Imaging based on Compton scattering: model uncertainty and data-driven reconstruction methods

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Abstract

The recent development of scintillation crystals combined with \gamma-rays sources opens the way to an imaging concept based on Compton scattering, namely Compton scattering tomography. The associated inverse problem rises many challenges: non-linearity, multiple order-scattering and high level of noise. Already studied in the literature, these challenges lead unavoidably to uncertainty of the forward model. This work proposes to study exact and approximated forward models and develops two data-driven reconstruction algorithms able to tackle the inexactness of the forward model. The first one is based on the projective method called regularized sequential subspace optimization (RESESOP). We consider here a finite dimensional restriction of the semi-discrete forward model and show its well-posedness and regularization properties. The second one considers the unsupervised learning method, deep image prior, inspired by the construction of the model uncertainty in RESESOP. The methods are validated on Monte-Carlo data.

Keywords: model uncertainty, Compton scattering tomography, sequential subspace optimization, deep image prior
1. Introduction

At first a tool for visualizing the inside of the human body using x-rays by the upcoming of computerized tomography (CT), the need for imaging affects nowadays astrophysics, homeland security, landscape and environment monitoring and of course manufacturing processes to cite only a few. This success is made possible by the technological progress in terms of detection—cameras, crystals, etc.—but also in terms of computing and storage capacities.

CT is a well-established and widely used technique which images an object by exploiting the properties of penetration of the x-rays. Due to the interactions of the photons with the atomic structure, the matter will resist the propagation of the photon beam of energy $E$ and intensity $I(x)$ according to the well-known Beer–Lambert law

$$I(y) = I(x)e^{-\mu \cdot t},$$

where $\mu$ stands for the lineic attenuation coefficient and $x \rightarrow y$ denotes the straight line $\{x + t(y - x), t \in [0, 1]\}$. To interpret the measurement of the intensity in a CT-scan is then possible with the help of the Radon transform in 2D and the x-ray transform in 3D, which maps the attenuation map $\mu(x)$ into its line integrals, i.e.

$$\ln \frac{I(s, \theta)}{I(d, \theta)} = R\mu(p, \theta) = \int_{\Omega} \mu(x)\delta(p - x \cdot \theta)dx$$

with $(p, \theta) \in \mathbb{R} \times S^1$ and where $s$ and $d$ stand for the position of the source and of the detection point. We refer to [31] for more information.

The energy constitutes an important variable made accessible by the recent development of scintillation crystals and semi-conductors detectors [24]. Currently the energy is exploited in multi-spectral CT as a supplementary variable split into several channels delivering a precise information on the attenuation coefficient at different energy levels. We refer to [2, 16, 17, 29, 35, 42, 44]. However the recently achieved energy resolution, more precisely the full width at half maximum (FWHM), of the current scintillation crystals opens the way to consider the energy as a reliable dimension along with viewpoints and detector positions. In particle physics, the question of the energy intersects with Compton scattering. Indeed, when one focuses on the physics between the matter and the photons, four types of interactions come out: Thomson–Rayleigh scattering, photoelectric absorption, Compton scattering and pair production. In the classic range of applications of the x-rays or $\gamma$-rays, $[50,1000]$ keV, the photoelectric absorption and the Compton scattering are the dominant phenomena which leads to a model for the lineic attenuation factor due to Stonestrom et al [43] which writes

$$\mu(x,E) = E^{-3}\lambda_{PE}(x) + \sigma(E)f(x)$$

where $\lambda_{PE}$ is a factor depending on the materials and symbolizing the photoelectric absorption, $\sigma(E)$ the total-cross section of the Compton effect at energy $E$ and $f$ the electron density (generally noted $n_e$) at $x$.

The Compton effect stands for the collision of a photon with an electron. The photon transfers a part of its energy $E_0$ to the electron. The electron suffers then a recoil and the photon is then scattered of an (scattering) angle $\omega$ with the axis of propagation. The energy of the photon after scattering is expressed by the Compton formula [11],

$$E = \frac{E_0}{1 + \frac{E_0}{m_e}(1 - \cos \omega)} =: E(\omega),$$
where $mc^2 = 511$ keV represents the energy of an electron at rest. Measuring accurately the variations of the energy can thus be interpreted as scattering events characterized geometrically by the scattering angle which is the foundation of Compton scattering tomography (CST), see [3, 4, 6, 8–10, 14, 15, 18–21, 32–34, 38, 45].

