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Chapter 5

Analysis and removal of offset and scaling artifacts in tomography

5.1 Introduction

Tomography is an imaging technique for determining three dimensional structures from two dimensional projection images. An object is illuminated, from various angles, by an X-ray or electron source and the unabsorbed intensity is recorded by a detector. After the projection acquisition, a reconstruction algorithm is applied to generate a 3D volume from the projection data. This volume can be interpreted as a stack of grayscale images, where the gray values are proportional to the attenuation of the corresponding materials in the physical object.

In X-ray tomography contrast is obtained through absorption of X-ray photons. Each material in the sample attenuates the X-ray beam, quantified by its thickness and attenuation coefficient. The path traveled through the sample and the materials on this path determine the photon count observed on the detector.

In electron tomography, a beam of electrons in vacuum is used to generate contrast (in an electron microscope) instead of X-rays. Electrons have a different interaction with matter. Part of the signal is scattered, either elastically or inelastically. Another part of the signal, referred to as direct beam, has no interaction with the material and passes freely through the (often very thin) sample. In Transmission Electron Microscopy (TEM), part of the transmitted electron signal is recorded. The most common imaging technique records the bright field image, which is the direct beam that is focussed on an imaging plane. Another approach is Scanning TEM (STEM), where the incoming electron wave is focussed on a spot. The sample is then scanned by moving this spot across the sample.

One of the major challenges within the field of tomography is the ability of obtaining quantitative information from the reconstructed projection images, concerning the size, shape and density of the 3D structures in the object. In order to do so, an additional, and currently subjective, segmentation step is required after the reconstruction to determine the correspondence between gray values in the reconstruction and different compositions in the original structure.
Quantitative interpretation of tomographic reconstructions is often hampered by the presence of reconstruction artifacts: structured distortions of the reconstructed volume. Most of these artifacts belong to one of the following categories:

- **Artifacts caused by structural data errors introduced during acquisition.** This category includes artifacts caused by nonlinear effects of the image formation process, such as diffraction contrast, as well as misalignment between the images in the projection data that cannot be fully corrected. Another common source is from detector inefficiencies, which cause ring artifacts.

- **Artifacts caused by the limited amount of measured data.** This category includes truncation artifacts that are introduced when the sample extends beyond the field-of-view of the detector, as well as missing wedge artifacts common in electron tomography, caused by the limited angular range of the microscope.

These artifacts cause subsequent segmentation problems.

This chapter deals with three types of similar reconstruction artifacts which mainly fall in the first category and are caused by:

- a **global offset** present in the projection data: a constant that has been added to each pixel in every projection image,

- a **local offset** on the projection data: a different constant added to each projection image,

- a **scaling** of the projection data: the intensity scaling of the projection images changes with each projection angle.

Note that we assume the projection images are linearized, meaning that a value of 0 for a pixel in the projection data should correspond to a line that only passes through free space and does not intersect with the object. Higher values correspond to lines that do intersect with the object. We will go into more detail about this in Section 5.2. In practice, the zero level of the projection data is affected by various acquisition parameters of the scanner or fluctuations in the radiation source intensity, which may result in an offset on the data. Manipulating the dataset using various image processing tools, *e.g.*, to align the projection images before reconstruction, may also result in offsets on the projection data.

A common approach to deal with a global offset in electron tomography is to subtract the minimum value of the projection data, which corresponds to the background intensity, if the background is visible in any of the projection images [Gon15]. However, this approach is not feasible the object is larger than the field of view of the detector (no background visible), or in case of a local offset. Therefore, in this chapter we introduce a method that can also be used in the latter, more challenging situation.

In this chapter we analyze the effect of a global offset on the reconstruction obtained by filtered backprojection and derive the reconstruction artifact analytically. Then we introduce an iterative algorithm for estimation of a global offset,
5.2 Origin of offsets and scalings in projection data

Based on algebraic reconstruction methods. Similar algorithms are derived for estimation of a local offset and scaling factors. In a series of simulation experiments we study the effects of certain reconstruction parameters on the estimation algorithms, such as the shape of the reconstruction area. Finally we apply the local and global offset estimation algorithms to an experimental dataset.

This chapter is structured as follows: in Section 5.2, offset and scaling artifacts are introduced and their causes are explained. In Section 5.3 we determine analytically the effect of a global offset on the reconstruction. In Section 5.4, we present an algorithm for estimating offsets based on the available projection data. The estimated offset can then be subtracted from the data before reconstruction, resulting in the reduction, or even removal, of offset artifacts. In Section 5.5 we present an algorithm for estimation of scale factors of the projection data. Section 5.6 presents a series of simulation experiments, aimed at validating the proposed estimation algorithms. The simulation experiments are followed by one example where the proposed local offset estimation algorithm has been applied to experimental datasets. Section 5.7 provides a discussion and concludes this chapter.

5.2 Origin of offsets and scalings in projection data

In this section we briefly introduce tomography, followed by a description of phenomena that introduce offsets or scaling in the acquired projection images. These offsets or scale factors can be introduced by physical instrument effects and by image manipulation after data acquisition.

