University of Tartu
Faculty of Science and Technology
Institute of Mathematics and Statistics

Kristel Saul

Investigation of resolution bounds of muon scattering tomography

Mathematics

Bachelor's Thesis (9 ECTS)

Supervisors: Artem Aksonov, MSc

Ella Puman, PhD

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MÜÜONTOMOGRAAFIA LAHUTUSVÕIME HINDAMINE

Bakalaureusetöö

Kristel Saul

Lühikokkuvõte

Selles bakalaureusetöös uuritakse müüontomograafia lahutusvõimet. Kasutatakse kahte erinevat jaotust müüonite hajumisnurkade kirjeldamiseks: tavalist normaaljaotust ning liitjaotust, mis kaasab täiendavalt müüonite energiajaotuse. Kummagi jaotuse parameetrit hinnati suurima tõepära meetodil ja võrreldi saadud tulemusi. Tõenäosusjaotuse parameetri hinnangul leiti parandusparameetrid, mis võimaldavad täpsemini määrata hinnangu usaldusintervalli.

CERCS teaduseriala: P190 Matemaatiline ja üldine teoreetiline füüsika, klassikaline mehaanika, kvantmehaanika, relatiivsus, gravitatsioon, statistiline füüsika, termodünaamika

Märksõnad: müüontomograafia, suurima tõepära meetod, normaaljaotus, liitjaotus

INVESTIGATION OF RESOLUTION BOUNDS OF MUON SCATTERING TOMOGRAPHY

Bachelor thesis

Kristel Saul

Abstract

This thesis investigates the resolution bounds of muon scattering tomography, a non-destructive imaging technique utilizing atmospheric muons. We use two muon scattering angle distributions: a simple Gaussian and a compound probability distribution which incorporates the distribution of particle momentum. By employing the maximum likelihood method, we derive parameter estimators for both distributions. Moreover, we introduce first-order correction parameters for the distribution parameter estimator, improving the accuracy of parameter estimates.

CERCS research specialization: P190 Mathematical and general theoretical physics, classical mechanics, quantum mechanics, relativity, gravitation, statistical physics, thermodynamics

Key Words: muon tomography, maximum likelihood, Gaussian distribution, compound probability distribution

Contents

Introduction

This bachelor's thesis presents an investigation of the muon scattering angle distribution parameters and how it affects the resolution of muon tomography. Tomography is the imaging of an object by taking multiple projections of it from different directions. It is a widely used tool in modern medicine, but also in various other fields such as archeology, geology, and security. [6] Muon tomography is a novel imaging technique that uses cosmic ray muons for passive imaging. It involves placing muon detectors on opposite sides of the object to be imaged and measuring the number of muons that pass through the volume of interest (VOI) at different angles. By detecting the entry and exit points of muons, their tracks and scattering angles can be calculated. Scattering information can be used to reconstruct a 3D map of the scanned volume because the scattering angles are dependent on the traversed material. This is an interesting difference between muon tomography and other image reconstruction methods - the image to be reconstructed is contained in the variance of the measured data. One of the challenges lies in the natural origin of muons: the source is not monochromatic and is not a collimated parallel beam that is a normal setup for X-ray CT. Thus, direct borrowing of reconstruction methods leads to a high level of background noise. [13]

Muon scattering angle distribution (not to be confused with "angular distribution") is typically assumed to be Gaussian with zero mean and variance parameterized by the particle's momentum, although the empirical distribution has heavier tails. Previous studies have either crudely presumed a constant momentum for muons [13] and used ray displacement as an additional source of data [12] or combined several Gaussians to better approximate the actual distribution [16]. In this thesis, we are using the scattering angle data and as a new approach, we take the momentum distribution into consideration and investigate the variance of a compound probability distribution.

The thesis is organized as follows. The first chapter provides an overview of cosmic rays, muon interactions and review of previous work on the subject by Larry J. Schultz [13]. After describing the details of muon flux and scattering tomography, we present a detailed description of the problem to be solved. In the second chapter, important definitions and the methodology for the investigation are presented. The third chapter delves into the derivation of parameter estimators and the statistical properties of these estimators are studied. The fourth chapter presents a discussion of the results obtained in the investigation, including potential limitations and future research areas. Finally, the fifth chapter provides a summary of the work presented in the thesis.

1 Literature review

This chapter gives an overview of cosmic rays, muon flux properties and interactions with matter. We introduce the principles of muon tomography and present Larry J. Schultz's work on this topic. With this preliminary knowledge, we can formally pose the main problem that will be investigated in this thesis.

1.1 Cosmic Rays and Muon Interactions

Primary cosmic rays are mainly composed of stable particles such as protons and nuclei. When they enter Earth's atmosphere and interact with atoms there, short-lived secondary particles are created, which further decay into much longer-lived elementary particles muons (μ). [3] The muon flux rate at sea level is 10,000 particles per square meter per minute [1]. Muons can be thought of as "heavy electrons": they are charged, although the charge may be positive or negative, and with a mass of 105.7 MeV (megaelectronvolts) [9], they are approximately 200 times heavier than electrons (0.511 MeV). Muons are easily detectable due to their charge.

The energy spectrum and angles at which muons arrive on Earth's surface vary for several reasons. Solar activity, altitude and geolocation can affect the primary cosmic ray spectrum, influencing muon energy [8]. Particle energies range from 0.1 GeV to over 100 GeV with a mean of 3-4 GeV (gigaelectronvolts). This means that most muons can penetrate a meter of dense materials such as rock and metal, whereas high-energy muons can penetrate Earth's crust as deep as 10 km [15]. Energy distribution follows power law E^{-n} [14]. For low-energy particles, the probability density function of the momentum p is approximated as

$$f_p(x) = \begin{cases} \frac{C}{x}, & x \in [p_a, p_b], \\ 0, & \text{elsewhere}, \end{cases} \tag{1.1}$$

where $C = \frac{1}{\ln(p_b/p_a)}$ is the normalization constant and p_a, p_b are the corresponding momentum values for the suitable energy range.

