Source term estimation via combined sparse convex optimization and maximum likelihood estimation for nuclear material accounting

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ABSTRACT

In this work we investigate the use of sparse convex optimization and maximum likelihood estimation for the specific problem of source term estimation for neutron sources. We simulate an experimental set up at Los Alamos National Laboratory (LANL), consisting of an array ^{3}He neutron detectors located in glove boxes containing nuclear materials of variable intensity and number. We demonstrate that under the correct conditions, the location, strength and number of sources can be recovered via this method, without prior knowledge of the number of sources present in the experiment. We investigate the effect of background strength, detector configuration, and optimization constraints on the robustness of the solutions obtained via our algorithm.

1. INTRODUCTION

In this paper we investigate the use of sparse convex optimization and maximum likelihood estimation (MLE) for source term estimation, or the estimation of the location and intensity of a radioactive source. Knowing the intensity of a radioactive source can provide information about the isotopic composition of material present. The motivation for this work is the application of a developed methodology to an experimental test bed at Los Alamos National Laboratory (LANL), which we refer to in this manuscript as the "DYMAC room". This set-up consists of an array of 16 ^{3}He detectors located within four glove boxes that can contain nuclear material of varying intensity and number. The problem of source localization in this context is crucial to nuclear material control and accounting (NMC&A) programs that track and verify the presence of specific nuclear material. The problem of source-term estimation is particularly challenging due to the sparsely situated detectors, and the fact that in the presence of multiple radiation sources, the radiation count at a given sensor is the sum of the contributions from all existing sources, leading to identifiabilty considerations. We note that all results in this manuscript are simulation based.

There exist several approaches to this problem: least squares,[1,2] genetic algorithms,[3] as well as Bayesian methods such as particle filtering.[4,5] Least squares and other gradient based methods suffer from the drawback that solutions may converge at local minima due to the non-convex nature of the problem. Heuristic optimization methods on the other hand are computationally expensive and thus not particularly suited to applications that aim to be "real-time".[6] Bayesian methods provide a simplistic probabilistic approach which aims to maximize the likelihood probability of measurement data; however, these do not directly address the source *number* estimation problem and may also be extremely sensitive to initial conditions. Ristic *et al.* propose the utilization of model selection criteria such as the Bayesian Information Criterion (BIC)[7] whereby models with different numbers of sources are compared in terms of both their accuracy and complexity in order to best select the number of sources.

Lee *et al.*[6] propose a two-step algorithm consisting of sparse convex optimization and then MLE in order to solve the source-term estimation problem. In this work we investigate the suitability of this method in solving the source-term estimation problem for the specific test bed configuration shown in Figure 1, with four glove boxes and sixteen total detectors, one on each corner of the globe boxes. We also investigate the effects of number of sources, source intensity strength, sampling time, and background effects on the methodology, as it applies to an analogous to DYMAC room simulated test bed.

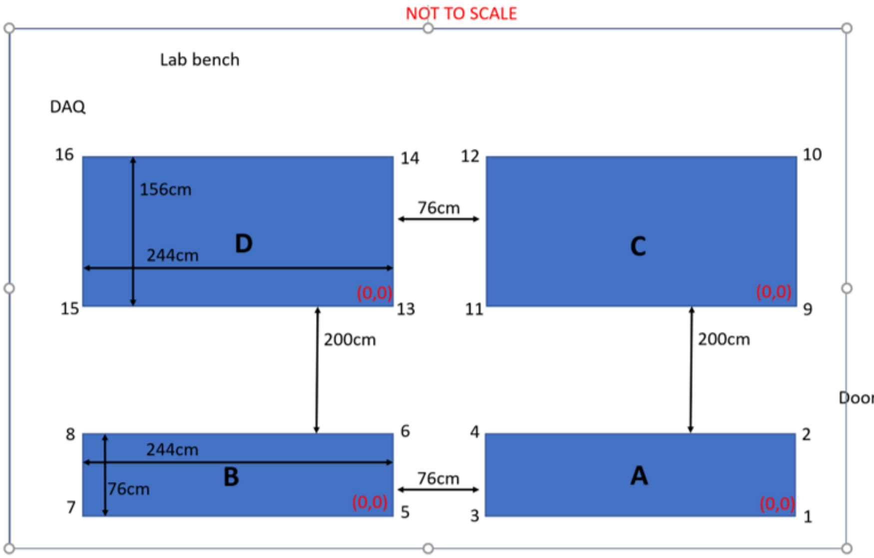

Figure 1: DYMAC room. Letters designate the glove boxes, and the numbers on the corners of the glove boxes represent the location of the 16 sensors.