5.2.1 Tomography

First we describe the mathematical model used for the reconstruction problem. Fig. 4.1 shows a schematic view of the parallel beam acquisition geometry for tomography. A detector measures the intensity of the radiation (e.g. X-ray) emitted from the source along a straight line

\[ \ell_{\theta,t} = \{(x, y) : x \cos \theta + y \sin \theta = t \} \]

where \( \theta \) indicates the rotation angle (with respect to the object) and \( t \) denotes the position of the detector pixel. Essentially each detector measurement approximates a line integral along the line \( \ell_{\theta,t} \)

\[ p_\theta(t) := \int_{\ell} f(x, y) \, ds. \]

where the object is presented by an image function \( f(x, y) \). This line integral can be rewritten by parameterization of the line \( \ell \) using the Dirac delta \( \delta(\cdot) \) function, which leads to the Radon transform [NW01],

\[ p_\theta(t) := \int_{-\infty}^{+\infty} \int_{-\infty}^{+\infty} f(x, y) \delta(x \cos \theta + y \sin \theta - t) \, dx \, dy. \]
To reconstruct the image function $f(x,y)$ from the projections $p_\theta(t)$ the Radon transform should be inverted, which can be achieved by the filtered backprojection method (FBP) [KS01], provided that infinitely many projections are acquired for the entire interval $\theta \in [0, \pi)$. In practice, due to a finite number of projections and discretization of the data, an inexact inversion is obtained using FBP.

In this chapter we focus on algebraic or iterative reconstruction methods which are based on a discretization of the image function $f(x,y)$ in pixels and of the projection images $p_\theta(t)$. The image is represented as vector $x \in \mathbb{R}^N$ and so is the projection data $p \in \mathbb{R}^M$. A single detector pixel measurement can be seen as a combination of the pixel values and the contribution of pixel $x_j$ to detector pixel $p_i$ is determined by the weight $w_{ij}$:

$$p_i = \sum_j w_{ij} x_j,$$

which we call the ray sum. The full set of equations leads to the following linear system:

$$W x = p \quad (5.1)$$

where $W \in \mathbb{R}^{M \times N}$ is called the projection matrix. Algebraic reconstruction methods such as SIRT, ART and LSQR typically compute a (weighted) least squares solution of Eq. (5.1) [KS01; GBH70; PS82].

### 5.2.2 Beer–Lambert’s law

In absorption contrast tomography, the intensity of the radiation $I$ that is measured on the detector is related to the intensity of the source $I_0$ by the Beer–Lambert law [IC88]:

$$I = I_0 e^{-\int \mu(\ell) d\ell} \quad (5.2)$$

assuming a monochromatic beam, where $\int \mu d\ell$ is the line integral of the attenuation coefficient in the direction of the ray. Therefore, the measured projection data are normalized prior to the reconstruction:

$$\int \mu(\ell) d\ell = -\log \left( \frac{I}{I_0} \right). \quad (5.3)$$

The source intensity is measured before scanning by taking an image without the object inside the beam. This so called flat field should be uniform, but often imperfections can be observed. Such imperfections can be caused by dust particles or nonlinearities of the detector pixels. By normalization (or flat field correction) such imperfections are partly removed.

In case the source intensity is not stable, the intensity of the flat field can vary with consecutive projections. However, the flat field correction will be applied using the initial source strength, which introduces an error. The recorded projections (in terms of photon counts) is

$$I = I_0 \lambda_k e^{-\int \mu(\ell) d\ell}, \quad k = 1, \ldots, K \quad (5.4)$$
where $\lambda_k$ describes the variations in the source intensity. After normalization, we obtain:

$$-\log \left( \frac{I}{I_0} \right) = \int_L \mu(\ell) \, d\ell - \log (\lambda_k).$$

(5.5)

So the measured projections after normalization (line integrals) now include an offset that depends on the $k$-th projection angle.

In modalities such as HAADF-STEM (High Angular Annular Dark Field Scanning Transmission Electron Microscopy) approximations of the line integrals are measured directly:

$$I = I_0 \int_L \mu(\ell) \, d\ell.$$  

(5.6)

In this case, any variations in the flat field lead to multiplicative errors in the measurements:

$$\frac{I}{I_0} = \lambda_k \int_L \mu(\ell) \, d\ell, \quad k = 1, \ldots, K.$$

Another common source for offsets is in the post-processing of the projection images, where several image manipulations may lead to a global scaling and offset of the projection data.

### 5.3 Analysis of global offset artifacts

To analyze the effect of a global offset on the reconstruction, we follow the analytical analysis that forms the basis of the filtered backprojection algorithm. An exact inversion formula for the Radon transform can be obtained as a composition of the following steps:

- **Fourier transform of the projections:**

  $$P_\theta(u) := \mathcal{F}\{p_\theta\}(u) = \int_{-\infty}^{\infty} p_\theta(t) e^{-2\pi i u t} \, dt$$

- **Application of a ramp filter in the Fourier domain:**

  $$Q_\theta(u) := P_\theta(u) |u|$$

- **Inverse Fourier transform of the filtered Fourier domain data:**

  $$q_\theta(t) := \mathcal{F}^{-1}\{Q_\theta\}(t) = \int_{-\infty}^{\infty} Q_\theta(u) e^{2\pi i u t} \, du$$

- **Backprojection of the filtered projections:**

  $$f(x, y) = \int_0^{\pi} q_\theta(x \cos \theta + y \sin \theta) \, d\theta$$
We consider a finite detector of length 1, therefore, the projection data are measured in the interval \( t \in [-\frac{1}{2}, \frac{1}{2}] \). The region outside this interval is set to zero.

