Deep Learning-based Compton Background Reduction in X-ray Fluorescence Spectrum

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1. Introduction

Gold nanoparticles (GNPs) are used for many research like targeting tumor cells, transferring medicine, imaging, and radiosensitization. Among these, we are investigating the development of imaging modality using X-ray fluorescence (XRF). XRF imaging makes it possible to get *in vivo* image and quantification of GNPs distributed within the tumor cells and other organs using two fluorescence X-ray (K-α1, K-α2) of gold [1]. Once a spectrum is obtained from the detector, only the counts detected within the energy range of fluorescence X-ray are used.

Therefore, in XRF, separating the fluorescence counts from the whole spectrum containing Compton background is one of the important work for improving XRF based imaging modality. To obtain the realistic background signals, we have to irradiate X-ray twice, first with GNPs and secondly without GNPs, which doubles the scanning time and the dose. For this reason, we have created artificial background signals by linear interpolation. However, this method cannot make a realistic background because it does not reflect any random noise.

We introduced 1D Convolutional Neural Network (CNN) deep learning model to reduce the background signals without additional experiments. CNN is a well-known neural network for the tasks related to the 2D image but sometimes is used for processing one-dimensional signal.

2. Materials and Methods

2.1. X-ray generator and detector

First, we used X-rad 320 (Precision X-ray Inc., US) for irradiating cone-beam X-ray of 320 kVp and 17 mA. And cadmium-telluride (X-123 CdTe) (AMETEK Inc., US) detector was used for measuring the photon counts coming from the object. To measure only fluorescence photon from GNP (Nanoprobe Inc., US), the CdTe detector is set in the 90° direction of the incident photon. The detailed setup is shown in Fig. 1. X-ray was irradiated for 30 s for each measurement.

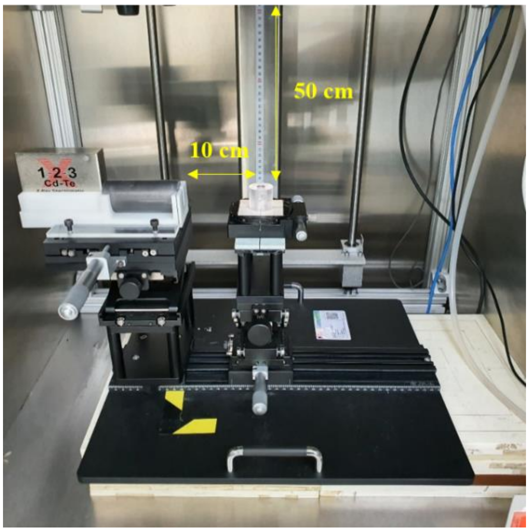

Fig. 1. CdTe detector and phantom setup. X-ray is irradiated from the top and fluorescence photons disperse in all directions. The CdTe detector measures theses photons in the 90° direction towards the incident X-ray.

2.2. Phantom and GNP solutions

To train the deep learning model, a lot of data and cases are required. GNPs of 0.0 (background), 0.125, 0.25, 0.5, 1.0, 2.0, and 4.0 wt% were contained in single-column polymethyl methacrylate plastic (PMMA) phantom shown in Fig. 2. In addition, combinations of 0.125, 0.25, 0.5, 1.0, and 2.0 wt% were contained in multi-column phantom shown in Fig. 2.

The distance from the beam source to the surface of the phantom is 50 cm and from the isocenter to the entrance of the collimator is 10 cm.

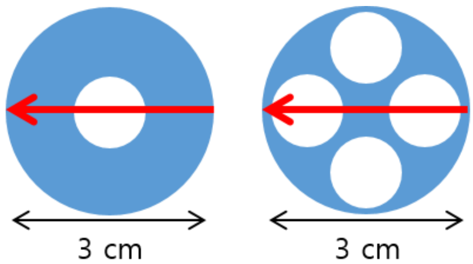

Fig. 2. Single-column phantom (left) and multi-column phantom (right). The detector and collimator was set at the center (red arrow) of the phantom to get the maximal fluorescence photons.