2. METHODS

2.1 Sensor Model

The sensor model formulation for this work is described by Lee *et al.*[6] as follows: the mean radiation count b_j at a given location (x_j, y_j) is determined by the inverse-squared distance law to be:

$$b_j = \sum_{k=1}^{N_s} \frac{\omega_k}{(x_k - x_j)^2 + (y_k - y_j)^2} + \omega_0 \tag{1}$$

where N_s is the number of sources, x_k, y_k are the coordinates of the k^{th} source with intensity ω_k and ω_0 is the background radiation. We can model a sensor measurement from this mean radiation count, and because we can model the radiation counts with a Poisson distribution, the variance is equal to the mean value (b_j). Let $\mathbf{z}_j = (z_{j,1}, z_{j,2}, \ldots, z_{j,m})$ be a vector of measurements from a stationary sensor from time $t = 1, 2, \ldots m$. As we are assuming that each of the m measurements are independent, the joint likelihood function at location j can be written as

$$p(\mathbf{z}_j | b_j) = \prod_{i=1}^{m} e^{-b_j} \frac{b_j^{z_j^i}}{z_j^i!} \tag{2}$$

where m is the number of measurements. Thus the source-term estimation problem is formulated as finding the set of source parameters (x_k, y_k, ω_k) and the number of sources N_s which maximize $p(\mathbf{z}_j | b_j)$ for all sensors, simultaneously.

2.2 Sparse Convex Optimization

In order to reduce this problem to a sparse convex optimization problem, Lee *et al.* exploit the fact that the sensor model described in Eq.1 is linear with source intensity, ω_k. We can model the DYMAC room as a discrete grid of N points, where each grid point is the potential location of a source. In addition we can compile the observations from the $M = 16$ sensors into $\mathbf{b}$, which is of dimension 16×1 and model the observed data at a given time point as

$$\mathbf{b} = \mathbf{A}\Omega + \omega_{\mathbf{0}} \tag{3}$$

where Ω is an $N \times 1$ vector describing the source strengths at the N grid points and the observation matrix $\mathbf{A}$ is an $M \times N$ matrix that describes the contributions of potential sources at locations on the discretized grid to the set of sensors.

$$\mathbf{A} = \begin{bmatrix} \frac{1}{(x_1^G - x_1)^2 + (y_1^G - y_1)^2} & \cdots & \frac{1}{(x_N^G - x_1)^2 + (y_N^G - y_1)^2} \\ \vdots & \ddots & \vdots \\ \frac{1}{(x_1^G - x_M)^2 + (y_1^G - y_M)^2} & \cdots & \frac{1}{(x_N^G - x_M)^2 + (y_N^G - y_M)^2} \end{bmatrix} \tag{4}$$

Since we expect there to be far fewer sources than grid points, Ω is a sparse vector: the majority of its entries are zero. Note that in the case of a distributed source, i.e., a source that covers multiple grid points, this assumption of sparsity would not hold. Since Ω cannot be uniquely determined from $\mathbf{b}$ (there are infinitely many Ω which can satisfy Eq.3), we define the best solution as one which achieves the optimal trade off between the sparsity of Ω and the residual of $\mathbf{A}\Omega + \omega_{\mathbf{0}} - \mathbf{b}$. In effect we are looking for the solution containing the fewest number of sources which still satisfactorily fits Eq.3. Thus the sparse convex optimization problem for source-term estimation follows the formulation

$$\hat{\Omega} = \min_{\Omega} \|\mathbf{D}\Omega\|_1 \tag{5}$$

$$\text{subject to } \mathbf{A}\Omega = \mathbf{b} - \omega_{\mathbf{0}} \tag{6}$$

$$\Omega \geq 0 \tag{7}$$

where $\mathbf{D}$ is a diagonal matrix of the 2-norms of the columns of $\mathbf{A}$, such that the formulation conforms to that suggest by Candès.[8] In order to enhance the sparsity of the solution, we follow the reweighted ℓ_1 minimization procedure suggested by Candès et al[9] and utilized specifically for the source-term estimation problem by Lee *et al.*[6] We refer throughout the rest of this manusciprt to this sparse convex optimization problem as SCOP.

