Development of a Markov chain Monte Carlo imaging algorithm for muon tomography

Pierre-Luc Drouin
DRDC – Ottawa Research Centre

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Abstract

The detection of Special Nuclear Material (SNM) represents one of the greatest challenges for radiation and nuclear defence, due to the very low emission of gamma rays and neutrons from Highly Enriched Uranium (HEU). Muon tomography systems constitute a promising avenue for SNM detection. These systems use measurements of muon deflection inside the analysed volume to estimate the scattering density of a set of voxels defined within this volume. In this document, a Bayesian model suitable to be used with a Markov Monte Carlo algorithm is investigated.

Significance for defence and security

Muon Tomography (MT) systems represent a promising technology for Special Nuclear Material detection. MT has the advantage of being a passive detection technique that can comply with the treaties for the non-proliferation of nuclear weapons. This report investigates a new algorithm which aims at measuring the scattering density of the material scanned by such a system. In the future, a muon tomography system could be used by the Canadian Armed Forces to scan suspect packages for SNM. Hardware and software development is currently ongoing at DRDC – Ottawa Research Centre.

Résumé

La détection de matières nucléaires spéciales (MNS) représente un des plus grands défis pour la défence dans le domaine du rayonnement et du nucléaire en raison du très faible taux d'émission de rayons gamma et de neutrons par l'uranium hautement enrichi (UHE). Les systèmes de tomographie muonique constituent une avenue prometteuse pour la détection des MNS. Ces systèmes utilisent des mesures de déviation de muons à l'intérieur du volume analysé afin d'estimer la densité de diffusion d'un ensemble de voxels tels que définis à l'intérieur de ce volume. Dans ce document, un modèle bayésien adapté pour être utilisé avec un algorithme Monte Carlo de Markov est étudié.

Importance pour la défense et la sécurité

Les systèmes de tomographie muonique (TM) représentent une technologie prometteuse pour la détection des matières nucléaires spéciales. La TM a l'avantage d'être une méthode de détection passive qui peut satisfaire les traités de non-prolifération des armes nucléaires. Ce rapport porte sur un nouvel algorithme qui permet de mesurer la densité de diffusion dans la matière analysée par un tel système. Dans le futur, un système de tomographie muonique pourrait être utilisé par les Forces armées canadiennes afin d'analyser des colis suspects pouvant contenir des MNS. Le développement de matériel et de logiciels est en cours au RDDC – Centre de recherches d'Ottawa.

Table of contents

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1 Introduction

In [1], a summary of the Metropolis-Hastings Markov chain Monte Carlo (MCMC) algorithm was presented and it was shown how such an algorithm can be used to sample the Probability Density Function (PDF) of the parameter space associated to an evaluated model. Because MCMC algorithms can be particularly well-suited for models that contain multiple parameters, including latent (hidden) variables, this class of algorithms is expected to be a good candidate for a muon tomography application, where one wants to estimate the scattering density of voxels inside a volume, based on the measured deflection of cosmic ray muons that scatter at unknown locations.

Other types of algorithms used for muon tomography include Point of Closest Approach (PoCA) [2, 3], Maximum Likelihood Expectation Maximisation (MLEM) [4, 5, 6, 7] and Maximum A Posteriori (MAP) [8, 9]. With the PoCA method, scattering density is estimated through the computation of a scattering angle distribution for each voxel, where a voxel is assigned to an event when the midpoint of the shortest segment linking the incoming and outgoing muon tracks (the point of closest approach) falls within that voxel. PoCA is thus a relatively simple method which is easily computable, but which assumes single muon scatter within the analysed volume. MLEM and MAP models are not based on this assumption and both aim at determining the most likely scattering densities. However, they do not provide a mechanism to evaluate parameter uncertainties. By contrast, MCMC can generate distributions for all parameters, including latent variables, which can then be used to compute desired estimator distributions.

2 Development of a general probability density function for muon tomography

As described in [1], a MCMC algorithm allows to sample the parameter space from a PDF $f(\vec{\theta}|\text{sample})$, where $\vec{\theta}$ is the set of parameters which characterise the model and whose probability space is constrained by a measured sample. In the case of a static scenario, where a parameter ν, part of $\vec{\theta}$, is used to represent the expected number of measured events for a sample which is collected during a fixed amount of time, the number of measured events is Poisson-distributed with a mean given by ν.

