Scatter Estimation and Correction for Experimental and Simulated Data in Multi-Slice Computed Tomography Using Machine Learning and Minimum Least Squares Methods

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Scatter Estimation and Correction for Experimental and Simulated Data in Multi-Slice Computed Tomography Using Machine Learning and Minimum Least Squares Methods

By
Tongyao Wang

A thesis presented to the McKelvey School of Engineering of Washington University in St. Louis in partial fulfillment of the requirements for the degree of

Master of Science

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Abstract

Scatter Estimation and Correction for Experimental and Simulated Data in Multi-Slice Computed Tomography Using Minimum Least Squares Methods and Machine Learning

By

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Master of Science in Electrical Engineering

Washington University in St. Louis, 2021

Research Advisor: Dr. Joseph A. O’Sullivan

Current research aims to reduce the stopping power ratio prediction error in the inputs to the proton therapy planning process to less than 1%, which allows for improved radiation therapy planning. Our present study on reducing SPR error neglects the effect of scattering, which can increase SPR error by as much as 1-1.5%. The idea is that for each source-to-detector pair, 24 mm collimation data is close to 3 mm collimation data but with increased signal due to scattering. The goal is to estimate 3 mm collimation data from 24 mm collimation data. Pairs of sinograms, both experimental data and simulated data, from 3 mm and 24 mm collimation data are used to derive methods for this scatter correction. One method uses a linear least-squares approach to derive a linear estimator. A second method uses a U-net structure in a machine learning approach. An experiment is run using Monte Carlo simulation data to predict the 3 mm scatter-only signal from the 24 mm scatter-only signal using least squares estimation. The current version of the U-net structure cannot predict scatter-corrected data successfully because more artifacts are introduced. The proposed least squares model can use local measurements to
estimate scatter locally. In 2 of 3 groups of phantom data, reconstructed images of scatter-corrected data show higher uniformity and structural similarity with the ground truth than uncorrected data. The highest Structural Similarity Index Measure reaches 0.9869, and the lowest nonuniformity index reaches 2.16%. My study found that using local measurements to estimate scatter locally, the least-squares model keeps corrected sinogram low error and significantly improves the quality of corrected images by observing fewer artifacts, lower nonuniformity index, and higher structural similarities.
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Chapter 1 Introduction

1.1 Motivation

X-ray fan-beam computed tomography is extensively used for imaging in clinical diagnosis tasks and radiation therapy, including proton therapy. It is important to reduce uncertainties in reconstructed values as much as possible. In current clinical practice, a 2-3.5% safety margin added to the distal boundary of the clinical target volume (CTV) in face of proton range uncertainties (Medrano et al., 2020). The proton stopping power ratio (SPR) is the dominant element of proton range. Current research has a goal of reducing the SPR prediction root mean squared errors to less than 1% for proton therapy planning (Zhang et al., 2018). Achieving this goal will allow for improved radiation therapy planning, with reduced margins that reduce the dose to nearby at-risk organs. SPR depends on tissue composition and electron density and DECT (Dual energy CT) technique is the promising method for more quantitative tissue characterization. However, our present study done by Zhang et al., and Evans et al., on reducing SPR error neglects the effect of scatter, causing residual cupping and image nonuniformity in the reconstructed images, which increases uncertainty of DECT SPR maps (Evans et al., 2013; Zhang, 2018). Medrano et al., investigated that with scatter considered, mean SPR percentage error will increased by 1.5% (Medrano et al., 2020). Thus, scattering may represent a limiting factor in achieving this ambitious goal of reducing SPR prediction errors to less than 1%. 

In the process of scanning objects, when x-ray photons interact with matter in the beam path, the trajectory of some of the photons is forced to change, while others stay on a straight path. Changes in the direction of motion and energy of x-ray quanta due to discrete interactions are
referred to as scattering. The measured signal without scattered photons will be due to unattenuated or primary photons incident on the detector that travels through the patient along straight-line paths without being scattered or absorbed. The primary signal is predicted by the Beer-Lambert law, averaged over the exit energy-fluence spectrum, and depends on the linear attenuation coefficients of the materials along the straight-line photon path. Moreover, the scattered profile depends on the energy of the incident beam and volumes of tissue irradiated by primary photons (Hangartner, 1987). Modern scanners reduce scattering effects by adding anti-scatter grids (Liu et al., 2021) to block scattered photons and by collimating the detectors precisely (Ohnesorge et al., 1999).

Scatter modeling and scatter correction are important to achieve accurate quantification models. Current scatter models are classified as analytical or Monte Carlo (Zhao et al., 2016). Analytical modeling estimates the scatter distribution in the raw CT data by convolving primary photon collision density with a scatter kernel. This method is computationally efficient when precalculated scatter kernels are used (Zhao et al., 2016). Monte Carlo modeling computes the scatter distribution directly by tracking the trajectories of photons (Lazos & Williamson, 2010). However, Monte Carlo simulation is computationally inefficient, and its potential for clinical use has not been confirmed yet, so Monte Carlo simulation is often combined with other methods (Baer & Kachelriess, 2012).

Scatter correction is classified as image-based scatter correction, which has high computational costs, and projection-based correction (Ruhrnschopf et al., 2011). In image-based scatter correction, the scatter profile is estimated from the reconstructed image and fed back for scatter correction of the projection data. In projection-based scatter correction, a scatter profile is
modeled from projection data first. Then projection data is processed with a correction algorithm to remove scatter from the measured data. In both methods, the reconstructed images based on corrected projection data can be used to check the performance of the correction algorithm.

Most published work is focused on scattering correction and scatter estimation using cone-beam computed tomography (CBCT) (Jiang et al., 2019; Lalonde et al., 2020; Lee & Lee, 2019; Maier et al., 2018; Nomura et al., 2019; Xu et al., 2017) which has a much larger scatter-to-primary ratio than multi-slice diagnostic CT. Recently, more work regarding medical imaging scattering has been done using learning-based methods whose ability to deal with a complex mapping relationship helps construct a non-linear predictive model of the scatter distribution. Nomura et al. (Nomura et al., 2019) used a U-net structured convolutional neural network to achieve scatter correction, showed that the U-net correction reduced and root mean squared error (RMSE) of images against scatter-free projections to 0.0862 compared to 0.278 for uncorrected images. Maier et al. (Maier et al., 2018) use a deep convolutional neural network to reproduce the scatter generated from MC simulations. Quantitatively, deep scatter estimation outperforms the reference approaches (Hybrid and kernel-based method), leading to scattering estimation with Mean Absolute Percentage Error (MAPE) between 0.6 % and 1.5%, with a maximum error between 5% and 13.2%. Xu et al. (Xu et al., 2017) use a novel neural network to achieve scatter estimation and correction, and the reconstructed Convolutional Neural Network (CNN) corrected signals are close to the reconstructed primary signal. From the previous literature, novel CNN architectures and U-net architectures have shown outperformance in scatter estimation and correction for CBCT.
Quantitative comparisons between FBCT and CBCT show that CBCT images, especially in face of large cone geometry, are prone to have more artifacts and scatter than convolutional fan-beam CT (Lechuga & Weidlich, 2016). For multislice FBCT, the magnitude of scatter radiation is only 1-4% of primary signal, and the impact of scatter produced by FBCT on diagnostic image quality is small (Liu et al., 2021). Therefore, scatter estimation and correction using multislice Fan Beam Computed Tomography (FBCT) has not been widely considered or studied.

However, in face of quantitative applications, e.g. DECT SPR mapping, scatter is a significant source of uncertainty. DECT model is sensitive to the error of reconstructed image, and 1% reconstructed image error will lead to 5% uncertainty through DECT process. Evans et al. (Evans et al., 2013) shared the same long-term work as goal discussed in this thesis. Their paper investigated the accuracy of two reconstruction algorithms, Filter Back Projection (FBP) and Alternating Minimizing (AM). The effects, scatter radiation and spectrum estimation, were studied and corrected to enhance the accuracy. Since spectrum estimation is not considered in my thesis, I will only focus on summarizing methods and results related to scattered radiation in the following. Four reconstructions of each data set were presented: AM algorithm with scatter correction, AM algorithm without scatter correction, FBP with beam-hardening correction, FBP without Beam Hardening correction. Signal intensity from scattered radiation was estimated by the beam-stop method and considered as constant for all detectors and all gantry angles in CT sinogram data space. Then scatter correction was achieved by subtracting constant scatter signal from a data model that was used to calculate expected data means from image estimate. Beam hardening correction was achieved by vendor-supplied empirical BH correction. Radial profile and uniformity index were used to assess the bias caused by scattered radiation. I used FBP with scatter correction in my thesis, so it is hard to compare the value of AM with the scatter
correction presented in Evans et al. The information of FBP I used is introduced in section 2.4.1. However, his paper concluded that scatter correction is necessary even in a low scatter environment for achieving target accuracy of 1% or better. Nonuniformity index (NUI) are worth checking for scatter corrected FBP and scatter uncorrected FBP.