2.3. Architecture

CNN uses the so-called 'kernel' so that fewer weights are trained and make the calculating time shorter. CNN originally was introduced for training 2D image data, but in our study, the data are one-dimensional [2]. The kernel usually is 2D like 2×2 and 3×3, which is changed to 1-dimensional as in the yellow box in Fig. 3.

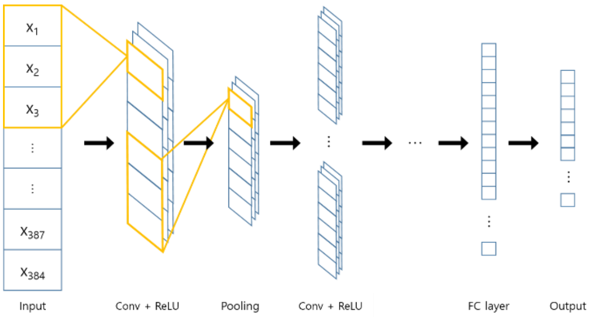

Fig. 3. One-dimensional CNN architecture. 1×3 kernel passes the input data of which the length is 384.

2.4 Dataset for training

For each GNP concentration, we obtained 250 data. The total counts are different for each experiment, so all data were normalized. We made targets by subtracting 0 wt% (background) data from each GNP concentration. We divided 250 data by 3:1:1 ratio for training, validation, and test.

2.5. Evaluation metric

To evaluate the results of the trained model, we calculated two metrics, the Pearson correlation coefficient (PCC) and peak signal to noise ratio (PSNR). It is well known that the model has good performance when the PCC value is closer to 1 and the PSNR value is higher than 20. The PCC means the degree of linearity between data X and Y. The PSNR means the ratio of the peak signal to the noise.

$$\mathrm{PCC} = \frac{\sum_i^n (X_i - \bar{X})(Y_i - \bar{Y})}{\sqrt{\sum_i^n (X_i - \bar{X})^2}\sqrt{\sum_i^n (Y_i - \bar{Y})^2}} \qquad (1)$$

$$\mathrm{PSNR} = 10 \cdot \log_{10}\left(\frac{MAX_I^2}{MSE}\right) \qquad (2)$$

X_i, Y_i : i^th^ data of each GNPs concentration
$\bar{X}, \bar{Y}$: Average of n data
$\mathrm{MAX}_\mathrm{I}^2$: Maximum value of the signal
MSE : Mean squared error

$$\mathrm{MSE} = \frac{1}{\mathrm{n}} \sum_{i=1}^n \left(Y_i - \hat{Y}_i\right)^2 \qquad (3)$$

In this case, data X is the inference, and data Y is the target. Mean squared error is the average squared difference between the target and inference. The PSNR is calculated with this value.

3. Results

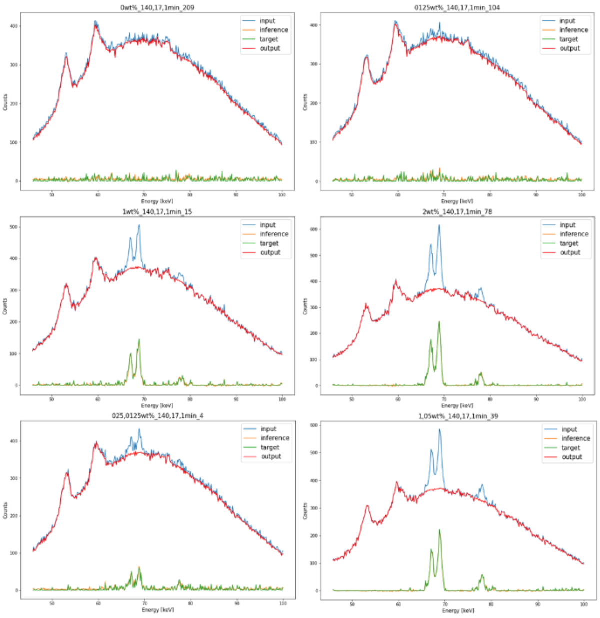

Fig. 4. Count spectra for some cases. Graphs in the first and second row are results of single-column phantom and the others in the third row are of multi-column phantom. The blue, green, orange, and red lines are the input data, target, inference by the trained model, and Compton background. The orange line almost overlaps with the green line.

