

Predicting ROC Curves for Source Detection Under Model Mismatch

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Abstract—Performance predictions and test thresholds for the task of detecting a gamma-ray source in background with a position-sensitive detector are often costly to compute empirically. The asymptotic distributions of test statistics for detecting a point-source in background give reasonable performance predictions in terms of the receiver operating characteristic curve (ROC) with less simulated or measured data than empirical methods. The asymptotic distributions also allow the user to determine the proper threshold to achieve a desired false alarm rate. Typically only approximate models are available or practical for complex gamma-ray imaging systems such as 3D position-sensitive semiconductor detectors. Applying standard formulas for the asymptotic distributions of maximum likelihood (ML) estimates in the presence of model mismatch can yield inaccurate and sometimes overly optimistic predictions of detection performance. We apply the theory of the asymptotic distribution of ML estimates under model mismatch to the case of detecting a point-source in background with a 3D position-sensitive CdZnTe detector employing an approximate model for the system response. We show that performance predictions computed using an asymptotic approximation that accounts for mismatch more closely match the empirical performance than predictions generated by an asymptotic approximation that ignores model mismatch.

I. INTRODUCTION

Statistical methods for gamma-ray source detection are often likelihood-based, meaning that the test statistic is a function of a maximum-likelihood estimate. The generalized likelihood ratio test (GLRT) is often used in the case where parameters, such as source intensity and position, are unknown [1]. The source intensity test (SIT) [2] compares the ML estimate of source intensity directly to a threshold, whereas the GLRT uses a function of the ML estimate.

The performance of likelihood-based tests is often difficult to estimate because one must simulate or record a large amount of data with and without a source present to generate an empirical receiver operating characteristic curve (ROC). The ROC measures detection performance by showing the probability of detection as a function of the probability of false alarm [3]. Empirical ROC curves have been used in nuclear material detection applications, e.g., [1] and [4]. Our previous work in [2] employed asymptotic approximations to the distributions of ML estimates to compute the ROC for detecting a source in background using less data than is needed for empirical calculation, but without accounting for model mismatch.

Likelihood-based tests are model-based, and their performance depends on the accuracy of the system model. Complex sensors, such as 3D position-sensitive gamma-ray detectors, are often difficult to model exactly due to the non-Gaussian uncertainties and nonlinear system response. The asymptotic

calculations in [2] do not account for mismatch between the model and the true system response. Our results show that applying the asymptotic formulas in [2] to 3D position-sensitive gamma-ray detectors with approximate system models can lead to overly optimistic performance estimates. We apply the methodology of [5] to compute the detection performance in terms of ROC with an asymptotic approximation that accounts for model mismatch.

We analyzed the asymptotic performance of gamma-ray imaging systems in [6] and [2], proving that position information always improves the detection performance when the detector sensitivity is uniform. In [6], we considered the detection performance of simplified 2D gamma-ray detectors with fully known system models. The asymptotic calculations that account for model mismatch allow us to extend the results of [2] and [6] to realistic 3D CdZnTe detectors.

The contribution of this work is a demonstration that asymptotic calculations of ROC that account for model mismatch can accurately detect empirical performance for a complex sensor with an unknown or intractable system response. This work is organized as follows: §II outlines the theory of asymptotic distributions of ML estimates under model mismatch, §III gives results demonstrating that the asymptotic performance calculations accurately predict actual performance for simulated 3D CdZnTe detectors, and §IV gives our conclusion and plans for future work.

II. BACKGROUND

A. System Model

This section describes the true distribution of a list of events recorded by a gamma-ray imaging system. This distribution is governed by physics and its exact form is typically unknown or difficult to compute in practice. We also describe a model distribution for a list of recorded events, which is often an approximation of the true distribution. We describe the model in general terms to allow adaptation to different types of gamma-ray detectors.