### 1.2 Proposed Idea and Goal

In the ideal case, wide collimation data is related to narrow collimation data, where collimation will be illustrated in section 1.3. In any single source-detector pair, the primary signal for 24 mm collimation is the same for 3 mm collimation. The scatter consists of random signals in each sinogram, but the mean scatter is larger for wide collimation data. Liu (Liu et al., 2021) investigated that, for 140kVp, simulated central axis scatter to primary ratio (SPR) at 3 mm collimation of 21.4 cm phantom is 0.321%, and SPR at 24 mm collimation is 2.154%. SPR at 3 mm collimation of 27 cm phantom is 0.558%, and SPR at 24 mm collimation is 3.940%. SPR at 3 mm collimation of 32 cm phantom is 0.709%, and SPR at 24 mm collimation is 5.120%. We can observe that SPR at 3 mm collimation is smaller than SPR at 24 mm collimation of those three types of phantoms. We treat 24 mm collimation data as primary plus scatter signal and 3 mm collimation data as primary signal. The assumption that scatter signal with 3 mm collimation can be ignored is that, without considering scatter radiation in narrow collimation, SPR can still be estimated successfully by referring to 0.35% RMS accuracy (Zhang, 2018).

In this thesis, all data used is in the projection domain. By using models that are designed for finding the mapping from 24 mm projection data to 3 mm projection data, narrow collimation data is expected to be estimated from wide collimation projection data. Three goals of this
projection-based method are 1) I designed the algorithm to estimate 3 mm collimation data from 24 mm collimation data. MSE between the ground truth and predicted output is expected be smaller than 1%. 2) As described in the proposed idea, 24 mm collimation data has the same primary signal as 3 mm collimation data but with higher mean scatter, so measured 24 mm collimation signal has larger value. Followed by Beer’s Law, signal can be derived by exponential term of negative linear attenuation coefficients. When investigating the scatter impacts, signal with scatter which is the non-negative value tends to have lower attenuation than primary signal or signal with less scatter. In the other words, in the attenuation profile, predicted data is expected to have higher value than 24 mm data. 3) The ultimate goal is to have more accurate reconstructed images and more accurate SPR estimation; in other words, scatter that appeared in reconstructed images in the image domain is expected to be reduced, so the impacts of scatter on mean SPR percentage error by 1-1.5% will be diminished as well (Medrano et al., 2020).

Two methods are investigated for obtaining the mapping. The first method is minimum least squares estimation, which implies the linear relationship between 24 mm collimation data and 3 mm collimation data. The motivation of using linear model is that B. Ohnesorge, et al. estimated scatter intensity distribution, which is subtracted from measured projection to achieve scatter correction, in fan beam projection using a convolution model. Scatter artifacts in three and fourth generation CT are found reduced by checking corrected reconstructed images (Ohnesorge et al., 1999).

The second method is a machine learning method, which has not been employed a lot in scatter estimation and correction in FBCT but has shown outperformance in this application in the
CBCT field as discussed in the previous literature review (Maier et al., 2018) (Xu et al., 2017) (Nomura et al., 2019). The machine learning structure used in this thesis was designed by Rui Liao and Tao Ge. In this thesis, the results produced by the machine learning structure are compared with results from linear least squares estimation. In previous work on scatter estimation or correction, the data used were mostly generated from Monte-Carlo simulations. Monte Carlo simulation is very accurate because the incorporated model is based on real physics concepts, but its computational complexity is high (Zhao et al., 2016). In this project, the performances of estimation and correction algorithms were evaluated both on phantom studies whose data were all collected from Philips Brilliance Big Bore CT scan experiments, and simulation studies produced from virtual CT which is designed based on geometry of Philips Brilliance Big Bore scanner.

1.3 Background

1.3.1 Fan Beam, Multi-slice Computed Tomography

The x-ray CT technique uses x-ray beams, traveling through a patient’s body, to image the anatomy and characterize tissue (Zhang, 2018). X-ray CT technology has undergone seven generations of development. In this thesis, I focus only on fan-beam, multislice CT scanners.

The x-rays generated by an x-ray tube are collimated in a fan shape, whose fan angle is usually between 30 to 60 degree (Prince & Links, 2006). The beam expands within the xy-plane and emanates from a slit along the z-axis. The object to be scanned is placed between the detector array and the x-ray source. The gantry holds the x-ray source and detectors so that they can rotate rapidly and repeatedly around the iso-center in the xy-plane (Zhang, 2018). Figure 1 shows the
geometry of projection of a fan-beam x-ray. The green arrow depicts that the x-ray tube and detector array rotate together in one complete cycle. Gantry positions are evenly distributed on a circle which is 360 degrees in total. Data acquired from one complete cycle of rotation are indexed by gantry positions and detectors.

![Illustration of projection of a fan-shaped x-ray beam on a single-slice CT. The green arrow represents the path of rotation. Figure source: Cone beam computed tomography in craniofacial imaging. by (Sukovic, 2003) Orthod Craniofac Res, 6 Suppl 1, 31-36; discussion 179-182. This figure has been modified by the author.](image)

Multislice CT was developed to overcome the heating problem caused by superfluous rotations needed when using single-slice CT. For single-slice CT, the slice thickness along z-axis is relatively small, so more rotations are needed to cover the targeted anatomy. Multislice CT increases the number of detector rows along the z-axis, so data can be collected for more than one slice at a time resulting in reducing the total number of rotations. Figure 2 shows the
differences between the geometries of the detector arrays of Single-slice CT (SSCT) and Multislice CT (MSCT). The figure on the left is the simplified geometry of SSCT. SSCT has a one-dimensional detector array consisting of many detectors placed in an arc along the x-axis but with a single element along the z-axis. The figure on the right shows the simplified geometry of MSCT. Each element along the z-axis of MSCT is not as monolithic as in SSCT, but is divided into several smaller detector elements forming multiple, parallel rows on the detector array. The right figure shown in Figure 2 shows an example of MSCT, consisting of 16 detector rows on the z-axis, each 1.25 mm long, for a total length of 20 mm. Data acquired from MSCT are indexed by gantry position, detector number and detector row. For instance, if there are 2640 gantry positions per rotation, 16 detector rows placed on the z-axis of the detector array, and 816 detectors per row, then, when the x-ray source and detectors rotate together for one circle, the dimension of the data will be $2640 \times 816 \times 16$.

Figure 2. Illustration of detector array of Single-slice CT (SSCT) (left) and Multislice CT (MSCT) (right). SSCT has monolithic detector elements along the z-axis. The MSCT detector array has multiple rows along the z-axis. Figure source: Principles of CT: multislice CT, by Goldman, L. W. (2008). J Nucl Med Technol, 36(2), 57-68; quiz 75-56. https://doi.org/10.2967/jnmt.107.044826
In MSCT, x-ray beam collimation is referred as the total length of the detector row along the z direction. Several detector elements along the z-axis can be linked together electronically to form different slice thickness. Figure 3 shows three different scanners: the middle one is close to the detector configuration used in this project. The Philips scanner can achieve 24 mm along z-direction formed by 16 0.75-mm-thick detector elements placed in the middle, and 4 of 8 1.5-mm-thick detector elements placed on the left and right ends respectively. The total slice thickness, or beam collimation length, is 24 mm. The slice thickness of the MSCT detectors can be adjusted by linking several detector elements in the z-axis as one monolithic detector. In this project, a 24 mm axial width x-ray beam can be utilized by linking each pair of adjacent 0.75-mm detectors into one 1.5-mm detector. So the number of detector rows is 16 instead of the 24 shown in the top two illustrations of Figure 3. The specific detector configuration and data formation used in this project will be introduced in detail in Section 2.1.

Figure 3. Diagram of 3 different scanners. Figure source: Principles of CT: multislice CT, by Goldman, L. W. (2008). J Nucl Med Technol, 36(2), 57-68; quiz 75-56. https://doi.org/10.2967/jnmt.107.044826
1.3.2 Scattering

Two important artifacts are caused by beam-hardening and photon scattering (Rodriguez-Granillo et al., 2015). According to the Beer-Lambert law, an x-ray beam will be attenuated exponentially when passing through a material. The low-energy X-rays are attenuated more than the high-energy ones, so the beam spectra attenuated by different path lengths of materials will have variable numbers low-energy photons. This is the cause of the beam-hardening effect. Scattered radiation and beam-hardening induce dark streaks in reconstructed images, especially between highly attenuating materials or along the long axis of a single highly attenuating object (Rodriguez-Granillo et al., 2015), and spatial low frequency gray value deformations, known as cupping artifacts (Ruhrnschopf & Klingenbeck, 2011). In many cases, especially for larger body parts, scattered radiation is a much more important source of artifacts than is beam hardening (Joseph & Spital, 1982). Scattered radiation also decreases soft tissue contrast and causes attenuation of highly attenuating substances to be underestimated.

