This is needed for calculating the gradient using the adjoint method described in 2.3.3.

### 2.3. Gradient Descent

In this report, the gradient descent method is used. This method allows finding the minimum of a convex function \( F(x) \) using the gradient \( \nabla F(x) \). The reason being that the fastest way to the minimum of a function is given by the direction and the magnitude of the gradient, which is also shown in figure 2.2. This method is needed to minimise the cost function, which will be described in 3.1. The gradient descent algorithm uses the following equation:

\[
x_{n+1} = x_n - \gamma_n \nabla F(x_n),
\]  
(2.16)

where \( x_n \) is the input of an arbitrary function \( F \), which in this case is the objective function described in 3.1, and \( \gamma_n \) is the step size, which scales the size of the step taken in the direction of the gradient and is initially chosen to be constant. Choosing the correct step size is important since a step size too small will be very slow and too large will make the solution diverge as shown in figure 2.3. This method itself is very popular and efficient and can be optimised in multiple ways [28]. For this report, the Barzilai-Borwein method has been used, which uses variable step sizes.

![Figure 2.2: This figure shows how gradient descent works on a convex function \( F(x) \). The steps are taken in the direction of the gradient, which takes the solution towards the minimum. This image was edited to match the functions and variables in this report [29].](image1)

![Figure 2.3: This figure shows the effect of different step sizes. Small steps converge slowly and big steps diverge. This image was edited to match the functions and variables in this report [14].](image2)

#### 2.3.1. Barzilai-Borwein method

The Barzilai-Borwein (BB) method is a method for determining fast and efficient step sizes \( \gamma_n^{BB} \), which speeds up convergence greatly compared to a constant step size [26], thus requires less computational time. Consider again equation 2.16. \( \gamma_n^{BB} \) is now calculated based on the information of points \( x_{n-1} \) and \( x_n \). Using \( s_{n-1} = x_n - x_{n-1} \) and \( y_{n-1} = \nabla F(x_n) - \nabla F(x_{n-1}) \), \( \gamma_n^{BB} \) is calculated as follows:

\[
\gamma_n^{BB} = \frac{s_{n-1}^T s_{n-1}}{s_{n-1}^T y_{n-1}}.
\]  
(2.17)

It should be noted that the first step size should still be chosen, this can be done arbitrary or very small since the next step size will be chosen by the BB method. The BB method has proven to be very useful in this report it did, however, diverge in some cases, which forces us to take a different, though similar approach in the next subsection.
2.3.2. Stabilised Barzilai-Borwein method

Going a step further to increase stability for the gradient descent the stabilised Barzilai-Borwein method was used. Step sizes were encountered which were too large and made the solution diverge, which the stabilised Barzilai-Borwein method should improve [4]. It goes as follows: The same step size in equation 2.17 is used and compared to a different step size which also makes use of the step size of equation 2.17:

\[
\gamma_{n}^{\text{stab}} = \frac{\|x_{n+1} - x_{n}\|}{\|\nabla F(x_{n})\|} = \frac{\|x_{n} - \gamma_{n}^{BB} \nabla F(x_{n})\|}{\|\nabla F(x_{n})\|},
\]

(2.18)

Then the step size \(\gamma_{n}\) is chosen by:

\[
\gamma_{n} = \min(\gamma_{n}^{BB}, \gamma_{n}^{\text{stab}}).
\]

(2.19)

2.3.3. Adjoint and Perturbation Theory

In order to calculate the gradient of the detector response (equation 3.1) with respect to the absorption or scatter coefficients, adjoint and perturbation theory are used. Adjoint theory is commonly applied to neutron transport in nuclear physics. The details are beyond the scope of this report, though the essentials in order to calculate the gradients are outlined in this subsection. A few concepts have to be introduced. When space and direction have been discretised, they can be rewritten into matrices. The Boltzmann transport equation can then, as actually already has been done, be written in its operator form. The equation then becomes:

\[
L \phi = s,
\]

(2.20)

with \(s\) being the source term of photons. The source term describes the creation of photons, which can be multiple things. In our case the source term is the incoming photons into the system by a transmitter on the border of the system, thus the photons transmitted into the system. When first order perturbation for the Boltzmann operator and the flux is used, the following is obtained [18]:

\[
L \phi = s \rightarrow (L_{o} + \Delta L)(\phi_{o} + \Delta \phi) = s,
\]

\[
L_{o} \phi_{o} + L_{o} \Delta \phi + \Delta L \phi_{o} + \Delta L \Delta \phi = s,
\]

with \(L_{o}\) and \(\phi_{o}\) being the reference flux. Since \(L_{o} \phi_{o} = s\) and second order pertubation terms are disregarded:

\[
L_{o} \Delta \phi = -\Delta L \phi_{o}.
\]

(2.21)

The detector response (or objective function) is equal to:

\[
R = < \Sigma, \phi >,
\]

(2.22)

with \(R\) being the detector response, \(\Sigma\) the to be reconstructed coefficient and \(<,>\) being the inner product over all 2D space \(S\) and all directions \(\Omega\) defined as:

\[
<,> = \int_{4\pi} d\Omega \int_{S} d\mathbf{r}.
\]

(2.23)

Then using adjoint theory the following needs to be solved:

\[
< \phi, L^{\dagger} \phi^{\dagger} > = s^{\dagger} = < \Sigma, \phi > = R,
\]

(2.24)

with \(L^{\dagger}\) being the adjoint of the Boltzmann operator defined in equation 2.15, \(\phi^{\dagger}\) being the adjoint flux, which is in simple words the flux moving in reverse, and \(s^{\dagger}\) being the adjoint of the source term, which is the opposite of the source term, photons leaving the system. Then for small changes in \(R\), due to small changes in \(\phi\):

\[
< \Delta \phi, L^{\dagger} \phi^{\dagger} > = \Delta R.
\]

(2.25)

Using equations 2.15 and 2.21, this can be rewritten as:
2.3. Gradient Descent

\[ \Delta R = - \langle \Delta L \phi_o, \phi^\dagger \rangle. \] (2.26)

In this case the change in the operator \( L \) is the change in the reconstructed coefficient \( \Sigma^a \) or \( \Sigma^s \).