We now investigate the result of an offset of 1 present in all projections. Ignoring the projections from the actual object (we focus on the artifact), we have, for any projection angle \( \theta \),

\[
p_\theta(t) = \text{rect}(t) = \begin{cases} 
1 & |t| \leq \frac{1}{2}, \\
0 & |t| > \frac{1}{2},
\end{cases}
\]

along with its Fourier transform

\[
P_\theta(u) = \mathcal{F}\{p_\theta\}(u) = \sin(\pi u) \frac{\sin(\pi u)}{\pi u}.
\]

Applying a ramp filter to the projection data in the Fourier domain results in

\[
Q_\theta(u) = P_\theta(u)|u| = \begin{cases} 
-\sin(\pi u) \frac{\sin(\pi u)}{\pi u} & u < 0 \\
\sin(\pi u) \frac{\sin(\pi u)}{\pi u} & u \geq 0
\end{cases},
\]

which yields, after applying the inverse Fourier transform:

\[
q_\theta(t) := \mathcal{F}^{-1}\{Q_\theta\}(t) = \frac{1}{(\frac{1}{2} - t)(\frac{1}{2} + t)2\pi^2}.
\]

Fig. 5.1 shows graphs of the functions \( p_\theta, P_\theta, Q_\theta \) and \( q_\theta \).

The backprojection of \( q_\theta(t) \) leads to

\[
f(x, y) = \int_0^\pi \frac{1}{(\frac{1}{2} - t)(\frac{1}{2} + t)2\pi^2} \, d\theta = \frac{4\pi}{2\pi^2 \sqrt{1 - 4(x^2 + y^2)}}
\]

with \( t = x \cos \theta + y \sin \theta \).

Two images of the function \( f \) are shown in Figs. 5.2b and 5.2c. They are the same, except that they show a different interval of intensities. The bright ring around the reconstruction corresponds to the poles of \( q_\theta \), at the edges of the detector. Fig. 5.2a illustrates that although the intensity variations within this circle are much smaller than at the boundary, the interior is not constant as well. Therefore, an offset on the projection data will result in a continuously varying, radially symmetric artifact in the reconstruction. Segmentation operations such as thresholding, that rely on the fact that similar structures have a gray level that is independent of their position in the sample, may therefore lead to erroneous results. The intensities of the offset artifact in the reconstruction are directly proportional to the value of the offset. For small offsets, its contribution is negligible, whereas major artifacts can be observed for large offsets with respect to the values of the actual projection data.

When using backprojection algorithms, such as filtered backprojection, the impact of offset artifacts is typically limited, as most of the structure of interest is contained in the slowly varying part of the offset intensity field. The effect of an offset on the projection data is more complicated for iterative reconstruction methods, such as ART or SIRT. Such algorithms reconstruct a certain area, where
5.3. Analysis of global offset artifacts

Figure 5.1: (a) Offset on the projection data; (b) Fourier transform of the offset; (c) Result of applying a ramp-filter in the Fourier domain (d) Offset on the projection data after filtering.

Figure 5.2: Filtered backprojection of an offset; (a) along the horizontal axis (b) full image: wide intensity window, which illustrates the bright circle formed at the edges of the detector (c) full image: narrow intensity window, which illustrates the gradual change in intensity in the interior of the circle.
the object function $f$ is assumed to be zero outside this area. Generally, it is advantageous to restrict this area as much as possible such that it still entirely contains the object. For flat objects, such as many electron microscopy samples, it is advantageous to reconstruct a flat rectangular area, instead of a full square. By using a rectangle, the entire area outside this rectangle is effectively constrained to be zero, which drastically reduces the number of unknowns in the reconstruction problem, thereby leading to a more accurate reconstruction. Fig. 5.3b shows a reconstruction computed by SIRT on a square which has been cropped, whereas Fig. 5.3c shows the same reconstruction computed by SIRT on a rectangle. The difference in quality can be clearly observed. Note that in this case no offset or scaling was applied to the projection data.

Figure 5.3: Comparison of two different reconstruction volumes for projection data without offset or scaling applied; (a) the flat phantom image of size $64 \times 512$; (b) a SIRT reconstruction on a square volume, $512 \times 512$, which has been cropped to the size of the phantom; (c) a SIRT reconstruction on a flat volume, $64 \times 512$.

The degrading effect of a projection data offset on the reconstruction becomes much stronger if the reconstruction area is made smaller than the outer circle of the basic offset artifact. This effect is demonstrated in Fig. 5.4, which shows two SIRT reconstructions of the offset on different reconstruction volumes. The $512 \times 512$ reconstruction corresponds to an offset of 1 on a detector 512 pixels wide for projection angles $\pm 90^\circ$, with $1^\circ$ increments. The $256 \times 512$ reconstruction corresponds to an offset of 1 on a detector 450 pixels wide for projection angles $\pm 60^\circ$, also with $1^\circ$ increments. SIRT was run for 100 iterations. The absolute values of the corresponding residual projections are shown in Figs. 5.4c and 5.4d, i.e. a forward projection of the reconstruction minus the original projections. Note that in Fig. 5.4a the size of the detector was 512 pixels, which means that the reconstruction size is just large enough to contain the full circular offset artifact. The corresponding residual is relatively small, see Fig. 5.4c, but some inconsistencies remain especially on the left and right sides. The circular artifact cannot be reproduced on a smaller reconstruction area of $256 \times 512$, as shown in Fig. 5.4b. Therefore, the residuals are larger in this case. The residuals in top and bottom of Fig. 5.4d are most prominent. So a numerical reconstruction of the offset artifact is not consistent (has nonzero residual), which is even more
5.4 Offset estimation algorithm

To reduce, or even remove offset artifacts when using iterative reconstruction methods such as SIRT, the unknown offset must be estimated from the available projection data. It can then be subtracted from the data before applying the reconstruction algorithm. In some cases, one or more projection images contain a region that is not occupied by the sample, where the beam (collection of rays) only intersects with vacuum. An example of such a region is shown in Fig. 5.5. In Section 5.6.3 we describe this dataset in detail. In such cases, the offset, which we denote as $\lambda \in \mathbb{R}$, can be determined directly from the projection image, e.g., by averaging the pixel values inside one or more of such regions or by simply determining the minimum value of the projections, as is done in [Gon15]. Here, we consider a more general case, where the offset cannot be estimated directly from the set of projection data.