X-ray scattering reduces image quality. It causes photons to change direction and to be detected in other detectors away from the correct ones (Hammer, 2014). Measured scatter increases as the number of detector rows is increased because the volume of irradiated tissue increases with increasing axial width of the subtending slice. Therefore, thinking of the multislice CT we are using, scatter effect in 24 mm collimation data is larger than scatter effect in 3 mm collimation data. Larger slice widths, like 24 mm, will scan a larger target area. Figure 4 illustrates how the target area changes when using wide and narrow collimation CT scanning through a human body. Especially when using computed tomography clinically on a patient’s body, fewer rotations are
necessary with wider collimation and motion artifacts are reduced. Therefore, using multiple
detector rows but with fewer effective scattered photons is desirable.

Figure 4. Illustrations of change in scanning target area with wide collimation (thick slice, on the right) and narrow collimation (thin slice, on the left). Figure source: https://quizlet.com/au/301301253/ct-flash-cards/(Tuckecr).

1.4 My Contributions on This Thesis:

The main contributions of this thesis are as follows:

- Designed the minimum least-squares estimation algorithm customized for finding the mapping from wide collimation data to narrow collimation data. This mapping was used to achieve scatter correction for wide collimation.
- Designed the algorithm used for truncating data so the number of inputs and outputs of the algorithm can be increased to better feed the model.
- Evaluated validation results from minimum least squares estimation using the chosen estimators (MSE). Evaluated testing results from minimum least squares estimation based on Structural Similarity Index Measure (SSIM), Nonuniformity Index (NUI), sinograms, and reconstructed images.
- Manipulated U-net Neural Network algorithms to produce validation results and test results trained on multiple groups of experimental data.
Investigated Geant4 based Virtual CT techniques and modified the code to add a Spherical Phantom with spherical inserts.

1.5 Outline

Chapter 2 describes the methods used to acquire and truncate the data. The mathematical derivation and the programming strategy of minimum least squares estimation are presented. The machine learning structure and Monte Carlo simulation methods are also introduced here. Chapter 3 presents the results produced by minimum least squares estimation and the machine learning algorithm. Chapter 4 is the Discussion and conclusion chapter. Chapter 5 is the References chapter.
Chapter 2 Methods

When using the Philips Brilliance Big Bore CT, it is difficult to collect scatter-only signal during experiments. With the proposed idea, we consider 3 mm collimation data as the scatter-corrected counterpart of 24 mm collimation data. Both minimum least squares estimation and a machine learning method are trained to derive 3 mm collimation measured projection signal \( (I_3) \), consisting of primary and scatter signal, from 24 mm collimation measured projection signal \( (I_{24}) \), consisting of primary and scatter signal. Scatter correction of 24 mm collimation data is achieved by finding the mapping and the successfully deriving the 3 mm signal utilizing prior knowledge of the mapping. Data collected from detector row 1 and row 2 in 4th 3 mm slice are used because they correspond to the middle row at 24 mm collimation. The information of data is introduced in section 2.1. The workflows of minimum least squares estimation and the learning-based scatter correction are summarized as Figure 5 (a) and (b).

The training process for the minimum least squares estimation is to estimate the matrix by feeding in pairs of 24 mm collimation \( (I_{24}) \) and 3 mm collimation data \( (I_3) \) from the training data set. To avoid overfitting, I partition the data into lower dimensional subsets to increase the number of data pairs. In the testing process, each predicted \( I_3 \) is derived by multiplying by each truncated \( I_{24} \) by the estimation matrix. The details of truncation are introduced in 2.2.2.

For simulation data produced by Geant4, I estimate the 3mm scatter-only signal \( (I_{s3}) \) from 24 mm scatter-only signal \( I_{s24} \). Previous learning-based literature (Xu et al., 2017) (Wang et al., 2021) start with deriving the scatter-only signal from primary plus scatter signal when using Monte Carlo simulation data because scatter to primary ratio is lower than 80%, and prediction
based on a scatter-only signal will be more accurate (Wang et al., 2021). In this project, since the proposed idea is that the 24 mm scatter signal is related to the 3 mm scatter signal, I choose to estimate the 3 mm scatter signal from the 24 mm scatter signal. The predicted scatter profile can be compared with the scatter profile of 24 mm collimation sinogram and the scatter profile of 3 mm collimation sinogram. The training model used is minimum least squares estimation, and the workflow is shown in Figure 5 (c).

The mathematics of least squares estimation is introduced in 2.2.3. The machine learning structure used in this thesis is a U-net neural network. This method is used for comparison with least squares estimation. Details of the U-net structure are introduced in Section 2.3. The evaluation method is explained in Section 2.4.
Figure 5. (a) is the workflow of minimum least squares estimation scatter correction, (b) is the workflow of the U-net learning-based correction, and (c) is the workflow of the scatter-only simulated data training and testing process.

2.1 Data

2.1.1 Experimental Data

The CT instrument we used to collect data is called the Philips Brilliance Big Bore Scanner, which is a multislice scanner. Each row consists of 816 detectors. The maximum energy of the x-
ray spectrum supported by the Big Bore Scanner is 140 kVp. The system is able to generate 3 mm, 12 mm and 24 mm collimation data by adjusting the collimator and the combination of detector rows and widths of the rows. In this project, we mainly focus on using 3 mm and 24 mm collimation data. The detector configuration for 3 mm collimation consists of 4 rows of detector elements, each 0.75 mm long in the z-direction. For a total z-axis length of 24 mm collimation data, the detector consists of 16 center rows, each 0.75 mm, and surrounded by 8 rows that are 1.5 mm long. Then adjacent pairs of detectors in the central rows get electronically linked together to yield 16 rows of 1.5 mm each. A diagram of the detector configuration of 24 mm collimation and 3 mm collimation is shown in Figure 6. The experiments were conducted using a scanning mode with 2640 views per rotation.

![Detector configurations of 24 mm collimation and 3 mm collimation along the z-axis.](image)

Raw data was exported to a PC for further preprocessing by using a proprietary software provided by Philips. The correction steps which were applied on the raw data included: Crosstalk, Threshold Check, DeltaR Normalization, Air Correction, Thresholding, Wedge
Subtract, Phantom Calibration, Bad Detector, Low Signal Streak, Lost Fan Interp, and Float to Ushort.

Five types of phantoms were scanned using the Philips Brilliance Big Bore Scanner. Table 1 lists the phantoms used in this thesis.

<table>
<thead>
<tr>
<th>Phantom name</th>
<th>Phantom Shape</th>
<th>With or without inserts</th>
</tr>
</thead>
<tbody>
<tr>
<td>Water Phantom</td>
<td>Cylindrical phantom</td>
<td>Water</td>
</tr>
<tr>
<td>Sample Head Phantom</td>
<td>Cylindrical phantom</td>
<td>Water, K$_2$HPO$_4$, propanol, ethanol, butanol</td>
</tr>
<tr>
<td>Body Phantom</td>
<td>Cylindrical phantom plus an elliptical ring</td>
<td>Water, K$_2$HPO$_4$, propanol, ethanol, butanol</td>
</tr>
<tr>
<td>Pelvis Phantom</td>
<td>Anthropomorphic phantom</td>
<td></td>
</tr>
<tr>
<td>Thorax Phantom</td>
<td>Anthropomorphic phantom</td>
<td></td>
</tr>
</tbody>
</table>

Table 1. Information about phantoms used in this thesis. The first column is the phantom names used in this thesis. The second column is the shape of the phantoms. The third column shows information about inserts in the phantoms.

Figure 7 shows pictures of (a) the Sample Head Phantom, (b) the Body Phantom, (c) the Thorax Phantom, and (d) the Pelvis Phantom. The dimension and shape of the Water Phantom is the same as the Sample Head Phantom but with no spherical inserts.

During the experiments, the scanner was set to axial scanning mode and scanned over 48 mm along the z-axis for the Water Phantom, Body Phantom and Sample Head Phantom. In other words, with the 24 mm collimation setting, data were acquired with 2 scans, each 24 mm long and consisting of 816 by 16 by 2640 measurements. With the 3 mm collimation setting, the data were collected with 16 scans, each 3 mm long and consisting of 816 by 4 by 2640 measurements. For the Pelvis and Thorax Phantoms, the total scanning coverage is 96 mm along the z-axis, so 4 scans are needed to acquire data with the 24 mm collimation setting, and 32 scans are needed to acquire data with the 3 mm collimation setting.
Figure 7. Pictures of experimental phantoms listed in Table 1. (a) Sample Head Phantom. (b) Body Phantom. (c) Thorax Phantom. (d) Pelvis Phantom.