### 2.3.4. Gradient of Absorption and Scatter coefficients

To conclude the theory chapter, the gradient of the objective function with respect to the absorption and scatter coefficients using adjoint theory is derived. The inner product \( \langle, \rangle \) is the same as the inner product of equation 2.24. The difference in detector response for the perturbation of \( \Sigma^a \) is derived as follows:

\[ \Delta R^a = - \langle \Delta L^a \phi_o, \phi^\dagger \rangle = - \sum_i \Delta \Sigma^a_i \langle \phi^o_i, \phi^\dagger_i \rangle \]

\[ = - \sum_i \Delta \Sigma^a_i \int d\Omega \int_S d\mathbf{r} \phi^o_i \phi^\dagger_i \]

\[ = - \sum_i \sum_k \Delta \Sigma^a_i \cdot \Delta x \cdot \Delta y \cdot w_k \cdot \phi^o_{l,k} \cdot \phi^\dagger_{l,k}, \]

with the gradient for \( \Sigma^a \) given as:

\[ \left( \frac{\Delta R^a}{\Delta \Sigma^a} \right)_i = - \sum_k \Delta x \cdot \Delta y \cdot w_k \cdot \phi^o_{l,k} \cdot \phi^\dagger_{l,k}. \] (2.27)

The same is done for the perturbation of \( \Sigma^s \):

\[ \Delta R^s = - \langle \Delta L^s \phi^o, \phi^\dagger \rangle. \]

\( \Sigma^s \) has two terms in the Boltzmann equation, which are linear in the inner product:

\[ \Delta R^s = - \langle \Delta \Sigma^s \phi^o, \phi^\dagger \rangle + \frac{\Delta \Sigma^s}{4\pi} \int_{4\pi} d\Omega' \phi^o(\Omega') \phi^\dagger(\Omega) \]

\[ = \sum_i \Delta \Sigma^s_i (\langle \phi^o_i, \phi^\dagger_i \rangle + \frac{1}{4\pi} \langle \int_{4\pi} d\Omega' \phi^o_i(\Omega'), \phi^\dagger_i(\Omega) \rangle) \]

\[ = \sum_i \sum_k \Delta \Sigma^s_i \cdot \Delta x \cdot \Delta y \cdot w_k \cdot (-\phi^o_{l,k} + \sum_{k'} \frac{w_{k'}}{4\pi} \phi^o_{l,k'}) \cdot \phi^\dagger_{l,k}, \]

with the gradient for \( \Sigma^s \) then given as:

\[ \left( \frac{\Delta R^s}{\Delta \Sigma^s} \right)_i = \sum_k \Delta x \cdot \Delta y \cdot w_k \cdot (-\phi^o_{l,k} + \sum_{k'} \frac{w_{k'}}{4\pi} \phi^o_{l,k'}) \cdot \phi^\dagger_{l,k}. \] (2.28)

To all gradients a L2 regularisation term is added, which is:

\[ (Reg)_i = \Delta x \cdot \Delta y \cdot \alpha \cdot \Sigma_i, \] (2.29)

with \((Reg)_i\) being the regularisation term and \(\alpha\) being the regularisation coefficient. This regularisation originates from the fact that regularisation is used in the objective function, which will also be explained in 3.1.3.
3 The Model and Its Implementation

What we’ve done in the previous chapter allows us to create a model to reconstruct the absorption and scatter coefficients using the discretised BTE and gradient descent with the gradient from the adjoint theory. This chapter will explain how we have constructed the model and how the implementation has been done in python.

3.1. Explanation of the Model
The model is explained in the following subsections.

3.1.1. Dimensions and Properties of the System
As described before we are using a \((L_x, L_y)\) 2D geometry. The system can have can have multiple cross sections representing different structures. This will be the system to be reconstructed. Since the goal was to try simulations for more patient-like geometries, absorption and scatter coefficients of a human body are used. As mentioned before, the coefficients in a human body range from \(\Sigma^a = 0.03-1.6\, \text{cm}^{-1}\) and \(\Sigma^s = 1.2-40\, \text{cm}^{-1}\) [30]. Which values are used in the simulations is explained in 3.3, but a general overview of the values for cross sections in a human body are given in table 3.1. The values of the wavelength to which the cross section corresponds do vary, however, they are not chosen outside 600\,nm and 700\,nm, otherwise, they cannot be properly compared and be used at the same time.

3.1.2. Detectors and Transmitters
In order to transmit photons into the system and measure the outward flux to reconstruct the cross sections of the system, detectors and transmitters have to be placed. Their positioning depends on their size. The size of an average optoelectronic transmitter and receiver, which are also used in practice, was found to be around 3mm [21][12][11][35]. They are placed alternating with some spacing between them (~0.5mm) and the amount depending on \(L_x\) and \(L_y\). Their exact placement is explained in the implementation in 3.2.2.

3.1.3. The Objective Function
The cross sections can be reconstructed using the detector response. The detector response is determined, by measuring the outward flux on the places of the detectors. The goal is to reconstruct the chosen coefficient to attain the same true flux. A measure of how close the reconstruction is to the true value is given by the objective function. The regulated least-squares objective function, to be minimised, for arbitrary \(\Sigma\) is given by:

\[
R = \frac{1}{2} \Delta x \cdot \left( \sum_{i_o} (\phi_{i_o} - \phi_{i_o}^{\text{meas}})^2 \right) + \frac{1}{2} \Delta y \cdot \left( \sum_{j_o} (\phi_{j_o} - \phi_{j_o}^{\text{meas}})^2 \right) + \frac{1}{2} \alpha \Delta x \cdot \Delta y \cdot \sum_{i,j} (\Sigma_{ij})^2,
\]  

(3.1)
where $\phi$ is the calculated outward flux for the guessed coefficient at indices where detectors are placed $i_D$ and $j_D$, $\phi^{\text{meas}}$ is the real measured flux at those same indices and the last term containing $\alpha$ is a L2 regularisation term, which is a dampening term to ensure a unique solution [31], with a sum over all $\Sigma$ in the system. The difference in the fluxes is squared, which makes the objective function a convex function for the gradient descent.

Table 3.1: This table contains relevant cross sections for parts of the human body [30] for a certain wavelength. The data has been filtered on wavelength to be not outside of [600,700]nm.