1.1. Spectral data

Given a monochromatic $\gamma$-ray source $s$ of energy $E_0$ and an energy-resolved detector $d$, the illumination of a specimen represented by its attenuation map $\mu$ leads by the Compton effect to a polychromatic response measured at $d$. This would also hold for a polychromatic source as studied in [26, 27] but for the sake of simplicity we consider in this work only monochromatic sources. Assuming only Compton scattering and photoelectric absorption events, we can decompose the spectrum $\text{Spec}(E, d, s)$ measured at a detector $d$ with energy $E$ as follows

$$\text{Spec}(E, d, s) = \sum_{i \in \mathbb{N}} g_i(E, d, s).$$

The data $g_i$ stands for the measured radiation without scattering events for $i = 0$ and after $i$-scattering events for $i > 0$. The ballistic data $g_0$ can be understood as the intensity $I(d, \theta)$ in equation (2). Studied in 2D [26] and 3D [37], the first-order scattered radiation can be modeled by weighted circular or toric Radon transform and shares similarities with $g_0$ in particular in terms of mapping properties. More generally, $g_i$, $i \geq 1$, can be seen as a special case of the integral transforms

$$\mathcal{L}_i(\mu, \bar{f})(E, d, s) := \int_{\Omega^2} \bar{f}(z) k_i(\mu; z, E, d, s) \, dz, \quad \bar{f} = \left( f \otimes \ldots \otimes f \right) \text{ i times}$$

with $k_i(\cdot)$ a singular kernel, $\Omega \subset \mathbb{R}^d$, $d = 2, 3$ and $(E, D, S)$ the domain of definition of $(E, d, s)$. The complexity to handle $k_i$ computationally, already for $i = 2$ studied in [26, 37], combined with its nonlinearity with respect to $f$ (already for the first-order scattering as $\mu$ is a function of $f$), makes the use of multiple-order scattering intractable in practice, at least with the current level of technology. The exploitation of scattering in imaging is thus extremely challenging at theoretical and computational level, so that in this work only the least complicated model, $\mathcal{L}_1$ for the first-order radiation $g_1$, will be used as a forward operator for reconstructing the electron density $f$ from the spectrum (5). As a consequence, $g_2$ and the higher-order radiation must be seen as a large noisy perturbation and therefore as a substantial part of the model inexactness we are dealing with in this study.

Studied in [37], the shape and disposition of the detector array is important to the structure of the forward models. We denote by $\mathbb{S}^d_1(d) \subset \mathbb{R}^d$ the half-sphere of dimension $d - 1$ and parametrized by angles $(\alpha_1, \ldots, \alpha_{d-1})$. We define the set of detector positions defined by $s$ and $t$ as

$$D(t) := \left\{ d = t(\alpha_1) \, \theta(\alpha_1, \ldots, \alpha_{d-1}), \, \theta \in \mathbb{S}^d_1(d) \right\}$$

with $t$ a smooth function. For the implementation, we consider here the case $t(\alpha) = \cos \alpha$ which characterizes the sphere passing through $\theta$ and will denote below $D(\cos)$ by $\mathbb{D}$ for the sake of readability.
1.2. Related work and contribution of this work

As mentioned above, the non-linear models for multiple order scattering $\mathcal{L}_i$ are difficult to deal with and iterative solution methods are very expensive due to the integration kernels, which makes the usage of $\mathcal{L}_i$ for $i \geq 2$ intractable. Also the non-linear operator $\mathcal{L}_1(\mu,f)$ for first-order scattering is difficult to handle, as we will discuss in section 2.2. This is the reason why it has been proposed in [26, 37] to split up the dependency on $f$ and study the linear approximation $\mathcal{L}_1^{*} := \mathcal{L}_1(\mu^{*},\cdot)$ instead, where $\mu^{*}$ is a known a priori approximation of the original $\mu(f)$. Although $\mathcal{L}_1^{*}$ is not the exact model for the first-order radiation $g_1$, the authors demonstrated that it is still possible to reconstruct an approximate of the contours of $f$ from

$$\mathcal{L}_1^{*} f = \mathcal{g}_1^0 \quad \text{or even} \quad \mathcal{L}_1^{*} f = \text{Spec}$$

where, in the latter, the multiple order scattering is seen as a large perturbation. Following on from the analysis of the forward operators and the observation that the first-order operator is less smoothing than the others, the idea to reduce the impact of the multiple order scattering consists in applying some pseudo-differential operator $\mathcal{P}$ on both sides of the inverse problem.

In this work we demonstrate that by involving information on the model uncertainty between $\mathcal{L}_1^{*}$ and the exact model $\mathcal{L}_1 := \mathcal{L}_1(\mu,\cdot)$ for the first-order radiation corresponding to $f$, it is not only possible to reconstruct the contour of $f$, but also its contrast is well preserved, even in presence of higher-order radiation data.

Before that, we also put light on some question that, to the best of our knowledge, has not been considered in the literature of CST, yet: it has been shown in [26, 37] that $\mathcal{L}_1^{*} : L^2(\Omega) \rightarrow L^2(\mathbb{R} \times \mathbb{R} \times \mathbb{R})$ are well-defined, see also theorem 2.4 later. In order to better reflect data acquisition it is necessary to consider semi-discrete versions of those operators, i.e. to sample the data space at finitely many source positions, detector positions and energy levels. However, in general, sampling $L^2$-functions is not well-defined, since it may not have a continuous representative. Fortunately, in [26, 37] it has been proven that the operators above fulfill some Sobolev-scale property, which, together with some Sobolev embedding theorem, enables us to derive a semi-discrete formulation in this work. Our approach is inspired from the semi-discrete Radon transform, see for example chapter 6.3 in [36]. The corresponding semi-discrete operators inherit continuity w.r.t. some suitable Sobolev-norms, but not w.r.t. $L^2$-norms. Therefore, we consider them on a finite dimensional subspace $X_j \subset L^2(\Omega)$ and work with these fully discrete operators in our numerical experiments.