The offset estimation problem becomes much more complicated when the entire field-of-view in all projection images is covered by the sample. If the structure of interest is contained within a supporting material of constant thickness,
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the thickness of the support in the direction of the beam is proportional to \( \frac{1}{\cos \theta} \), where \( \theta \) is the incidence angle of the beam. If regions can be identified in each projection image that contain only the supporting material, the offset can be estimated by fitting the function \( \lambda + \frac{k}{\cos \theta} \) to the average projection values in these regions, where both the offset parameter \( \lambda \) and the proportionality constant \( k \) are estimated simultaneously.

5.4.1 Global offset estimation

It was shown analytically in Section 5.3 that a global offset on the projection data leads, after filtering with the ramp filter, to a filtered projection that tends to infinity at the boundaries of the detector. After backprojection, this results in a reconstruction that cannot be represented as a grid of finite pixel values. This is not exactly the case for the SIRT reconstructions of the global offset as shown in Fig. 5.4a, but still parts of the residual do not converge to zero and inconsistencies remain. If one dimension of the reconstruction grid is smaller than the detector width, these inconsistencies are more pronounced. Therefore, the presence of an offset in the projection data can lead to an inconsistent reconstruction problem: there exists no reconstruction that matches the data.

The result of applying a reconstruction algorithm to inconsistent projection data depends quite heavily on the particular reconstruction algorithm. Here, we restrict the discussion to the case of SIRT as it allows for a clear mathematical analysis.

We denote the SIRT reconstruction of a vector \( p \) of projection data by \( S(p) \). SIRT converges to a reconstruction \( \tilde{x} = S(p) \) for which

\[
\| W \tilde{x} - p \|_R
\]

is minimal, where \( \| x \|_R = \sqrt{x^t Rx} \) denotes a norm based on a weighted sum of squares [GB08].

Figure 5.5: Background intensity of an experimental HAADF-STEM dataset, from EMAT (Electron Microscopy for Materials Science, Antwerp).
So, SIRT converges to a reconstruction that corresponds as closely as possible with the given projection data. If the data is inconsistent, due to noise or an offset on the data, this property will still hold, but the projection distance,

$$d(x, p) = \|Wx - p\|_2,$$

will become larger. This property can be used to estimate the offset, by computing the offset for which \(d(S(p_\tau), p_\tau)\) is minimal, where \(p_\tau = p - \tau e\). Each element of the vector \(e\) is \(1\) (where \(e\) has the same length as \(p\)). Note that \(p\) is the set of recorded projection data including an unknown offset and \(p_\tau\) is the projection data with a correction term for the global offset. This leads to the following formal model of the offset estimation problem:

$$\min_{\tau} \|W(S(p_\tau)) - p_\tau\|_2 \tag{5.7}$$

Computing \(d(S(p_\tau), p_\tau)\) for a single offset requires the computation of a SIRT reconstruction, which may take considerable time. Searching an entire interval of potential offsets \(\tau\) is computationally unfeasible. Fortunately, Eq. (5.7) can be solved by computing only two SIRT reconstructions, by exploiting the linearity of the SIRT algorithm.

As demonstrated in [KS01], every iteration of the SIRT algorithm performs a linear transformation on the output of the previous iteration. Therefore, the result after a finite number of SIRT iterations is the composition of a finite number of linear transformations, which is again a linear transformation:

$$S(\lambda p + \gamma b) = \lambda S(p) + \gamma S(b).$$

The forward projection operation \(W\) is also a linear transformation. Therefore, we can write the objective of the minimization problem as:

$$d(S(p_\tau), p_\tau) = \|W(S(p - \tau e)) - (p - \tau e)\|_2$$

$$= \|WS(p) - \tau WS(e) - p + \tau e\|_2$$

$$= \|\bar{p} - \tau \bar{e}\|_2, \tag{5.8}$$

where \(\bar{p} = WS(p) - p\) and \(\bar{e} = WS(e) - e\). The vector \(\bar{p}\) corresponds to the difference between the measured data (including the offset) and the computed projections based on its SIRT reconstruction. The vector \(\bar{e}\) corresponds to the difference between an offset of 1 and the computed projections based on its SIRT reconstruction. Note that the expression in Eq. (5.8) is minimal if \(\bar{e}\) and \(\bar{p} - \tau \bar{e}\) are perpendicular. That is, we can compute \(\tau\) by a vector projection of \(\bar{p} - \bar{e}\) onto \(\bar{e}\):

$$\tau = \frac{\bar{p} \cdot \bar{e}}{\bar{e} \cdot \bar{e}}, \tag{5.9}$$

where we assume that \(\bar{e} \neq 0\), meaning that the SIRT reconstruction of the offset is inconsistent (has nonzero residual). If \(\bar{e} = 0\), then Eq. (5.8) is independent of \(\tau\) and we cannot retrieve it in this manner.
To compute $\tilde{e}$ and $\tilde{p}$ we indeed need only two SIRT reconstructions. However, there is an alternative approach for solving Eq. (5.7) that is more efficient. First note that the following equation

$$Wx = p - \tau e,$$

is consistent if $\tau$ equals the true offset on the projections $\tau^*$, where

$$p = p^* + \tau^* e,$$

and $p^* = Wx^*$ are the projections of the ground truth image $x^*$. If we move the offset correction term to the left-hand side, we obtain the following linear system:

$$Wx + \tau e = p,$$

$$[W, e] \begin{bmatrix} x \\ \tau \end{bmatrix} = p,$$  \hspace{1cm} (5.10)

which can be solved by a least squares solver. In this way, the reconstruction and the offset parameter can be estimated simultaneously, which reduces the amount of computations substantially when compared to Eq. (5.9). In our experiments of section Section 5.6 we use the least squares method LSQR [PS82] to solve Eq. (5.10).