2.1.2 Simulation Data

The virtual CT is designed based on specifications of the Philips Brilliance Big Bore CT scanner. The detector layouts are the same as described in the specifications of the real CT. The energies of x-ray spectra available to use are 140 kVp and 90 kVp. The number of gantry views per rotation of this virtual CT is set as 360. Due to long computation time, photon history is set to track only 100 million photons at each gantry angle. The Monte Carlo Simulation method based on the Geant4 package is used to produce the simulation data. The code was designed and written by Ruirui Liu (Liu et al., 2021), and for this project, the code was modified to increase the number of detector rows from 1 to 16. Two types of simulated phantoms are used. The first phantom, named the Simulated Sample Head Phantom in this thesis, is modeled after the cylindrical phantom with inserts and has the same dimensions and insert materials as the experimental Sample Head Phantom. The background material of this phantom is water, and the
walls of the Lucite container are not simulated. The diagram of the Simulated Sample Head Phantom is shown in Figure 8(a). The second phantom, called the Spherical Phantom, is a water sphere of diameter is 180 mm. It is filled with 16 ethanol spherical inserts with diameter of 12 mm, 11 ethanol spherical inserts with diameter of 24 mm, 72 butanol spherical inserts with diameter of 6 mm, and 45 butanol spherical inserts with diameter of 3 mm. The center of the Spherical Phantom is at the origin (0,0,0). Inserts with diameter of 12 mm are placed in the upper half of this sphere. The centers of these inserts are placed along positive y axis. The 24 mm-diameter inserts are placed in the left half of this sphere. Inserts with diameter of 6 mm are placed in the lower half of the sphere. Inserts with diameter of 3 mm are placed in the right half of the large sphere. The front and lateral views of this spherical phantom are shown in Figures 8(b) and 8(c), respectively. The name and characteristics of the simulated phantoms are listed in Table 2.

<table>
<thead>
<tr>
<th>Name</th>
<th>Shape</th>
<th>Inserts</th>
</tr>
</thead>
<tbody>
<tr>
<td>Simulated Sample Head</td>
<td>Cylindrical Phantom</td>
<td>Water, K$_2$HPO$_4$, propanol, ethanol, butanol</td>
</tr>
<tr>
<td>Phantom</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Sample Spherical Phantom</td>
<td>Spherical Phantom</td>
<td>Water, ethanol, butanol</td>
</tr>
</tbody>
</table>

Table 2. List of simulated phantoms and their characteristics.

Figure 8. Illustrations of simulated phantoms built by Geant4 code. (a) is the Simulated Sample Head Phantom. The large circles (red and green) represent the outer and inner of the cylindrical phantom. The small circles inside represent different inserts. (b) is the front view of Spherical Phantom. (c) is the lateral view of Spherical phantom.
2.2 Minimum Least Squares Estimation

2.2.1 Workflow of Scatter Correction Based on Minimum Least Squares Estimation

Firstly, I will evaluate the feasibility of structure and parameters chosen for the algorithm by evaluating the performance on the same training data set. The predicted output was generated as the product of the estimation matrix and the 24 mm collimation data that is used for training. By comparing the predicted sinogram with the training 3 mm sinogram, which is taken as ground truth, the performance of minimum least squares estimation on training data in transmission domain is estimated. The standard of evaluation is that MSE (mean squared error) of the predicted output against the input should be smaller than 1%. Once MSE is smaller than 1%, initial guesses and parameters are settled for use in the next step; training data and testing data are independent.

In the independent data training and testing processes, independent training data and test data set is required to test the generalization of the model for new data. Training data and test data should be collected from different phantoms. For example, training data can be 24 mm collimation and 3 mm collimation from the thorax phantom, and testing data can be data collected from the pelvis phantom.

2.2.2 Processing Data

Our method for processing pairs of measurements is to use “windows” of data. The purpose of processing the data is to avoid overfitting by increasing pairs of input and output, and shrink the size of each training datum. For each group of data, if we treat the measurements as a 3-D
matrix, there are \( n \) by 816 by 2640 measurements, where \( n \) represents the number of detector rows (16 for 24 mm collimation and 2 for 3 mm collimation), 816 represents the number of detectors per row, and 2640 represents the total number of source locations. For each source location, I select \( M \) columns of data to get an \( n \) by \( M \) matrix. This matrix is what we refer to as a “window.” A virtual cursor is used to monitor the steps that the window slides. Locate the cursor at the beginning of the window and move by \( K \) columns to get the next window until all 816 detectors have been used. There are two options when implementing the window selection. The first is to choose non-overlapping windows, which means \( K = M \). The other option is to choose overlapping windows, with \( K < M \). In the testing process, overlapping data selection method shows superiority on 1) increasing number of data points, 2) being prone not to miss information appears at the edge at each non-overlapping function. Based on this rationale, the non-overlapping method was also applied on the same phantom data for comparison. These window-selection strategies are shown in Figure 9.

*Figure 9. Diagram of the window-selection process. The upper arrow points to the non-overlapping method and the lower arrow points to the overlapping method.*
This window-selection method applied to 24 mm collimated data produced the input data and applied to 3 mm collimation data produced the output data. For the non-overlapping selection, I chose $K = 48 = M$. For the 24 mm collimation data, there are 16 detector elements (rows) along the z-axis. The window is 16 by 48, and there are 17 windows per source location; considering 2640 total source locations, there are $17 \times 2640$ total windows. For the 3 mm data, originally, there are 4 detectors per row, and each detector is 0.75 mm long. For consistency with the length of detector elements in the 24 mm collimation design, which is 1.5 mm long per detector, I combined the first two rows into one by taking the average of them, then combined the third and fourth rows into one by taking the average.

After nonoverlapping window selection, dimension of 24 mm collimation data is (48, 16, 17) for each gantry position. I denoted 17 as layers, 48 as rows and 16 as columns. Then reshape (48, 16, 17) to $(48 \times 16, 17)$ by row-wise order, which means, after reshaping, in each layer, the last element from the previous row resides by the first element of the next row. The illustration of row-wise reshaping method is shown in Figure 10. Counting in all gantry positions, the data dimension is (768, 17, 2640), where 2640 becomes layers, 768 represents rows and 17 represents columns. Then apply the row-major reshaping method, the data becomes (768, 44880). Same procedure will be repeated on 3 mm collimation data to form dimension of (96, 44880).

In the overlapping window selection, stride $K$ is chosen as 12, which is 25% of the window size. Then dimension of 24 mm collimation data is (768, 179520) and of 3 mm collimation data is (96, 179520).
2.2.3 Mathematics Derivation and Computational Procedure for Minimum Least Squares Estimation

Minimum least squares estimation provides the linear mapping relationship between 24 mm and 3 mm collimation data. To recover the linear mapping, minimum least squares estimation became the first choice. It aims to find the best-fit estimators by minimizing the squared differences between the observed data and their corresponding expected data.

\[ \mathbf{A} = \min_{\mathbf{A}} \sum_{n=1}^{N} \| \mathbf{y}_n - \mathbf{A} \mathbf{x}_n \|^2. \]  

(A is the linear mapping relationship of interest. If denote 24 mm collimation as \( \mathbf{X} \), whose dimension is \((768, N)\), where \( N \) will vary in terms of overlapping and non-overlapping window selection. \( \mathbf{x}_n \) is each row vector of \( \mathbf{X} \), whose dimension is \((768,1)\). Similarly, if denote 3 mm collimation as \( \mathbf{Y} \), whose dimension is \((96, N)\). \( \mathbf{y}_n \) is each row vector of \( \mathbf{Y} \), whose dimension is \((96,1)\).)

We seek the matrix \( \mathbf{A} \) according to

\[ \mathbf{A} = \min_{\mathbf{A}} \sum_{n=1}^{N} \| \mathbf{y}_n - \mathbf{A} \mathbf{x}_n \|^2. \]  

(Figure 10. Illustration of row-wise reshaping method. \( r \) represents row, \( c \) presents column.)
Equation (1) is the general form of minimum least squares and $\mathbf{A}$ is the coefficient matrix used for minimization, which is the crucial element that must be estimated. Expanding the squared terms in (1) gives
\[
\min_{\mathbf{A}} \sum_{n=1}^{N} (\mathbf{y}_n - \mathbf{A}\mathbf{x}_n)^T (\mathbf{y}_n - \mathbf{A}\mathbf{x}_n). \tag{2}
\]
A necessary condition for the minimization is that the gradient be zero, which yields
\[
\sum_{n=1}^{N} (\mathbf{y}_n - \mathbf{A}\mathbf{x}_n)(\mathbf{x}_n)^T = 0 \tag{3}
\]
or
\[
\mathbf{A} = (\sum_{n=1}^{N} \mathbf{y}_n\mathbf{x}_n^T)(\sum_{n=1}^{N} \mathbf{x}_n\mathbf{x}_n^T)^{-1}. \tag{4}
\]
Anticipating the recursive least squares (RLS) algorithm discussed below, the matrix $\mathbf{A}$, which we also will call a filter, recursively finds the coefficients that minimize a weighted linear least squares cost function according to:
\[
\mathbf{A}_N = (\sum_{n=1}^{N} \mathbf{y}_n\mathbf{x}_n^T)(\sum_{n=1}^{N} \mathbf{x}_n\mathbf{x}_n^T)^{-1}, \tag{5}
\]
\[
\mathbf{A}_{N+1} = (\sum_{n=1}^{N+1} \mathbf{y}_n\mathbf{x}_n^T)(\sum_{n=1}^{N+1} \mathbf{x}_n\mathbf{x}_n^T)^{-1}. \tag{6}
\]
Where in Equation (6), $N+1$ represents $\mathbf{A}$ is updated recursively. A key mathematical tool of this algorithm is the matrix inversion lemma. The coefficient is updated recursively once the input data are updated at each step. The matrix inversion lemma is also known as the Woodbury matrix formula and states the identity that the inverse of a rank one update of the matrix can be computed by doing a rank one update of the inverse of the original matrix.