2.3 Maximum Likelihood Estimation

An observation to make concerning the algorithm described in 2.2 is that the accuracy of estimation is bound by the resolution of the grid chosen. The method used in this paper further refines the original estimates of the source locations (and source intensities) by using MLE. For this problem formulation, we refer back to the joint likelihood described in Eq.2: we seek to find the parameter vector $\boldsymbol{\theta}$, size N_s (the number of sources), containing the locations and strengths of the sources which maximises the likelihood described in Eq.2 for each sensor:

$$\hat{\boldsymbol{\theta}}_{MLE} = \arg\max_{\hat{\boldsymbol{\theta}}} \; \log[p(\mathbf{z}|\boldsymbol{\theta})] = \arg\min_{\hat{\boldsymbol{\theta}}} \{-\log p(\mathbf{z}|\boldsymbol{\theta})\} \tag{8}$$

where $\mathbf{z}$ corresponds to the vector of measurements collected by the sensors. In this optimization problem we impose the constraint that the source strengths should be non-negative. In this work we implement the MLE problem in the JULIA programming language[10] , and the optimization problem is solved using the IPOPT solver.[11]

3. RESULTS

3.1 Small Test Case

We first begin with a smaller, representative test case in order to examine the suitability of the SCOPMLE method for source term estimation. We reduce the DYMAC room to a 41 × 41 grid, with 16 detectors placed in 10 × 10 glovebox corners, as shown in Figure 2. The sensor readings are then simulated by sampling a Poisson distribution as described in Eq.2. Unless otherwise stated, for the sake of computational ease the experiments described in this section will be based on variations of this test case.

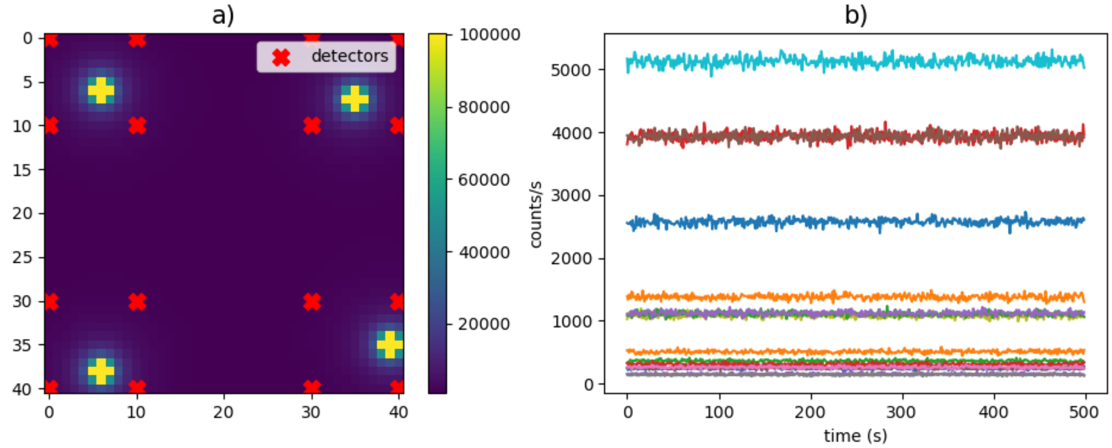

Figure 2: a) Test case (41×41 grid) with four 10^5 counts/s sources (yellow crosses) placed in four glove boxes with 16 detectors (red x's). b) 16 sensor readings, generated by sampling from a Poisson distribution.

3.2 Number of sources

We first perform an experiment to determine the number of sources that can be accurately located using this methodology. Given that each source is characterized by three parameters (x-coordinate, y-coordinate and intensity), we would expect the maximum number of sources which can be successfully localized with 16 detectors to be 5. Since the MLE estimation is particularly sensitive to initial conditions provided by the sparse convex optimization, we simply examine if the larger grid points in Ω coincide with the true source locations for each experiment. We note that we have constrained the problem so that the discrete grid of possible source locations is only located within the glove boxes, implying that the material location will not be estimated outside of a glove box. This is a valid assumption, as most nuclear material of interest will be handled exclusively within a glove box. We note that despite restricting the SCOP to the gloveboxes (i.e constraining all values outside the gloveboxes to 0.), during the optimization process these constraints may be violated, resulting in small non-zero values in the constraint regions.