Fig. 4 shows the counts spectra of test results. The blue line is the input signal, green and orange lines are target and inference by the model each. The red line is calculated by subtracting the orange from the blue line, so this is the background signal. The inference (orange) matches well with the target (green).

All numerical values are in Table I. PCC values are better and show almost linearity in high concentration cases.

Table I: PCC and PSNR for test dataset results

Concentration (wt%)	PCC	PSNR
0	0.733	16.76
0.125	0.774	17.77
0.25	0.856	21.68
0.5	0.945	27.26
1	0.986	33.33
2	0.997	39.39
4	0.999	40.35
0.125, 0.25	0.930	25.81
0.125, 0.5	0.974	30.81
0.125, 1	0.994	36.93
0.125, 2	0.998	42.53
0.25, 0.5	0.981	32.04
0.25, 1	0.994	37.28
0.25, 2	0.998	41.35
0.5, 1	0.996	38.17
0.5, 2	0.998	42.62
1, 2	0.999	42.24
Overall	0.950	33.31

We did the same experiment with another GNPs concentrations set of 0, 0.0313, 0.0625, 0.125, 0.25, 0.5, 1, and 2 wt%. For each case, we irradiated 10 times and obtained peak counts using linear interpolation and our deep learning model. The peak counts are the summation of counts in the energy range from 65.84 to 69.86 keV in which the XRF peak signal is remarkable. The black and red points and lines are the results calibrated by linear interpolation and deep learning model each. There is an obvious linearity between X-ray photon counts and GNP quantity.

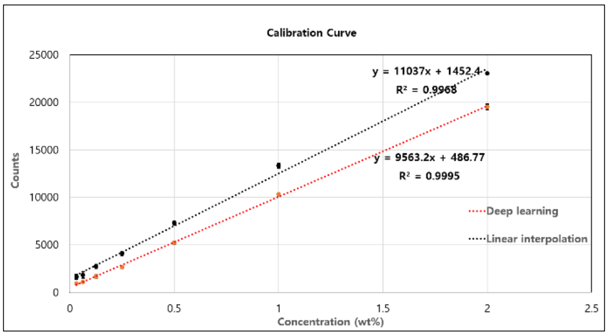

Fig. 5. Calibration curve calculated with additional data (0, 0.0313, 0.0625, 0.125, 0.25, 0.5, 1, and 2 wt%).

4. Discussion

The Spectra in Fig. 4 shows that the inference by deep learning model matches well with the target. In addition, the average PCC and PSNR values mean the good performance of this model.

The metrics of 0 wt% and 0.125 wt% in Table I also mean not that great performance compared to the others. The peak signal in 0.125 wt% is not large enough and there is no peak signal in 0 wt%. Furthermore, the random noise from Compton background increases so that the numerator in the equation (2) decreases and the denominator increases. For this reason, metrics of these two cases are less than of others. However, the first and second spectrum in Fig. 4 clearly shows that the model effectively reduces the Compton background.

The calibration curve in Fig. 5 shows that overall count from our model is lower than from the linear interpolation method, but has better linearity. R square values are better in our model, and points of 1 and 2 wt% are closer to the calibration curve.

Besides, linear interpolation only makes approximated Compton background that contains no random noise, but Compton background inferred by deep learning is more realistic which shows random noise like the red spectrum in Fig. 4. To confirm the strength of our model, we will do further research, for example, make a sinogram and a reconstructed CT image using a simple phantom.

5. Conclusion

Our 1D CNN based deep learning model has great performance at reducing the Compton background in the X-ray fluorescence spectrum, and we expect that our model makes a better 2D CT image than the existing methodology.

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