There are two main reasons why we want to use RLS instead of computing $\mathbf{A}$ according to Equation (4) are 1) If dimension of $\mathbf{A}$ is large, implementing matrix inverse and multiplication
would be very expensive. By applying the RLS filter, we are able to reduce the high computational cost. Since input pairs are all non-negative values, the matrix which is obtained by summing them up will be large in values and the inverse of it will be extremely small. By doing matrix multiplication between those two, there could be numerical instability. By doing RLS, we are able to avoid this situation.

To better show the process of recursive updates, separating the terms from (4) is necessary. Let

\[ R_N = \sum_{n=1}^{N} x_n x_n^T, \]  
\[ R_{N+1} = R_N + x_{N+1} x_{N+1}^T, \]  
\[ Q_N = R_{N}^{-1}, \]

where the subscript \( N \) represents each stage and \( N+1 \) represents the updated one. \( Q_N \) is the inverse correlation matrix

\[ Q_{N+1} = (Q_N^{-1} + x_{N+1} x_{N+1}^T)^{-1} \]

\[ = Q_N(I + x_{N+1} x_{N+1}^T Q_N)^{-1}. \]

In Equation (10), \( I \) represents the identity matrix. A simple form of the Woodbury matrix identity is given as

\[ (I + ab^T)^{-1} = I - \frac{1}{1 + b^T a} ab^T. \]

Applying this to the expression in (10),

\[ Q_{N+1} = Q_N - \frac{1}{1 + x_{N+1}^T Q_N x_{N+1}} Q_N x_{N+1} x_{N+1}^T Q_N \]

The part inside the parentheses of Equation (10) is expanded according to Equation (12). Then

the recursive update to matrix \( A \) is given by

\[ A_{N+1} = (\sum_{n=1}^{N} y_n x_n^T + y_{N+1} x_{N+1}^T) Q_{N+1}. \]
Since $Q_{N+1}$ is shown as (12), apply (12) to the updated matrix $A$. There are two parts of the update to this matrix. The first term has the primary matrix plus the rank one term, which is given by

$$\left(\sum_{n=1}^{N} y_n x_n^T + y_{N+1} x_{N+1}^T\right) Q_N = A_N + y_{N+1} x_{N+1}^T Q_N . \quad (14)$$

The derivation of the second part is

$$-\left(\sum_{n=1}^{N} y_n x_n^T + y_{N+1} x_{N+1}^T\right) \frac{1}{1 + x_{N+1}^T Q_N x_{N+1}} Q_N x_{N+1} x_{N+1}^T Q_N$$

$$= - A_N x_{N+1} \frac{1}{1 + x_{N+1}^T Q_N x_{N+1}} x_{N+1}^T Q_N - y_{N+1} \frac{x_{N+1}^T Q_N x_{N+1}}{1 + x_{N+1}^T Q_N x_{N+1}} x_{N+1}^T Q_N . \quad (15)$$

Combining Equation (15) and Equation (14), the final expression for the updated $A_n$ is given by

$$A_{n+1} = A_n + (y_{n+1} - A_n x_{n+1}) \frac{1}{1 + x_{n+1}^T Q_n x_{n+1}} x_{n+1}^T Q_n . \quad (16)$$

The RLS computational algorithm is summarized as follows:

Initial guess $A_0$

Input pairs of examples: $(y_n, x_n)$

Initialize the inverse correlation matrix: $Q_0$

For each input pair $(y_n, x_n)$, $n=1,2,\ldots,N$

Compute prediction error: $e_n = y_n - A_{n-1} x_n$

Compute update vector: $\gamma_n = Q_{n-1} x_n$

Compute scale factor: $\rho_n = \frac{1}{1 + x_{n+1}^T Q_n x_{n+1}}$

Update estimation matrix: $A_n = A_{n-1} + \rho_n e_n \gamma_n^T$

Update inverse correlation matrix: $Q_n = l^{-1} (Q_{n-1} - \rho_n \gamma_n \gamma_n^T)$
Based on the expression derived in Equation (16), the computation of estimating the matrix \( A \) starts with a guess of the initial \( A_0 \), which is often very small, and I chose a matrix of all zeros here. According to Equation (8), the correlation matrix and the inverse correlation matrix are determined by the input vectors. The initial guess for either the correlation matrix or its inverse requires knowledge of prior input history, which is hard to define. In order to prevent the matrix \( Q_n \) from becoming singular after a finite number of iterations, \( Q_0 \) is usually defined as \( \alpha \mathbf{I} \), where \( \mathbf{I} \) is the identity matrix and \( \alpha \) is the coefficient that controls the value of \( Q_n \). Conventionally, the choice of \( \alpha \) is given as \( \alpha > 100 \sigma^2 \), where \( \sigma^2 \) is the variance of the input data (Rowell, 2008).

Therefore, the initial coefficient of the inverse correlation matrix should be large; I chose at least 100000. In the algorithm, the additional parameter that is not shown in the mathematical derivation, called the forgetting factor, is represented as \( \lambda \). This parameter controls the relative weight of more recent examples to the previous examples. A small value of \( \lambda \) can lead to rapidly changing values of the inverse correlation matrix and of the resulting filter \( A \). A value of \( \lambda \) closer to 1 leads to a slowly changing inverse correlation matrix and therefore a slowly changing value of the filter. Since the number of iterations is very large in this project, choosing \( \lambda \) wisely will make the matrix more sensitive to recent input data instead of converging early to a barely changeable value. Typically, \( \lambda \) is chosen between 1 and 0.98 (Ifeachor & Jervis, 2002).

However, if I randomized the order of the pairs of \((x_n, y_n)\), it leads to stable values of the inverse correlation matrix and the resulting filter. In that case, the value of the forgetting factor may not be as important, but we still choose it to be close to 1 in order to further stabilize the value. Also,
the forgetting factor makes the final values almost independent of the initial condition. As discussed above, the initial condition of the inverse correlation matrix is chosen to be large because it has larger eigenvalues than the converged final matrix. This is because, predominantly, the inverse correlation matrix decreases in size at all early and many late iterations.

### 2.2.4 Methods of Obtaining The Predicted Output

We applied two ways to derive the predicted output. The first is: Multiply A matrix with 24 mm collimation data separated into multiple 16 by 48 blocks by overlapping window selection. For instance, if the overlapping fraction is 75% (36 out of 48 are overlapped), then the number of blocks is 65. To combine these blocks into the desired (2,816) dimension, I selected 30 columns from the first and the last blocks and only kept the middle 12 columns, columns 19 to 30, of the remaining 63 blocks. Of course, the number of blocks and column selection could vary according to a different overlapping fraction. In this thesis, the results presented are using overlapping fraction 98%, which means every time, the block is shifted by 1 column.

The second method is to use a reduced-size A matrix. The dimension of the whole A matrix is (96,768), where odd rows represent elements from the 1st row of the 3 mm collimation data, and even rows represent elements from the 2nd row; every 16 columns out of 768 columns represent one column of the 16 detector rows of the 24 mm collimation data, and 768 are composed of 48 columns of 16 detector rows. Separate the large A matrix into two smaller matrices by selecting odd rows or even rows. We selected the first (16,16) block from each smaller A matrix, shifted the block by 1 row and 16 columns to select the next one, and the rest can be done in the same
manner. In this case, averaging 16 by 16 matrix shows that the 24 mm collimation data make the most contribution on the seventh element of 3 mm collimation. The plots of the reduced-size A matrix are shown in section 3.1. To keep the 7th element in the middle, we reduced the A matrix to (13,16). Then we multiplied 24 mm collimation data, whose dimension is (16,816), with each of reduced-size A matrix respectively, and for each gantry position, the dimension of each of output is (13, 816), where 13 means 13 columns from either detector row 1 or detector row 2 in 3 mm collimation data. To recover the row 1 in 3 mm collimation from the output, firstly, we separated the output into three parts, the first part is the first six columns, the second part is from column 7 to 810, and the third part is the last six columns. The computational recovery algorithm is summarized below for convenience. The algorithm is designed by Joseph O’Sullivan.