Note that the solutions found by Eq. (5.9) and Eq. (5.10) are inherently different. The vector projection method using SIRT solves the problem in two optimization steps:

$$\bar{x} = \arg \min_x \|Wx - p\|_R,$$

and subsequently

$$\min_{\tau} \|W\bar{x} - p\|_2.$$  

Note that the SIRT reconstruction $\bar{x}$ does not necessarily have a minimum residual in the $\ell_2$-norm, due to the weighted norm $\|\cdot\|_R$. Also, SIRT is known to converge slowly and might be terminated early in practice. The method using LSQR applied to the system in Eq. (5.10) solves the following optimization problem,

$$\min_{x, \tau} \|Wx + p\|_2.$$  

Furthermore, LSQR has the property that it computes the smallest norm solution, i.e., it finds a solution for which $\|(x^T, \tau)\|_2$ is smallest. In Section 5.6.1 we will explore the difference between these two approaches.

### 5.4.2 Local offset estimation

The same idea can be applied if the offset is different for every projection. First we order all equations corresponding to a each projection angle:

$$Wx = p - \begin{pmatrix} \lambda_1 e \\ \lambda_2 e \\ \vdots \\ \lambda_K e \end{pmatrix},$$  \hspace{1cm} (5.11)
where \( e \) is a column vector of \( D \) ones, where \( D \) is the number of pixels per projection image. If we move the offset correction to the left-hand side, the linear system is written as:

\[
\begin{pmatrix}
W_1 \\
W_2 \\
\vdots \\
W_K
\end{pmatrix}
x + \begin{pmatrix}
\lambda_1 e \\
\lambda_2 e \\
\vdots \\
\lambda_K e
\end{pmatrix} = \begin{pmatrix}
p_1 \\
p_2 \\
\vdots \\
p_K
\end{pmatrix} = p,
\]

which leads to:

\[
\begin{pmatrix}
W_1 & e \\
W_2 & e \\
\vdots & \ddots \\
W_K & e
\end{pmatrix}
\begin{pmatrix}
x \\
\lambda_1 \\
\lambda_2 \\
\vdots \\
\lambda_K
\end{pmatrix} = \begin{pmatrix}
p_1 \\
p_2 \\
\vdots \\
p_K
\end{pmatrix}.
\]

The least squares solution will yield both a vector of offsets and the corresponding reconstructed image.

### 5.5 Scale estimation algorithm

As discussed in Section 5.2, for certain projection acquisition methods, source intensity fluctuations can lead to a scaling of projection data. An approach similar to the local offset estimation can be applied to the estimation of scalings. However, some modifications are necessary to ensure the estimation algorithm works reliably in this case. In this section we discuss these modifications.

Note that a scaling \( \alpha \) applied to all projection images results in a scaling of the gray values in the SIRT reconstruction:

\[
S(\alpha p) = \alpha S(p).
\]

due to the linearity of SIRT. The same holds for the solution of least squares methods:

\[
\min_x \| Wx - \alpha p \|_2^2 \equiv \min_y \alpha^2 \| Wy - p \|_2^2 \quad (5.13)
\]

for \( x = \alpha y \). Therefore, if the projection vector \( p \) is scaled by a single factor, i.e., a global scaling, we cannot determine this scaling \( \alpha \) based on the residuals of a reconstruction (obtained by SIRT, LSQR, or another method). Both the original and scaled variants of the projections have the same residual after reconstruction, up to a scaling. Note that if each projection image is scaled by a different factor, there is no reconstruction that matches this projection data, because a reconstruction pixel would have different projections (in intensity) depending on the projection angle. Therefore, we can fix this local scaling and change it to a global scaling where artifacts in the reconstruction are removed.
Let $\kappa_1^*, \ldots, \kappa_K^*$ be a set of scale factors applied to the original projections $p^*$ (which is in the column space of $W$ in Eq. (5.1)):

$$
\begin{pmatrix}
p_1 \\
\vdots \\
p_K
\end{pmatrix} = 
\begin{pmatrix}
\kappa_1^* p_1^* \\
\vdots \\
\kappa_K^* p_K^*
\end{pmatrix},
$$

The goal is to retrieve these scale factors from the scaled projection data $p$.

Let $\sigma_1, \sigma_2, \ldots, \sigma_K$ be a set of scale factors which we use to correct the scaled projections,

$$
Wx =
\begin{pmatrix}
\sigma_1 p_1 \\
\sigma_2 p_2 \\
\vdots \\
\sigma_K p_K
\end{pmatrix},
$$

(5.14)
i.e., $\sigma_i = 1/\kappa_i^*$ is optimal, where we assume that $\kappa_i \neq 0$ for any $i = 1, \ldots, K$. Note that the estimation problem in Eq. (5.14) has a trivial solution, $x = 0$ and $\sigma_i = 0$, for $i = 1, \ldots, K$. If each projection is scaled by zero, the projection data is consistent to a reconstruction that is zero everywhere. The least squares solver LSQR applied to Eq. (5.14) finds the smallest norm solution $\| (x^T, \sigma_1, \ldots, \sigma_K) \|_2$. Therefore, it will converge to this trivial solution. To avoid the trivial solution we introduce the parameter:

$$
\tau_i = 1 - \sigma_i.
$$

The introduction of this parameter leads to the following linear system, after we move the unknowns to the left-hand side:

$$
\begin{pmatrix}
W_1 & p_1 \\
W_2 & p_2 \\
\vdots & \vdots \\
W_K & p_K
\end{pmatrix}
\begin{pmatrix}
x \\
\tau_1 \\
\tau_2 \\
\vdots \\
\tau_K
\end{pmatrix} = 
\begin{pmatrix}
p_1 \\
p_2 \\
\vdots \\
p_K
\end{pmatrix}.
$$