In order to involve the model uncertainty between the inexact and exact linear forward operators, two approaches appear suited and are considered in this work.

The first one is the regularized sequential subspace optimization (RESESOP)-Kaczmarz method developed in [7] for dealing with model inexactness, which occurs when considering an approximate version $\mathcal{A}^0$ instead of the true forward operator $\mathcal{A}$. The principle of this method is to split the inverse problem into subproblems and to iteratively project onto stripes containing the solution set. The thickness of those stripes is then controlled by a parameter of model uncertainty between $\mathcal{A}$ and $\mathcal{A}^0$. In this work we inspect the regularization capability of RESESOP applied to the fully discrete version of the inexact operator $\mathcal{L}_1^{*}$. Since the fully discrete operator is defined on a subspace $X_j$, we extend the RESESOP theory and inspect in theorem 3.13 under which circumstances the reconstructions are stable with respect to $X_j$, which might also be a valuable contribution for solving other inverse problems with RESESOP.

As a second approach for dealing with an inexact forward operator we design a suitable loss function for the widely used deep image prior (DIP) unsupervised learning technique, which
was presented in [28] for denoising and inpainting problems. The reason to use this approach is twofold:

(a) It does not require datasets which are at the moment inexistant for CST.
(b) It provides a very flexible architecture while sharing interesting properties from optimization.

1.3. Outline

The paper is organized as follows. Section 2.1 recalls the forward models associated to the first- and second-order scattered part of the spectrum. After that, in section 2.2 we have a closer look at the non-linearity of $\mathcal{L}_1$ and observe that its Fréchet derivative is computationally expensive and might not fulfill the tangential cone condition in general. In section 2.3 we recall mapping properties of the linear operators $\mathcal{L}_{\mu_i}$ for $i = 1, 2$ and further present well-defined semi-discrete and fully discrete formulations. We also discuss in section 2.4 how the model uncertainty between $\mathcal{L}_{\mu_1}^*$ and $\mathcal{L}_{\mu_1}$ can be defined and measured. The first reconstruction method involving information on the model uncertainty, RESESOP, is recalled in detail in section 3.1. Section 3.2 consists of two parts. First, we settle down the notation for the case of RESESOP being applied to the fully discrete problem, in order to distinguish between the fully and semi-discrete problem. Second, we analyze the stability of RESESOP applied to restricted operators. More precisely, we prove that the RESESOP reconstructions for the fully discrete problems converge to the SESOP reconstruction of the semi-discrete problem, under some assumptions. Inspired by the RESESOP approach, we then recall the DIP algorithm in section 4 and present an appropriate loss function that takes the model uncertainty into account. Simulation results for the fully discrete inverse problem are presented in section 5 for synthetic data and Monte-Carlo data for the second-order scattered radiation. We also show the effects of using bad estimates for the model uncertainty, which will illustrate the central challenge for further development of the RESESOP algorithm in the future, namely to find accurate model uncertainty estimates. A conclusion ends the manuscript.

2. Formulation of the mathematical problem

As explained in the Introduction, the measured spectrum is the sum of the primary radiation and of the scattered radiation of different orders. From a physical point of view, the lower the energy the lower is the probability of a scattering event. It follows that high-order scattering events, typically $\geq 3$, represent a marginal part of the scattered radiation and by the stochastic nature of the emission of photons will be highly noisy. To reflect this physical point of view, we consider that

$$\text{Spec} = g_0 + g_1 + g_2 + \epsilon$$

with $\epsilon$ a noisy perturbation. In this section, we recall the modeling of the first- and second-order scattered radiation, their properties and detail the computation of the spectral data for a specific scanning architecture. The section ends with the presentation of a general reconstruction strategy.

2.1. The forward problem

Let us consider a photon beam traveling from $\mathbf{s}$ to $\mathbf{x}$ and from $\mathbf{x}$ to $\mathbf{d}$ after a scattering event of angle $\omega = \angle(\mathbf{x} - \mathbf{s}, \mathbf{d} - \mathbf{x})$ with $\angle(\cdot, \cdot)$ the angle between two vectors. Such a beam is subject
One time scattered photons arriving \( d \) from \( s \) with energy \( E(\omega) \) have been scattered on \( \Sigma(\omega, d, s) \), two opposite circular-arcs in 2D.

Given a point detector \( d \) and an ionizing point source \( s \) with energy \( E_0 \) and photon beam intensity \( I_0 \), the variation of photons \( N_c \) scattered at \( x \) and detected at \( d \) with energy \( E_\omega \), see [13], can be expressed as

\[
\frac{dN_c(x, d, s)}{d\Omega} = I_0 \left( \frac{d\sigma_c}{d\Omega} \right) A(\mu(\cdot, E_0))(s, x)A(\mu(\cdot, E_\omega))(x, d)f(x)dx,
\]

where \( \frac{d\sigma_c}{d\Omega} \) stands for the Klein–Nishina probability [23]. Due to the Compton formula equation (4), the loci of scattering events can be uniquely represented by a scattering angle \( \omega \). Now, one can integrate equation (8) w.r.t. \( x \in \Omega \) to estimate the measured scattered flux. As proven in [38, 39], the first-order scattered radiation \( g_1 \) can be modeled by the integration of the electron density \( f \) along spindle tori (in 3D) or circular-arcs (in 2D) expressed as

\[
\Sigma(\omega, d, s) = \{ x \in \mathbb{R}^d : \angle(x - s, d - x) = \omega \}, \quad d = 2, 3.
\]