1) *True Distribution of Recorded Events*: We assume that the true distribution of recorded events follows the list-mode model of [7] for Poisson measurements. During a fixed-duration scan, the system will record attribute vectors, such as interaction locations within the detector and deposited energy, for each photon interaction event. Let the list of attribute vectors recorded by the system be $\mathbf{x} = (x_1, x_2, \dots, x_J)$. The random number of measurements is $J \sim \text{Poisson}(\bar{J})$, where $\bar{J} = \lambda_s \tau$, λ_s is the rate of recorded events in counts per unit

time, and τ is the deterministic scan time chosen by the user. Each $x_j \in \mathcal{R}$ where \mathcal{R} is the set of all possible event attributes.

Let $p(x)$ be the true density of the attributes of a single recorded event. We do not parameterize this true density because it represents the true physical process. Provided that the count rate is low enough to avoid dead-time effects [7], the true probability density of the list of event attributes \mathbf{x} is given by

$$p(\mathbf{x}) = e^{-\bar{J}} \bar{J}^J / J! \prod_{j=1}^J p(x_j). \quad (1)$$

2) *Measurement Model*: For detecting a point-source in background, we consider a modeled attribute distribution similar to that of [2]. The parameters characterizing the source are the intensity α with units of counts emitted per unit time and source position¹ $\phi \in \Phi$. In the 3D far-field with a known source energy, the set Φ could be $[0, 2\pi] \times [0, \pi]$, representing all possible azimuth and polar angles on a sphere. We parameterize the possibly unknown background intensity by the background count rate λ_b with units counts recorded per unit time. Let θ be the vector of all parameters, where θ lies in the d -dimensional parameter space Θ . We also define the modeled sensitivity $\tilde{s}(\phi)$ to be the probability that a photon emitted from a source positioned at ϕ is recorded. Throughout, we use superscript “ \sim ” to denote functions or distributions that are part of the model and might differ from the true underlying functions or distributions that they represent.

Since the mean number of emissions \bar{J} is unknown, we model it by $\tilde{J}(\theta)$, where $\tilde{J}(\theta) = \tilde{\lambda}(\theta)\tau$, and $\tilde{\lambda}(\theta)$ is the modeled photon emission rate in counts per unit time. For example, when the source and background intensities and position parameters are unknown,

$$\theta = (\alpha, \phi, \lambda_b). \quad (2)$$

We model the rate of recorded photons by

$$\tilde{\lambda}(\theta) \triangleq \lambda_b + \alpha \tilde{s}(\phi). \quad (3)$$

Let $\tilde{p}(x; \theta)$ be the modeled attribute density, which should approximate the true density $p(x)$. When model mismatch exists, $\tilde{p}(x; \theta) \neq p(x)$ for some values of $x \in \mathcal{R}$ for each $\theta \in \Theta$ [8]. This definition means that there is no parameter in the parameter space such that the modeled and true distributions are identical.

Let $\tilde{p}_S(x; \phi)$ and $\tilde{p}_B(x)$, denote the modeled distributions of recorded event attributes x given that they are detected and come from the source and background, respectively. Note that $\tilde{p}_S(x; \phi)$ depends only on the source position, and $\tilde{p}_B(x)$ does not depend on any of the parameters in (2). The overall modeled distribution of recorded attributes is a mixture of $\tilde{p}_S(x; \phi)$ and $\tilde{p}_B(x)$ given by

$$\tilde{p}(x; \theta) = \frac{\lambda_b \tilde{p}_B(x) + \alpha \tilde{s}(\phi) \tilde{p}_S(x; \phi)}{\lambda_b + \alpha \tilde{s}(\phi)}. \quad (4)$$

¹ ϕ could also denote a vector containing both spatial position and energy

Under the above assumptions, we model the likelihood as follows [2], [7]:

$$\tilde{p}(\mathbf{x}; \theta) \triangleq e^{-\tau \tilde{\lambda}(\theta)} [\tau \tilde{\lambda}(\theta)]^J / J! \prod_{j=1}^J \tilde{p}(x_j; \theta). \quad (5)$$

B. Estimator definition

Because the maximizer of the modeled likelihood in (5) differs from the ML estimate in general, it is called a quasi maximum likelihood estimator (QMLE) [8]. Under the model (5), we find the QMLE by solving

$$\tilde{\theta}_\tau \triangleq \arg \max_{\theta \in \Theta} \log \tilde{p}(\mathbf{x}; \theta). \quad (6)$$

In the next section, we examine the asymptotic properties of $\tilde{\theta}_\tau$ as $\tau \rightarrow \infty$, i.e., as one records more events by increasing the scan time. § III shows that the asymptotic approximation can accurately characterize the distribution of $\tilde{\theta}_\tau$, even for a finite scan time.

