INVERSE PROBLEM FOR LIGHT SPREADING APPLIED TO MEDICAL TOMOGRAPHY

Project Report Version 1

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Sommaire

[redacted]CONTEXT

Inverse problems ar+e some of the most important problems in science and mathematics because of their wide range of applications in medical imaging, computer vision, radar, etc. These are problems that, given a set of observations, tell us the parameters that cause them, parameters that we cannot directly observe. In general, numerically solving an inverse problem requires advanced optimization algorithms. However, those can be difficult to implement. That is why we are introducing an approach based on machine learning and neural networks.

The problem to solve is a medical tomography inverse problem by infrared. This project will prepare to study a neural network-based method for finding the optical properties of an organ. It was suggested and is run by the MOCO ("Modélisation et Contrôle") team at IRMA ("Institut de Recherche Mathématique Avancée"). This team is made up of specialists in PDE analysis, control theory, high-performance scientific computing, and statistics (IRMA, n.d.). This specific project is under the guidance of IRMA researchers Emmanuel Franck, Laurent Navoret, and Vincent Vigon.

[redacted]DESCRIPTION

We send an infrared light beam through an organ and we measure the signal on part of that organ. Knowing the initial conditions and the signal at all times, we can infer the influence of the organ's properties. Namely the influence of the density, the scattering opacity, and the absorption opacity. Using a P1 model for the radiative transfer equation (1), we will implement a splitting scheme to compute the signal's value (its evolution on the boundaries of the 1-dimensional domain, and the complete signal at the end of the simulation). Then we will visually inspect the data to understand the influence of the domain's properties on the signal.

1. Objectives

Main objective:

- Understand how the optical properties of an organ affect a signal traveling through it.

Specific Objectives:

- Describe the mathematical model for radiative transfer used.
- Numerically solve the model
- Analyse the data

2. Tasks

This is a nonexhaustive list of the tasks that were completed during the project.

- Read about the mathematical model to be used
- Implement the splitting scheme using a finite volumes method
- Run test cases
- Run benchmarking tests
- Analyse the model

3. Ressources

The choices made to use C++ to solve the RTE relies on it being a compiled progamming language, giving us more speed, which are critically important when doing the data dump. Python was chosen as the language for data visualization because it is the best for that. Ressources used are as follows:

- muParser library for parsing expressions into functions
- Computing power via Atlas is available at v100.math.unistra.fr
- Coogle Colab for bulk data visulisation in Python

4. Delivrables

What was be delivered at the end of this project are:

- A software named ***transfer*** that solves the numerical model
- A notebook that analyses meaningful trends in the data generated
- A typewritten report named **rapport_v1.pdf**
- A presentation named **presentation.pdf** (*yet to be completed*)

All these files can be found on the GitHub repository feelpp/csmi-m1-2020-moco-inverse along with instructions on how to run the software.

[redacted]ROADMAP

1. Mathematical basis

i. The radiative transfer equation (RTE)

Light traveling in a straight line through a medium interacts is modified and vice-versa:

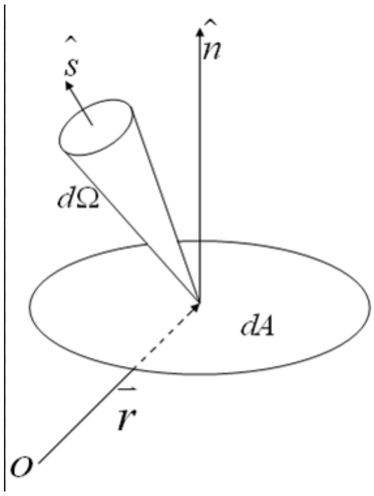
- Emission: photons of light are emitted as a result of electrons in the matter jumping to a less excited state. This phonome is characterized by the opacity of emission σ_e. It is the inverse of the mean length between two consecutive emissions. The matter loses energy to the light beam.
- Aboortion: photons are abosorbed by atoms and an electron (in an excite state is released). The matter is heated by this gain of energy.
- Scatering: Some photons are shifted from their direction. Energy is conserved in the traveling light beam.

