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SPECTRAL RECONSTRUCTION FOR FACET-II COMPTON SPECTROMETER*

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Abstract

The Compton spectrometer under development at UCLA for FACET-II is a versatile tool to analyze gamma-ray spectra in a single shot, in which the energy and angular position of the incoming photons are recorded by observing the momenta and position of Compton scattered electrons. We present methods to reconstruct the primary spectrum from these data via machine learning and the EM Algorithm. A multi-layer fully connected neural network is used to perform the regression task of reconstructing both the double-differential spectrum and the photon energy spectrum incident with zero angular offset. We present the expected performance of these techniques, concentrating on the achievable energy resolution.

INTRODUCTION

Gamma-ray Compton scattering has been used in measuring the energy and incident angle of the gamma-ray photons in the past [1]. The scattering probability of electrons have a distinct angle and energy dependence on the incoming photon, so by carefully measuring the information of the electrons, one may reconstruct the gamma-ray spectrum. The Compton spectrometer under development at UCLA deploys this idea. We bend the trajectories of the scattered electrons in magnetic fields, and thereby convert energy information to position information. Those scattered electrons then hit a scintillator where their energy is deposited in the screen.

The main objective of this paper is to provide an overview of various methods we use to reconstruct the gamma-ray spectrum based on energy deposited by electrons in a scintillator screen. Section Reconstruction Algorithms provides the background and implementation of EM Algorithm and machine learning, and reconstruction results are presented in the Section Results.

RECONSTRUCTION ALGORITHMS

Both EM Algorithm and machine learning are used in reconstructing the energy spectrum with no angular dependence, and machine learning was also used in an earlier attempt to reconstruct the double differential spectra.

The variables used in the reconstruction are as follows:

- Energy deposited on the scintillator is summed across the vertical (angular) axis and binned into a histogram

of a fixed width with bin index d . 128 scintillator bins cover the range from 0 to 225 mm.

- The gamma-ray spectrum to be constructed is placed into bins with logarithmic bin widths and indexed by the parameter b . 128 energy bins cover the range from 0.16 MeV to 7 MeV. The designed working region for the spectrometer is set to be from 0.2 MeV to 7 MeV at coil current 4500 A, which is the range used in the Results Section.
- The total energy emitted in gamma rays in each energy bin is $n(b)$.
- The energy deposited in scintillator is $n^*(d)$.
- Taking into account the geometry of the Compton spectrometer, there is a coefficient associated with the energy deposition in scintillator bin d of photons coming from energy bin b . We denote this coefficient as $p(b, d)$.

We may now state our problem: it is, given $n^*(d)$ and $p(b, d)$, one must extract $n(b)$.

EM Algorithm

We have adapted the expectation-maximization (EM) algorithm by Vardi, Shepp, and Kaufman [2], which was originally concerned with image reconstruction in positron emission tomography (PET). Our problem is similar to the challenge of PET imaging in that we seek to extract a source signal from an observed data set that has a complex relationship with source properties. Vardi, Shepp, and Kaufman provided a simplified derivation for the iterative process of their EM Algorithm, and here we select a few key steps from their derivation.

The Expectation step (E step) Suppose we have a guess of an emission rate associated with $n(b)$ to be $\lambda^{old}(b)$. Then we can estimate the energy of the photons emitted in energy bin b to be $\hat{n}(b)$:

$$\hat{n}(b) \sum_{d=1}^D p(b, d) = \sum_d \mathbb{E}[n(b, d) | \lambda^{old}(b), n^*(d)]. \quad (1)$$

$\sum_{d=1}^D p(b, d)$ is present because not all photons are detected. Now $n(b, d)$ are a set of Poisson random variables with sum $n^*(d)$, so each of them follows the binomial distribution with probability $\lambda^{old}(b, d) / \sum_{b'} \lambda^{old}(b', d)$. We can evaluate the expectation value:

$$\hat{n}(b) \sum_{d=1}^D p(b, d) = \lambda^{old}(b) \sum_d \frac{n^*(d)p(b, d)}{\sum_{b'} \lambda^{old}(b')p(b', d)}. \quad (2)$$

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The Maximization step (M step) If $\hat{n}(b)$ is our estimate for energy emitted in energy bin b , it is also the estimate for the corresponding emission rate $\lambda(b)$, because $n(b)$ is a Poisson process with rate $\lambda(b)$. In other words, $\lambda(b) = \hat{n}(b)$ makes it most likely to observe $\hat{n}(b)$.