Let us define a muon tomography system where muon position and direction is measured when the particles enter and leave the analysed volume. The volume is divided into a set of voxels whose scattering densities[1] are estimated through the measurements of muon scatters. We define the set of model parameters $\vec{\theta}$ as

$$\vec{\theta} \equiv \left(\vec{\phi}, \nu, \vec{\Theta}\right), \tag{1}$$

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[1] The scattering density depends on both the density and the Z number of the material causing the scattering.

where $\vec{\phi}$ contains all voxel scattering densities, ν is the expected number of analysed muons and where $\vec{\Theta}$ contains all muon positions, directions and energies for all defined track segments for all analysed events. If the set of measured positions and directions for all analysed muons is provided by $\vec{\mu}$, $f(\vec{\theta}|\text{sample})$ can be expressed as

$$\begin{aligned} f(\vec{\theta}|\text{sample}) =& f(\vec{\phi},\nu,\vec{\Theta}|\vec{\mu}) \\ =& f(\nu|\vec{\phi},\vec{\Theta},\vec{\mu})f(\vec{\phi},\vec{\Theta}|\vec{\mu}) \\ =& f(\nu|n_{\text{events}})\frac{f(\vec{\mu}|\vec{\phi},\vec{\Theta})f(\vec{\phi},\vec{\Theta})}{f(\vec{\mu})} \\ =& f(\nu|n_{\text{events}})f(\vec{\mu}|\vec{\Theta})f(\vec{\Theta}|\vec{\phi})\frac{f(\vec{\phi})}{f(\vec{\mu})}, \end{aligned} \tag{2}$$

where n_{events} is provided by the number of events in $\vec{\mu}$ and where $f(\vec{\mu}|\vec{\Theta})$ is provided by the position and angular resolution of the apparatus. The dependence of the PDF $f(\vec{\mu}|\vec{\phi},\vec{\Theta})$ on $\vec{\phi}$ was dropped because the measured positions and orientations solely depend on the initial and final track segments as defined through $\vec{\Theta}$. In a scenario where significant material is located between the voxelised volume and the locations of position and orientation measurements, extra voxels with defined and fixed scattering densities can be added for proper modeling. The PDF $f(\vec{\Theta}|\vec{\phi})$ evaluates the probability density for all muon tracks through the detector, while $f(\vec{\phi})$ and $f(\vec{\mu})$ are prior PDFs. As explained in [1], the Metropolis-Hastings algorithm is insensitive to a scaling parameter that does not depend on the sampled parameters, such that the $f(\vec{\mu})$ can be ignored. However, it is not the case for $f(\vec{\phi})$, which can be used to define an expected scattering density configuration for the analysed volume.

In this section, an exact muon tomography parameter space PDF expression suitable for the Metropolis-Hastings algorithm has thus been derived, which can be expressed as

$$f(\vec{\phi},\nu,\vec{\Theta}|\vec{\mu}) \propto f(\nu|n_{\text{events}})f(\vec{\mu}|\vec{\Theta})f(\vec{\Theta}|\vec{\phi})f_{\text{p}}(\vec{\phi}), \tag{3}$$

where a subscript was added to identify the scattering density prior PDF. In the above expression, ν and $\vec{\Theta}$ represent nuisance parameters, as $\vec{\phi}$ is ultimately the only parameter of interest. However, the $\vec{\phi}$ distribution is easily obtained, as it is provided by simply considering this parameter in the reduced Markov chain resulting from the Metropolis-Hastings algorithm, which is equivalent to computing the marginal PDF for $\vec{\phi}$. In the next section, an expression for the $f(\vec{\Theta}|\vec{\phi})$ muon track PDF is developed.

3 Development of the muon track PDF

In the previous section, $\vec{\Theta}$ was defined as a parameter that contains all muon positions, directions and energies for all defined track segments for all analysed events. If it is now subdivided in a set of Θ subcomponents as

$$\vec{\Theta} \equiv (\Theta_1, \Theta_2, \ldots, \Theta_{n_\text{events}}), \tag{4}$$

one for each event. Since these parameters are only correlated with $\vec{\phi}$, the $f(\vec{\Theta}|\vec{\phi})$ PDF can be rewritten as

$$f(\vec{\Theta}|\vec{\phi}) = \prod_{e=1}^{n_\text{events}} f(\Theta_e|\vec{\phi}), \tag{5}$$

where $f(\Theta|\vec{\phi})$ is the muon track PDF for a given event. The Θ subcomponents are then further divided as

$$\Theta \equiv \left(\vartheta_0, \vartheta_1, \ldots, \vartheta_{n_\text{seg.}}\right), \tag{6}$$