These opacities depend on multiple parameters among which ρ, T and ν respectively defined as the density of the medium, the temperature, and the frequency of the photon interacted with.

We denote by $I(t, x, \Omega, \nu)$ the specific radiative intensity. As we can see, at any time t, it depends on 6 variables:

- 3 for the position x
- 2 for the direction of propagation on the photon Ω
- 1 more for the frequency of the photon ν

This quantity is proportianlly linked to the number of photons found at time t in the volume dx, having a frequency in the interval of length d\nu, and flowing in the solid angle $d\Omega$. (Turpault, 2003).



A good example of an homogenuous and isotropic intensity is given by Placks law:

$$B(\nu, T) = \frac{2h\nu^3}{c^2}\left[e^{\frac{h\nu}{kT}} - 1\right]^{-1}$$

Where h isPlanks constats, c is the speed of light and k is the Boltmann constant.

A few number of simplications still have to be made before we can write the equation we need. Namely that we are at the local thermodynamic equilibrium (LTE). That is, the local medium (around a phton)medium is at chemical and thermal equilibrium. In this state, the opacities $\sigma_e, \sigma_e, \sigma_e$ become function of only ρ and T.

Le'ts also define the radiative equilibrium, when the matter and the radiation are at equilibrium (namely T_radiation = T). In this latter state, photons are distributed according to Planck's function at the mediums temperature. Also

The radiative transfer equation is obtanined by making a summary with all the terms that affect the intensity of the light beam, at the microscopic level. We get (Franck, p.21):

$$\begin{aligned}\frac{1}{c}\frac{\partial}{\partial t} I(t, x, \Omega, \nu) + \Omega \cdot \nabla_{\mathrm{x}} I(t, x, \Omega, \nu) \\ = \sigma_a(\rho, \Omega, \nu)(B(\nu, T) - I(t, x, \Omega, \nu)\ ) \\ + \frac{1}{4\pi}\int_0^{\propto}\int_{S^2} \sigma_c(\rho, \Omega, \nu) p(\Omega' \rightarrow \Omega)\big(I(t, x, \Omega', \nu) - I(t, x, \Omega, \nu)\big)\, d\Omega' \mathrm{d\nu}\end{aligned}$$

(RTE)

In this equation, c is the speed of light, and p is the scatering's angular redistribution function. It is such that:

$$\oint p(\Omega' \rightarrow \Omega)\, d\Omega' = 1$$

It represents the probability of a photon being deviated from its origin direction Ω' into our direction of focus Ω.

In order to obtain a P1 model, we nee dto define 3 macroscopic quantities (the radiative energy, flux and pressure) respectively as follows (Franck, p.16):

$$E(t,x) = \int_0^{\infty} \frac{4\pi}{c} \int_{S^2} I(t,x,\Omega,\nu)\, d\Omega d\nu$$
$$F(t,x) = \int_0^{\infty} \frac{4\pi}{c} \int_{S^2} \Omega\, I(t,x,\Omega,\nu)\, d\Omega d\nu$$
$$P(t,x) = \int_0^{\infty} \frac{4\pi}{c} \int_{S^2} \Omega \otimes \Omega\, I(t,x,\Omega,\nu)\, d\Omega d\nu$$

By computing the moment of order 1 of the RTE and taking into account that:

- Planck function (B) 's flux is zero (since B is isotropic)
- B's integral on all frequencies ν equals aT^4 (a being the Stefan constant),

We also need to link to pressure to energy; we then get the P1 model (equations (1) and (2) below).