C. Asymptotic Distribution of the QMLE

Let ∇_θ denote the $d \times 1$ gradient with respect to θ , and let ∇_θ^2 denote the $d \times d$ Hessian with respect to θ . By the definition in (6), assuming that the log-likelihood is differentiable and the maximizer is in the interior of the parameter space, the QMLE $\tilde{\theta}_\tau$ satisfies

$$\nabla_\theta \log \tilde{p}(\mathbf{x}; \tilde{\theta}_\tau) = \mathbf{0}. \quad (7)$$

We also define

$$\tilde{g}(\theta) \triangleq \mathbb{E}[\nabla_\theta \log \tilde{p}(\mathbf{x}; \theta)] = \int_{\mathcal{R}} \nabla_\theta \log \tilde{p}(\mathbf{x}; \theta) p(\mathbf{x}) d\mathbf{x}, \quad (8)$$

where the expectation is with respect to the true distribution $p(\mathbf{x})$, which need not be known analytically, as discussed further below.

1) *Convergence*: Let $\tilde{\mu} \in \Theta$ be the solution to

$$\tilde{g}(\theta)|_{\theta=\tilde{\mu}} = \mathbf{0}, \quad (9)$$

assuming that such a solution exists and is unique. Under suitable conditions, $\tilde{\mu}$ is the limit of the sequence of estimates $\tilde{\theta}_\tau$ as $\tau \rightarrow \infty$. One possible set of regularity conditions that guarantees existence, uniqueness, and convergence is given in [5]. The convergence of the QMLE is stated in Theorem 1, which extends Theorem 2.2 of [8] to the case of a Poisson number of measurements. The proof is given in [5].

Theorem 1. *Under suitable regularity conditions, $\tilde{\theta}_\tau \xrightarrow{\text{a.s.}} \tilde{\mu}$ as $\tau \rightarrow \infty$.*

D. Asymptotic normality

A QMLE may also be asymptotically normal if certain conditions on the model and true distributions are met. Theorem 2 is an extension of Theorem 3.2 of [8] to the case of a Poisson number of measurements.

Theorem 2. Under suitable regularity conditions, asymptotically as $\tau \rightarrow \infty$,

$$\sqrt{\tau} \left(\tilde{\boldsymbol{\theta}}_\tau - \tilde{\boldsymbol{\mu}} \right) \xrightarrow{d} \mathcal{N}(\mathbf{0}, \Sigma(\tilde{\boldsymbol{\mu}})), \quad (10)$$

where

$$\Sigma(\boldsymbol{\theta}) = \tilde{\mathbf{H}}^{-1}(\boldsymbol{\theta}) \tilde{\mathbf{G}}(\boldsymbol{\theta}) \tilde{\mathbf{H}}^{-1}(\boldsymbol{\theta}), \quad (11)$$

$$\tilde{\mathbf{G}}(\boldsymbol{\theta}) \triangleq \lambda_s \mathbf{E} \left[\left(\begin{array}{c} \left(\nabla_{\boldsymbol{\theta}} \log \tilde{p}(x; \boldsymbol{\theta}) + \nabla_{\boldsymbol{\theta}} \log \tilde{\lambda}(\boldsymbol{\theta}) \right) \\ \left(\nabla_{\boldsymbol{\theta}} \log \tilde{p}(x; \boldsymbol{\theta}) + \nabla_{\boldsymbol{\theta}} \log \tilde{\lambda}(\boldsymbol{\theta}) \right)^T \end{array} \right) \right], \quad (12)$$

and

$$\tilde{\mathbf{H}}(\boldsymbol{\theta}) \triangleq \lambda_s \nabla_{\boldsymbol{\theta}}^2 \log \tilde{\lambda}(\boldsymbol{\theta}) - \nabla_{\boldsymbol{\theta}}^2 \tilde{\lambda}(\boldsymbol{\theta}) + \lambda_s \mathbf{E} \left[\nabla_{\boldsymbol{\theta}}^2 \log \tilde{p}(x; \boldsymbol{\theta}) \right]. \quad (13)$$