There are two distinct ways muons interact with matter: energy loss through electromagnetic interaction and deflection due to multiple Coulomb scattering (illustrated in Figure 1). The nature of these interactions depends on the atomic number of the material. By measuring the magnitude of said interactions, it is possible to probe objects with muon flux and analyze the object's material composition. This is discussed in the next chapter. Multiple Coulomb scattering is mainly used for tomographic purposes. [13]

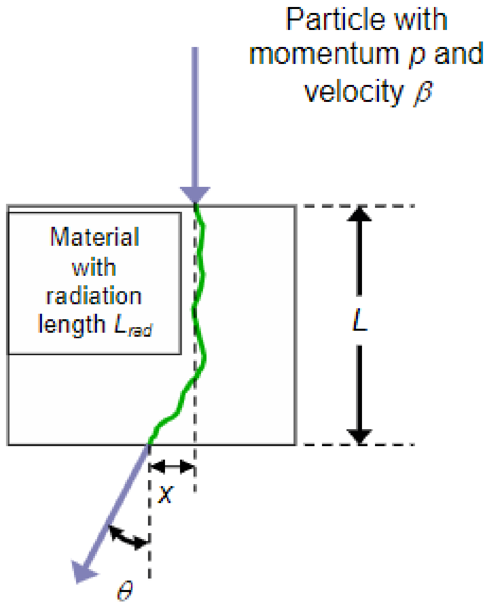

Figure 1: Multiple Coulomb scattering of a charged particle through a homogeneous material. The magnitude of scattering is exaggerated for illustrative purposes. [13]

Multiple Coulomb scattering is a phenomenon when a charged particle experiences small deviations on its path while traversing an object due to Coulomb interactions. The distribution of these scattering angles was approximated by Moliere as a zero mean Gaussian with a probability density function

$$f_\theta(x) \approx \frac{1}{\sqrt{2\pi\sigma_\theta^2}} \exp\Big(-\frac{x^2}{2\sigma_\theta^2}\Big) \tag{1.2}$$

for which the standard deviation is approximated to be

$$\sigma_\theta \approx \frac{15}{p}\sqrt{\frac{L}{L_{rad}}}. \tag{1.3}$$

Here L is the depth of the material, and L_{rad} is the radiation length of the material. Radiation length is a characteristic of a material. It is related to the energy loss of high-energy particles electromagnetically interacting with it. [7] These approximations result from particle physics, and the details are out of the scope of this thesis.

The magnitude of scattering angles is in milliradians (1 mrad $\approx 0.057°$): for a 3 GeV muon, the scattering angles in water and uranium are approximately 2.6 mrad and 28 mrad, respectively [13].

1.2 Muon tomography

Because of the muons' effective penetrating properties, the idea of muon tomography was born. One of the leading authors in muon tomography is Larry J. Schultz, whose PhD dissertation [13] is an important source for this thesis. Influenced by the formula (1.3), the scattering density λ of a material is defined as a function of radiation length

$$\lambda(L_{rad}) = \left(\frac{15}{p_0}\right)^2 \frac{1}{L_{rad}}, \tag{1.4}$$

which is essentially the mean square scattering angle of muons with nominal momentum p_0 passing through a unit depth of that material. Nominal momentum is a fixed value for particle momentum. In [13], a simplification is made, assuming that all muons have the same energy with $p_0 = 3$ GeV.

By combining equations (1.3) and (1.4), the variance of scattering angle θ can be represented as a function of scattering density

$$\sigma_\theta^2 = \lambda(L_{rad})L. \tag{1.5}$$

If the material depth L and scattering angle variance σ_θ^2 are known, equation (1.5) is just a linear equation, and the value of λ can be easily calculated. The main objective of muon tomography is to reconstruct the irradiated object inside the volume of interest (inside the scanner device) and determine its material composition. This can be done if the scattering density distribution in the volume of interest is known. For that, the volume of interest is discretized by dividing it into voxels (3D pixels) (Fig. 2a).

Inside each voxel, the material is assumed to be homogeneous (Fig. 2b). The optimal size of a voxel is another interesting topic, but we will not investigate it in this thesis and assume it to be appropriate. The relation (1.5) is now written for the j-th voxel as

$$\sigma_j^2 = \lambda_j L_{ij}, \tag{1.6}$$

where L_{ij} is the path length of i-th muon in j-th voxel. These equations form a system of linear equations. By solving this system and finding all λ_j values, a 3D scattering density map can be reconstructed, which gives us the desired image of the scanned object. For that, σ_j^2 values must be known. Maximum likelihood estimation is usually applied. Now, we can finally present the problem setup.

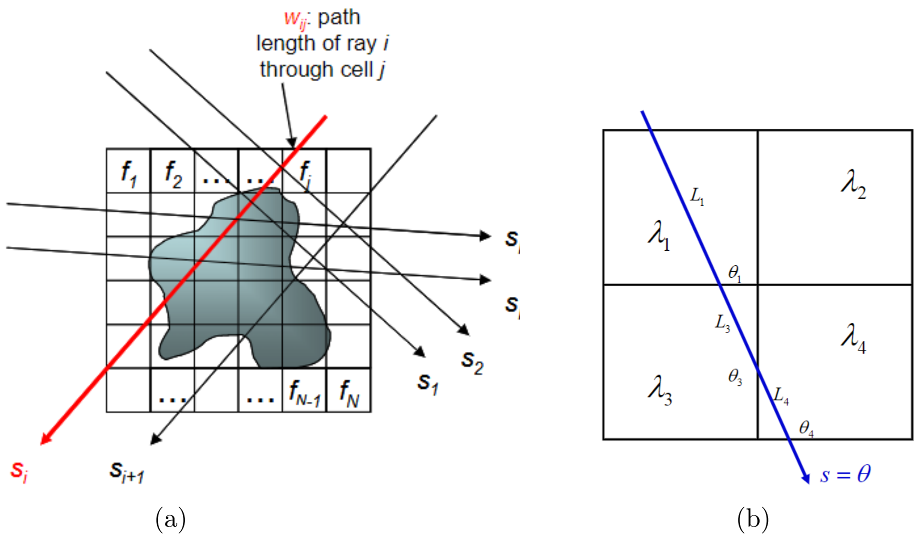

Figure 2: Discretized volume of interest. Slightly different notations are used for (a): w_{ij}, s_i and f_j correspond to L_{ij}, θ_i and λ_j, respectively. Subfigure (b) illustrates the ray's passage through the pixelized grid with different scattering densities and path lengths in each pixel. [13]

1.3 Problem setup

We start with the following conditions. We are given an $n \times n \times n$ volume of interest with a total number of elements $N = n^3$ that represent individual voxels and a set of "rays" (muons) that pass through the VOI. The number of rays is M. For each ray, there exists a nonempty set S_r of voxels that the r-th ray passes. Each ray can be represented as a random variable

$$\eta_r = \sum_{v \in S_r} \xi_v, \tag{1.7}$$

where ξ_v is the v-th individual voxel value. Random variables ξ_v are independent of each other, and they have Gaussian distribution that depends on material and energy spectrum

$$\sigma^2_{\xi_v} = \left(\frac{p_0}{p}\right)\sigma^2_{0\xi_v}. \tag{1.8}$$

Here, p_0 is nominal momentum, which would be the particle momentum when the source is monochromatic, and σ_0^2 is the nominal variance, a constant parameter for each voxel. We assume that the particle's momentum p is a random variable with a probability density function described in equation (1.1).