Since the radiation pehnomena alone doest not conserve energy, (1) and (2) need to be coupled with the evolution of the matter get the conservation of energy. Luckily, we are only interested in the effects of the radiation on the matter, therefore we only need not to consider terms that are not affected by the radiation. Remembering that the probability of a photon being emitted is the same as it being absorbed (i.e $\sigma_a = \sigma_e$ at LTE). This should give us equation (3):

$$\begin{cases} \partial_t E + c\partial_x F = c\sigma_a(aT^4 - E) & (1) \\ \partial_t F + \frac{c}{3}\partial_x E = -c\sigma_c F & (2) \\ \rho C_v \partial_t T = c\sigma_a(E - aT^4) & (3) \end{cases} \qquad \text{(P1)}$$

Where:

- a is the Stefan constant
- C_v is the thermal capacity of the medium
- c is the speed of light
- $T(t,x) > 0$ is the temperature of the medium
- $E(t,x) \in \mathbb{R}$ is the energy of the photons
- $F(t,x) \in \mathbb{R}$ is the flux of the photons
- $\rho(x) > 0$ is the density of the medium
- $\sigma_a(\rho,T) > 0$ is the absorption opacity
- $\sigma_c(\rho,T) > 0$ is the scattering opacity

b. Scheme's strnght

The P1 scheme has numerous advantages, it generalizes well under limiting conditions:

1. Transport limit

Ithe opacities are very weak, the photons travel thourgh the medium without any interaction. The P1 model has that property.

2. Diffusive limit

When the scattering opacity σ_c and the absorption opacity σ_a are high enough to be close to the speed of light c (which is far larger than the observed phenomenon's speed), the model in (1) is reduced to the following:

$$\partial_t(aT^4 + \rho C_v T) - \partial_x\left(\frac{c}{3\sigma_c}\partial_x aT^4\right) = O\left(\frac{1}{c}\right) \qquad (2)$$

This model is called the **diffusion approximation** (Franck, 2020, p.7). It matches a diffusion equation with a diffusion coefficient of $\frac{c}{3\sigma_c} \approx O(1)$. But more importantly, it gives us a good way of testing our program.

2. Solving the PDE with Finite Volumes

Due to the hyperbolic nature of the PDE (1), the constraints of our domain, and the need to deal with discontinuities, the **finite volumes** method is well suited to solving it. However, the well-known Rusanov scheme is not accurate enough, especially when the opacities are very high. Therefore, we will use a finite volume scheme with a splitting strategy (Franck, 2012, p. 160).

First, we must discretize our domain to form a mesh. Let a and b be the two real numbers such that $b > a$, and $N > 0$ an integer. We split the domain $[a, b]$ into N cells of equal length to obtain a uniform mesh. At the two edges, we add two "ghost" cells. In total, we have $N + 2$ cells. Let's denote by Δx the length of the intervals (the volume of the cells). For each cell $j \in [\![0, N + 1]\!]$, we write x_j its center, $x_{j-\frac{1}{2}}$ its left edge, and $x_{j+\frac{1}{2}}$ its right edge.

Next, we write the splitting scheme. Two steps are required here.

i. Step 1: The equilibrium part

We consider the "equilibrium" part of (1). That is, the photons are not moving, and we only take into account the relaxation terms in temperature (Franck, 2012, p. 160). This leads to all the terms with ∂_x in (1) to be equal to 0. The equation becomes:

$$\begin{cases} \partial_t E = c\sigma_a(aT^4 - E) \\ \partial_t F = 0 \\ \rho C_v \partial_t T = c\sigma_a(E - aT^4) \end{cases} \tag{3}$$

Writing $\Theta = aT^4$, we solve (3) on each independent cell. The numerical scheme is given below.

$$\begin{cases} \dfrac{E_j^{q+1} - E_j^n}{\Delta t} = c\sigma_a\left(\Theta_j^{q+1} - E_j^{q+1}\right) \\ \dfrac{F_j^{q+1} - F_j^n}{\Delta t} = 0 \\ \rho_j C_v \mu_q \dfrac{\Theta_j^{q+1} - \Theta_j^n}{\Delta t} = c\sigma_a(E_j^{q+1} - \Theta_j^{q+1}) \end{cases}$$