The results of the sparse optimization are shown in Figure 3. The true source locations are depicted with the red circles and the estimates are shown as black boxes. In panels a)-e), there is exactly one black box within each red circle and no where else on the grid, demonstrating the method's ability to accurately estimate the location for up to five sources. However, when there are six sources in panel f), the methodology estimates a larger number of sources than are actually present. We note that the color scale is logarithmic in all of the figures, thus thresholding the grid and recovering the source locations is an easy task in most of these examples.

3.3 Dynamic Range

In the following experiment, we fix the number of sources in our test case to 4, with 3 of the source intensities fixed at 10^5 counts/s. We then proceed to vary the intensity of the fourth source, in order to determine how sensitive the test case is to the range of source intensities present in the room. We run the full SCOPMLE algorithm, and then evaluate the total intensity estimation errors for all four sources. The results shown in Figure 4 indicate that the error on estimates are reasonable if the fourth source emits between 10^3 and 10^7 neutrons per second. We note that the estimated error is also likely dependent on the distance between the fourth source and the closest set of sensors.

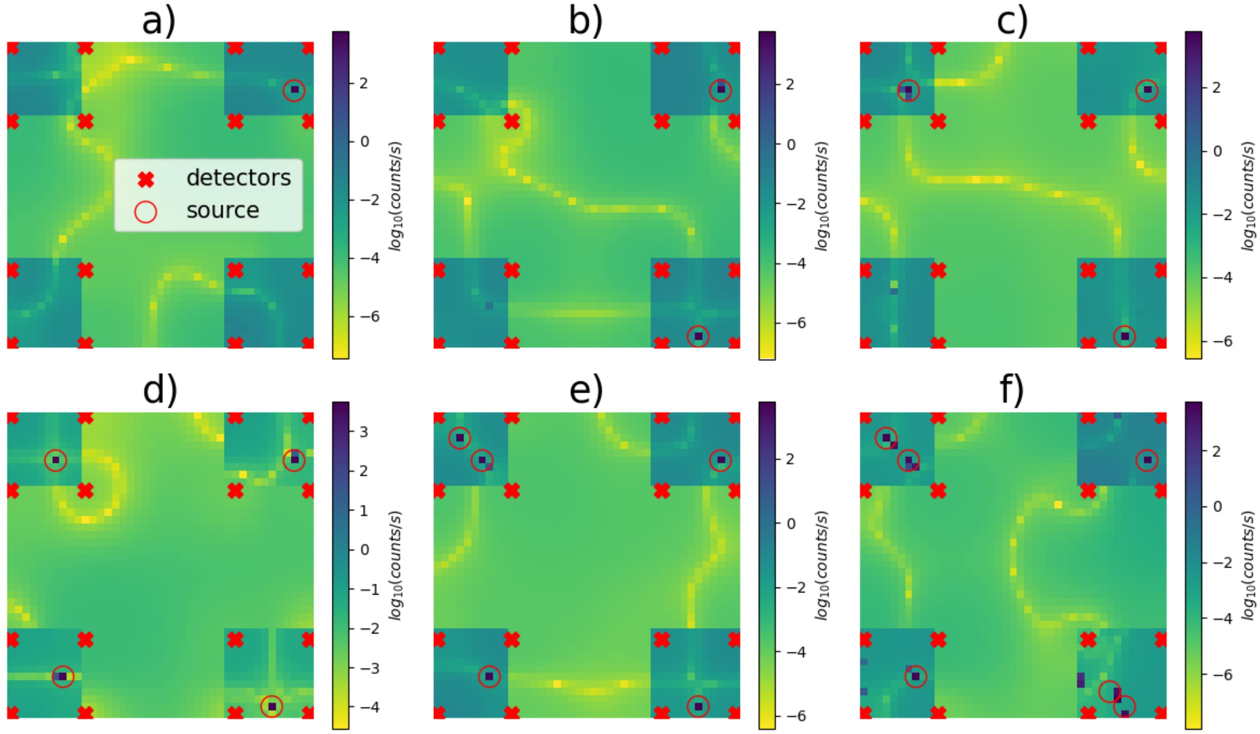

Figure 3: Sparse convex optimization results: grid point intensities (counts/s) are shown on the log-scale for clarity for 1-6 (a-f) sources. True source locations are shown as red circles and source location estimates are shown with black boxes. We note that the test case is able to successfully locate up to 5 sources: adding the 6th source introduces large location estimation errors.