(5.15)
We use LSQR to solve Eq. (5.15). If the parameter $\tau_i$ tends to zero, due to LSQR finding a smallest norm solution, the corresponding scaling $\sigma_i$ tends to 1, which corresponds to projections that are not scaled. In this way, the trivial solution of zeros is avoided and the least squares solution is close to unity, which is reasonable if we assume that the scale factors are close to 1.

5.6 Experiments and results

In this section we perform a series of simulation experiments on 2D and 3D simulation datasets. We quantify the accuracy of our method for retrieving global and local offsets and scaling factors of projections. Finally we apply our proposed method on an experimental dataset obtained by HAADF STEM microscopy which exhibits offset and/or scaling artifacts.
5.6. Experiments and results

5.6.1 Slice-based simulation experiments

In this section we compare results of the global offset, local offset and scale estimation algorithms. If we refer to a global offset, local offset or scale problem then we have applied one of the following to the projection data (not combined and unless specified otherwise):

- a global offset of 100,
- a random local offset sampled uniformly from (5, 55),
- a linear scaling uniformly distributed from 0.1 to 2 (not random).

Note that for the phantom that we consider, shown in Fig. 5.7, the average intensity of the projection data without offsets is approximately 60. The gray values in the ground truth are 0.5 (background) and 1 for the object. Projection data is generated for the angles ±60°, with 1° increments, by using the projection matrix from Eq. (5.1). We use the ASTRA toolbox to generate the projection matrix on-the-fly using the CPU [PBS13], without storing the matrix elements for memory considerations. The strip model is used to generate the projection matrix, the matrix elements are based on the area of intersection between one ray (part of the beam corresponding to a detector pixel) and a pixel [Zhu+08].

Note that we have two different ways to estimate a global offset: one involves computing a vector projection from Eq. (5.9) using two SIRT reconstructions, the other involves solving Eq. (5.10) using LSQR. In Fig. 5.4, we investigated the effect of the height of the reconstructed volume on the SIRT reconstruction of a global offset. The height is defined as the $y$-component of the reconstruction volume, as shown in the schematic of the geometry in Fig. 5.6. It seems that on a square reconstruction area, with sides as large as the detector, the residual of the offset artifact is close to zero. Therefore, we expect that it is difficult to recover offsets in this case by minimizing the residual compared to a case where the reconstruction domain is rectangular.

Note that in practice a reconstruction volume might not be particularly flat. First of all, the sample might not be very thin (size in the $y$-direction of Fig. 5.6). Secondly, if the sample thickness is only known approximately, it is safer to have a reconstruction height that is slightly larger than the thickness of the sample. If the height of the reconstruction area is smaller than the actual thickness of the sample, severe artifacts will be generated on the upper and lower boundaries of the reconstruction. Therefore, in the first experiment we investigate the effect of the height of the reconstruction area on the accuracy of the offset and scale estimation algorithms.

We apply the proposed estimation algorithms to the corresponding datasets described previously. We used a detector size of 310 pixels to generate the projections and a reconstruction size of $64 \times 512$. LQSR applied to global offset estimation (Eq. (5.10)), is iterated 250 times. SIRT for computing the vector projection for determining a global offset (Eq. (5.9)), is iterated 250 times. LSQR applied to local offset estimation (Eq. (5.12)), is run for 300 iterations. LSQR applied to the scale estimation algorithm (Eq. (5.15)), is iterated 400 times.
Figure 5.6: Representation of the geometry for flat reconstruction areas. The detector is placed at $\theta = 0^\circ$, and the rotation axis is the $z$-axis (perpendicular to $x$- and $y$-axes). Note that in 3D the reconstruction volume and detector also have a component in the $z$-direction. Typical rotation angles are $\theta \in [-s_\theta, +s_\theta]$ and $s_\theta < 90^\circ$.

Figure 5.7: Ground truth image of size $64 \times 512$, representing a part of a slice of a cylinder block.

The relative errors are shown in Fig. 5.8, meaning relative to the true offset/scaling:

$$|\lambda - \lambda_{\text{true}}| / |\lambda_{\text{true}}|.$$ 

As can be seen from Fig. 5.8 the height of the reconstruction has a significant impact on the accuracy of these methods. Up to 50% of the image width, the accuracy is still acceptable, but for larger heights some accuracy is lost. This is probably due to the effect we saw in Fig. 5.4, where the smaller reconstruction area has larger residuals from the global offset artifact. Therefore, on a smaller reconstruction area, an improvement in the global offset estimation has a larger reduction of the residual. This might explain why the global offset estimation is most accurate if the reconstruction domain matches the phantom size. A similar reasoning can be applied to the accuracy of the local offset estimation. These results suggest that the reconstruction height is not very crucial for the offset retrieval, provided that the reconstruction height is smaller than 60% of the reconstruction width.