Rewritten as:

$$\begin{cases} E_j^{q+1} = \alpha E_j^n + \beta \Theta_j^{q+1} \\ F_j^{q+1} = F_j^n \\ \Theta_j^{q+1} = \gamma \Theta_j^n + \delta E_j^{q+1} \end{cases}$$

Applying Cramer's rule, we get:

$$\begin{cases} E_j^{q+1} = \dfrac{\alpha E_j^n + \beta\gamma\Theta_j^n}{1-\beta\delta} \\ F_j^{q+1} = F_j^n \\ \Theta_j^{q+1} = \dfrac{\gamma\Theta_j^n + \alpha\delta E_j^n}{1-\beta\delta} \end{cases} \tag{4}$$

Where

- E_j^n, F_j^n and Θ_j^n are the value values of E_j, F_j and Θ_j on the cell at the beginning of the step.
- $\alpha = \frac{1}{\Delta t}\left(\frac{1}{\Delta t} + c\sigma_a\right)^{-1}$, $\beta = c\sigma_a\left(\frac{1}{\Delta t} + c\sigma_a\right)^{-1}$, $\gamma = \frac{\rho_j C_v \mu_q}{\Delta t}\left(\frac{\rho_j C_v \mu_q}{\Delta t} + c\sigma_a\right)^{-1}$, and $\delta = c\sigma_a\left(\frac{\rho_j C_v \mu_q}{\Delta t} + c\sigma_a\right)^{-1}$
- σ_a written above is a function of ρ_j and T_j^n. Thus, it is actually $\sigma_a(\rho_j, T_j^n)$.
- μ_q is such that $\mu_q = \dfrac{1}{T^{3,n} + T^n T^{2,q} + T^q T^{2,n} + T^{3,q}}$

Since this step is a fixed point method, we iterate on q until we get close enough to the fixed point $(E_j^*, F_j^*, \Theta_j^*)$, or more precisely (E_j^*, F_j^*, T_j^*). We then move to the next step.

ii. Step 2: Solving the rest

Once the first step converges, we move to this step with the values of $E, F,$ and T on each cell updated. We write:

$$\begin{cases} \dfrac{E_j^{n+1} - E_j^*}{\Delta t} + c\dfrac{F_{j+\frac{1}{2}} - F_{j-\frac{1}{2}}}{\Delta t} = 0 \\ \dfrac{F_j^{n+1} - F_j^*}{\Delta t} + c\dfrac{E_{j+\frac{1}{2}} - E_{j-\frac{1}{2}}}{\Delta t} = cS_j \\ \rho_j C_v \mu_q \dfrac{T_j^{n+1} - T_j^*}{\Delta t} = 0 \end{cases} \tag{5}$$

With

$$F_{j+\frac{1}{2}} = M_{j+\frac{1}{2}}\left(\frac{F_{j+1}^n + F_j^n}{2} - \frac{E_{j+1}^n - E_j^n}{2}\right), \quad F_{j-\frac{1}{2}} = M_{j-\frac{1}{2}}\left(\frac{F_j^n + F_{j-1}^n}{2} - \frac{E_j^n - E_{j-1}^n}{2}\right)$$

$$E_{j+\frac{1}{2}} = M_{j+\frac{1}{2}}\left(\frac{E_{j+1}^n + E_j^n}{2} - \frac{F_{j+1}^n - F_j^n}{2}\right), \quad E_{j-\frac{1}{2}} = M_{j-\frac{1}{2}}\left(\frac{E + E_{j-1}^n}{2} - \frac{F_j^n - F_{j-1}^n}{2}\right)$$