where ϑ_0 and $\vartheta_{n_\text{seg.}}$ are the initial muon positions, directions and energies at the entrance and at the exit of the voxelised space, respectively, and where $n_\text{seg.}$ is the number of muon track segments used in the model. For a given analysed muon event, the $f(\Theta|\vec{\phi})$ PDF can thus be expressed as

$$\begin{aligned} f(\Theta|\vec{\phi}) =& f(\vartheta_0|\vec{\phi}) f(\vartheta_1|\vec{\phi}, \vartheta_0) f(\vartheta_2|\vec{\phi}, \vartheta_0, \vartheta_1) \cdots f(\vartheta_{n_\text{seg.}}|\vec{\phi}, \vartheta_0, \ldots, \vartheta_{n_\text{seg.}-1}) \\ =& f_\text{p}(\vartheta_0|\vec{\phi}) \prod_{j=1}^{n_\text{seg.}} f(\vartheta_j|\vec{\phi}, \vartheta_{j-1}), \end{aligned} \tag{7}$$

where the second line was obtained after noticing that the PDF for a given muon track segment depends only on the state of the immediately preceding segment, and where a subscript was used to indicate that $f_\text{p}(\vartheta|\vec{\phi})$ is a prior PDF for the incident state of the muon when entering the voxelised space. From Equations (5) and (7), the muon track PDF can thus be expressed as

$$f(\vec{\Theta}|\vec{\phi}) = \prod_{e=1}^{n_\text{events}} f_\text{p}(\vartheta_{0e}|\vec{\phi}) \prod_{j=1}^{n_\text{seg.}} f(\vartheta_{j_e}|\vec{\phi}, \vartheta_{j-1_e}). \tag{8}$$

4 Expansion of the muon measurement PDF

The parameterisation defined in the previous section can be used to expand and simplify the $f(\vec{\mu}|\vec{\Theta})$ PDF. If $\vec{\mu}$ is expressed as

$$\vec{\mu} \equiv \left(\mu_{\text{i}1}, \mu_{\text{f}1}, \ldots, \mu_{\text{i}n_\text{events}}, \mu_{\text{f}n_\text{events}}\right), \tag{9}$$

where μ_{i_e} and μ_{f_e} are the measured initial and final states for the analysed muon e, respectively, then $f(\vec{\mu}|\vec{\Theta})$ is given by

$$\begin{aligned} f(\vec{\mu}|\vec{\Theta}) &= \prod_{e=1}^{n_\text{events}} f(\mu_{\text{i}e}, \mu_{\text{f}e}|\Theta_e) \\ &= \prod_{e=1}^{n_\text{events}} f(\mu_{\text{i}e}|\vartheta_{0e}) f(\mu_{\text{f}e}|\vartheta_{n_\text{seg.}e}), \end{aligned} \tag{10}$$

because of the statistical independence of the different analysed events and because the measured initial and final states are independent, given that true initial and final states are known.

5 An expanded expression for the general muon tomography PDF

Combining Equations (3), (8) and (10), a general expression for a muon tomography PDF suitable to be used with a Markov chain Monte Carlo technique has thus been found to be given by

$$f(\vec{\phi},\nu,\vec{\Theta}|\vec{\mu}) \propto f(\nu|n_{\text{events}}) f_{\text{p}}(\vec{\phi}) \times \prod_{e=1}^{n_{\text{events}}} f(\mu_{\text{i}_e}|\vartheta_{0e}) f(\mu_{\text{f}_e}|\vartheta_{n_{\text{seg.}}e}) f_{\text{p}}(\vartheta_{0e}|\vec{\phi}) \prod_{j=1}^{n_{\text{seg.}}} f(\vartheta_{j_e}|\vec{\phi},\vartheta_{j-1_e}), \quad (11)$$

where $f_{\text{p}}(\vec{\phi})$ and $f_{\text{p}}(\vartheta_0|\vec{\phi})$ are prior PDFs for voxel scattering densities and initial muon states, respectively. If there is prior knowledge of the analysed volume, the information can thus be provided through $f_{\text{p}}(\vec{\phi})$, or a flat prior could be otherwise used. In the case of $f_{\text{p}}(\vartheta_0|\vec{\phi})$, the dependence on $\vec{\phi}$ arises only through the dependence of muon acceptance on the analysed volume scattering density. For applications where this dependence is weak, then

$$f_{\text{p}}(\vartheta_0|\vec{\phi}) \approx f_{\text{p}}(\vartheta_0). \quad (12)$$