We should note that we cannot directly compare the recovered scaling and the true scaling of the projection data, because we can only find it up to a global
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Figure 5.8: Influence of the height of the reconstruction volume on the offset and scale estimation algorithms. The relative error is shown of the recovered offset and scale factors with respect to the true offset and scale factors.

scaling. Therefore, we remove this common global scaling between the recovered scaling and true scaling for computing the relative error. A correction should also be applied to the error of the local offset. In Fig. 5.9a we plotted the recovered local offset and the true local offset. Note that it seems the difference between the two is a global offset. However, in Fig. 5.9b we see that this is not the case, a very smooth curve remains. This curve corresponds approximately to projections of a constant volume. Note that for a volume of height $\delta_x$, the length $L$ of a ray through the center of the volume is

$$L = \delta_x / \cos \theta,$$

which holds in a certain range of angles (at least $\theta < 90^\circ$, depending on the size of the volume). The same holds approximately for rays that do not go through the center of the volume, except for rays that intersect with the left or right edges of the volume. Therefore, it is likely that the local estimation algorithm using LSQR applied to Eq. (5.12) finds the reconstruction up to a constant. This constant does not increase the residual of Eq. (5.12) since its projections are then subtracted by the local offset estimate. This explains why the local offset estimation is smaller than the true local offset. Fortunately, a constant added to the reconstruction does not change the structure of the reconstruction. In the computation of the local offset estimation error we therefore correct for this offset on the reconstruction (which we already applied in Fig. 5.8).

Most datasets obtained from flat samples in electron microscopy have a gap in the angular range (leading to missing wedge artifacts) and the projection images are truncated, meaning that only a part of the sample is visible on the detector [ATM06]. Therefore, we performed experiments to see the effect of these limited data problems on the offset and scale retrieval algorithm. From this point forward, we do not include the vector projection method using SIRT for retrieving a global offset, since the method using LSQR is more accurate in the results in Fig. 5.8. In Fig. 5.10a the effect of a missing wedge is shown for the same dataset we used in
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Figure 5.9: (a) Comparison of the recovered local offset and true offset; (b) The absolute difference; (c) Average projection values of a constant volume (where each image pixel is 1), not the similarity to the absolute error of the recovered local offset; (d) Final absolute error after subtracting a multiple of the curve in (c).

the previous experiment, except for a different angular range. Note that the angle on the horizontal axis indicates the maximum rotation angle, e.g. 90° indicates an angular range of [−90°, 90°] with 1° increments. The missing wedge does not seem to be influencing the results for realistic rotation angles.

In case of truncation, the local and global offset estimation fails if the detector is smaller than the height of the reconstruction volume, see Fig. 5.10b. Note that the size of the detector determines the size of the circular offset artifact and in this case the offset artifact fully fits inside the reconstruction area. The local offset and scale retrieval are slightly more susceptible to the amount of truncation, but a detector size of 100 pixels seems sufficient.

In experimental data from electron microscopy a missing wedge and truncation are both present. In Fig. 5.11 we show the effect of a combination of these. In this case we see that the effect is more severe. The global offset and scale estimation do not seem to be influenced much. For certain combinations of detector size and angular range the error of the local offset estimation increases considerably, but if the truncation is not severe for a relatively large angular range, this is not a
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Figure 5.10: Influence of limited data on the offset and scale estimation algorithm.

Figure 5.11: Relative error of the retrieved offset-scalings in case a limited angular range is combined with truncation. Truncation is indicated by detector size and missing wedge by the maximum tilt angle.
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Figure 5.12: Slice in the $z$-direction of the particle phantom of size $460 \times 256 \times 64$.

problem. The scale retrieval algorithm is not very sensitive to the missing wedge, but the truncation can be an issue in extreme cases.

5.6.2 3D simulation experiments

We consider a particles in substrate phantom of size $460 \times 256 \times 32$ of which a central slice is shown in Fig. 5.12. A total of 121 projections were simulated for a detector of $256 \times 256$ pixels using parallel beam geometry and an angular range of $\pm 60^\circ$. The same offsets and scalings were applied as described in the beginning of Section 5.6.1. The datasets are reconstructed on a volume of size $460 \times 256 \times 32$ pixels. For the implementation of the algorithms we use the ASTRA toolbox for the GPU accelerated forward and backprojection operations [PBS13]. The hardware we used consists of a workstation with an Intel Core i7-2600K@3.4 GHz CPU, 16 GB of system RAM and an NVIDIA GTX 570 GPU.

First we compare the results of the global and local offset and scale estimation on the reconstructions qualitatively using LSQR with 250, 400 and 600 iterations respectively. After obtaining the offsets or scale factors we reconstruct the corrected projection data using 100 iterations of LSQR. In Fig. 5.13 central slices of the reconstructions before and after correction are shown. We show the part of the reconstruction that is in the field of view of the detector for every projection image. The proposed methods are able to significantly reduce the artifacts due to offsets on, and scaling of, the projection images. Some vertical smearing effects can be observed, but this is expected due to the limited angular range of $\pm 60^\circ$ (missing wedge artifacts).

In the next experiment we test the effect of the number of projection angles on the offset or scale retrieval. It is not directly clear if increasing the number of projection images results in a better estimation of the offset and scales, because we add equations to the systems in Eq. (5.12) and Eq. (5.15) and at the same time introduce another unknown (local offset or scale factor). For this experiment we use a subset of the projection images used in the previous experiment, such that the projection images are approximately equiangular distributed in the interval $\pm 60^\circ$. The results shown in Fig. 5.14a indicate that the offsets and scale factors can be found more accurately if the number of projections is increased, except for
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Figure 5.13: Qualitative comparison of corrected and uncorrected reconstructions. Central slices in the \( z \)-direction are shown of size \( 256 \times 256 \) (the part that is always in the field of view of the detector).
the global offset. However, the accuracy is not dependent to a great extent on the number of projection angles, even for a limited number of projection images the result of the offset and scale estimation is accurate up to 2 significant digits or more.