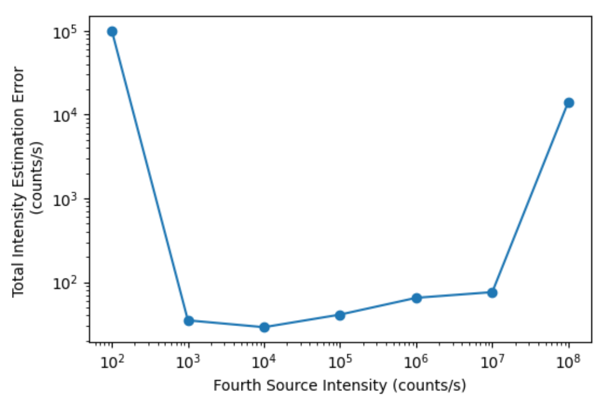

Figure 4: Total intensity estimation error by SCOPMLE with varying dynamic range. The source intensities are recovered to an acceptable tolerance (<100 counts/s) in the $10^3 - 10^7$ range.

3.4 Full Test Case

Figure.1 shows the dimensions of the DYMAC test bed we hope to eventually deploy our methodology to estimate the number, intensity, and location of sources in real-time. Thus we perform another round of experiments on a grid which more closely resembles that room of interest. We note that if modelled as a square grid, the dimensions of this room (576×576) are much larger than our initial, small test case. When attempting to run the sparse convex optimization algorithm on this grid of this size we note that often times the algorithm did not converge to a satisfactory answer, or at all. In order to mitigate this issue, we simply down sample the room to a 28×28

grid. Since the purpose of the sparse convex optimization is to provide initial guesses to the MLE algorithm, a high spatial resolution is not required. In all of the following experiments, we use the source locations shown in Figure 5 and set all source intensities to 10^5 counts/s.

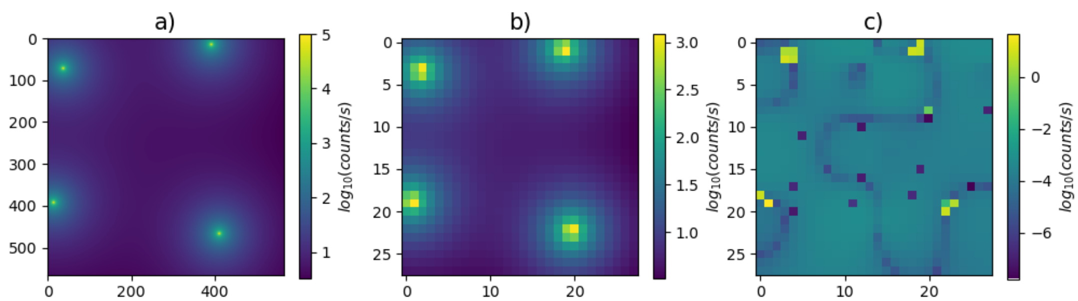

Figure 5: a) Full room with four 10^5 counts/s sources in the glove boxes b) Down sampled room with sources c) sparse convex optimization result for down sampled room using 16 sensors.

We observe a drawback of utilising a low-resolution grid in Figure.5 c): even with the iterative re-weighting scheme used by Lee *et al.*,[6] the sparse convex optimization does not localize high values to single pixels, but rather spreads them out in neighborhoods of contiguous pixels: a single source can result in up to 4 high value grid points. This indicates there may be some tuning required due to the trade-off between computational cost and precision of the sparse convex optimization process. In order to account for this and still provide the MLE with reasonable initial inputs, we simply perform "neighborhood merging": for a given high value pixel over some threshold we take the maximum value within a one pixel-radius, as shown in Figure 6. This results in clean, single-pixel initial guesses for the MLE. In order to select the correct number of sources based on the MLE, we utilize the Aikaike Information Criterion,[12] which we observe consistently returns the correct number of sources in our experiments.