Recall that a charged particle experiences multiple stochastic scatterings. The precise location or the number of scattering events cannot be observed nor measured. Instead, by measuring the entering and exiting points (and directions) of a particle, the total scattering angle θ_i of

i-th muon can be calculated, which we consider to be the ray signal η_r. It is well-known that the sum of normally distributed independent random variables is also a normally distributed random variable with a mean and variance as the sum of its components means and variances. Since the voxel values ξ_v are normally distributed independent random variables, the sum (1.7) is also a normally distributed random variable with mean 0 and variance

$$\sigma_r^2 = \sum_{v \in S_r} \sigma_v^2, \tag{1.9}$$

where S_r is the set of voxels v that the r-th muon crosses.

The aim of this thesis is to investigate the statistical properties of muon scattering angle parameter $\sigma_{0\xi_v}^2$ estimates. This will be done through maximum likelihood method. We will not investigate the scattering density as it is done in Schultz's dissertation [13], but rather the variance since this is the source for estimating scattering densities. By understanding properties such as the expected value, variance, and confidence interval of the estimated variance $\hat{\sigma}_{0\xi_v}^2$, we can also estimate the resolution of the 3D density plot.

We assume the number of muons M is large enough for sufficient statistics. Before getting to the real-life scenario with a large number of voxels N, we first investigate the properties of σ_0^2 in the simple scenario where $N = 1$.

2 Methodology

This chapter serves as a foundation for the work that is done in the main chapter of this thesis. In order to understand the context and implications of the research question, it is essential to establish a common understanding of key terms and concepts. We present a series of propositions in this chapter that will guide the analysis and interpretation of the findings. By clarifying these concepts, this chapter aims to provide a clear framework for the research that follows. First, we introduce two important probability distributions: the well-known Gaussian distribution and the compound probability distribution.

2.1 Probability distributions

Definition 2.1. A random variable X is said to be *normally distributed* if it has a probability density function

$$f_X(x) = \frac{1}{\sqrt{2\pi}\sigma} e^{\frac{-(x-\mu)^2}{2\sigma^2}},$$

where $-\infty < x < \infty$, $-\infty < \mu < \infty$ and $\sigma > 0$. The parameters μ and σ^2 are the mean value and variance of X, respectively. This is also called the Gaussian distribution. [11]

Recall that the muon scattering angle distribution is approximated as a zero mean Gaussian, but with a variance that depends on a parameter that also has its own distribution. If we don't want to make the assumption that all muons have nominal momentum p_0, then we need a distribution that takes into account the momentum distribution.

Definition 2.2. Suppose we have a continuous random variable X with probability density function h, and that h is parameterized with p, which also has its own distribution g. We define the probability density function f of a *compound probability distribution* as

$$f_X(x) = \int_{-\infty}^{\infty} h_{X,p}(x,y) g_p(y) dy.$$

The idea behind this distribution is similar to marginalizing a joint probability distribution or creating a scale mixture model where h is the mixing distribution.

Proposition 2.1. Suppose we have a normally distributed random variable ξ with zero mean and parameterized variance $\sigma^2(p) = \frac{p_0^2\sigma_0^2}{p^2}$. Here p_0^2 and σ_0^2 are constants. If the distribution of parameter p is

$$g_p(y) = \begin{cases} \frac{C}{y}, & y \in [p_a, p_b], \\ 0, & \text{elsewhere}, \end{cases}$$

where C is the normalization constant $C = \frac{1}{\ln \frac{p_b}{p_a}}$ and $p_a > 0$, then the compound probability density function f is

$$f_\xi(x) = \int_{p_a}^{p_b} \frac{1}{\sqrt{2\pi\sigma^2(y)}} \exp\left(\frac{-x^2}{2\sigma^2(y)}\right) \frac{1}{\ln \frac{p_b}{p_a}} \frac{1}{y} dy = \frac{1}{\sqrt{2\pi} \ln \frac{p_b}{p_a} p_0 \sigma_0} \int_{p_a}^{p_b} \exp\left(- \frac{x^2 y^2}{2 p_0^2 \sigma_0^2}\right) dy. \tag{2.1}$$

Because the integral in equation (2.1) has finite bounds, we cannot express it with elementary functions [4]. Instead, this kind of integral can be asymptotically approximated by Laplace's method.

2.2 Moments of random variables

The investigation of statistical properties of probability distributions usually requires calculating the moments of random variables. Here, we give two important definitions which are taken from John Rice's book [11].

Definition 2.3. The *i-th moment* of a random variable X is

$$m_i = EX^i.$$

Definition 2.4. The *moment-generating function* of a random variable X is

$$M_X(t) = Ee^{tX}.$$

It can be used to calculate the i-th moment of X by taking the i-th derivative with respect to t and finding its value at $t = 0$:

$$EX^i = M_X^{(i)}(0).$$

Now we calculate the moment-generating functions for the two distributions that are important for our work.