<table>
<thead>
<tr>
<th>Tissue</th>
<th>$\lambda$(nm)</th>
<th>$\Sigma^a$(cm$^{-1}$)</th>
<th>$\Sigma^s$(cm$^{-1}$)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Bladder</td>
<td>630</td>
<td>0.28-0.76</td>
<td>2.5-6.37</td>
</tr>
<tr>
<td>Bone</td>
<td>650</td>
<td>0.09-0.14</td>
<td>12.5-15.8</td>
</tr>
<tr>
<td>Brain</td>
<td>630</td>
<td>0.02-0.50</td>
<td>3.72-21.97</td>
</tr>
<tr>
<td>Breast</td>
<td>660</td>
<td>0.037-0.110</td>
<td>11.4-13.5</td>
</tr>
<tr>
<td>Tumour</td>
<td>690</td>
<td>0.070-0.10</td>
<td>14.7-17.3</td>
</tr>
<tr>
<td>Small Bowel</td>
<td>630</td>
<td>0.19-0.21</td>
<td>8.95-10.05</td>
</tr>
<tr>
<td>Large Bowel</td>
<td>630</td>
<td>0.12-0.18</td>
<td>10.11-10.42</td>
</tr>
<tr>
<td>Diaphragm</td>
<td>661</td>
<td>0.15-1.08</td>
<td>9.65-21.7</td>
</tr>
<tr>
<td>Heart</td>
<td>630</td>
<td>0.03-1.55</td>
<td>17.56-75.06</td>
</tr>
<tr>
<td></td>
<td>661</td>
<td>0.12-0.18</td>
<td>5.22-90.80</td>
</tr>
<tr>
<td>Liver</td>
<td>630</td>
<td>1.15-1.56</td>
<td>21.6-30.4</td>
</tr>
<tr>
<td>Lung</td>
<td>630</td>
<td>0.16-1.36</td>
<td>1.07-83.81</td>
</tr>
<tr>
<td></td>
<td>661</td>
<td>0.49-0.88</td>
<td>21.14-22.52</td>
</tr>
<tr>
<td>Pericardium</td>
<td>630</td>
<td>0.13-0.33</td>
<td>13.0-21.9</td>
</tr>
<tr>
<td>Prostate</td>
<td>630</td>
<td>0.05-1.0</td>
<td>3.41-17.02</td>
</tr>
<tr>
<td></td>
<td>650</td>
<td>0.14-0.61</td>
<td>5.24-22.68</td>
</tr>
<tr>
<td></td>
<td>672</td>
<td>0.09-0.72</td>
<td>3.37-29.8</td>
</tr>
<tr>
<td>Skin</td>
<td>630</td>
<td>0.05-1.11</td>
<td>2.26-20.95</td>
</tr>
<tr>
<td></td>
<td>661</td>
<td>0.51-0.64</td>
<td>2.24-5.77</td>
</tr>
</tbody>
</table>

### 3.2. Implication of the Model in Python

In this section the implication in python is explained in more detail. The steps in python are outlined and when extra explanation is needed, they are given in subsections.

#### 3.2.1. Steps of the Implication

1. Set the spatial and directional properties of the system and the regularisation term.
   
   (a) Set the values for $L_x$, $L_y$, $N_i$ and $N_j$.
   
   (b) Set the number of directions ($n$) and calculate the weights ($w_k$) using the discrete ordinate method $S_N$.
   
   (c) An array of length $(N_i \times N_j \times n)$ is initialised to contain information of the fluxes in all directions of the discrete ordinates for each block.
   
   (d) Set the regularisation term $\alpha$

2. Apply the true, to be guessed, absorption and scatter coefficients to the system.
   
   (a) An $(N_i \times N_j)$ array is initialised for these values.
   
   (b) These coefficients can be uniform over the field or be applied per block to recreate certain structures within the system.

3. Place detectors and transmitters based on values of step 1a and according to the explanation given in 3.2.2.

4. Solve the BTE for the whole system.
3.2. Implication of the Model in Python

(a) A flux on the border at positions where transmitters are placed in all directions of the ordinates towards the inside of the system is set to 1. This is the flux of photons given by a transmitter.

(b) The true, reference, flux of the system is then determined by calculating the total flux in the system using the discrete BTE in each block and each direction.

5. Then the objective function is calculated, which is equation 3.1, using only the outward flux where detectors are placed as described in 3.2.2.

6. Set the system to guessed absorption or scatter coefficients. Only one of each is reconstructed, this was a limitation of the implication. So one of the coefficients will be the true value.

7. Solve the BTE again and determine the detector response and in turn the objective function.

8. Update the coefficient using the gradient, derived in 2.3.4, and the gradient descent method.

9. Repeat step 5, 6, 7 and 8 and stop after set iterations or reached goal of objective value.

10. (Optional): An extra step can be taken to determine if the minimum of the solution was found. This is simply done by perturbing the coefficient block per block and checking if the objective function becomes larger.

11. If wanted try for the other coefficient, using the true value for the current one.

These are the steps, the following subsection explains some extra details.

3.2.2. Detector and Transmitter Placement

The way the realistic placement of detector and transmitters was implemented in python is as follows: First, the code gets inputs of the length \(L_x\) and \(L_y\) of the edge and the number of discrete blocks \(N_x\) and \(N_y\). The lengths are then divided by 3mm to see how many detectors of 3mm would fit and then divided by 3 to get the number of detectors \(N_{det}\) to be placed on the edge with enough room in for transmitters and space in between. This is rounded to an integer using NumPy round. Then the number of blocks to be assigned per sensor \(n_{det}\) is determined by dividing 0.3mm by \(\Delta x\) or \(\Delta y\), this should also be rounded to an integer. We then have the following information: Amount of blocks on the edge, number of detectors, number of blocks per detector and from this also the number of empty blocks and also the number of empty spacing, which is always the number of detectors plus 1 to ensure empty spacing at the beginning and end of the edge. Then we will use truncating integer division to divide number \(n\) (number of empty blocks) into \(p\) parts (number of empty spacing) [27]:

\[
d = \text{int}(n/p),
\]

\[
r = \text{int}(n\%p),
\]

\[
(d + 1, \ldots, d + 1), (d, \ldots, d)\]

\[
times \frac{n}{r} \text{ times} \quad \frac{n}{p} \text{ times}
\]