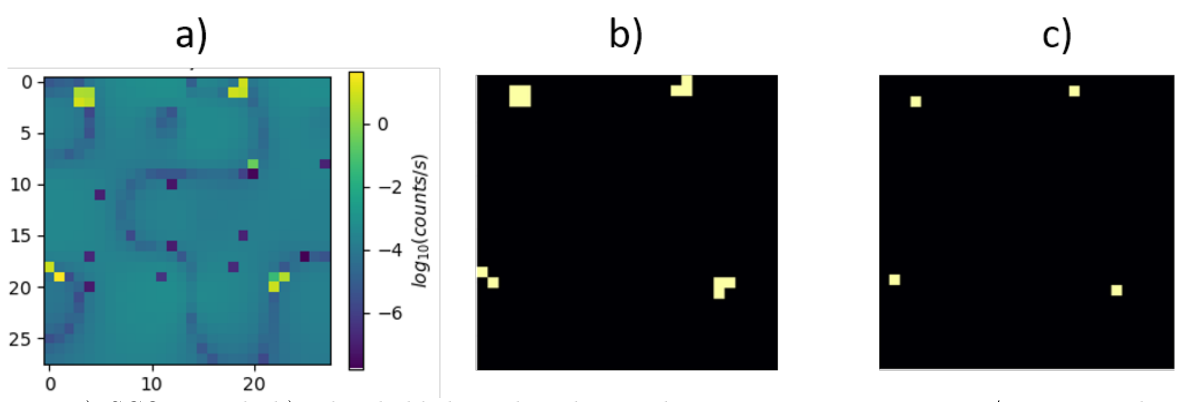

Figure 6: a) SCOP result b) Thresholded result, where only intensities over 1 counts/s are considered, c) neighborhood merging, this is the input into MLE.

We highlight the importance of good initialization for the MLE in Table 1, where we show the total location and intensity estimation errors for the four sources in this problem with and without SCOP initialization.

Initialization	x-error (cm)	y-error (cm)	intensity-error (%)
SCOP	2.69	3.99	0.04 %
Random	723.3	469	54.5 %

Table 1: MLE source term estimation errors with initialization method

3.5 Sampling

An important consideration for algorithms aimed at real-time applications is the length of time a source must be measured, i.e., number of measurements, necessary for accurate source-term estimation. Since we model our sensors using the Poisson distribution described in Eq.2, the confidence in the estimation of the true mean neutron count is dependent on the number of samples used in this estimation: longer measurement times (more samples) will result in narrower confidence estimates on the true mean of the Poisson distribution. We thus examine the effect of the sampling time on the location and intensity estimation errors, as shown in Figure.7, where we show a) the location estimation error in MLE for all 4 sources, and b) the intensity estimation error as a percentage of the total source intensity in the room (4×10^5 counts/s). Although these are point estimates, and more trials are needed to establish bounds on these error estimates, we note that with a sampling time exceeding 100 seconds is required to achieve location errors below 10 cm.