Proposition 2.2. The moment-generating function of a normal random variable ξ with $\mu = 0$ and variance σ^2 is

$$M_\xi(t) = Ee^{t\xi} = \int_{-\infty}^{\infty} e^{tx} \frac{1}{\sqrt{2\pi\sigma^2}} e^{\frac{-x^2}{2\sigma^2}} dx = e^{\frac{\sigma^2 t^2}{2}}. \tag{2.2}$$

Proposition 2.3. The moment generating function of a random variable ξ with probability density function (2.1) is

$$M_\xi(t) = \int_{-\infty}^{\infty} e^{tx} \frac{1}{\sqrt{2\pi}\ln\frac{p_b}{p_a} p_0\sigma_0} \int_{p_a}^{p_b} \exp\left(-\frac{x^2y^2}{2p_0^2\sigma_0^2}\right) dydx = \tag{2.3}$$

$$\frac{1}{\sqrt{2\pi}\ln\frac{p_b}{p_a} p_0\sigma_0} \int_{p_a}^{p_b}\int_{-\infty}^{\infty} \exp\left(tx - \frac{x^2y^2}{2p_0^2\sigma_0^2}\right) dxdy = \tag{2.4}$$

$$\frac{1}{\ln\frac{p_b}{p_a}} \int_{p_a}^{p_b} \frac{1}{y} \exp\left(\frac{p_0^2\sigma_0^2t^2}{2y^2}\right) dy. \tag{2.5}$$

With these moment-generating functions at hand, we can find the formulas for the moments of a random variable, first with a normal distribution and then with the compound distribution. We start by calculating the derivatives of (2.2) and (2.5). For the normal distribution:

$$M_\xi''(t) = \sigma^2 e^{\frac{\sigma^2t^2}{2}}(\sigma^2t^2+1), \tag{2.6}$$

$$M_\xi^{(4)}(t) = \sigma^4 e^{\frac{\sigma^2t^2}{2}}(\sigma^4t^4+6\sigma^2t^2+3), \tag{2.7}$$

and so it is easy to see that the second and fourth moments are

$$E\xi^2 = \sigma^2, \tag{2.8}$$

$$E\xi^4 = 3\sigma^4. \tag{2.9}$$

Now, for the compound distribution. The first, second and fourth derivatives of (2.5) are

$$M_\xi'(t) = \frac{p_0^2\sigma_0^2}{\ln\frac{p_b}{p_a}} \int_{p_a}^{p_b} \frac{t}{y^3} \exp\left(\frac{p_0^2\sigma_0^2t^2}{2y^2}\right) dy, \tag{2.10}$$

$$M_\xi''(t) = \frac{p_0^2\sigma_0^2}{\ln\frac{p_b}{p_a}} \int_{p_a}^{p_b} \exp\left(\frac{p_0^2\sigma_0^2t^2}{2y^2}\right)\left(\frac{1}{y^3} + \frac{p_0^2\sigma_0^2t^2}{y^5}\right) dy, \tag{2.11}$$

$$M_\xi^{(4)}(t) = \frac{p_0^2\sigma_0^2}{\ln\frac{p_b}{p_a}} \int_{p_a}^{p_b} \exp\left(\frac{p_0^2\sigma_0^2t^2}{2y^2}\right)\left(\frac{p_0^2\sigma_0^2t}{y^5} + \frac{p_0^4\sigma_0^4t^3}{y^7} + \frac{2p_0^2\sigma_0^2}{y^5}\right) dy. \tag{2.12}$$

The corresponding moments can be easily found:

$$E\xi = M_\xi'(0) = 0, \tag{2.13}$$

$$E\xi^2 = M_\xi''(0) = \frac{p_0^2\sigma_0^2}{\ln\frac{p_b}{p_a}} \int_{p_a}^{p_b} \frac{1}{y^3} dy = \frac{p_0^2\sigma_0^2}{2\ln\frac{p_b}{p_a}}\left(\frac{1}{p_a^2} - \frac{1}{p_b^2}\right), \tag{2.14}$$

$$E\xi^4 = M_\xi^{(4)}(0) = \frac{p_0^2\sigma_0^2}{\ln\frac{p_b}{p_a}} \int_{p_a}^{p_b} \frac{2p_0^2\sigma_0^2}{y^5} dy = \frac{p_0^4\sigma_0^4}{2\ln\frac{p_b}{p_a}}\left(\frac{1}{p_a^4} - \frac{1}{p_b^4}\right). \tag{2.15}$$

These calculations will be useful later when we have figured out the estimator of the muon scattering angle distribution parameter. This will be done using the maximum likelihood method.

2.3 Maximum likelihood estimator

The following definitions are also from Rice's book [11].

Definition 2.5. The *likelihood function* of a parametric model $\{f(x|\theta) : \theta \in \Omega\}$ with given observed values $X_1, \ldots, X_n$ is

$$L(\theta) = \prod_{i=1}^{n} f(X_i|\theta).$$

The *maximum likelihood estimator* (MLE) of θ is the value of $\hat{\theta} \in \Omega$ that maximises $L(\theta)$. Often the *log-likelihood function*

$$l(\theta) = \ln L(\theta) = \sum_{i=1}^{n} \ln f(X_i|\theta)$$

is used since it is easier to work with a sum than with a product.

Definition 2.6. An estimator $\hat{\theta}$ for a parameter θ is said to be *unbiased* when

$$E\hat{\theta} = \theta.$$

Definition 2.7. An estimator based on a sample size of n $\hat{\theta_n}$ for a parameter θ is said to be *consistent* if $\hat{\theta_n}$ converges in probability

$$\hat{\theta_n} \to \theta \text{ as } n \to \infty.$$

Definition 2.8. The *Fisher information* of a random variable's parameter is the variance of the partial derivative of log-likelihood θ

$$I(\theta) = -E\left(\frac{\partial^2}{\partial\theta^2} l(X|\theta)\right) = -\frac{1}{n} E(l''(\theta)).$$

Essentially, it describes how much information a random variable carries about its parameter.

Proposition 2.4. The Fisher information can be used to find the *Cramer-Rao lower bound* for the variance of an unbiased parameter estimator $\hat{\theta}$ as

$$D(\hat{\theta}) \geq \frac{1}{nI(\theta)} = -\frac{1}{E(l''(\theta))}.$$

When the variance of an estimator reaches the lower bound, the estimator is said to be *efficient*.

Proposition 2.5. The $100(1-\alpha)\%$ confidence interval for maximum likelihood estimator is

$$\hat{\theta} \pm \bar{z}_{\frac{\alpha}{2}} \left(\frac{1}{\sqrt{nI(\hat{\theta})}} \right) \tag{2.16}$$

where $\hat{\theta}$ is the estimator, n is the number of observations and $I(\hat{\theta})$ is the Fisher information of the estimator.