Now the order of \(d + 1\) and \(d\) is randomised using NumPy random shuffle. This is done to ensure an evenly distributed amount of blocks. Then an array is created with alternating False for empty spaces and True for detector spaces. The detector response is then only checked at blocks where there is a True for a detector. For simplicity, transmitters are placed on the empty blocks. This was done since the empty spacings are also around 3-4 mm and this prevents writing another large piece of code in a short time. This was also sufficient for the goal to place realistic detectors and transmitters. The indices \(i_D\) and \(j_D\) in equation 3.1 are then only the indices where there is a True for detector. In order to clarify this, an example is given:

Consider \(L_x=2\text{cm}\) and \(N_x=30\), thus \(\Delta x=\frac{2\text{cm}}{30}\):

\[
N_{det} = \text{round}(\frac{2\text{cm}}{0.3\text{cm}}) = \text{round}(6.67) = 2,
\]

\[
n_{det} = \text{round}(\frac{0.3\text{cm}}{\Delta x}) = \text{round}(\frac{30 \times 0.3\text{cm}}{2\text{cm}}) = \text{round}(4.5) = 5,
\]
\[ N_{\text{empty}} = N_{\text{det}} + 1 = 2 + 1 = 3 \]

\[ n_{\text{empty, tot}} = N_x - N_{\text{det}} \times n_{\text{det}} = 30 - 2 \times 5 = 20. \]

These empty blocks are then evenly distributed according to the truncated integer division method:

\[ d = \text{int} \left( \frac{n_{\text{empty, tot}}}{N_{\text{empty}}} \right) = \text{int} \left( \frac{20}{3} \right) = 6, \]

\[ r = \text{int} \left( n_{\text{empty, tot}} \cdot \% N_{\text{empty}} \right) = \text{int} \left( 20 \cdot \% 3 \right) = 2, \]

Empty spacings : (7, 7, 6) random (7, 6, 7).

The distribution of detectors and empty spacings is then shown in figure 3.1. For the simplification all empty spacings are then used for the transmitters. To show how a 2D square grid would look like: the example is shown in figure 3.2.

Figure 3.1: The distribution of detectors and empty spacings for the example in 3.2.2.

Figure 3.2: The distribution of detectors and transmitters for the example in 3.2.2. This shows the whole 2D square grid.
3.3. Cases Studied

This section is dedicated to outline the cases on which the model will be tested.

3.3.1. Validating the Derived Adjoint Gradients

In order for the simulations to work, the derived gradients in 2.3.4 need to be checked. This will be done in the following way [16]: Use settings \( L_x = L_y = 1.0\, \text{cm}, N_x = N_y = 9, \Sigma_{\text{init}} = \Sigma_{\text{init}} = 5\, \text{cm}^{-1}, N = (2, 4, 6, 8) \) and \( \alpha = 0 \). Then the to be checked cross section will be set to guess \( 3\, \text{cm}^{-1} \), except for the inner block of \( \Omega^a \) or \( \Omega^s \). This inner block is set to \( 2.999\, \text{cm}^{-1} \) and \( 3.001\, \text{cm}^{-1} \), such that \( \Delta \Sigma = 0.002\, \text{cm}^{-1} \). \( \Delta R \) is then calculated by taking the difference in objective function at the guessed cross sections. Now \( \Delta R / \Delta \Sigma \) is known. To test if this is correct, the guessed inner block is set to \( 3\, \text{cm}^{-1} \) and the gradient is calculated with the formulas of 2.3.4. These gradients should be approximately equal.

3.3.2. Speedup Using the Stabilised Barzilai-Borwein Method

Though already explained in 2.3.2, it should be tested if the model works with the stabilised Barzilai-Borwein step size implementation, which should speedup the computation significantly. A few cases have been selected to check the speeds of both methods. These cases are cubical 2D grids of 20, 30 and 40 blocks per side, the number of discrete ordinates using \( L_x = L_y = 1.0\, \text{cm} \), \( N_x = N_y = 9 \), \( \Sigma_{\text{init}} = \Sigma_{\text{init}} = 5\, \text{cm}^{-1} \), \( N = (2, 4, 6, 8) \) and initial step size 5, 25 and 50. The step size is initial for both methods and thus is it also the step size used in the constant method. The cross sections are: \( \Sigma_{\text{init}} = 0.2\, \text{cm}^{-1} \), \( \Sigma_{\text{init}} = 1\, \text{cm}^{-1} \) and \( \Sigma_{\text{guess}} = 1.5 \times \Sigma_{\text{init}} \). Both grid size and number of ordinates majorly decide the computational time since the number of computations depends directly on the number of blocks and number of ordinates. Since comparing the speeds with a single initial step size could create an unfair BB favoured scenario multiple initial step sizes were chosen. It should be noted that a high initial step size could make the constant method faster than a lower step size, however, this might cause a non-convergent solution, because the gradient descent might overshoot the solution, causing a divergence also shown in figure 2.3. A divergence is defined here as when the objective function has not decreased after 1000 iterations. The time was determined by timing steps 5, 6, 7, 8 and 9 from 3.1 and stopping the timer when the objective function was below \( 10^{-6} \). This is not necessarily the perfect solution but does give an indication of speed. A small section about this speedup is dedicated in the results in 4.2.

3.3.3. Test Case

Before we take on some practical cases to test the possibilities of optical tomography, it is important to test whether the model produces a solution or not. The model will be tested with and without realistic detector and transmitter placement for the following case: \( (L_x, L_y) = (1.0, 1.0), (N_x, N_y) = (20, 20), N = (2, 4, 6) \), initial step size 5, \( \alpha = 10^{-6} \), \( \Sigma_{\text{init}} = 0.5 \), \( \Sigma_{\text{guess}} = 0.5 \) and the guessed cross sections are 1.5 times the initial value. The true solution will be compared to the computed solution and the computed solution will be tested whether the objective function is minimal or not. The minimum is reached when a perturbed cross section in a single block with 0.999 and 1.001 times the best solution value for the cross section in that block yields a higher objective function or an objective function which is above 0.999 times the best objective function.