The Complete Algorithm We update $\lambda^{new}(b)$ for 50 iterations with the following update rule:

$$\lambda^{new}(b) = \frac{\lambda^{old}(b)}{\sum_{d=1}^D p(b, d)} \sum_d \frac{n^*(d)p(b, d)}{\sum_{b'} \lambda^{old}(b')p(b', d)}. \quad (3)$$

Choices for $p(b, d)$ One option for $p(b, d)$ is the energy deposition of monoenergetic gamma-rays, i.e. energy emitted in energy bin b that is detected in scintillator bin d . $n^*(d)$ is generated by a Geant4 simulation.

We also used a smoothed basis for $p(b, d)$, i.e. replacing the original delta function in energy bin b with a Gaussian function centered at b with $\sigma = 6$ bins. Under such condition, $p(b, d)$ is modified to be the scintillator output of one such Gaussian-distributed beam.

Machine Learning

Machine learning allows the machine to capture important features of an arbitrary function so that it becomes a copy of the function and generates correct outputs based on new inputs. A model is an instance of a learned version of the arbitrary function.

Here the input for our model is the output of the spectrometer, namely, $n^*(d)$. The machine's task is to learn to output the correct gamma-ray spectrum, $n(b)$. This task was implemented with a fully connected network.

A fully connected network is a series of matrix multiplications plus bias, passing through activation functions.

$$\begin{aligned} \text{Out} &= \text{Act}(\mathbf{W}_1 \text{hid}_1 + b_1) \\ &= \text{Act}(\mathbf{W}_1 \text{Act}(\mathbf{W}_2 \text{hid}_2 + b_2) + b_1) = \dots \end{aligned}$$

The shape of the hidden layers and the number of hidden layers can be freely chosen. Activation functions can also be freely chosen when appropriate. The model learns by adjusting the values in the matrices so that the error in the output is minimized.

Training Data Generation Training data and labels are generated based on a set of scintillator outputs with monoenergetic inputs. Due to the nature of machine learning, a large number of training samples is needed far beyond the 400 samples provided, so I combined the outputs from monoenergetic beams and feed them through the machine. This approach is valid because energy deposition is a linear process and a superposition of the monoenergetic outputs is a valid output from the scintillator.

It is known that only reasonably balanced and sufficiently random training sets may teach the model anything useful. The ground truth for the model output to approximate, i.e. the energy spectra used as training "labels", should not be

biased towards certain shapes in order to ensure the full flexibility of model.

To achieve uniform, random, yet reasonably smooth truth labels, we used trajectories of particles diffusing with a drag force in a bounded box. Those trajectories were simulated with Python step-wise with the following velocity update rule:

$$v_{i+1} = 0.95 \times (v_i + 0.01 \times (\text{Uniform}[0, 1] - 0.5))$$

and the elastic reflection at the bottom and top boundary is enforced (Fig. 1).

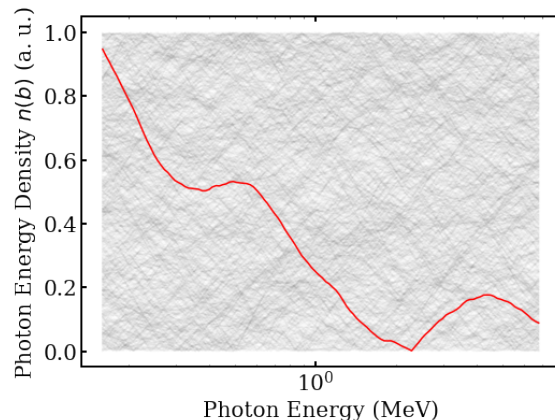


Figure 1: 1000 generated raw labels for machine learning, plotted with their physical units in x axis against a magnitude in y that will become the weight of one corresponding monoenergetic output in a combined training input. The 1000 labels are plotted in black with transparency 2%, and one such label is plotted in solid red. The uniformity of the labels is visualized by the even shades of grey.

Search of Network Parameters The exact architecture of the fully connected network was determined by training many models with varying parameters. The free parameters of the models are: the number of layers, the size of each layer, the activation function of each layer, whether or not to add bias to the layer, learning rate of the model, the maximum label value we normalize to, and the maximum data value we normalize to.

We wrote scripts to generate all combinations of these parameters, trained all the different models with these parameter sets, and selected the best performing model based on the final mean squared error.

Our final selected model has three hidden layers of 128, 128, and 512 nodes, no bias, and all the activation functions are ReLU (Rectified Linear Unit) activation.

RESULTS

Here we present the results of the three reconstruction algorithms: EM Algorithm with the original monoenergetic basis, the smoothed EM Algorithm, and machine learning (Fig. 2). The spectrum used to test the three reconstruction algorithms is the dataset 'E300 PWF/Matched

Trailing ($s=0.06$)/both', a simulated spectrum for the PWFA experiment at FACET-II.