Some of these definitions and propositions can be generalized to multivariate cases. When the estimated parameter is $\vec{\theta} \in \mathbb{R}^k$, then the log-likelihood function will be

$$l(\vec{\theta}) = \ln L(\vec{\theta}) = \ln \prod_{i=1}^{n} f(X_i|\vec{\theta}) = \sum_{i=1}^{n} \ln f(X_i|\vec{\theta}).$$

2.4 Asymptotic approximations for integrals

We have already seen how prevalent are the integrals of e^{-x^2} (or some similar forms of it). There are a few special occasions where there exist elegant solutions. These integrals are listed in the table [17]. We will present some of them here as well.

$$\int_{-\infty}^{\infty} e^{-ax^2} dx = \sqrt{\frac{\pi}{a}}, \tag{2.17}$$

$$\int_{-\infty}^{\infty} x^2 e^{-ax^2} dx = \frac{1}{2}\sqrt{\frac{\pi}{a^3}}, \tag{2.18}$$

$$\int_{-\infty}^{\infty} e^{-ax^2-2bx} dx = \sqrt{\frac{\pi}{a}} e^{\frac{b^2}{a}}, \tag{2.19}$$

where the constant a is positive.

With finite bounds, these integrals cannot be expressed with elementary functions. A way to deal with them is using Laplace's method.

Proposition 2.6. Suppose we want to approximate the integral

$$\int_{a}^{b} e^{kf(x)} dx,$$

where $f(x)$ is a twice differentiable function with a maximum at x_0, $k > 0$ and the bounds a, b can be finite or infinite. Laplace's method suggests we find the Taylor series of $f(x)$ around x_0. It is usually sufficient to drop the terms after the second-order term. [5]

Two cases should be considered: one where $x_0 \in [a, b]$ (local maximum) and one where it is outside of the bounds (global maximum). If x_0 is inside the bounds then the first-order term disappears and, according to [2], we get the approximation

$$\int_a^b e^{kf(x)} dx \approx e^{kf(x_0)} \int_{-\infty}^{\infty} \exp\left(\frac{k}{2} f''(x_0)(x - x_0)^2\right) dx. \tag{2.20}$$

If x_0 falls outside of the bounds, then the maximum is equal to either a or b and thus the first-order term in the Taylor series does not disappear. Therefore the approximation formula is

$$\int_a^b e^{kf(x)} dx \approx e^{kf(x_0)} \int_{-\infty}^{\infty} \exp\left(kf'(x_0)(x - x_0) + \frac{k}{2} f''(x_0)(x - x_0)^2\right) dx. \tag{2.21}$$

3 Results

This chapter is organized as follows. In the first subchapter, we analyze the scenario of multiple rays M crossing one voxel. First, we assume the distribution of scattering angles to be just Gaussian and calculate the estimator for the parameter σ^2. Then, we attempt to find the parameter estimator using the compound probability distribution (2.1). This will be done using the maximum likelihood method. In the second subchapter, we generalize to the real-life scenario where the number of voxels N is also large and arrive at a system of equations to find estimators for each voxel's parameter. The results we obtain will be discussed in the next chapter. The tools for the work done here were presented in Chapter 2.

3.1 One voxel scenario

We first analyze the simple scenario of M rays crossing just one voxel, meaning there is only one parameter σ^2 to be estimated and $\eta_r = \xi_1$.

3.1.1 Maximum likelihood estimator using Gaussian distribution

We start with the Gaussian distribution. If we have M rays measurements x_r, we can construct the likelihood function

$$L(\sigma^2) = \prod_{r=1}^{M} P(x_r|\sigma^2) = \prod_{r=1}^{M} \frac{1}{\sqrt{2\pi\sigma^2}} e^{-\frac{x_r^2}{2\sigma^2}} = \left(\frac{1}{\sqrt{2\pi\sigma^2}}\right)^M \exp\left(\frac{-1}{2\sigma^2}\sum_{r=1}^{M} x_r^2\right) \tag{3.1}$$

and the log-likelihood is therefore

$$l(\sigma^2) = \ln L(\sigma^2) = -\frac{M}{2}\ln 2\pi\sigma^2 - \frac{1}{2\sigma^2}\sum_{r=1}^{M} x_r^2. \tag{3.2}$$

To find the value for σ^2 that maximizes expression (3.2), the derivative with respect to σ^2 must be taken

$$l'(\sigma^2) = -\frac{M}{2\sigma^2} + \frac{1}{2\sigma^4}\sum_{r=1}^{M} x_r^2, \tag{3.3}$$

set equal to zero and then the estimator can be expressed as

$$\hat{\sigma}^2 = \frac{1}{M}\sum_{r=1}^{M} x_r^2. \tag{3.4}$$

This estimator result is well-known and can be easily analyzed. If we assume that we can replicate the measurement of x_r-s - that number of muons is always M, that each muon arrives with the same energy and with the same direction in each experiment, but scatters randomly in the voxel - it means that our estimator becomes a random variable itself. Because of this, the values x_r now behave as random variables, too. And since we have only one voxel, we can say that $x_r = \xi_1$. This means that we can calculate the expected value and variance of $\hat{\sigma}^2$.

First, we find the expected value:

$$E(\hat{\sigma}^2) = E\Big(\frac{1}{M}\sum_{r=1}^{M} x_r^2\Big) = \frac{1}{M}\sum_{r=1}^{M} E(x_r^2) = \frac{1}{M}\sum_{r=1}^{M} E(\xi_1^2) = E(\xi_1^2). \tag{3.5}$$

Using equation (2.8) for the second moment, we receive

$$E(\hat{\sigma}^2) = E(\xi_1^2) = \sigma^2, \tag{3.6}$$

meaning that the estimator is unbiased. The variance of parameter estimator $\hat{\sigma}^2$ is

$$D(\hat{\sigma}^2) = E(\hat{\sigma}^2)^2 - (E(\hat{\sigma}^2))^2 = E\Big(\frac{1}{M}\sum_{r=1}^{M} x_r^2\Big)^2 - \sigma^4. \tag{3.7}$$