Initialize row 1 in 3 mm collimation to an all zero matrix (1,816)

For k from 1 to 816:

if k < 7  % the first part of output
    row1(1,1:6+k) = row1(1,1:6+k) + transpose of output(8-k:13,k)
if k > 810 % the third part of output
    row1(1,k-6:816) = row1(1,k-6:816)+transpose of output(1:823-k,k)
else: % the middle part of output
    row1(1,k-6:k+6) = row1(1,k-6:k+6) + transpose of output(:,k)
end
end
2.3 Machine Learning

The structure of U-net has been proved effective for the scatter correction problem (Lalonde et al., 2020; Maier et al., 2018; Nomura et al., 2019; Wang et al., 2021). The architecture of the U-net based neural network used in this project is shown as Figure 11. There are two paths in this network design: downsampling paths and upsampling paths. In the downsampling paths, each step consists of two 3 by 3 convolution layers, followed by a Rectified Linear Unit (ReLu). We chose the input size as $816 \times 16$ to allow for future dimension reduction and increase. On the downsampling path, the size of each feature map was reduced by 2. For instance, the first feature map after the first step of convolution layers and max pooling became $408 \times 8$. Then, after the max pooling operation, the size of features was decreased, and the number of features was doubled. In the upsampling path, the upsampled features were merged with the prior downsampled features each time before experiencing $3\times3$ convolution layers. The other steps are analogous to the downsampling path. Finally, the dimension of the output is $816 \times 2$. The loss function here is defined as the function to minimize the error. Here we chose mean squared error as the loss function and the optimizer is stochastic gradient descent.
2.4 Evaluation

2.4.1 Experimental Data

Sinograms of 24 mm collimation data, predicted output and true 3 mm collimation data are presented to evaluate the performance of the model, and to assess similarities and differences between true 3 mm collimation data and the predicted output.

The MSE is calculated to evaluate the predictive capability of the model. The equation of MSE is

$$MSE = \frac{1}{n} \sum_{i=1}^{n} (Y_i - \hat{Y}_i)^2.$$
$Y_t$ represents each measurement from the second row of 3 mm collimation sinogram (2640 $\times$ 816), and $\hat{Y}_t$ represents measurements from the second row of predicted sinogram (2640 $\times$ 816).

A filtered back projection (FBP) algorithm was used to reconstruct images. The code was written for Object Constrained Computed Tomography (OCCT) research, and written by David G. Politte.

Since phantom background, water, are known to be uniformity, nonuniformity index (NUI) will be used to assess the quality of corrected and uncorrected images. The equation of NUI is defined by Lazos et al., (Lazos & Williamson, 2010):

$$NUI = 100 \frac{\mu_{98\%} - \mu_{2\%}}{\mu_{98\%}}$$

$\mu_{98\%}$ is the minimum intensity value that exceeds the value of 98% of the water ROI, and $\mu_{2\%}$ is the maximum intensity value that exceeds no more than 2% of the water ROI. I chose the circular water ROI with diameter of 23 pixel, and computed cumulative histogram of the pixel intensities within the region. In the end, selected 2% and 98% quantile as $\mu_{2\%}$ and $\mu_{98\%}$.

The other metric is used to assess similarities between predicted image and ground truth image is structural similarities index measurements (SSIM). SSIM quantifies the perceptual differences between two images, and is not a common metric analyzing image quality prepared for radiation therapy. I use SSIM because NUI is only measure image quality within the selected region while SSIM is able to quantify the image globally. Moreover, I used MSE to quantify similarities.
between predicted results and ground truth in sinogram domain, and SSIM quantifies this similarities in image domain.

2.4.2 Simulated Data

When analyzing Monte Carlo Simulation data, a normalized scatter profile of 24 mm collimation data, 3 mm collimation data, and the predicted output will be plotted. The normalized scatter profile (NSP) is energy imparted to each detector by scattered photons divided by the energy imparted to the central-axis (middle detector) by primary photons exiting the scanned object (Liu et al., 2021). In the other words, the 24 mm and 3 mm scatter profiles will be normalized by the corresponding primary signal in the middle detector. The predicted signal is normalized by the 3 mm primary signal in the middle detector. The denoising method, modified by Liu et al. (Liu et al., 2021), is used to eliminate noise of normalized scatter signal. The assumption of this method is that the signal follows by Poisson random process with the mean produced by convolution of true scatter profile and gaussian kernel. Maximum likelihood estimation technique is used to design this denoising method.
Chapter 3 Results

3.1 A Matrix

Figure 12 shows plots of the estimation matrix $A$ produced by training with the thorax phantom and the body phantom. The horizontal axes of Figures 12(a), 12(b), and 12(c) have been vectorized to include all 48 detectors in a truncation window times 16 detector rows to yield 768 distinct indices. Similarly, the vertical axis of Figure 12(a) has been vectorized to include all 48 detectors in a truncation window times 2 detector rows to yield 96 distinct indices. In Figure 12(a), we can observe a diagonal line, which represents that the x and y axes have a linear relationship. The bright spots along the line represent which elements along the x-axis (detector rows of 24 mm collimation sinogram) make the largest contributions to elements along the y-axis (columns of the 3 mm collimation sinogram). Figure 12(b) and Figure 12(c) show how matrix $A$ contributes to columns in row 1 and row 2 of the 3 mm collimation sinogram, respectively. For better illustration, we vertically sheared Figure 12(b) to create Figure 12(d) and vertically sheared Figure 12(c) to create Figure 12(e). This shearing converted the diagonal lines into horizontal lines. Then we took the element-by-element average of $16 \times 16$ non-overlapping sub-blocks in Figures 12(d) and 12(e) to create Figures 12(f) and 12(g), respectively, to indicate which rows in the 24 mm collimation data make the largest contributions to the 3 mm collimation data. The bright spot appeared in Figure 12(f) shows that, for row 1 of the 3 mm collimation data, on average, the row 9th of the 24 mm collimation sinogram makes the largest contribution to the 7th column of the 3 mm collimation sinogram. Similarly, Figure 12(g) shows that for row 2 of the 3 mm collimation data, on average, the 10th row of the 24 mm collimation sinogram makes the largest contribution to the 7th column of the 3 mm collimation sinogram.
Ideally, if the 24 mm collimation and 3 mm collimation data are aligned, the brightest spot should appear at the center. Therefore, this plot is the evidence of the misalignment along the z-axis between the 3 mm collimation data and the 24 mm collimation data.
Figure 12. Plot of A matrix. (a) Plot of matrix A trained with thorax and body phantom data. (b) Contributions of matrix A to row 1 of the 3 mm collimation sinogram. (c) Contributions of matrix A to row 2 of the 3 mm collimation sinogram. (d) Vertically sheared version of panel (b) to convert the diagonal relationship of matrix A contributions on row 1 to a horizontal one. (e) Vertically sheared version of panel (c) to convert the diagonal relationship of matrix A contributions on row 2 to a horizontal one. (f) Averaging weighting for row 1 contributions on columns in the 24 mm collimation sinogram. (g) Averaging weighting for row 2 contributions on columns in the 24 mm collimation sinogram.
3.2 Least Squares Estimation

Whole A Matrix:

The training data needs to be normalized by corresponding air scan data. Unnormalized training data does not affect MSE too much but can cause a linear attenuation coefficient of predicted air to increase by 2.5% than it should be. The overlapping blocks used to multiply with the A matrix are shifted by one column.

Training data is 24 mm and 3 mm of thorax phantom. The evaluation of how well the matrix can predict training data is presented here. Figure 13 shows 3 mm sinograms of thorax phantom, predicted sinogram, and their differences. The main differences appear at the edge between the phantom and the air. The MSE between 3 mm sinogram, which is considered ground truth, and the predicted sinogram is 0.00357%.

![Figure 13](image)

*Figure 13. (a) 3 mm sinogram of thorax phantom for 2rd detector row. (b) Predicted sinogram derived by thorax phantom-trained matrix and input data (24 mm data of thorax phantom) for 2rd detector row. (c). Difference between 3 mm and predicted sinogram.*
Figure 14 shows 24 mm, 3 mm, and predicted attenuation profile for gantry position 600. In most locations, predict attenuation profile is between 24 mm and 3 mm, although there are fluctuations due to noise. There is one prominent anomalous high peak appearing in the 24 mm attenuation profile. The high peak also appears in other 24 mm attenuation profiles for other gantry positions but at different detector locations.

![Measured and predicted attenuation profile](image)

*Figure 14. Measured and predicted attenuation profile of Thorax Phantom for gantry position 600.*

Figure 15(a) indicates: when applied the whole A matrix on deriving predicted output, even though MSE between the three and predicted sinogram is smaller than 1%, unknown black streaks are existing on the top of the predicted thorax slice, which does not appear in the same area of either the 24 mm or the 3 mm reconstructed image. Besides, the unknown high-attenuation artifact surrounds the boundary, and the same artifact also appears in other reconstructed images of predicted body phantom and predicted pelvis phantom. These unknown artifacts motivated us to use a reduced-size A matrix to derive predicted output.
Figure 15. (a) Reconstructed image of predicted Thorax phantom for row 2. (b) Reconstructed image of 24 mm collimation data for row 10. (c) Reconstructed image of 3 mm collimation data for 3 mm collimation data for row 2.