Typically, the $f_{\text{p}}(\vartheta_0)$ PDF could be expressed as

$$f_{\text{p}}(\vartheta_0) = f_{\text{p}}(E_0) f_{\text{p}}(\vec{x}_0,\vec{u}_0|E_0), \quad (13)$$

where $\vec{x}_0$, $\vec{u}_0$ and E_0 are the initial muon position, direction and energy when entering the voxelised volume, respectively, that is

$$\vartheta_0 \equiv (\vec{x}_0,\vec{u}_0,E_0). \quad (14)$$

Also, the $f_{\text{p}}(E_0)$ energy prior would be provided through the knowledge of the energy spectrum of the muons incident on the detector, with some possible distortion due to an energy dependence of the muon acceptance. On the other hand, the $f_{\text{p}}(\vec{x}_0,\vec{u}_0|E_0)$ prior would strongly depend on the detector geometry, in addition to the spatial distribution of the incident muons.

In Equation (11), the $f(\mu_{\text{i}}|\vartheta_0)$ and $f(\mu_{\text{f}}|\vartheta_{n_{\text{seg.}}})$ PDFs are provided through the characterisation of the detector's position and angular resolutions, while $f(\nu|n_{\text{events}})$ is the Poisson PDF. The remaining PDF, $f(\vartheta_j|\vec{\phi},\vartheta_{j-1})$ is to be provided from a scattering model, which is discussed in the next section.

6 Muon scattering model

In order to estimate voxel scattering densities, muon tomography requires the reconstruction of the analysed muon tracks. The model that was elaborated in the previous sections relies on the computation of a muon scatter PDF, $f(\vartheta_j|\vec{\phi},\vartheta_{j-1})$, to accomplish this task. This PDF must provide the following information:

- the distribution of scatter angle,
- the distribution of lateral displacement for the muon, and
- the energy loss associated to the muon propagation.

Most simulation algorithms use multiple scattering theories from Molière [10], Goudsmit and Saunderson [11], and Lewis [12]. Although these methods provide scatter angle distributions, none of them provide the required lateral displacement distribution. A popular formula for the width of a Gaussian approximation has been provided by Highland [13] and Lynch and Dahl [14], which is recommended in the Review of Particle Physics [15]:

$$\theta_0 = \frac{13.6\,\mathrm{MeV}}{\beta c p} z\sqrt{x/X_0}\Big[1 + 0.038\log(x/X_0)\Big], \tag{15}$$

where βc, p, z and x/X_0 are the velocity, the momentum, the charge number of the incident particle and the thickness of the scattering medium in radiation lengths, respectively. In addition to the Gaussian approximation which can lead to poor accuracy in some cases, this equation was formulated for a model where the scatter particles are perpendicularly incident on a medium of constant thickness. This model is not the most appropriate for muon tomography, where muons are modeled to scatter while traveling through a voxelised space. These muons are thus incident on the individual voxels at different angles, and they are likely to exit some voxels from a side which is not parallel to the side where they penetrated.

A more appropriate multiple scattering model developed by L. Urbán [16] is described in the Physics Reference Manual for Geant4 [17]. This model uses the true path length of the scattered particle to provide a non-Gaussian angular distribution $g(u)$ (where $u \equiv \cos\theta$ and θ is the scatter angle), an expression for the average lateral displacement, the lateral correlation for this displacement and an expression to convert the geometrical path length to the expected true path length. Although [17] provides sufficient information for a general understanding of the model used by Geant4, there are discrepancies between the model described in the document and the implementation of the algorithm in the Geant4 code (it seems the implemented algorithm was subjected to some improvements, which are not captured in the document). The currently implemented algorithm should thus be used as a basis for the calculation of the muon scatter PDF.

7 Looking forward

Throughout this document, a Bayesian model for muon tomography suitable for a Metropolis-Hastings MCMC algorithm, such as described in [1], has been derived. This model was designed using minimal approximations and naturally allows for the full propagation of the incident muon source and detector uncertainties. By their nature, MCMC algorithms are well suited for problems that involve large number of nuisance parameters, such as the muon paths and their true initial and final states. Parameter transition PDFs are not uniquely defined though, and there is freedom in defining the algorithm that performs parameter updates. Mixed sampling schemes can also be used, using a combination of Metropolis-Hastings and Gibbs sampling, for example. Different MCMC advanced ideas are discussed in [18]. During the further development of a MCMC-based muon tomography algorithm, the optimisation of the parameter transition PDF and sampling schemes will be important to ensure proper convergence step acceptance rates. Proper tuning of these components should reduce computation time by orders of magnitude. Nonetheless, extensive optimisation within the implementation of the algorithm is expected, and it is anticipated that an implementation of the algorithm for a GPU architecture will be required to lower the computation time sufficiently.

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