For an illustration of the geometry of a circular-arc see figure 1. It follows that

\[
g_1 \sim \Sigma_1(\mu, f)(E, d, s) := \int_{\Omega} \frac{\omega}{\mu} \delta(E - \phi(x, d, s)) d\mathbf{x}
\]

where \( \frac{\omega}{\mu} \) quantifies the physical factors (attenuation and photometric dispersion) in equation (8) between \( s, x \) and \( d \), and \( \phi \) stands for the level-set function associated to the inside (resp. outside) spindle torus when positive (resp. negative) and is given by

\[
\phi(x, d, s) = E \left( \frac{\cot^{-1}(\kappa(x, d, s) - \rho(x, d, s))}{\sqrt{1 - \kappa^2(x, d, s)}} \right)
\]
where
\[
\kappa(x, d, s) = \frac{(x - s) \cdot (d - s)}{\|x - s\|_2 \|d - s\|_2} \quad \text{and} \quad \rho(x, d, s) = \frac{\|x - s\|_2}{\|d - s\|_2}
\]
(11)
with \(\|\cdot\|_2\) the Euclidean norm.

Regarding the second-order scattering, equation (8) can be extended naturally by adding a second scattering event at \(y\) between \(x\) and \(d\). The key is to see the first scattering locus as a local polychromatic source where the energy is a function of the aperture of a cone at vertex \(x\) and direction \(x - s\). The second scattering event is then modeled similarly to \(g_1\) but w.r.t. to the source \(x\). Given two scattering angles \(\omega_1\) and \(\omega_2\), it holds by the Compton formula (4)
\[
\cos \omega_1 + \cos \omega_2 = 2 - mc^2 \left( \frac{1}{E} - \frac{1}{E_0} \right) =: \lambda(E) \in (0, 2).
\]
Following on from [26, 37], the second-order scattering points \(y\) can then be represented as the intersection between the cone at vertex \(x\) and direction \(x - s\) and the spindle torus \(\Sigma(x, d, s)\)
which leads to the following characteristic function
\[
\psi(y, x, d, s) := \frac{y - x}{\|y - x\|} \cdot \frac{x - s}{\|x - s\|} + \cos (\cot^{-1} \phi(y, x,d)) .
\]
Following the same scheme as for \(g_1\), the second-order scattered radiation \(g_2\) can be represented by a nonlinear integral transform
\[
g_2 \sim \mathcal{L}_2(\mu, f) (E, d, s) := \int_{\Omega^2} \mathcal{M}_2(z, d, s) \tilde{f}(z) \delta(E - \lambda^{-1}(\psi(z, d, s))) \, dz
\]
(12)
where \(\mathcal{M}_2(\mu)\) quantifies the physical factors between \(s, z\) and \(d\) with \(z = (x, y), \tilde{f} = f \otimes f\). We refer to [26, 37] for more details.

2.2. A look on the nonlinear problem

The operators \(\mathcal{L}_1\) and \(\mathcal{L}_2\) are nonlinear w.r.t. \(f\) and \(\tilde{f}\) respectively but also difficult to handle numerically. The Fréchet (or Gâteaux) derivative is then essential in the construction of reconstruction schemes. Focusing on the first-order scattering, we can compute the corresponding Fréchet derivative where we neglect the photoelectric absorption in \(\mu\) in equation (3), i.e. \(\mu(\cdot, E) = \sigma(E)f\), and consider, for the sake of simplicity, the operator \(\mathcal{L}_1(\mu, f) := \mathcal{L}_1(\mu, f) : X \to Y\) with \(X, Y\) two suited Hilbert spaces equipped with their respective norms. Furthermore, the weight \(\mathcal{M}_1\) (see [26, 37] for more details) can then be written as
\[
\mathcal{M}_1(f) = C \exp \left(-\frac{\|f\|}{\|x - s\|_2 \|d - x\|_2^2} \right), \quad C > 0
\]
where \(X\) denotes the x-ray transform applied on the electron density \(f\) along the scattering path \(s\) to \(x\) and \(x\) to \(d\) (see equation (1)).

**Theorem 2.1.** \(\mathcal{L}_1\) is Fréchet-differentiable with
\[
(\mathcal{L}_1)'h(E, d, s) = \int_{\Omega^2} \left( \mathcal{M}_1(f) h(z, d, s) f(z) + \mathcal{M}_1(f) (z, d, s) h(z) \right) \delta(E - \phi(z, d, s)) \, dz
\]
and \((\mathcal{L}_1)'\) is bounded for every \(f \in L_2(\Omega)\) bounded.