Reduced-size A Matrix

When we used normalized training data to train the A matrix, the full-size A matrix maintains the expectation of producing reasonable air value. When taking the 24 mm collimation data into
the matrix, since the value in the air is roughly 1, the predicted air value needs to be 1 as well. This normalized characteristic makes the constant input produce the constant output. However, this characteristic disappears in reducing the A matrix size even though using normalized data to train; consequently, we need to normalize the reduced-size A again by its summation to recover the function.

### 3.2.1 Performance on Training Data

Training data is 24 mm and 3 mm of thorax phantom. The evaluation of how well the reduced-size matrix can predict training data is presented here. Figure 16 shows 3 mm sinograms of thorax phantom, predicted sinogram, and their differences. The differences between the 3 mm sinogram and predicted sinogram are very small according to the small MSE value, 0.0087%.

![Figure 16](image)

**Figure 16.** (a) 3 mm sinogram of thorax phantom for 2rd detector row. (b) Predicted sinogram derived by thorax phantom-trained matrix and input data (24 mm data of thorax phantom) for 2rd detector row. (c) Difference between 3 mm and predicted sinogram.
Figure 17 shows 24 mm, 3 mm, and predicted attenuation profile for gantry position 600. Figure 17(b) shows the attenuation profile in the detector range 350-550, the area subtended by the phantom. Like what was observed in the attenuation profile when using the whole A matrix, in most locations, the predicted attenuation profile is between 24 mm and 3 mm attenuation profile, although there are fluctuations due to noise. This situation also appears in other attenuation profiles for different gantry positions.

Figure 17. (a) Measured and predicted attenuation profile of Thorax Phantom for gantry position 600. (b) Zoom-in version of (a), select range of detector 350-550.

Figure 18 shows reconstructed images of predicted, 24 mm, and 3 mm sinograms. The predicted image using the reduced-size A matrix has fewer unknown artifacts than the last predicted image, whose sinogram is derived by the whole A matrix; the black streaks and surrounding high-attenuation artifacts disappear in Figure 18(a). Spinal volume tends to have higher attenuation in the predicted image than in 3 mm and 24 mm collimation images. An unknown object appeared on the right of the thorax phantom to produce a high-attenuation spot, and in the 24 mm image, streaks artifacts originate from this spot. Low-intensity horizontal artifacts at \( Y=290 \) may result from slits on the phantom. Except for the horizontal artifacts, these are
reduced in reconstructed images of 24 mm sinogram for detector row 11. The non-uniformity index (NUI) of the predicted output is 2.16%. The NUI of the 24 mm image is 3.22%, and the NUI of the 3 mm image is 3.19%. The NUI of the 3 mm image is close to the NUI of the 24 mm image. Omitting beam hardening correction during preprocessing step may be the reason. NUI of 24 mm image (scatter-uncorrected image) is decreased by 32% after correction. NUI of the 3 mm is higher than the predicted image's NUI because the image is too noisy to discern cupping artifacts. A matrix is designed to map the mean of scattering instead of noise, besides the computational algorithm introduced in section 2.2.4 involves the function of smoothing the data by keeping the window overlapped. SSIM between the predicted image and the ground truth is 0.9869, and SSIM between uncorrected image and the ground truth is 0.9860. SSIM shows that the predicted image has higher similarities with the 3 mm collimation image globally.

![Figure 18. (a) Reconstructed image of predicted Thorax phantom for row 2. (b) Reconstructed image of 24 mm collimation data for row 10. (c) Reconstructed image of 3 mm collimation data for 3 mm collimation data for row 2.](image)

**3.2.2 Independent Training and Testing Data**

In this section, all data collected from one phantom will be used for training. The performance of the same training data and independent testing data will be evaluated. Independent testing data
sets collected from phantoms that are distinguished from training phantoms are used to evaluate the generalization capability of the least-squares estimation method for totally new data, such as would be encountered in newly acquired clinical data. There are three types of phantom involved: Thorax phantom, Body phantom, and Pelvis phantom. I used Thorax phantoms to train the model and the other two as test data. The pairs of independent data sets used for training and testing are summarized as two groups listed in Table 3.

<table>
<thead>
<tr>
<th>Group</th>
<th>Training</th>
<th>Scan mode</th>
<th>Energy</th>
<th>Testing</th>
<th>Scan mode</th>
<th>Energy</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>Thorax phantom with 24 mm, 3 mm collimation</td>
<td>Axial</td>
<td>140 kVP</td>
<td>Body phantom with inserts with 24 mm, 3 mm collimation</td>
<td>Axial</td>
<td>140 kVP</td>
</tr>
<tr>
<td>2</td>
<td>Thorax phantom with 24 mm, 3 mm collimation</td>
<td>Axial</td>
<td>140 kVP</td>
<td>Pelvis Phantom with 24 mm, 3 mm collimation</td>
<td>Axial</td>
<td>140 kVP</td>
</tr>
</tbody>
</table>

*Table 3. Phantoms used for collecting training and testing data.*

**Group 1:**

Figure 19 shows 3 mm sinograms of the body phantom, predicted sinogram, and their differences. The MSE between the 3 mm sinogram, the ground truth, and the predicted sinogram is 0.0088%, which is very similar to the MSE in the training sinogram.
Figure 19. (a) 3 mm sinogram of body phantom for 2rd detector row. (b) Predicted sinogram derived by body phantom-trained matrix and input data (24 mm data of body phantom) for 2nd detector row. (c) Difference between 3 mm and predicted sinogram.

Figure 20 shows 24 mm, 3 mm, and predicted attenuation profile of body phantom for gantry position 600. In most locations, the predicted attenuation profile is between 24 mm and 3 mm.

Figure 20. (a) Measured and predicted attenuation profile of Body Phantom for gantry position 600. (b) Zoom-in version of attenuation profile. Select the range of detector 350-550 from (a).
In Figure 21 (a), a circular artifact appears in the middle of the phantom. Besides, the blur circle (294,273) may be caused by the high-intensity circle lower-Z plastic sample container. UI of the predicted image is 2.70%, NUI of 24 mm image is 3.24%, and NUI of 3mm collimation image is 3.21%. When testing on the Body phantom, the NUI of the uncorrected image is decreased by 16% after correction. SSIM between the predicted image and the ground truth is 0.9781, and SSIM between 24 mm image and 3 mm image is 0.9723. With the circular artifacts appearing on the water insert, the predicted image still shows higher similarities with the ground truth. This SSIM is decreased by 0.8% comparing with the previous one on the thorax phantom image. The lower SSIM and NUI are due to lower accuracy when recovering the predicted output from testing data.

Figure 21. (a) Reconstructed image of predicted Body phantom for row 2. (b) Reconstructed image of 24 mm collimation data for row 10. (c) Reconstructed image of 3 mm collimation data for 3 mm collimation data for row 2.

**Group 2:**

The MSE of the predicted sinogram against the 3 mm sinogram is 0.00705%, which is smaller than the MSE in the body phantom and the MSE in the thorax phantom. Similarly, the attenuation profile of predicted data is between 3 mm and 24 mm at most places, though fluctuation makes the attenuation profile of 24 mm collimation higher than 3 mm at some places.
Figure 22. (a) 3 mm sinogram of pelvis phantom for 2rd detector row. (b) Predicted sinogram derived by pelvis phantom-trained matrix and input data (24 mm data of body phantom) for 2rd detector row. (c). Difference between 3 mm and predicted sinogram.

Figure 23. (a) Measured and predicted attenuation profile of Pelvis Phantom for gantry position 600. (b) Zoom-in version of attenuation profile. Select the range of detector 350-550 from (a).
The reconstructed image of the predicted pelvis phantom shows artifacts whose center locates at (230,265). While when we select the water ROI covering artifacts, the NUI of the predicted (corrected) image is 9.13%, which is three times larger than the previous NUI of the corrected image. When the water ROI is not in the artifacts range, the NUI of the predicted (corrected) image, 2.21%, is lower than the NUI of 24 mm (uncorrected), 2.64%. The NUI of the 3 mm image is 2.40%. The NUI of 24 mm and 3 mm within the same ROI increases; the NUI of the 24 mm image is 3.72%, and the NUI of the 3 mm image is 3.15%. Here, with the artifacts in the predicted image, the SSIM between the predicted image and the ground truth, 0.9821, is lower than the SSIM between the 24 mm image and the ground truth, 0.9832. The SSIM between the predicted image and the ground truth is higher than the one in body phantom but still lower than SSIM in the training data set.

![Reconstructed image of predicted Pelvis phantom for row 2.](a) Reconstructed image of 24 mm collimation data for row 10. (b) Reconstructed image of 3 mm collimation data for row 2.