We measured the point-wise root mean squared error (RMSE) between the truth that is normalized to have maximum of 1, and the prediction that is divided by the same factor. The machine learning result had RMSE of 0.0555. The RMSE for the original EM Algorithm is 0.0878, and that for the smoothed EM Algorithm is 0.0354.

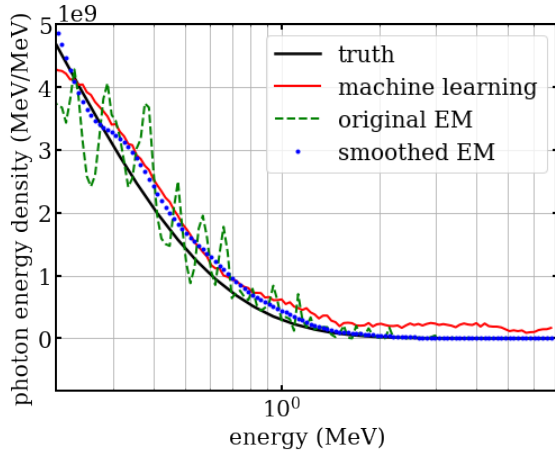


Figure 2: Comparison of three different reconstruction algorithms. The true PWFA spectrum is plotted in solid black. The red curve is the predicted spectrum from machine learning. The dashed green curve corresponds to the original EM Algorithm, and the blue dotted line is the result from the smoothed EM Algorithm. The dotted line agrees the best with the truth.

Due to smoothing in the basis as well as the smooth training data fed into the machine learning model, the ability to resolve sharp peaks of the smoothed EM Algorithm and of the machine learning model is limited, as shown in Fig. 3.

DISCUSSION

Reconstruction algorithms with a certain degree of complexity is needed because Compton scattered electrons have angular and energy distributions. Our task involves extracting source information based on mixed output, so two schools of methods were investigated in this work.

The EM Algorithm features an iterative process to find the emission rate in each energy bin, thereby equating that with the gamma-ray spectrum. In its original form with the monoenergetic basis, EM Algorithm performed well with locating peaks, but was susceptible to noise and undesirable fluctuations given smooth data. The smoothed basis reduced the fluctuation as well as the ability to discern nearby peaks. For the PWFA spectrum, RMSE for the original EM Algorithm is 0.0878 and that for the smoothed EM Algorithm is 0.0354. Machine learning with a fully connected network is a flexible tool to map outputs to inputs. Trained with carefully synthesized data, the model learned the function of the spectrometer. For the PWFA spectrum, RMSE for the

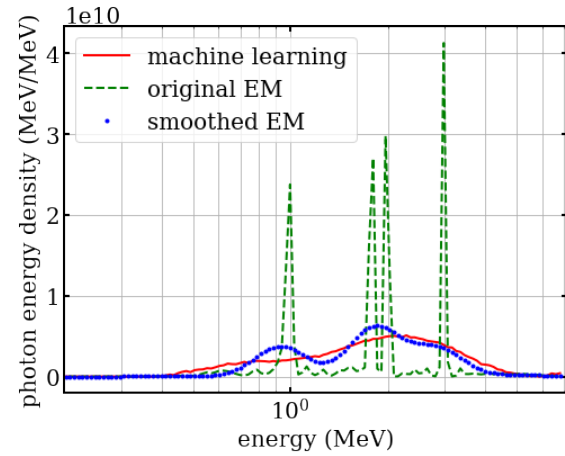


Figure 3: Comparison of three different reconstruction algorithms for a spectrum with 4 monoenergetic peaks. The dashed green curve corresponds to the original EM Algorithm, which is a good reference for the true spectrum. The red curve is the predicted spectrum from machine learning, and the blue dotted line is the result from the smoothed EM Algorithm.

machine learning model is 0.0555, better than the original EM Algorithm.

Based on the discussion above, smoothness in the target spectra seems to be an important factor to consider in choosing the reconstruction algorithm. Smooth training data as well as smooth bases will limit the ability to resolve peaks in the spectra, but will greatly improve performance of the algorithms to reproduce smooth spectra. It is therefore advised that we choose the smoothing based on analytic knowledge or simulation of an unknown spectrum.

Similarly, efforts has been put into recovering the angular information with a fully connected neural network. Due to the computing power needed to generate a full set of patterns produced by monoenergetic gamma photons at different angular positions, the earlier work with an outdated spectrometer design may not be illuminating to be presented here. However, the success with the energy reconstruction convinced us about the feasibility of reconstructing double differential spectra with EM Algorithm and machine learning.

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