**Proof.** The Fréchet derivative for \(\mathcal{L}_1\) is defined as
\[
\mathcal{L}_1(f + h) = \mathcal{L}_1(f) + (\mathcal{L}_1)'h + o(h).
\]
Inspecting $\mathcal{M}_1$ closer, we note that it is the composition of a smooth function and of a linear operator which implies that $\mathcal{M}_1$ is Fréchet-differentiable. Given the Fréchet derivative of $\mathcal{M}_1$, it holds

$$\mathcal{M}_1(f + h) = \mathcal{M}_1(f) + (\mathcal{M}_1)' h + o(h)$$

leading to

$$\mathcal{L}_1(f + h) = \mathcal{L}_1(f) + \int_\Omega (\mathcal{M}_1)' h(z,d,s) f(z) \delta(E - \phi_1(z,d,s)) \, dz$$

$$+ \int_\Omega \mathcal{M}_1(f)(z,d,s) h(z) \delta(E - \phi_1(z,d,s)) \, dz$$

$$+ \int_\Omega h(z) (\mathcal{M}_1)' h(z,d,s) \delta(E - \phi_1(z,d,s)) \, dz$$

$$+ \int_\Omega f(z) o(h) \delta(E - \phi_1(z,d,s)) \, dz.$$  

The linear part w.r.t. $h$ on the righthand side, i.e. its Fréchet derivative, reads now

$$(\mathcal{L}_1)' h = \int_\Omega \left( (\mathcal{M}_1)' h(z,d,s)f(z) + \mathcal{M}_1(f)(z,d,s)h(z) \right) \delta(E - \phi_1(z,d,s)) \, dz.$$  

For $\Omega$ compactly supported and for $f$ being bounded, it is clear that the linear operator $f(z) (\mathcal{M}_1)' + \mathcal{M}_1(f)\delta$ is bounded and consequently the property holds for $(\mathcal{L}_1)'$.

We observe that the computation of the Fréchet derivative of $\mathcal{L}_1$, for instance within the Kaczmarz’s method, would require the computation of $(\mathcal{M}_1)'$ and $\mathcal{M}_1(f)$ at each iterate which constitutes, especially in 3D, an expensive task.

Besides the computation cost, the Fréchet derivative needs to satisfy the so-called tangential cone condition which would read as

$$\|\mathcal{L}_1(f + h) - \mathcal{L}_1(f) - (\mathcal{L}_1)' h\|_Y \leq c_1\|\mathcal{L}_1(f + h) - \mathcal{L}_1(f)\|_Y,$$

with some constant $c_1 < 1$, in order that most of the iterative schemes applied on $\mathcal{L}_1$ converge. Using the expression of $\mathcal{M}_1$, it holds with symbolic notations

$$\mathcal{L}_1(f + h) - \mathcal{L}_1(f) - (\mathcal{L}_1)' h$$

$$= \int_\Omega \left[ (\mathcal{M}_1(f + h) - \mathcal{M}_1(f)) (f + h) - (\mathcal{M}_1)' h f \right]$$

$$= \int_\Omega \left[ (\mathcal{M}_1(f + h) - \mathcal{M}_1(f)) (f + h) - (\mathcal{M}_1)' h f \right]$$

$$= \int_\Omega (\mathcal{M}_1(f + h) (1 - \mathcal{M}_1(-h)) (f + h) + (\mathcal{M}_1(f)) (f + h)$$

$$= \int_\Omega (-Xh) (\mathcal{M}_1(f + h) (f + h) + \mathcal{M}_1(f) f) - \int_\Omega \sum_{n=2}^{\infty} \frac{(\mathcal{M}_1)^n}{n!} (f + h) (f + h).$$

We observe that the tangential cone condition might not hold for ‘large’ $h$ as the second term explodes for $h$ large. Therefore, dealing with the nonlinear problem might require an a priori initial value close to the solution which is not always possible to guarantee.
2.3. Linear approximations and discretization

As discussed above, the non-linearity is difficult to tackle, which encourages to split up the dependency on \( f \) and therefore study instead linear approximations \( \Sigma_1(\mu^*, \cdot) \) and \( \Sigma_2(\mu^*, \cdot) \) with \( \mu^* \) a known a priori smooth approximation to the original \( \mu \). In the following we recall some properties of these approximations on the Sobolev scale. Beforehand, we settle some notation.

The Schwartz space is denoted by \( S(\mathbb{R}^d) \), whereas its dual space, the space of tempered distributions, by \( S'(\mathbb{R}^d) \), see e.g. chapter I.1 in [46] for more information. A tempered distribution \( T : S(\mathbb{R}^d) \rightarrow \mathbb{R} \) is called regular if it is induced by a function \( t \in L^1_{\text{loc}}(\mathbb{R}^d) \), i.e. \( T \varphi = \int_{\mathbb{R}^d} t(x) \varphi(x) \, dx \) holds for every \( \varphi \in S(\mathbb{R}^d) \). For simplicity, we do not distinguish between \( T \) and \( t \) in the following.

Definition 2.2 (definition I.5.1, [46]). For \( \alpha \in \mathbb{R} \), the Sobolev space of order \( \alpha \) is defined as

\[
H^\alpha(\mathbb{R}^d) := \left\{ f \in S'(\mathbb{R}^d) : \hat{f} \text{ regular and } \| \hat{f} \|_{L^2}^2 = \int_{\mathbb{R}^d} |\hat{f}(\xi)|^2 (1 + |\xi|^2)^\alpha \, d\xi < \infty \right\},
\]

where \( \hat{f} \in S' \) denotes the distributional Fourier transformation of \( f \in S' \), see chapter I.1.9 in [46].