In the absence of model mismatch, $\tilde{\mathbf{G}}(\boldsymbol{\theta})$ and $\tilde{\mathbf{H}}(\boldsymbol{\theta})$ are equal to the ‘‘per unit time’’ Fisher information matrix [8]. This allows us to make the simplification $\Sigma(\boldsymbol{\theta}) = \mathbf{F}^{-1}(\boldsymbol{\theta})$, where $\mathbf{F}(\boldsymbol{\theta})$ is the time-normalized Fisher information matrix [8]. Thus, Theorem 2 reduces to the classic asymptotic normality and asymptotic efficiency of ML estimation [9].

A consequence of Theorem 2 is that one can approximate the distribution of $\tilde{\boldsymbol{\theta}}_\tau$ by

$$\tilde{\boldsymbol{\theta}}_\tau \stackrel{\text{approx}}{\sim} \mathcal{N}\left(\tilde{\boldsymbol{\mu}}, \frac{1}{\tau} \Sigma(\boldsymbol{\theta})\right).$$

This essential fact is the basis of the asymptotic approximations used to compute the results in §III.

E. Detection Problem

We wish to decide between the two hypotheses:

$$\begin{aligned} H_1 &: \alpha > 0, \quad \phi \in \Phi \\ H_0 &: \alpha = 0, \quad \phi \in \Phi, \end{aligned}$$

using the source intensity test (SIT)

$$\tilde{\alpha} \underset{H_0}{\overset{H_1}{\geq}} \gamma, \quad (14)$$

where $\tilde{\alpha}$ is the QML estimate of source intensity. The analysis in this work can also be used to analyze other tests, such as the generalized likelihood ratio test (GLRT). In our results, we only consider the SIT. A comparison between the SIT and the GLRT is given in [2] in the absence of model mismatch.

III. RESULTS

We used the predicted asymptotic distributions to create an ROC curve that one can use to set the threshold and to estimate the probability of detection for a given false alarm rate. We state some results in terms of area under the ROC curve (AUC) [10], which is a measure of detector performance that does not depend on the threshold or a chosen false alarm rate.

In §II, we made no assumption about the form of the true distribution of attributes $p(x)$. In our simulations, we assume that the true attribute distribution follows the mixture model

$$p(x) = \frac{\alpha^t p_S(x; \phi) + \lambda_b^t p_B(x)}{\alpha^t + \lambda_b^t}, \quad (15)$$

where α^t and λ_b^t are the true mean number of source and background counts recorded, respectively. This assumption is not needed to estimate the asymptotic ROC or AUC using our method, but it is needed for simulation. Real measurements are typically a mixture of source and background events, so the assumption is often valid in practice.

Throughout this section, we compare predicted performance accounting for and ignoring model mismatch. The predicted performance accounting for model mismatch uses the result of Theorem 2 to compute the asymptotic ROC. The predicted performance ignoring mismatch applies the asymptotic normality result that does not account for model mismatch, which was used in [2]. In the notation of this paper, the asymptotics when model mismatch is ignored are based on [2] with $\Sigma(\tilde{\boldsymbol{\mu}})$ replaced by $\mathbf{F}^{-1}(\boldsymbol{\theta}_{\text{true}})$, and $\tilde{\boldsymbol{\mu}}$ replaced by $\boldsymbol{\theta}_{\text{true}}$. When model mismatch is ignored, we evaluate $\mathbf{F}(\boldsymbol{\theta})$ using the Monte Carlo expressions in [2], where the Monte Carlo expectation is computed with respect to the true distribution. The true distribution is naively and incorrectly assumed to be equal to the model distribution at the true parameter value.