The expected value of the sum squared term needs to be analyzed on its own:

$$E\Big(\frac{1}{M}\sum_{r=1}^{M} x_r^2\Big)^2 = D\Big(\frac{1}{M}\sum_{r=1}^{M} x_r^2\Big) + \Big(E\Big(\frac{1}{M}\sum_{r=1}^{M} x_r^2\Big)\Big)^2 =$$
$$\frac{1}{M^2}\sum_{r=1}^{M} D(x_r^2) + \Big(\frac{1}{M}\sum_{r=1}^{M} E(x_r^2)\Big)^2 =$$
$$\frac{1}{M^2}\sum_{r=1}^{M}\big(E(\xi_1^4) - E(\xi_1^2)^2\big) + \frac{1}{M^2}\big(\sum_{r=1}^{M} D\xi_1\big)^2 =$$
$$\frac{1}{M}(E\xi_1^4 - \sigma^4) + \frac{1}{M^2}(M\sigma^2)^2 = \frac{1}{M}E\xi_1^4 - \frac{1}{M}\sigma^4 + \sigma^4.$$

Using equation (2.9), we receive

$$D\hat{\sigma}^2 = \frac{1}{M}3\sigma^4 - \frac{1}{M}\sigma^4 + \sigma^4 - \sigma^4 = \frac{2}{M}\sigma^4. \tag{3.8}$$

3.1.2 Confidence intervals for the maximum likelihood estimator

To find confidence intervals (uncertainty) for the estimated $\hat{\sigma}^2$ value we use the formula (2.16) from a previous chapter. First, the Fisher information (recall definition 2.8) of σ^2 needs to be calculated. For that, we take the second derivative of equation (3.2) with respect to σ^2

$$l''(\sigma^2) = \frac{M}{\sigma^4} - \frac{3}{\sigma^6}\sum_{r=1}^{M} x_r^2 \tag{3.9}$$

and find the expected value of that expression

$$E\big(l''(\sigma^2)\big) = E\Big(\frac{M}{\sigma^4}\Big) - E\Big(\frac{3}{\sigma^6}\sum_{r=1}^{M} x_r^2\Big) = \frac{M}{\sigma^4} - \frac{3M}{\sigma^6}E\xi_1^2 = \frac{-2M}{\sigma^4}. \tag{3.10}$$

The Fisher information of $\hat{\sigma}^2$ is

$$I(\hat{\sigma}^2) = \frac{2}{\sigma^4} \tag{3.11}$$

and the Cramer-Rao lower bound is therefore

$$D\hat{\sigma}^2 \geq \frac{\sigma^4}{2M}. \tag{3.12}$$

As we saw from the variance calculations in equation (3.8), this lower bound is reached. Finally, the 95% confidence interval for the parameter estimator is

$$\hat{\sigma}^2 \pm \frac{1.96\sigma^2}{\sqrt{2M}}. \tag{3.13}$$

3.1.3 Maximum likelihood estimator using compound probability distribution

In the first subchapter, we derived a new probability density function that incorporates momentum distribution. The next attempt is to get similar results to what we obtained for a simple Gaussian distribution. First, we make use of the compound distribution in the form of equation (2.1) and construct the likelihood function to estimate nominal variance σ_0^2:

$$L(\sigma_0^2) = \prod_{r=1}^{M} \frac{1}{\sqrt{2\pi}\ln\frac{p_b}{p_a}p_0\sigma_0}\int_{p_a}^{p_b} \exp\Big(-\frac{x^2y^2}{2p_0^2\sigma_0^2}\Big)dy =$$
$$\left(\frac{1}{\ln\frac{p_b}{p_a}\sqrt{2\pi p_0^2\sigma_0^2}}\right)^M \prod_{r=1}^{M}\int_{p_a}^{p_b} \exp\Big(-\frac{x^2y^2}{2p_0^2\sigma_0^2}\Big)dy.$$

The log-likelihood is therefore

$$l(\sigma_0^2) = M \ln \left(\frac{1}{\sqrt{2\pi p_0^2 \sigma_0^2}} \frac{1}{\ln \frac{p_b}{p_a}} \right) + \sum_{r=1}^{M} \ln \int_{p_a}^{p_b} \exp\left(-\frac{x_r^2 y^2}{2p_0^2\sigma_0^2} \right) dy = \tag{3.14}$$

$$-\frac{M}{2} \ln 2\pi p_0^2 \sigma_0^2 - M \ln \ln \frac{p_b}{p_a} + \sum_{r=1}^{M} \ln \int_{p_a}^{p_b} \exp\left(-\frac{x_r^2 y^2}{2p_0^2\sigma_0^2} \right) dy. \tag{3.15}$$

We continue by taking the derivative of this with respect to σ_0^2. In equation (3.17), we change the order of differentiation and integration. This can be done because we are differentiating and integrating with respect to different variables and the bounds are constant [10]. The likelihood function is

$$l'(\sigma_0^2) = -\frac{M}{2\sigma_0^2} + \sum_{r=1}^{M} \frac{d}{d\sigma_0^2} \ln \int_{p_a}^{p_b} \exp\left(-\frac{x_r^2 y^2}{2p_0^2\sigma_0^2} \right) dy = \tag{3.16}$$

$$-\frac{M}{2\sigma_0^2} + \sum_{r=1}^{M} \frac{1}{\int_{p_a}^{p_b} \exp\left(-\frac{x_r^2 y^2}{2p_0^2\sigma_0^2} \right) dy} \int_{p_a}^{p_b} \frac{d}{d\sigma_0^2} \exp\left(-\frac{x_r^2 y^2}{2p_0^2\sigma_0^2} \right) dy = \tag{3.17}$$

$$-\frac{M}{2\sigma_0^2} + \frac{1}{2p_0^2\sigma_0^4} \sum_{r=1}^{M} x_r^2 \frac{\int_{p_a}^{p_b} y^2 \exp\left(-\frac{x_r^2 y^2}{2p_0^2\sigma_0^2} \right) dy}{\int_{p_a}^{p_b} \exp\left(-\frac{x_r^2 y^2}{2p_0^2\sigma_0^2} \right) dy}. \tag{3.18}$$

Both of these integrals under the sum cannot be expressed with elementary functions, but they can be estimated using Laplace's method (see Proposition 2.6). However, preliminary bounds for that expression can be found like this:

$$p_a^2 \leqslant y^2 \leqslant p_b^2,$$

$$p_a^2 e^{-cy^2} \leqslant y^2 e^{-cy^2} \leqslant p_b^2 e^{-cy^2},$$

$$\int_{p_a}^{p_b} p_a^2 e^{-cy^2} dy \leqslant \int_{p_a}^{p_b} y^2 e^{-cy^2} dy \leqslant \int_{p_a}^{p_b} p_b^2 e^{-cy^2} dy,$$

$$p_a^2 \leqslant \frac{\int_{p_a}^{p_b} y^2 e^{-cy^2} dy}{\int_{p_a}^{p_b} e^{-cy^2} dy} \leqslant p_b^2.$$