Given some open set \( \Omega \subseteq \mathbb{R}^d \), the space of infinitely times differentiable functions \( \Omega \rightarrow \mathbb{R} \) with compact support in \( \Omega \) is denoted by \( \mathcal{D}(\Omega) \), its dual space \( \mathcal{D}'(\Omega) \) is defined in the usual sense, see e.g. definition I.1.1 in [46]. According to theorem I.1.18 in [46], each tempered distribution can be extended to a distribution in \( \mathcal{D}'(\mathbb{R}^d) \).

Definition 2.3 (definition I.5.2, [46]). Let \( \Omega \subseteq \mathbb{R}^d \) be open and \( \alpha \in \mathbb{R} \). The space \( H^\alpha(\Omega) \) is defined as

\[
H^\alpha(\Omega) := \left\{ R_\Omega f : f \in H^\alpha(\mathbb{R}^d) \right\},
\]

where \( R_\Omega \) denotes the restriction operator \( R_\Omega : \mathcal{D}'(\mathbb{R}^d) \rightarrow \mathcal{D}'(\Omega) \) to the domain \( \Omega \). Note that \( R_\Omega \) is the adjoint of the extension operator \( \mathcal{D}(\Omega) \rightarrow \mathcal{D}(\mathbb{R}^d) \) —extension by zero outside of \( \Omega \).

Furthermore, \( H^\alpha_{\text{loc}}(\Omega) \) is defined as the closure of \( \mathcal{D}(\Omega) \) in the topology of \( H^\alpha(\mathbb{R}^d) \) and we define for \( \alpha \geq 0 \) the space

\[
H^\alpha_{\text{loc}}(\Omega) := \left\{ f \in L^2_{\text{loc}}(\Omega) : f\varphi \in H^\alpha_0(\Omega) \text{ for all } \varphi \in \mathcal{D}(\mathbb{R}^d) \right\}
\]

and equip it with the topology induced by the system of semi-norms \( f \mapsto \| f\varphi \|_{L^2} \) for \( \varphi \in \mathcal{D}(\mathbb{R}^d) \). Its topological dual space is then denoted by \( H^{-\alpha}_{\text{loc}}(\Omega) \). Having this notation on hand, we recall some smoothness properties of the operators \( \Sigma_1(\mu, \cdot) \) and \( \Sigma_2(\mu, \cdot) \), which play an essential role in the derivation of semi-discrete models.

Theorem 2.4 ([26, 37]). We let \( h \in C^\infty(\Omega) \) with \( \Omega \subseteq \mathbb{R}^d \), \( d = 2, 3 \). Then, for the detector set \( \mathcal{D} \) defined in equation (6) where the domain of the parameters \((\alpha_1, \ldots, \alpha_d)\) is open and \( s \in \mathcal{D} \) fixed, the operators \( \Sigma_1(h, \cdot) \) and \( \Sigma_2(h, \cdot) \) are Fourier integral operators of order

\[
\tau_1 := \frac{1 - d}{2} \quad \text{and} \quad \tau_2 := \frac{2 - 3d}{4}
\]

respectively and it exists \( E \subseteq \mathbb{R}^+ \) where they are continuous mapping from \( H^\alpha_{\text{loc}}(\Omega) \) to \( H^{\alpha-\tau_1}(E, \mathbb{D}) \) and \( H^\beta_0(\Omega^{\beta}) \) to \( H^{\beta-\tau_2}(E, \mathbb{D}) \) respectively for all \( \alpha \in \mathbb{R} \) and \( \beta \in \mathbb{R}^+ \).

Proof. See [37] for \( d = 3 \) and [26] for \( d = 2 \).
In the next sections, we consider a semi-discrete and a fully discrete setting for the spectral data in order to better reflect data acquisition. To this end, we consider a set of source and detector positions \((s_k, d_k)_{k=1,...,K}\) as well as a set of energy \((E_p)_{p=1,...,P}\). The sampling step on the energy will in practice depend on the energy resolution (called FWHM) of the detector.

We also aim to connect these both settings in terms of representation. However, similarly to the semi-discrete Radon transform, see e.g. in [36, chapter 6.3.], we face the problem that sampling \(\mathcal{L}_1(\mu, f)\) on a finite set is not well-defined for arbitrary \(f \in L^2(\Omega)\), as its equivalence class may not have a continuous representative. Indeed, for \(s\) fixed, the operator

\[
\mathcal{L}_1 : L_2(\Omega) \rightarrow H^\alpha(\Omega, \mathbb{D})
\]

\[
f \mapsto \mathcal{L}_1(\mu, f)(\cdot, s)
\]

is not well-defined in the semi-discrete setting, as \(\mathcal{L}_1(\mu, f)\) would have no continuous representative, and therefore discretizing \((E, d, s)\) would be improper regarding the continuous case. However, we can exploit an embedding property of Sobolev spaces.