3.3.4. Practical Cases

Now we are going to focus on trying the reconstruction model on practical cases. Based on the ranges of values in table 3.1 some conclusions can already be drawn using equation 2.4. Some tissues have high absorption and scatter cross section and also lie deep within the body, such that they are deemed impossible to reconstruct. The cases chosen are beforehand considered potentially possible or cases in the practice. Cases in practice are, but not limited to: Infant neuroimaging [13], neuroimaging [32] [9] [8], finding breast cancer [9] [8], imaging oxygenated \( (\text{HbO}_2^+) \) and deoxygenated \( (\text{Hb}) \) blood flow [9] [8], imaging finger joints for detection of arthritis [9] and muscle function imaging. With the data from table 3.1 the brain, breasts and tumours can be modelled. We are thus interested in imaging the brain of an adult and an infant and possible tumours if reconstruction is possible and finding breast tumours. It should be noted that all the upcoming cases will be reconstructed using guessed coefficients which is twice the average of the whole system for absorption and half the average of the whole system for scatter. These values were chosen based on the magnitude of the true values, which is low for absorption and high for scatter. All the reconstructions will be tested for a minimal solution as also
described in 3.3.3. All the reconstructions will be done using two different regularisation terms: $\alpha=10^{-6}$ and $\alpha=10^{-9}$. All initial step sizes are chosen to be 5. The choice for $N$ will be determined by the results of the test cases for the gradient (3.3.1) and the reconstruction in general (3.3.3). The models of the body parts will be made using data from medical research or averages from other literature. All these models will use the simplification that they are square shaped. The to be reconstructed models in python are shown along the results in the results chapter.

First, we will try to reconstruct an adult brain with and without tumour. The average thickness of the adult male skull is taken as the average of the frontal (6.3mm), parietal (5.8mm), temporal (3.9mm) and occipital (7.7mm) parts of the skull [22], thus $(6.3+5.8+3.9+7.7)/4=6.5$ mm. These parts of the skull are shown in figure 3.3. The thickness of the scalp is taken as the sum of the thickness of the epidermis $(44.70\pm13.99\mu m)$ and dermis $(1200.93\pm297.23\mu m)$, which are two parts of the skin, of the upper medial forehead, being 1.25mm [6]. The average head circumference of an adult male is 55.90 ±1.85 cm [24]. There is a huge variety in brain tumours and we have chosen a type that grows on the surface of the brain since this is easier to detect. This type of brain tumour is called a Meningioma and can reach the size of 5cm in diameter [36]. Since the model is taken to be square we take $(L_x, L_y)$ as $(14\text{cm},14\text{cm})$ of which the outer layer is 0.14cm skin followed by a layer of 0.56cm bone, a square with sides of 4.48cm of tumour directly against the skull wall on the middle of the left inside and the rest is considered all brain. These numbers have been chosen such that the grid size can be chosen as $(N_x, N_y)=(100,100)$. For the cross sections the average values in table 3.1 are taken with most overlapping wavelength, which was 630nm, 650nm and 630nm respectively, being $\Sigma_{\text{Skin}}^a=0.58\text{cm}^{-1}$, $\Sigma_{\text{Bone}}^a=0.12\text{cm}^{-1}$, $\Sigma_{\text{Tumour}}^a=0.09\text{cm}^{-1}$, $\Sigma_{\text{Brain}}^a=0.26\text{cm}^{-1}$, $\Sigma_{\text{Skin}}^b=11.61\text{cm}^{-1}$, $\Sigma_{\text{Bone}}^b=14.15\text{cm}^{-1}$, $\Sigma_{\text{Tumour}}^b=15.8\text{cm}^{-1}$ and $\Sigma_{\text{Brain}}^b=12.85\text{cm}^{-1}$.

For the infant head with and without tumour we take the 50th percentile of the head circumference of a 6.5-month infant, which is 44cm [15]. $(L_x, L_y)$ is then $(11\text{cm},11\text{cm})$. The thickness of the skin and bone will scale with comparison to the adult head considering the same grid size, thus $11/14$ of the adjusted adult size. Skin is 0.11cm thick, the skull 0.44cm and the tumour has sides of 3.52cm. This can also be done by keeping the same system as the adult brain and scaling only $L_x$ and $L_y$.

Finally, to simulate the breast with and without a tumour we need to create a model of the breast. This will again be a square. The circumference is taken as four times the nipple to infra-mammary fold (N-IMF) distance of 6.45cm [34]. The skin thickness of the breast will be taken as 2mm, being in the normal range and easy to discretise [25]. The model with the tumour will use a T2 tumour of size 35mm [34]. The model can then be made as follows: $(L_x, L_y)$ is $(6.5\text{cm},6.5\text{cm})$, with the outer layer being 0.2cm skin, an eventual tumour of size 3.5cm placed directly under the skin and the rest being breast tissue. These values have again been adjusted to reduce grid size, which is $(N_x, N_y)=(65,65)$. For the cross sections the average values in table 3.1 are taken with most overlapping wavelength, which was 661nm, 690nm and 660nm respectively, being: $\Sigma_{\text{Skin}}^a=0.58\text{cm}^{-1}$, $\Sigma_{\text{Tumour}}^a=0.09\text{cm}^{-1}$, $\Sigma_{\text{Breast}}^a=0.07\text{cm}^{-1}$, $\Sigma_{\text{Skin}}^b=4.0\text{cm}^{-1}$, $\Sigma_{\text{Tumour}}^b=15.8\text{cm}^{-1}$ and $\Sigma_{\text{Breast}}^b=12.45\text{cm}^{-1}$.
4.1. Results of the Derived Adjoint Gradients

The first section is dedicated to the validation of the gradient from the adjoint theory. The results are shown in table 4.1. As can be seen the error is zero for all cases except for $\Sigma^s$ for $N = 2$.

<table>
<thead>
<tr>
<th>$N$</th>
<th>$\Delta R/\Delta \Sigma^a$</th>
<th>error (%)</th>
<th>$N$</th>
<th>$\Delta R/\Delta \Sigma^s$</th>
<th>error (%)</th>
</tr>
</thead>
<tbody>
<tr>
<td>2</td>
<td>-0.014614441</td>
<td>0%</td>
<td>2</td>
<td>-5.421010e-20</td>
<td>-399900%</td>
</tr>
<tr>
<td>4</td>
<td>-0.010766541</td>
<td>0%</td>
<td>4</td>
<td>1.766986e-05</td>
<td>0%</td>
</tr>
<tr>
<td>6</td>
<td>-0.010219079</td>
<td>0%</td>
<td>6</td>
<td>1.806524e-05</td>
<td>0%</td>
</tr>
<tr>
<td>8</td>
<td>-0.009966936</td>
<td>0%</td>
<td>8</td>
<td>1.810905e-05</td>
<td>0%</td>
</tr>
</tbody>
</table>

Table 4.1: The results of the comparison between the gradient calculated using adjoint theory and the true gradient. Table (a) shows the results for the absorption coefficient and table (b) shows the results for the scatter coefficient.