We also considered the effect of Poisson noise. We simulated the noise and varied the intensity of the noise, which is indicated by the simulated photon counts (lower photon counts means lower signal-to-noise ratio). The results are shown in Fig. 5.14b. The noise does have an effect on the global offset and scale retrieval for datasets with low signal-to-noise ratio. For the global offset estimation, the results are accurate for all noise levels. For the scale factors the noise level has a larger influence. The local estimation algorithm is far less influenced by the noise level and achieves a good accuracy overall.

**5.6.3 Experimental electron tomography dataset**

In the final experiment we test the offset estimation algorithm on an experimental dataset obtained with an electron microscope, using the HAADF-STEM technique. In Fig. 5.15 a projection image of size $512 \times 512$ is shown. The object consists of PbSe/CdSe core/shell nanocrystal particles that are studied in materials science [Bal+11; Cas+12]. The dataset consists of 151 projections from tilt angles between $\pm 75^\circ$ (1° tilt increments) and was obtained by a FEI TITAN³ 50–80 electron microscope using a parallel beam geometry. Because we assume that the offsets are constant for a single projection image, we can simply restrict the reconstruction to a few slices (in the $x$-direction, see Fig. 5.6). This saves a lot of memory and computation time. In this experiment we reconstruct 50 slices in the $x$-direction. We choose a total of 150 slices in the $z$-direction, which results in a reconstruction volume of $50 \times 512 \times 150$.

The background intensity of the dataset is negative, which suggests that the projection data is not scaled, but has a negative offset. Because we do not know if the projections contain a global or local offset, we apply the local offset estimation algorithm as described in Section 5.4.2. The result of a local offset estimation is shown in Fig. 5.16. The retrieved offset indeed indicates a negative offset. The

![Figure 5.14: (a) Error with respect to the number of projection angles; (b) Error with respect to noise level (expressed in simulated photon counts).](image-url)
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Figure 5.15: Projection image of size 512 × 512.

Figure 5.16: The retrieved offset.

core-shell particles are supported by a carbon grid, which has very low contrast in the projection images. Note that the thickness of this support (i.e. the path length of the electrons through the support) is inversely proportional to the cosine of the projection angle. This might explain why we the offset behaves like $1/\cos \theta$, because it is a superposition of the offset caused by the support material and a negative global offset. As a result, simply subtracting (the mean of) the background intensity would not be sufficient. Note that the local offset estimation can therefore also be used to reduce the effect of the support material on the reconstruction.

We subtract the retrieved offset from the projection data and compute an LSQR reconstruction, see Fig. 5.17c. We compare this with a reconstruction where the minimum value is subtracted from the projections (an estimate of the background intensity), shown in Fig. 5.17b. The difference in quality can be seen especially on the top and bottom part of the reconstruction, where artifacts are still visible in Fig. 5.17b. The reconstruction after local offset removal is much improved. Compared to an LSQR reconstruction that is not corrected for offset, see Fig. 5.17a, the reconstruction has improved significantly. These results show
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![Figure 5.17](image)

(a) Original LSQR reconstruction

(b) LSQR reconstruction with background value subtracted

(c) LSQR reconstruction after offset correction

Figure 5.17: Comparison of the slices in the x-direction of the original reconstruction and corrected reconstructions, by removing the minimum value from the projection data (background), and after local offset estimation.

that the proposed offset estimation is an effective technique for removing offset artifacts, without the need for manual estimation of the background intensity.

5.7 Discussion and conclusions

During the acquisition of the projection images for tomography, an offset on or scaling of the gray values of the projection images can be introduced by fluctuations in the radiation source's intensity. The offset can be a constant added to each gray value of each projection image, which is a global offset, or the offset can be constant only for the pixels in a single projection image, which is referred to as a local offset. In our analysis of the filtered backprojection reconstruction of a global offset, we found that the offset causes an additive artifact in the reconstruction that has the shape of a disk. By enforcing a rectangular reconstruction domain, the global offset causes an inconsistency in the reconstruction and by minimizing inconsistency of the reconstruction with respect to a negative correction term, the offset can be found accurately.

We extended the algorithm such that it can be applied to retrieve a local offset and scaling of projection data. We assume that each scale factor scales the gray values of one projection image. These algorithms work in a similar way
as the global offset estimation: a least squares solver (LSQR) is employed to simultaneously compute a reconstruction and find the unknown offsets or scale factors.

In a series of simulation experiments we investigated the effect of limited data problems that are typically encountered in electron tomography, such as a limited angular range or truncation of projections (if the sample is not contained in the field of view of the detector). Moreover, we determined how strongly the results of the offset and scale estimation algorithms depend on the shape of the reconstruction, in particular the height. Our conclusions are that a missing wedge or truncation should not pose a problem, if the severity of these effects is not too large. The effect of a missing wedge was less strong, even for a very small tilt range of $\pm 20^\circ$ accurate results could be obtained. The effect of truncation was much larger: for the test image that was 512 pixels wide, results were not so accurate if the detector was smaller than 100, 200 and 300 pixels for the global offset, scaling and local offset estimation respectively. We observed that the offset and scale estimation algorithms yield more accurate estimations if the height of the reconstruction domain is small. On this smaller reconstruction domain the influence of the offset or scaling of the projections is much more pronounced in the residuals of the corresponding reconstructions. Therefore, the offset and scale estimation algorithms are able to retrieve the offsets or scalings more accurately in this case, compared to the case where the reconstruction area is square.

The result of the experimental electron tomography dataset shows that offsets can be found which significantly improve the reconstruction even in cases where no background is visible. The effect of offset artifacts can be substantially reduced.