**Theorem 2.5.** Let \(\Omega \subset \mathbb{R}^d\) be a region, i.e. open and path-connected. Further, let \(m \in \mathbb{N}_0\). Then for every \(\alpha - m > d/2\) the space \(H^\alpha_0(\Omega)\) is continuously embedded into \(C^m(\Omega)\). The latter is the space of \(m\) times differentiable functions vanishing at the boundary of \(\Omega\), and whose derivatives are uniformly continuous.

**Proof.** In chapter I.5.1 in [46] it has been stated that for \(\alpha \geq 0\) the space \(H^\alpha_0(\Omega)\) is isomorphic to the Sobolev-Slobodeckii space \(W^{\alpha, \infty}_0(\Omega)\)—see chapter I.3.1 in [46] for a definition, which can be continuously embedded into \(C^m_0(\Omega)\) according to corollary I.6.2. in [46], given that \(\alpha - m > d/2\).

In order to exploit this result, it is important to relax the locality constraint in theorem 2.4. To this end, we consider a suited smooth cut-off \(\chi \in C^\infty(\mathbb{E}, \mathbb{D})\) with compact support in \((\mathbb{E}, \mathbb{D})\), so that \(\chi \mathcal{L}_1(\mu, f) \in H^{\alpha - \tau}_0(\mathbb{E}, \mathbb{D})\) for \(h \in C^\infty(\Omega), f \in H^\alpha_0(\Omega)\). Choosing \(k = 0\), it follows that the operator

\[
\chi \mathcal{L}_1 : H^\alpha_0(\Omega) \rightarrow H^{\alpha - \tau}_0(\mathbb{E}, \mathbb{D})
\]

\[
f \mapsto \chi \mathcal{L}_1(\mu, f)(\cdot, \cdot, s)
\]

has a continuous representative for

\[
\alpha - \frac{1 - d}{2} > \frac{d}{2} \iff \alpha > \frac{1}{2}.
\]

The result holds similarly for \(\mathcal{L}_2\). Therefore, assuming \(\mu \in C^\infty(\Omega)\) and \(f \in H^\alpha_0(\Omega)\) with \(\alpha > 1/2\), we can now define the forward operators for the semi-discrete first-order and second-order scattering by

\[
\mathcal{L}^\mu_1 : H^\alpha_0(\Omega) \rightarrow \mathbb{R}^{P \times K}
\]

\[
f \mapsto \left(\chi \mathcal{L}_1(\mu, f(E_p, d_k, s_k))\right)_{p=1,...,P, k=1,...,K}
\]

\[
\mathcal{L}^\mu_2 : H^\alpha_0(\Omega^2) \rightarrow \mathbb{R}^{P \times K}
\]

\[
f \mapsto \left(\chi \mathcal{L}_2(\mu, f(E_p, d_k, s_k))\right)_{p=1,...,P, k=1,...,K}.
\]

Letting aside the ballistic radiation \(g_0\) which contributes in only one value at \(E_0\) in the spectrum, the spectral problem (7) becomes then

\[
\mathcal{L}^\mu_1 f + \mathcal{L}^\mu_2 f = \text{Spec.}
\]

(13)
Most reconstruction techniques require the computation of the adjoint operator, here of $L^1_\mu$ and $L^2_\mu$, and consider the topology of the $L_2$-space in order to take into account perturbations in the measurement. However, akin to the semi-discrete Radon transform, see [36], the adjoint of $L^1_\mu$ is not continuous w.r.t. the $L_2$-topology and its computation in the $H^\alpha$-topology can be a hard analytic and computational task. A way to circumvent this obstacle is to restrict the domain space to a finite dimensional subspace allowing us to use for instance the $L_2$-topology, by equivalence of the norms. Therefore, we consider for the implementation the fully-discrete case which can be formulated by restricting the forward domain space into a subspace $\mathcal{X}_j \subset H^\alpha_0(\Omega)$ with $\dim(\mathcal{X}_j) < 1$, i.e.

$$
(L^1_\mu)_j : \mathcal{X}_j \rightarrow \mathbb{R}^{P \times K} \\
(f_j) \mapsto L^1_\mu f_j \\
(L^2_\mu)_j : \mathcal{X}_j \times \mathcal{X}_j \rightarrow \mathbb{R}^{P \times K} \\
(f_j, f_j) \mapsto L^2_\mu f_j.
$$

Since $\mathcal{X}_j$ is finite dimensional, $(L^1_\mu)_j$ and $(L^2_\mu)_j$ are bounded with respect to the $L_2$-norm and more standard approaches can be used to solve

$$
(L^1_\mu)_j f_j + (L^2_\mu)_j f_j = g_1 + g_2
$$

where $g_i, i = 1, 2$, denotes the sampled version of $g_i$. An interesting question is how to relate the solution to all subproblems (14) to the solution of (13). This is answered in section 3.

### 2.4. Model uncertainty and reconstruction strategies

Focusing on the Compton part, the spectral problem (7) can be reformulated with the fully discrete setting in equation (14) by

$$
\text{Find } f \text{ from Spec with } \| (L^1_\mu)_j f_j + (L^2_\mu)_j f_j - \text{Spec} \|_2 \leq \epsilon, \ j \in \mathbb{N}
$$

in which $\text{Spec} \in \mathbb{R}^{P \times K}$ is the sampled version of Spec.