4.2. Speedup of the Barzilai-Borwein Gradient Descent Method

This section is about the computational speedup of using the stabilised Barzilai-Borwein method instead of using constant step sizes in the gradient descent. The results of the speeds are shown in figure 4.1. The raw results are shown in table A.1 in the appendix. As can be seen from figure 4.1, the BB method was faster in all cases, except for $N_x = N_y = 30$, $N=6$ and step size 50, which was still comparable. The constant step size diverged in the case for the step size 50 and grid $N_x = N_y = 20$, while the BB method never did. It has to be mentioned that after a while both methods eventually diverge when left to run indefinitely without goal objective, though they are considered converged when a minimum was reached.

4.3. Simple Test Case

It is also important to check whether the model produces correct results. Using the Barzilai-Borwein method and the settings described in 3.3.3. The results of $N=(2,4,6)$ are given in figures 4.2, 4.3 and 4.4, respectively.

As can be seen, the ideal reconstruction of $\Sigma^a$ is almost identical to the reference case, however, $\Sigma^s$ is not perfectly reconstructed, though still reached a minimum, for all tested $N$. The reconstructions with the realistic detector and transmitter placement also reached a minimum, with $\Sigma^a$ being a better reconstruction of the reference than $\Sigma^s$, also for all $N$. The reconstruction for realistic detector and transmitter placement is similar to the true system and the shapes in the results are effects of the detectors and transmitters being positioned on parts of the edge and the number of discrete ordinates.
The higher \( N \), the better the reconstruction in general, especially for the scatter coefficient. The results of the practical cases studied are outlined in the next section.

![Figure 4.1: The speed comparison for different \( N \) in \( S_N \). Each figure has a different initial step size. (a) has initial step 5, (b) has 25 and (c) has 50. For initial step 50 (c), the method without BB diverged for a 20x20 grid. All plots have the y-axis in log scale. The labels only contain the sides of the cubical grids. The dashed lines are with the BB method and the non dashed lines are without the BB method.](image-url)
Figure 4.2: These are the results of the simple test cases for N=2. On the top side the reference cases are shown and on the bottom the reconstructions, with on top without detector and transmitter placement and on the bottom with detector and transmitter placement as described in 3.2.2. On the left $\Sigma^n$ is shown and $\Sigma^T$ is on the right.
Figure 4.3: These are the results of the simple test cases for \(N=4\). On the top side the reference cases are shown and on the bottom the reconstructions, with on top without detector and transmitter placement and on the bottom with detector and transmitter placement as described in 3.2.2. On the left \(\Sigma^a\) is shown and \(\Sigma^s\) is on the right.
Figure 4.4: These are the results of the simple test cases for N=6. On the top side the reference cases are shown and on the bottom the reconstructions, with on top without detector and transmitter placement and on the bottom with detector and transmitter placement as described in 3.2.2. On the left $\Sigma^0$ is shown and $\Sigma^+$ is on the right.
4.4. Results of Cases Studied

Here the results of the cases studied are given. The cases studied are reconstructed using $N=4$, since this accurate enough and still quite fast, based on the results of the previous sections. They have also been reconstructed using $N=2$, these results, though incorrect according to the previous results, are shown in the appendix for potential comparison, which will not be made in this report.

4.4.1. Adult Head With and Without Tumour

The adult head without and with tumour has been reconstructed without and with detector placement, for absorption and scatter and for $\alpha=10^{-6}$ and $\alpha=10^{-9}$. The results are shown in figures 4.5, 4.6, 4.7 and 4.8, respectively.

As can be seen in these figures, the absorption coefficient could be reconstructed, except for the case with tumour and realistic detector and transmitter placement, which did not converge. When the case with and without tumour is compared, a significant difference could not be discovered. The scatter coefficient was more successful. Despite that the case with realistic detector and transmitter placement could not be reconstructed, there was a difference when a tumour is in the head. The difference, however, is not that noticeable. It should be mentioned that changing $\alpha$ did not change this outcome much for both coefficients and even though the solution reached a minimum, the reconstructions did not match the initial system in terms of coefficient value. The next case is the infant head, which is the same system with scaled size.

4.4.2. Infant Head With and Without Tumour

The infant head without and with tumour has been reconstructed without and with detector placement, for scatter and absorption and for $\alpha=10^{-6}$ and $\alpha=10^{-9}$. The results are shown in figures 4.9, 4.10, 4.11 and 4.12, respectively.

To begin, the cases where the realistic detector and transmitter placement was tried all did not converge. The following results will therefore only compare the cases with the ideal detector and transmitter placement (on the whole border). The absorption coefficient reconstruction did not yield useful information. The reconstruction did not correspond to the true system, though similar in shape. For the scatter coefficient the results were the same as for the adult head. A small difference can be seen. Again the regularisation did not make a significant difference and the solutions were at a minimum. The next reconstruction is the reconstruction of the breast. The breast reconstruction is again smaller in size and also different in coefficients.

4.4.3. Breast With and Without Tumour

The breast without and with tumour has been reconstructed without and with detector placement, for scatter and absorption and for $\alpha=10^{-6}$ and $\alpha=10^{-9}$. The results are shown in figures 4.13, 4.14, 4.15 and 4.16, respectively.