$$S_j = -\frac{1}{2}\left(M_{j+\frac{1}{2}}\sigma_{j+\frac{1}{2}} + M_{j-\frac{1}{2}}\sigma_{j-\frac{1}{2}}\right)F_j^{n+1}$$

$$M_{j+\frac{1}{2}} = \frac{2}{2 + \Delta x \sigma_{j+\frac{1}{2}}}, \quad M_{j-\frac{1}{2}} = \frac{2}{2 + \Delta x \sigma_{j-\frac{1}{2}}}$$

$$\sigma_{j+\frac{1}{2}} = \frac{1}{2}\left(\sigma_c(\rho_j, T_j^n) + \sigma_c(\rho_{j+1}, T_{j+1}^n)\right), \quad \sigma_{j-\frac{1}{2}} = \frac{1}{2}\left(\sigma_c(\rho_{j-1}, T_{j-1}^n) + \sigma_c(\rho_j, T_j^n)\right)$$

We must also include the CFL condition below to ensure the scheme's stability.

$$\Delta t < \frac{\Delta x}{c}$$

We can rewrite (5) as:

$$\begin{cases} E_j^{n+1} = E_j^* - \mathrm{A}\left(F_{j+\frac{1}{2}} - F_{j-\frac{1}{2}}\right) \\ F_j^{n+1} = \mathrm{B}F_j^* - \Gamma\left(E_{j+\frac{1}{2}} - E_{j-\frac{1}{2}}\right) \\ T_j^{n+1} = T_j^* \end{cases} \tag{6}$$

With

$$\mathrm{A} = \frac{c\Delta t}{\Delta x}, \mathrm{B} = \frac{1}{\Delta t}\left(\frac{1}{\Delta t} + \frac{c}{2}\left(M_{j+\frac{1}{2}}\sigma_{j+\frac{1}{2}} + M_{j-\frac{1}{2}}\sigma_{j-\frac{1}{2}}\right)\right)^{-1} \text{ and } \Gamma = \frac{c}{\Delta x}\left(\frac{1}{\Delta t} + \frac{c}{2}\left(M_{j+\frac{1}{2}}\sigma_{j+\frac{1}{2}} + M_{j-\frac{1}{2}}\sigma_{j-\frac{1}{2}}\right)\right)^{-1}$$

Once all of this is done, we move back to step 1, then back to step 2 and so on until we reach a predefined time at which we want the solution.

3. Phase 2: Descriptive statistics

i. Step 1: Data analysis

After exporting the data from simulations in the previous step, we will need to study them using appropriate descriptive statistics tools. We will then have to find meaningful correlations between the variables. During this step, we will try to show the results that the neural network will later find by itself. The step will serve as a preparation for the AI training and predicting phase, to be completed during the internship.

b. Step 2: Finding the density

Here we will make the AI understand the trends we found in the previous step. Knowing not only the signals $E(t,x)$, $F(t,x)$, and $T(t,x)$ at all times, but also the scattering and absorption opacities ($\sigma_c(\rho,T)$ and $\sigma_a(\rho,T)$), we will rebuild the domain's density $\rho(x)$. We can see that the inputs for the neural network will be 2D tensors (indexed by t and x) while the output will be 1D (indexed only by x).

First, we will train and validate the neural network with the data obtained from solving the PDE (1) in the first phase. Second, we will test it hoping it generalizes well.

c. Step 3: The absorption and scattering opacities

This step is quite similar to the previous step with the only difference that we will be trying to predict $\sigma_c(\rho,T)$ and $\sigma_a(\rho,T)$ knowing $\rho(x)$ this time. However, it requires a more complex neural network.

Just as the previous step, this part is no longer part of the project, we will cover it during the internship.

[redacted]RESULTS

1. Test cases

a. Case 1: transport limit

b. Case 2: diffusion approximation

c. **Case 3: Olson-Auer-hall test case**

2. Dataframes

[redacted]BENCHMARKING

Ask if there are some enchmarking cases!