Therefore, for every ray r there exists some value $p_r \in [p_a, p_b]$ such that

$$p_r^2 = \frac{\int_{p_a}^{p_b} y^2 e^{-cy^2} dy}{\int_{p_a}^{p_b} e^{-cy^2} dy}. \tag{3.19}$$

Here we have made the reasonable assumption that $p_a \geqslant 1$, we know that $e^{-cy^2} \geqslant 0$ (where $c = \frac{x_r^2}{2p_0^2\sigma_0^2}$) and that it is integrable. Using this we arrive at a compact formula for the derivative of the log-likelihood function

$$l'(\sigma_0^2) = -\frac{M}{2\sigma_0^2} + \frac{1}{2p_0^2\sigma_0^4}\sum_{r=1}^{M} x_r^2 p_r^2. \tag{3.20}$$

We set this equal to zero and get an estimation for parameter

$$\hat{\sigma_0}^2 = \frac{1}{p_0^2 M}\sum_{r=1}^{M} x_r^2 p_r^2. \tag{3.21}$$

Notice that if p_r is equal to nominal momentum, this estimator would be the same as in equation (3.4). The value p_r can be thought of as the "weight" of the r-th ray. It's interesting that it is dependent not only on the ray it itself, but also on the voxel it traverses. The expected value and variance of $\hat{\sigma_0}^2$ should be calculated similarly as it was done previously:

$$E(\hat{\sigma_0}^2) = E\left(\frac{1}{p_0^2 M}\sum_{r=1}^{M} x_r^2 p_r^2\right) = \frac{1}{p_0^2 M}\sum_{r=1}^{M} E(x_r^2 p_r^2), \tag{3.22}$$

$$D(\hat{\sigma_0}^2) = D\left(\frac{1}{p_0^2 M}\sum_{r=1}^{M} x_r^2 p_r^2\right) = \frac{1}{p_0^4 M^2}\sum_{r=1}^{M} D(x_r^2 p_r^2). \tag{3.23}$$

Because x_r and p_r are not independent random variables, the expected value and variance of their product are not trivial to calculate. We can see from equation (3.19) that the "weights" p_r are also dependent on voxel values through σ_0^2. Therefore, we continue as follows.

- Find the zero-order approximation for $\hat{\sigma_0}^2$ from equation (3.4).
- Use that value to calculate ray "weights" p_r with (3.19). Laplace's method can be used. Two cases must be considered: one where the maximum lies inside the given bounds and one where it is outside of the bounds.
- Use the received p_r values as correction parameters to the $\hat{\sigma_0}^2$ value with equation (3.21) and receive the first-order approximation.

This process could be iterated several times to find better estimations for σ_0^2, but we stop at the first-order approximation and continue analyzing the received estimator's expected value and dispersion. If we assume that we have the values of p_r and since we're dealing with one voxel scenario ($\eta_r = \xi_1$) we can move further in the equations (3.22) and (3.23):

$$E(\hat{\sigma_0}^2) = \frac{E\xi_1^2}{p_0^2 M} \sum_{r=1}^{M} p_r^2, \tag{3.24}$$

$$D(\hat{\sigma_0}^2) = \frac{D\xi_1^2}{p_0^4 M^2} \sum_{r=1}^{M} p_r^4 = \frac{E\xi_1^4 - \left(E\xi_1^2\right)^2}{p_0^4 M^2} \sum_{r=1}^{M} p_r^4 \tag{3.25}$$

Using equations (2.14) and (2.15) for the moments, we find that

$$E(\hat{\sigma_0}^2) = \frac{\sigma_0^2}{2M \ln \frac{p_b}{p_a}} \left(\frac{1}{p_a^2} - \frac{1}{p_b^2} \right) \sum_{r=1}^{M} p_r^2, \tag{3.26}$$

$$D(\hat{\sigma_0}^2) = \frac{\sigma_0^4}{2M \ln \frac{p_b}{p_a}} \left(\frac{1}{p_a^4} - \frac{1}{p_b^4} - \frac{1}{2 \ln \frac{p_b}{p_a} p_a^4} + \frac{1}{2 \ln \frac{p_b}{p_a} p_b^4} + \frac{2}{\ln \frac{p_b}{p_a} p_a^2 p_b^2} \right) \sum_{r=1}^{M} p_r^4. \tag{3.27}$$

3.2 Multiple voxel scenario

In this subchapter, we generalize the previous cases to a multiple voxel scenario.

3.2.1 Maximum likelihood estimator using Gaussian distribution

In [13], the scattering density values are estimated through maximum likelihood estimation. The conditional probability of the r-th muon with respect to parameter σ_r^2 is

$$P_{\eta_r}(x_r|\sigma_r^2) = \frac{1}{\sqrt{2\pi\sigma_r^2}} e^{-\frac{x_r^2}{2\sigma_r^2}}, \tag{3.28}$$

where σ_r^2 is defined by equation (1.9). Since all muons are independent random variables, the likelihood function is constructed as a product of M normal probability density functions, all with different parameters

$$L_{\vec{\eta}}(\vec{x}|\vec{\sigma}^2) = \prod_{r=1}^{M} \frac{1}{\sqrt{2\pi\sigma_r^2}} e^{-\frac{x_r^2}{2\sigma_r^2}}. \tag{3.29}$$

By taking the log of both sides, the log-likelihood function is obtained:

$$l_{\vec{\eta}}(\vec{x}|\vec{\sigma}^2) = -\frac{1}{2} M \ln(2\pi) - \frac{1}{2} \sum_{i=1}^{M} \left(\ln \sigma_r^2 + \frac{x_r^2}{\sigma_r^2} \right). \tag{3.30}$$

From here, Schultz starts to work with scattering densities as they are connected through equation (1.5), but we are interested in finding confidence intervals for the voxel parameters

σ_v^2-s. Instead, we substitute σ_r^2-s with equation (1.9) and arrive at the equation

$$l(\vec{x}|\vec{\sigma}^2) = -\frac{1}{2}M\ln(2\pi) - \frac{1}{2}\sum_{r=1}^{M}\Big(\ln\sum_{v\in S_r}\sigma_v^2 + \frac{x_r^2}{\sum\limits_{v\in S_r}\sigma_v^2}\Big). \tag{3.31}$$