The MSE of the new predicted pelvis sinogram against the 3 mm collimation sinogram is 0.00548%, which is reduced by 22% comparing with the old predicted pelvis sinogram. The attenuation profile looks roughly the same as before. However, artifacts in the reconstructed image of the new predicted pelvis sinogram are not reduced, and the same NUI of the new
predicted image is produced. SSIM between this new image and the ground truth keeps the same as well.

![Predicted Image](image)

*Figure 25. Reconstructed image of predicted Pelvis phantom for row 2. This predicted data is derived by Body and Thorax-trained A matrix.*

### 3.3 Machine Learning

To compare to Least squares estimation, this learning-based method used the same training and testing data pairs. Table 4 is the summary list of training, and testing data set pairs.

<table>
<thead>
<tr>
<th>Group</th>
<th>Training</th>
<th>Scan Mode</th>
<th>Energy</th>
<th>Testing</th>
<th>Scan Mode</th>
<th>Energy</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>Thorax</td>
<td>Axial</td>
<td>140kVp</td>
<td>Body Phantom</td>
<td>Axial</td>
<td>140kVp</td>
</tr>
<tr>
<td>2</td>
<td>Thorax</td>
<td>Axial</td>
<td>140kVp</td>
<td>Pelvis</td>
<td>Axial</td>
<td>140kVp</td>
</tr>
<tr>
<td>3</td>
<td>Thorax, Body Phantom</td>
<td>Axial</td>
<td>140kVp</td>
<td>Pelvis</td>
<td>Axial</td>
<td>140kVp</td>
</tr>
</tbody>
</table>

*Table 4. List of training and testing data sets.*

Figure 26 (a) is the reconstructed image of output derived from a Thorax trained U-net model and Body Phantom 24 mm collimation test data. Figure 26 (b) is the reconstructed image of output derived from a Thorax trained U-net model and Pelvis 24 mm collimation test data, and Figure 26 (c) is the reconstructed image of output derived from Thorax and Body Phantom
trained U-net model and Pelvis 24 mm collimation test data. Each reconstructed image of the predicted output shows blur inside the phantom, and the first image shows strong circular artifacts. From observation of reconstructed images, the U-net trained model we designed cannot produce output data whose reconstructed images have clear image structures and fewer artifacts.

Figure 26. (a) Reconstructed image of the 2nd detector row from the predicted output derived from Body Phantom test data and a Thorax trained U-net. (b) Reconstructed image of the 2nd detector row from the predicted output derived from Pelvis Phantom test data and a Thorax trained U-net. (c) Reconstructed image of the 2nd slice from the predicted output derived from Pelvis Phantom test data and a Thorax and Body Phantom trained U-net.

3.4 MC Simulation Data with Least Squares Estimation

In our Monte Carlo simulations, the training data is the scatter-only signal generated from a spherical phantom, and the testing data is the scatter-only signal generated by a simulated sample
head phantom. The corrected 3 mm scatter-only signal is derived by multiplying the estimation matrix by the 24 mm collimation scatters signal generated from the sample head phantom; here, the estimation A matrix is the whole A matrix instead of reducing the size. The following figures are shown to analyze the 24 mm, and 3 mm collimation scatter profiles collected from the simulated sample head phantom and the corrected 3 mm scatter-only signal.

Figure 27 shows the normalized scatter profile (NSP) on the scatter-only signal of 24 mm collimated simulated sample head phantom, 3 mm collimated simulated sample head phantom, and corrected output, each of which is averaged over 360 gantry positions. The denoising function used here is introduced in section 2.4.2. NSP is obtained by normalizing scattered photon energy deposited to each detector by the primary photon energy deposited in the middle detector (Liu et al., 2021). From Figure 27, we can observe that the NSPs of the 3 mm collimated data and the corrected output is lower than the NSP of the 24 mm collimated data, and the NSP of the corrected output data is very close to that of the 3 mm collimation data. As expected, NSP increases with wider collimation.

![Figure 27. NSPs of the 24 mm and 3 mm collimation scatter signal, as well as the corrected data.](Image)
Chapter 4 Discussion and Conclusions

Our initial goal is to estimate 3 mm sinograms from 24 mm sinograms using the whole A matrix, and the predicted output is considered as scatter-corrected output; 24 mm collimation data is considered as scatter-uncorrected. Even though the MSE between the scatter-corrected sinogram and the ground truth is lower than 1%, the unknown high-attenuated artifacts around the boundary appear in every reconstructed image of corrected data but are not found in 3 mm image or 24 mm image. Since the same algorithm, filtered back projection, is applied on reconstructing all images in this thesis, the unknown artifacts motivate us to modify the initial goal from using the whole A matrix to a reduced-size A matrix to derive new scatter-corrected output.

Using a reduced-size A matrix, the MSE of each new scatter-corrected sinogram against the corresponding ground truth remains low. The highest MSE is 0.00880%, which is calculated when comparing scatter-corrected body phantom and 3 mm phantom body sinogram, and the lowest MSE is 0.00705% in scatter-corrected pelvis phantom and the actual 3 mm pelvis phantom. With increasing phantoms used for training data, the MSE of the corrected pelvis phantom against its ground truth is reduced by 22%, reaching 0.00548%. Artifacts around the boundary disappear in all scatter-corrected images, and the nonuniformity index in scatter-corrected body phantom and thorax phantom is lower than the nonuniformity index in corresponding uncorrected images. The lowest nonuniformity index of the corrected image is 2.16%. Higher SSIM demonstrates that scatter-corrected images in group 1 and group 2 have higher structural similarities with the corresponding ground truth than scatter-uncorrected images have. However, the corrected pelvis phantom shows more artifacts, quantitatively displayed as
three times higher NUI than the uncorrected image and higher SSIM than the uncorrected one. Increasing training data does not reduce the blur artifacts, NUI, or SSIM. In the next paragraph, misalignment between 3 mm and 24 mm collimation data will be introduced, and this misalignment may lead to more effects on the pelvis phantom since it has a more complex structure and more variations along the z-axis than body phantom. Future study on pelvis phantom data is necessary.

During analyzing the reduced-size A matrix, we found that 3 mm collimation experimental data is misaligned with 24 mm collimation data in the z-axis. Theoretically, the area that two detector rows in the 3 mm collimation setting from scan four scan over is 9 mm to 12 mm along the z-axis. The detector rows in 24 mm collimation setting scanning over the same range of area are row 7 and row 8 because each width is 0.75 mm. However, by comparing reconstructed images of projection data acquired with 3 mm collimation using data from row 1 and row 2 with reconstructed images from data acquired with 24 mm collimation using the middle row, and by observation on averaged reduced-size A matrix, we found that row 1 in 3 mm collimation is aligned with row 9 in the 24 mm collimation. Row 2 in 3 mm collimation data is aligned with row 10 in the 24 mm collimation; the alignment is shifted by one detector row. In axial scanning, the patient bed is translated between scans along the z-axis to scan over the desired area, but the table positions are not recorded and cannot be extracted from raw data. During the scanning process, if 24 mm collimation scanning and 3 mm collimation scanning does not start with the position, then detector rows will not be aligned perfectly along the z-axis. In the future, we would like to do more experiments on the same type of phantom and analyze whether this situation is related to phantom placement. In future work, if using experimental data collected
from the Philips Brilliance Big Bore, we need to develop methods for extracting the starting position information from raw data.

Our assessments of the performance of the machine learning U-net structure do not show improved results. The training data set is not large enough. Neural Networks are more effective with large training data sets (but not so large as to "overtrain"). With limited time available to conduct experiments, there were only 4 or 5 types of phantoms used to collect data. Varying the data window size is an excellent way to increase the number of pairs of training input and output, but this is not a workable strategy because our chosen U-net structure needs to shrink the size of arrays used internally many times during the downsampling steps. In future work, more experiments will be performed.

Conclusively, with the initial goal, the errors between predicted data and ground truth in the sinogram domain are low. However, we do not see advantages of using global measurements to estimating the value locally by using the whole A matrix, and we do not see improvement in image quality but seeing more artifacts in corrected images. However, the modified goal, using local measurements to estimate scattering locally, keeps low error in the sinogram domain and makes a significant improvement on image quality by observing fewer artifacts. This least-squares model is designed to reduce the scatter in the sinogram domain, but the ultimate goal is to reduce scatter on images and calculate accurate SPR. The current work shown in this thesis is a promising start, while future work needs to be done. DEAM (Dual-energy alternating minimizing algorithm) need to be involved in matching with the previous work done by Medrano et al. (Medrano et al., 2020) and Zhang (Zhang et al., 2018), and the future goal will involve taking the 24 mm projection data and estimating the data corresponding to the images.
reconstructed from 3 mm projection data using DEAM. In this goal, data recovered from reconstruction algorithms will take source spectrum, two bases, and background knowledge (e.g., scatter) into account.
Chapter 5 References