[redacted]MILESTONES CHECK

This section gives a summary for the roadmap, the objectives and the deadlines for the project. Original estimates are written in black, and actual tasks done and time spent are in red.

Milestone		Details	Tools needed	Deadline	Estimated number of hours	Actual number of hours
Understanding the model		We will seek to understand the PDE (1) and its numerical model on a slightly theoretical basis. This has already been done, but new information keeps coming every day.		April 2, 2020	8 hours	12 hours
Report version 0		A report indicating the context and the roadmap for the project. This milestone is currently under completion.	Microsoft Office Word	April 15, 2020	16 hours	
Phase 1: Finite Volumes	Solving the scheme	Using the finite volumes method in 1D, we need to solve the PDE (1). This has milestone has already been completed.	VS Code, GitHub, Eigen, Cparse	April 15, 2020	40 hours	
	Verification	Verify that the finite volume method is correctly implemented and solves a direct problem on a given domain. A good way to verify our splitting scheme is to test it on the diffusion approximation in (2). Tests will be put in place for continuous integration. We will need to find and correct all the bugs that appear in the code.	VS Code Matplotlib	April 29, 2020	16 hours	
	Benchmarking	Compare our algorithm to known solutions in order to optimize our code for speed. This step might be done multiple times depending on the changes we make to the algorithm during verification.	VS Code	April 29, 2020	4 hours	
	Validation	Making sure the problem solves the correct direct problems linked to medical tomography.	VS Code, Matplotlib	April 29, 2020	4 hours	

	Data export	Writing and running a script that exports thousands of instances of a correctly solved direct problem. We will make sure to export the data one state of the model at a time. This requires us to run the above-optimized program a great number of times, which is the reason we need to get it right on the first try.	Altas	May 5, 2020	8 hours	
Phase 2: Descriptive statistics	Studying the data	Using the exported data, we will seek to learn new information, finding interesting correlations, creating new variables, deleting outliers, cleaning out the data, and so on. During the internship, our goal will be to make the AI understand these correlations.	Pandas	May 19, 2020	24 hours	
	Verification	Verify that the model is properly studied. A positive indicator might be that when generating new instances of the data, we continue seeing the same trends.	Google Colab	May 19, 2020	16 hours	
	Validation	Check that the trends we find are effectively the trends from light spreading in medical tomography. We will compare our data trends to known databases in the same area of study.	Google Colab	May 19, 2020	4 hours	
	Benchmarking	Check that our algorithms for analysis are fast enough to be easily repeatable on other systems.	Google Colab	May 19, 2020	4 hours	
Report version 1		The task is to write a more complete version of the report.	MS Word	May 19, 2020	8 hours	
Report version 2		The final version of the report, incorporating corrections indicated by the supervisors.	MS Word	May 19, 2020	4 hours	
Presentation		A slideshow to be written in PowerPoint.	MS PowerPoint	May 19, 2020	8 hours	

This represents **164 hours** (approximately 7 full days) working on the project. Of course, these are just estimations and they will be appropriately adjusted in the following weeks to better fit the reality.

[redacted] CONLUSIONS

The project has let us to see how their ebergy is affected when photons travel thourgh a medium (test case 1 and 2). We have also been able to observe how the radiative temperature evolves as it travels through the medium at radiative equilibrium (test case 3). This gives us satifyng results to generate more data to train a neural network that will then predict the optical properties the medium.

However, this our numerical schem still depends on the P1 model for the radiative tranfer equation. While not costly and relatively easy to solve, a P1 model has amajor disadvantage: it only gives predictions when the anisotropy factor (normally) is reduced. Ie:

$$f = \frac{\|F\|}{eE} \leq \ 0.57 \qquad \text{normaly, we only have } f \leq 1$$

This shortcoming wil be addressed during an internship and other methods like Pn, or M1 will be tested..

[redacted] REFERENCES

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