Recall that the set S_r contains all voxels that the r-th ray traverses. To find the maximum likelihood estimate, the gradient of equation (3.31) has to be taken:

$$\nabla l(\vec{x}|\vec{\sigma^2}) = \Big(\frac{\partial l(\vec{x}|\vec{\sigma^2})}{\partial\sigma_1^2},\ldots,\frac{\partial l(\vec{x}|\vec{\sigma^2})}{\partial\sigma_N^2}\Big) \tag{3.32}$$

and set equal to zero, meaning that each component is equal to zero. Now let's define R_v as the set of all rays that cross the v-th voxel. The k-th component of the gradient is

$$\frac{\partial}{\partial\sigma_k^2}\Big(-\frac{1}{2}\sum_{r=1}^{M}\Big(\ln\sum_{v\in S_r}\sigma_v^2 + \frac{x_r^2}{\sum\limits_{v\in S_r}\sigma_v^2}\Big)\Big) = -\frac{1}{2}\sum_{r\in R_k}\frac{\partial}{\partial\sigma_k^2}\Big(\ln\sum_{v\in S_r}\sigma_v^2 + \frac{x_r^2}{\sum\limits_{v\in S_r}\sigma_v^2}\Big) = \tag{3.33}$$

$$-\frac{1}{2}\sum_{r\in R_k}\Big(\frac{1}{\sum\limits_{v\in S_r}\sigma_v^2} - \frac{x_r^2}{\Big(\sum\limits_{v\in S_r}\sigma_v^2\Big)^2}\Big). \tag{3.34}$$

By going under the sum with the partial derivative operator, we reduce the number of summands and sum only over the rays that cross the k-th voxel (and therefore contribute to the value of σ_k^2). By switching back to σ_r^2 notation and setting the gradient components (3.33) equal to zero we obtain

$$\sum_{r\in R_k}\left(\frac{x_r^2}{\sigma_r^4} - \frac{1}{\sigma_r^2}\right) = 0. \tag{3.35}$$

To verify that this is indeed the right expression, we check if it holds for the one voxel scenario. Then $S_r = 1$, $R_k = M$ and the left side of expression (3.35) takes the form

$$\sum_{r=1}^{M}\Big(\frac{x_r^2}{\sigma^4} - \frac{1}{\sigma^2}\Big) = \frac{1}{\sigma^4}\sum_{r=1}^{M}x_r^2 - \frac{M}{\sigma^2}. \tag{3.36}$$

By setting this equal to zero and then multiplying both sides with $\frac{\sigma^4}{M}$, the same expression as (3.4) is obtained

$$\hat{\sigma}^2 = \frac{1}{M}\sum_{r=1}^{M}x_r^2. \tag{3.37}$$

The investigation of equation (3.35) and deriving formulas for parameter estimator is not a trivial task and will not be done in this thesis. Therefore, we will also not include the maximum likelihood estimator calculations for a multiple voxel scenario with compound probability distribution since it requires further knowledge of solving systems of non-linear equations. This is an area of future research.

4 Discussion

In Chapter 3, we used the maximum likelihood method to analyze the statistical properties of the muon scattering angle distribution parameter. The one voxel scenario with Gaussian distribution gives a preliminary idea of the confidence interval for the parameter estimator. The interval becomes narrower when the number of muons increases. This means that more precise results can be obtained with a longer exposition time. However, since the relation is $\frac{1}{\sqrt{M}}$, it must be kept in mind that for a 10 times better resolution (going from 1 cm resolution to 1 mm resolution for example), the exposure time has to be a 100 times longer. This is one of the limitations of using cosmic radiation for tomographic purposes and drives the research for different approaches. When analyzing the multiple voxel scenario, we arrived at a system of non-linear equations. We did not solve the system for estimators of individual voxel values, but we validated that the system is correct by checking whether it holds for the one voxel scenario.

As for the results regarding the compound probability distribution, we only presented results for the one voxel scenario. We found out that each ray contributes differently to the estimator, and that the correction parameters ("weights") p_r depend both on x_r-s and σ_0^2. We presented an iterative method to find the first-order approximation for σ_0^2 estimator. If the "weights" are calculated, for example with Laplace's method, the expected value and variance of parameter estimator $\hat{\sigma_0}^2$ could be found. The analysis of multiple voxel scenario, both with Gaussian distribution and compound distribution, is currently out of the scope of this thesis and needs more knowledge on the topic of solving systems of non-linear equations.

If we compare the expected values of $\hat{\sigma_0}^2$ (Equations (3.8) and (3.23)), we see that for the Gaussian distribution, we have an unbiased estimator, but with the compound distribution, the estimator is biased. To find the confidence interval of a biased estimator, the bias correction must first be done. Since the estimator has "weights" p_r (defined by Equation (3.19)) which we cannot calculate precisely, but could estimate with Laplace's method, the confidence interval for the parameter is expected to be even wider. This is also subject to future research.

Conclusion

In this thesis, we have investigated the statistical properties of muon scattering angle distribution parameter σ_0^2. Two different scenarios were considered - multiple rays crossing one voxel and multiple voxels. We started by considering a single Gaussian distribution to model the voxel values in an imaging system. We derived a maximum likelihood estimator for the parameter, σ_0^2, and calculated its expected value and dispersion in the one voxel scenario. The results demonstrated that the estimator is unbiased and consistent.

To improve the accuracy of our estimations, we incorporated momentum distribution and developed a compound probability density function. We derived a maximum likelihood estimator for σ_0^2 and obtained similar results to those for the simple Gaussian distribution. We also proposed a method to iteratively refine the estimation of σ_0^2 by considering ray correction parameters, p_r, which depend on both the ray itself and the voxel it traverses. This was also done in the one voxel scenario.

To find parameter σ_v^2 estimations in the real-life scenario with multiple voxels, we derive a system of non-linear equations. The solution for that requires additional knowledge on the topic.

We have taken important steps that open up new possibilities for future research. One key area to explore is extending the results we found for the estimator with compound probability distribution to situations involving multiple voxels. This would help us better understand the resolution of muon tomography systems, which was the main goal of this thesis. We have laid the groundwork for this kind of research. Moreover, by developing faster algorithms for the iterative process and testing our methods on real-world data, we can make our research more relevant for practical applications.

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