Unfortunately, a lot of the breast reconstructions did not converge, even though this model is a lot smaller than the previous. Not only were there a lot of non convergent cases, the reconstructions were far from the true system. Again regularisation did not make a significant difference and the successful cases reached a minimum.
4.4. Results of Cases Studied

Figure 4.5: Absorption coefficient reconstruction for the adult brain without tumour for N=4. On the top the to be reconstructed system is shown. Then the second row is the reconstruction with idealised detector and transmitter placement and the last is with realistic placement. On the left $\alpha=10^{-6}$ is used and $\alpha=10^{-9}$ on the right. When an image says “DNC” it did not converge and the simulation was not able to produce a solution.
Figure 4.6: Absorption coefficient reconstruction for the adult brain with tumour for N=4. On the top the to be reconstructed system is shown. Then the second row is the reconstruction with idealised detector and transmitter placement and the last is with realistic placement. On the left $\alpha=10^{-6}$ is used and $\alpha=10^{-9}$ on the right. When an image says "DNC" it did not converge and the simulation was not able to produce a solution.
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Figure 4.9: Absorption coefficient reconstruction for the infant brain without tumour for N=4. On the top the to be reconstructed system is shown. Then the second row is the reconstruction with idealised detector and transmitter placement and the last is with realistic placement. On the left $\alpha=10^{-6}$ is used and $\alpha=10^{-9}$ on the right. When an image says "DNC" it did not converge and the simulation was not able to produce a solution.
Figure 4.10: Absorption coefficient reconstruction for the infant brain with tumour for N=4. On the top the to be reconstructed system is shown. Then the second row is the reconstruction with idealised detector and transmitter placement and the last is with realistic placement. On the left $\alpha=10^{-6}$ is used and $\alpha=10^{-9}$ on the right. When an image says "DNC" it did not converge and the simulation was not able to produce a solution.
4.4. Results of Cases Studied

Figure 4.11: Scatter coefficient reconstruction for the infant brain without tumour for N=4. On the top the to be reconstructed system is shown. Then the second row is the reconstruction with idealised detector and transmitter placement and the last is with realistic placement. On the left $\alpha=10^{-6}$ is used and $\alpha=10^{-9}$ on the right. When an image says “DNC” it did not converge and the simulation was not able to produce a solution.
4.4. Results of Cases Studied

Figure 4.12: Scatter coefficient reconstruction for the infant brain with tumour for N=4. On the top the to be reconstructed system is shown. Then the second row is the reconstruction with idealised detector and transmitter placement and the last is with realistic placement. On the left $\alpha=10^{-6}$ is used and $\alpha=10^{-9}$ on the right. When an image says “DNC” it did not converge and the simulation was not able to produce a solution.
Figure 4.13: Absorption coefficient reconstruction for the breast without tumour for N=4. On the top the to be reconstructed system is shown. Then the second row is the reconstruction with idealised detector and transmitter placement and the last is with realistic placement. On the left $\alpha=10^{-6}$ is used and $\alpha=10^{-9}$ on the right. When an image says “DNC” it did not converge and the simulation was not able to produce a solution.
Figure 4.14: Absorption coefficient reconstruction for the breast with tumour for N=4. On the top the to be reconstructed system is shown. Then the second row is the reconstruction with idealised detector and transmitter placement and the last is with realistic placement. On the left $\alpha=10^{-6}$ is used and $\alpha=10^{-9}$ on the right. When an image says "DNC" it did not converge and the simulation was not able to produce a solution.
4.4. Results of Cases Studied

Figure 4.15: Scatter coefficient reconstruction for the breast without tumour for N=4. On the top the to be reconstructed system is shown. Then the second row is the reconstruction with idealised detector and transmitter placement and the last is with realistic placement. On the left $\alpha=10^{-6}$ is used and $\alpha=10^{-9}$ on the right. When an image says "DNC" it did not converge and the simulation was not able to produce a solution.
4.4. Results of Cases Studied

Figure 4.16: Scatter coefficient reconstruction for the breast with tumour for N=4. On the top the to be reconstructed system is shown. Then the second row is the reconstruction with idealised detector and transmitter placement and the last is with realistic placement. On the left \( \alpha=10^{-6} \) is used and \( \alpha=10^{-9} \) on the right. When an image says "DNC" it did not converge and the simulation was not able to produce a solution.
5.1. Validation of Adjoint Gradient
As could be seen in table 4.1 all the gradients for the test cases matched, except for the N=2 scatter coefficient. The scatter coefficient is highly dependent on the number of angles since it determines the probability that a photon will be redirected into a different angle, thus it might be the result of the fact that a small grid has been used and N=2 has 4 discrete angles. It can be assumed that the adjoint theory can be applied to find the gradient in the test cases. As mentioned before, the test cases have been executed using N=4 using these findings.

5.2. Speedup using the Barzilai-Borwein Method
The speedup using the Barzilai-Borwein method was mainly caused by the number of iterations it took to get to the solution, which was significantly less for the BB method. These iterations can be seen in table A.1. The BB method was thus able to reduce computational time for at least a variety of settings. Only the constant step method was unable to reach convergence for higher step sizes at which the speeds became closer to the BB method. This could imply that fine-tuning the step size might increase the efficiency of the constant step method, but this is considered a disadvantage since the simulation has to be run multiple times to fine-tune. The BB method never diverged for these tests. The BB method was also barely affected by the initial step size. Being quicker and always convergent, without having to guess the step size makes the BB method a very useful method for the model.

The eventual divergence for running indefinitely can have multiple reasons. For the constant step size this most likely the result of the step size eventually becoming too large. For the BB method, it is more difficult to figure out. It should automatically adjust the step size to be correct for all gradients. It might be that the BB method is not perfectly suited for this model, but working very well in simple test cases up to a certain level of precision. It might also be caused by the fact that the derived step size is the same for all blocks, making a part of the solution diverge because of the size of the other gradients, though this would be the same without the BB method. Both methods eventually diverged, thus it can not be the result of using the BB method. The gradient itself could also be incorrect, however, we have validated the gradient, which was found to be correct. It is still unclear why this was the case and it should be investigated more thoroughly in an eventual follow-up research. Since the minimum of the objective function was still reached and the solution only diverged after a lot of iterations, this will not be regarded as an issue for the rest of the research.