A. Results with simulated 3D position-sensitive CdZnTe detector

1) *Methods:* We used Monte-Carlo simulation to compute $\Sigma(\tilde{\boldsymbol{\mu}})$ in using (11)-(13) with 10^6 events. The detector is 1.5cm×2.0cm×2.0cm of CdZnTe. The events were simulated using GEANT4 [11] for a far-field point source of 662 keV and a spatially uniform monoenergetic background of 662 keV. The source position estimator $\hat{\phi}_{\text{ML}}$ used exhaustive search over a fixed grid of 90×90 position bins. The event probabilities are modeled using the model proposed in [12]. The background is monoenergetic with the same energy as the source because this represents the most difficult detection problem. One can also use the proposed framework to evaluate detection performance in polyenergetic backgrounds. We generated the empirical ROC by computing $\tilde{\alpha}$ for simulated scans with 330 mean counts each.

2) *Results:* Figure 1 shows the ROC for source-to-background ratio of 1:10 and 330 mean total counts. The proposed predicted ROC that accounts for model mismatch is much closer to the empirical ROC than the previous predicted in ROC in [6] and [2] that ignores model mismatch. Even with this small number of source counts per trial, the asymptotic approximation appears to be reasonable. Note that the ROC predicted by asymptotics not accounting for model mismatch is an overly optimistic estimate of the true performance.

Figure 2 shows the area under the ROC curve (AUC) for a source-to-background ratio of 1:10 as a function of the scan time τ . When the scan time is small, the AUC computed using asymptotics is not a good approximation to the empirical AUC. This is because the asymptotic approximation improves as the mean number of counts increases. If the mean number of counts per scan is small, the normal approximation to the distribution of the MLE is not accurate, and thus the asymptotic detection performance predictions are poor. The small difference between the AUC predicted accounting for

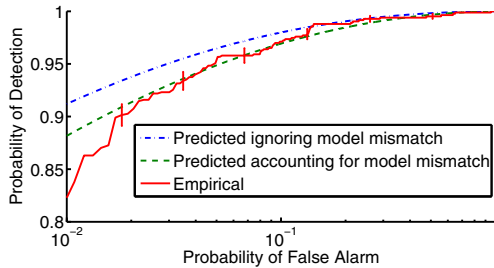


Fig. 1. Empirical and theoretical ROC curves of the SIT for a point source with mean source counts $\tau\alpha^t = 30$ counts/sec and mean background counts $\tau\lambda_b^t = 300$ counts/sec using a simulated 3D position-sensitive CdZnTe detector. Error bars denote standard error.

and not accounting for model mismatch indicates that the model used in this experiment is relatively close to the true distribution of recorded event attributes. The AUC computed using asymptotics that account for model mismatch is closer to the empirical AUC for scan times large enough for the asymptotic approximation to be valid.

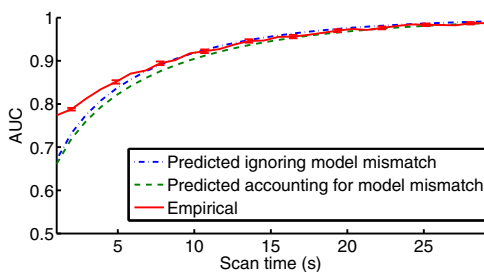


Fig. 2. Empirical and theoretical AUC of the SIT for source intensity $\alpha^t = 1$ counts/sec and background intensity $\lambda_b^t = 10$ counts/sec using a simulated CdZnTe detector. Error bars denote standard error.

IV. CONCLUSION

We presented asymptotic formulas for predicting ROC curves that one can evaluate using Monte Carlo methods and used them to evaluate the performance of a 3D CdZnTe detector for detecting a point-source in background. We found that asymptotic approximations that account for model mismatch accurately predict detection performance in terms of the ROC for a sufficiently large mean number of recorded counts per scan.

Future work will use asymptotic analysis to compare detection performance between situations where the source position and background intensity are known and unknown, and to explore the effects of commonly used sources of model mismatch, such as assuming that all observed events deposit all of their energy in the detector. Future work will also use asymptotic analysis accounting for mismatch to compare the performance of position-sensitive detectors, such as CdZnTe, to the performance of less-expensive spectrometers, such as NaI. We also plan to use the asymptotic framework to quantify the effect of detector size on detection performance.

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