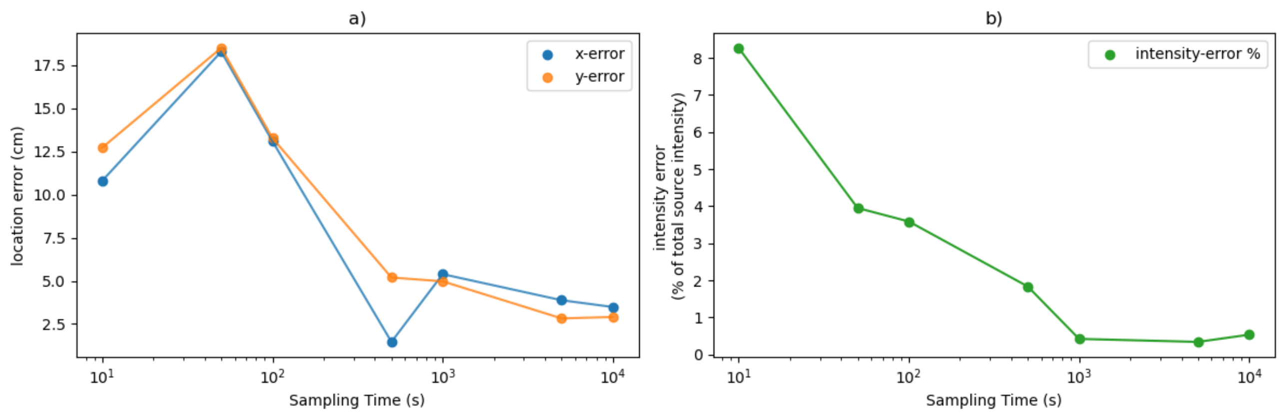

Figure 7: a) x and y coordinate estimation errors and b) intensity estimation errors as a percentage of total intensity with increasing sampling time.

3.6 Background Strength

Finally, we can also estimate how robust this method is to the background strength. In the following experiment we vary the background strength between 1-10 counts/s and examine how this translates to localization and intensity estimation errors: we note that even with a background of 2 counts/s the estimation results in 20 cm errors in location in both the x and y axis, and close to 20% intensity estimation errors, highlighting the sensitivity of the method to background strength for this test case. This demonstrates the importance of understanding and estimating the background radiation levels in a room so that its impact on the counts at the detectors can be accounted for, leading to more accurate estimates of location and intensity.

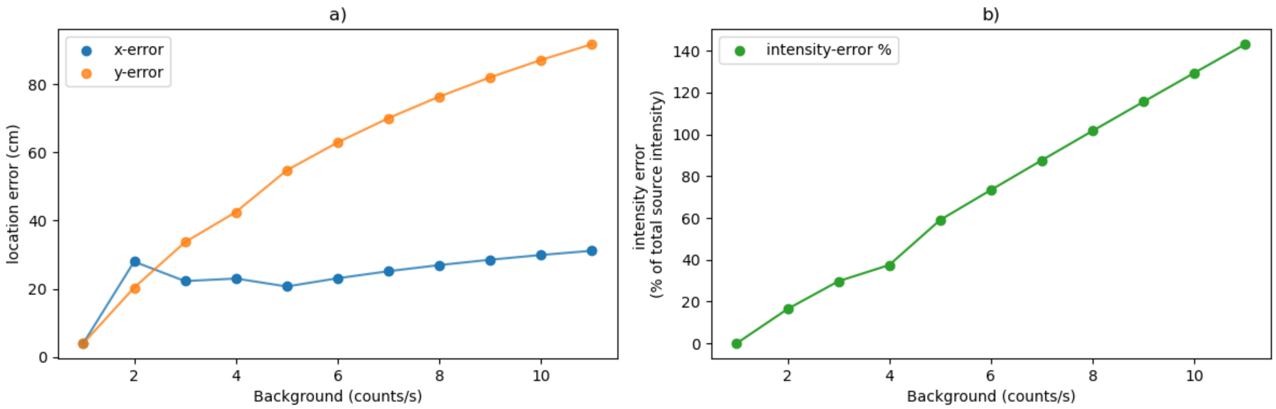

Figure 8: a) x and y coordinate estimation errors and b) intensity estimation errors as a percentage of total intensity with increasing background strength.

4. DISCUSSIONS

In this work we have implemented the SCOPMLE method suggested by Lee[6] in order to investigate its applicability to the DYMAC test bed at LANL. We demonstrate that for a small test problem, the 16 sensor configuration allows for the localization of up to 5 sources, and estimates of source intensity with reasonable error for source strength ratios ranging from 10^{-2} - 10^{3} when considering sources of strength 10^{5} counts/s. When expanding the analysis to a test case more analogous to the test bed, we note that it is necessary to down sample the initial grid used for the SCOP, whilst also performing thresholding and max neighborhood merging on the SCOP result before feeding this as an input to the MLE. Finally, we perform experiments which examine the robustness of the method to sampling time and background strength, and note that even small background radiation (2 counts/s) can greatly reduce the accuracy of the source localization and intensity estimation. Future work will move towards applying the method to experimental data collected in the test room.

ACKNOWLEDGMENTS

This work was supported by the Laboratory Directed Research and Development (LDRD) program at Los Alamos National Laboratory.

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