5.3. Simple Test Case
We saw from the results of the simple test case that this method is able to reconstruct small homogeneous cases. The scatter coefficient for N=2 appears to be incorrect, which we have already seen to be the case in the validation of the gradients. This confirms those results. The rest seems to be correct. So for at least N≥4 the reconstruction method works for small simple cases.
5.4. Cases Studied

First, it should be mentioned that almost all of the reconstructions with realistic detector and transmitter placement, as described in 3.2.2, did not converge. It is not clear why. The placement itself seems proper, though it does not work. The gradients were validated, the method did work on smaller cases and all cases before did converge. The reconstruction might simply be too complex or there might be some errors. The model only checks the detector response on certain parts of the edge, which might lead to overcompensation on the rest of the system which in turn might lead to artefacts in the reconstruction. This might especially be a problem when the system is too large in size, thus when the middle of the system cannot be properly reconstructed. The model might only focus on reconstructing a small part of the border, which is difficult when the border is alternating detector and transmitter. The skin in our models of the head and breasts are also one or two blocks wide, this could also mean that when the borders themselves are not reconstructed properly, this part is not reconstructed properly either and is a problem in itself. There are a few things that can still be tried to figure out what might be wrong. First, the limitations can be researched by trying multiple grid sizes and lengths. When do the reconstructions for the realistic detector and transmitter placement work and when do they stop working? Then different placements can be tried. Will it work better when transmitters are placed entirely or partly on a single edge with detectors placed on the rest of the borders of the system, then moving the transmitters around the system and combining the results? The ratio of detectors and transmitters could also be changed. Does increasing the grid size, thus increasing the number of blocks for small parts of the system such as the skin, give better reconstructions, though increasing computation time significantly? Does the reconstruction simply not work this way? These might be things that could be researched in a follow-up research.

Now aiming the rest of the discussion on the results that did converge, which were mainly the reconstructions with detectors and transmitters placed everywhere. Since three different body parts were tried with and without tumours it could be determined if the reconstruction method is effective in detecting tumours on the surface of the adult brain, infant brain and directly underneath the skin of a breast. These comparisons could be made for the absorption and scatter coefficient. If we compare the two for the idealised detector placement, a small difference can be seen, though not huge. Since the difference is small and you also need an image without a tumour, which you do not have in reality, to see this difference the method might not be efficient in detecting tumours on the surface of the adult brain and infant brain. We can not say this for the breast, since this reconstruction could not always be made and there was no difference to be seen in the reconstruction. This might be the case since the scatter coefficient in all cases is very high and the size of the system is very large. When we look at the reconstructions themselves the validity of the solutions are also questionable since the reconstructions were not close to the real solution. They did sometimes match the shape, which was skin (and bone) on the outside and soft tissue on the inside, but the values were very off. Is the method even capable of handling such large systems? It seems from the figures that the method is only capable of reconstructing the edges of the system. When we look at the values of the coefficients, the absorption coefficient is quite low, but still, a lot of the photons might be absorbed when travelling a large distance. The scatter coefficient is quite high and after a short distance, a large portion of the photons might have already lost their initial direction. It might be the case that only scattered photons on the edge of the system might be detected when they have not travelled very far. When the photons are not capable of travelling through the system, the coefficients can not be reconstructed for the inner part of the system since the objective function will only change a very small amount. Thus a thing that could be further investigated could be reconstructing even smaller systems. Arthritis in fingers and oxygenated and deoxygenated blood in the skin was mentioned before, though proper coefficient values could not be found. Having photons travelling only a small part in the surface and bouncing back might also mean that this method is more suitable for surface imaging like the skin. It could also be that the reconstruction method contains errors. We have slowly build up the reconstruction method by validating the gradients, testing simple cases, testing the gradient descent and checking different values for regularisation. All these tests gave positive results and what is truly wrong is difficult to say. A different kind of regularisation or even no regularisation could still be tried. It is too soon to conclude from these results that this method is incapable of detecting tumours since the validity of the results is questionable.
Conclusion

In this paper a model to reconstruct the absorption and scatter coefficients for optical, near infrared, photons using the Boltzmann transport equation and gradient descent has been researched. This has been done by discretising the system, determining the gradients using the adjoint theory, speeding up the gradient descent using the stabilised Barzilai-Borwein method, creating realistic detector and transmitter placement and then testing this method on test cases and more realistic patient like cases. We saw that the gradients were correct for $N \geq 4$, that the Barzilai-Borwein method reduced computation time significantly in all cases and that the simple test cases were successfully reconstructed using the realistic detector and transmitter placement. From the results we can conclude that this method is capable of reconstructing small homogeneous cases for $N \geq 4$, with small coefficients, using the Barzilai-Borwein method and the realistic detector and transmitter placement as described in this report. For larger and more complex realistic cases this method was unable to create a valid reconstruction and the realistic detector and transmitter cases did not converge. Therefore it can not be concluded whether or not this method is able to detect surface tumours in the adult brain, infant brain and the breast. It is unclear what caused the divergence for the realistic detector and transmitter case, but multiple things can be tried: The placement itself can be adjusted such that they are alternating in a different way, images can be combined of detectors on different positions, the ratio of detectors and transmitters could be adjusted or larger grid sizes might be used. To try and find out why the rest of the reconstructions for the realistic case studies were not similar to the true system, using idealised detector and transmitter placement, these things can be tried in a follow-up research: Reconstructing smaller systems such as arthritis in fingers and different kinds of blood flow in the skin, reevaluating the reconstruction method by trying different kinds of regularisation or trying even smaller systems. Another thing to research might be if the method is suitable for surface imaging like the skin since it might be the case that photons are able to travel short distances through the surface and bouncing back due to the high scatter coefficients, thus being able to reconstruct the surface with higher accuracy than the inner parts of the system.
Bibliography


[34] *Tumor size chart: How does tumor size affect breast cancer staging?* URL: https://www.medicalnewstoday.com/articles/325669#measuring-tumors.


Appendix: Raw results for the speed comparison

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Table A.1: This table contains the raw results for the speed comparison. These cases are cubical 2D grids of 20, 30 and 40 blocks per side, number of discrete ordinates using N=(2,4,6) and initial step size 5, 25 and 50. The test was stopped when an objective function of $10^{-6}$ was reached. DNC means that the solution Did Not Converge, thus was not able to produce a correct solution. That condition was no decreasing objective function after 1000 iterations.
Appendix: N=2 reconstructions for cases studied
Figure B.1: Absorption coefficient reconstruction for the adult brain without tumour. On the top the to be reconstructed system is shown. Then the second row is the reconstruction with idealised detector and transmitter placement and the last is with realistic placement. On the left $\alpha=10^{-6}$ is used and $\alpha=10^{-8}$ on the right. When an image says "DNC" it did not converge and the simulation was not able to produce a solution.
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