Deep learning-based Monte Carlo dose prediction for BNCT: A feasibility study

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1. Introduction

Boron neutron capture therapy (BNCT) is a radiation therapy that employs boron-10-containing compounds, which can be selectively accumulated in tumor cells. Once sufficient uptake occurs, the tumor is irradiated with a thermal neutron beam, causing the neutron capture reaction $^{10}\mathrm{B}(n,~\alpha)^7\mathrm{Li}.$ This reaction produces high linear energy transfer (LET) charged particles that can effectively kill tumor cells. Unlike conventional radiation therapy, BNCT requires the Monte Carlo method for accurate particle transport calculations, as neutron interactions are more complex than photon interactions [1]. However, this leads to substantially longer dose calculation times compared to other radiation therapies. In this study, we propose a deep learning-based dose prediction algorithm for BNCT, which enables significantly faster dose estimation than conventional Monte Carlo-based approaches.

2. Methods and Results

2.1. Dataset and pre-processing

The dataset was obtained from the GLIS-RT open dataset [2], which includes CT, MRI, and structural data such as gross target volume (GTV) and organs at risk (OAR). The complete cohort comprised 229 patients. To generate 3D dose distributions for training the dose prediction network, two-port cylindrical neutron beam configurations with randomly sampled beam weights were selected and simulated for each patient using the GPU-accelerated Monte Carlo algorithm RT² [3]. In total, 250 random two-port beam simulations were performed per patient. During preprocessing, all data were resized to 128x128x64. The intensities in the CT and structural mask data were normalized to a range of [-1, 1]. For the 3D dose distribution data, normalization was performed with respect to the maximum dose value, followed by standardization using the Z-score method. The dataset was then divided into training, validation, and test sets with a ratio of 7:2:1, respectively.

2.2. Network architecture and training details

In this study, a 3D U-Net backbone architecture was employed, incorporating several attention modules in the bottleneck. The network input consists of concatenated CT images, structural masks, and beam masks along the channel dimension. To incorporate additional beam information, beam parameters were encoded using sinusoidal positional encoding and integrated between the 3D U-Net blocks via two consecutive Linear-SiLU layers. The mean absolute error (MAE) was used as the loss function. Training was performed for 20 epochs with a mini-batch size of 4, utilizing the Adam optimizer with a learning rate of 0.0001 and a weight decay of 0.002. Model training required 9 days on a single NVIDIA A100 GPU.

2.3. Results of BNCT dose prediction

The quantitative results of the mean absolute error (MAE) on the test set are presented in Table I. These results include dose-volume histogram (DVH) criteria for the target volume as well as the average metrics for organs at risk (OAR). The findings demonstrate that the overall performance of our dose prediction network is comparable to that of Monte Carlo-based dose calculations. Fig. 1 and 2 provide a comparison of the DVH and 3D dose distributions for a randomly selected patient.

Table I: MAE results

	D95	D50	D5	D1	Avg
Target	2.104	3.269	3.654	3.380	0.001
OAR	0.443	1.115	2.607	3.322	

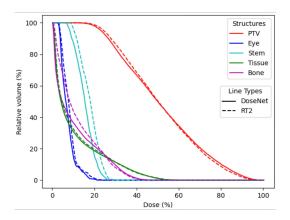


Fig. 1. Comparison of dose-volume histogram between deep learning-based method and Monte Carlo based method

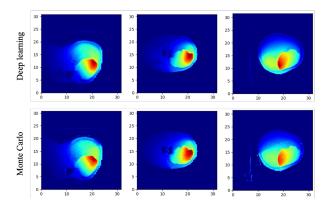


Fig. 2. Comparison of 3D dose distribution between deep learning-based method and Monte Carlo based method

3. Conclusions

In this study, we introduced a deep learning-based dose prediction network for BNCT that effectively addresses the time-consuming nature of conventional Monte Carlo-based dose calculations. Our proposed model accurately predicts the 3D dose distribution resulting from complex neutron interactions. The results demonstrate the feasibility of using the dose prediction network for particle transport calculations in BNCT treatment planning.

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