**Remark 2.6.** Using $g_0$ in the reconstruction process is sensible. For instance, it is possible to reconstruct under sparsity constraints a first approximation of the attenuation map which can help to refine the forward model, in particular the weight functions, see [26, 27]. However, we discarded this part of the spectrum as we wanted to stress the model uncertainty using a weaker a priori of the attenuation map.

This inverse problem is in particular challenging regarding the following two aspects:

- **Complexity:** While the computational cost regarding $L^1_\mu u$ is similar to the one of the semi-discrete Radon transform (assuming the weight function is precomputed), evaluating $L^2_\mu$ is much more expensive. Given a grid of $N^d$ elements, then the complexity of $L^1_\mu$ is of order $O(N^2) \times J \times K)$ while $L^2_\mu$ is of order $O(N^{2d} \times J \times K)$. In two dimensions and $N = 100$, it means that the computation of the second order scattering is 10000 times more expensive! This represents an important obstacle which encourages us to focus on the first-order scattered radiation and forces us to use different simulators such as a Monte-Carlo approach for the second-order.
model uncertainty: the linearization of the forward models by assuming a prior attenuation map $\mu^*$ leads to an inaccuracy in the model i.e. we have with some $\eta_j > 0$

$$\left\| (L\mu_1^r) f_j - \left( L\mu_1^r \right)^* f_j \right\|_2 \leq \eta_j.$$ 

The issue of the model uncertainty further increases when focusing on the first-order scattering as proposed above. In this case, the second-order (and larger order in practice) has to be treated as model error as well, which yields

$$\left\| (L\mu_1^r) f_j + (L\mu_2^r) f_j - \left( L\mu_1^r \right)^* f_j \right\|_2 \leq \eta_j,$$

where $\eta_j$ can be expected large.

Another reason to focus on the first-order part is the smoothness properties given in theorem 2.4. Since the $L_2$ is a smoother Fourier integral operator (FIO) than $L_1$, it tends to spread the features of $f$ and therefore the first-order part is richer for encoding $f$. A way to emphasize the smoothness scale, it is possible to add to the inverse problem a discretized differential operator (finite difference for example), $\mathfrak{P} : \mathbb{R}^{P \times K} \to \mathbb{R}^{P \times K}$ acting on the energy variable, leading to solve

$$\mathfrak{P} (L\mu_1^r) f_j = \mathfrak{P} \text{Spec}_j \text{ with } f \in \mathcal{X}_j \text{ for some } j \in \mathbb{N}.$$ 

and to the model uncertainty

$$\left\| \mathfrak{P} \left( (L\mu_1^r) f_j + (L\mu_2^r) f_j - \left( L\mu_1^r \right)^* f_j \right) \right\|_2 \leq \eta_j^\mathfrak{P}.$$ 

We observe empirically that the use of a differential operator reduces the model uncertainty, i.e. $\eta_j^\mathfrak{P} < \eta_j$, but this remains to be proven. This strategy was successfully applied: in 3D using FBP-type algorithm for the extraction of the contours in [37] and in 2D using iterative total-variation (TV) regularization in [26, 27]. However errors and artifacts due to an inaccurate model can appear and need to be addressed using data-driven algorithm.

In [7] the authors consider a CT problem affected by motion of the patient, which leads to an inexact forward operator, as the motion is not explicitly known. They proposed to apply the RESESOP for solving inverse problem subject to model uncertainty and studied how the method is well-posed and regularizing for the exact inverse problem. In section 3, we propose to adapt this strategy for solving the semi-discrete and fully-discrete problems associated to CST. We also prove that the fully-discrete RESESOP is a regularization method for the semi-discrete SESOP solution.

A second approach consists in implementing the DIP unsupervised learning method in order to address our inexact inverse problem. Discussed in section 4 and in section 5, the standard loss function does not succeed to compensate for the model uncertainty in CST. Inspired from the RESESOP approach, we propose to adapt the loss function by incorporating the model uncertainty in the loss function which leads to similar results with the RESESOP method.

3. Study and construction of a RESESOP algorithm for CST

As discussed in section 2, we are facing the issue of solving an inverse problem without explicitly knowing the forward operator. In order to get a valid reconstruction, we need to take the
model uncertainty between the exact operator $L_\mu^\mu_1$ and the inexact forward operator $L_\mu^{\mu^*}_1$, into account, where these are the semi-discrete operators from section 2.3, respectively. Clearly, there is some $\eta > 0$ such that

$$
\| L_\mu^\mu_1 - L_\mu^{\mu^*}_1 \| \leq \eta,
$$

where $\| \cdot \|$ here denotes the operator norm of linear bounded mappings $H^\alpha_0(\Omega) \to \mathbb{R}^{n \times k}$. Admittedly, this would be a natural but coarse way to quantify the model uncertainty between those operators. In CST, the model uncertainty between $L_\mu^\mu_1$ and $L_\mu^{\mu^*}_1$ highly depends on the different source and detector positions, but also on the energy of the scattered photons. Therefore, it would be more accurate to consider these operators coordinate-wise, which leads to a system of inverse problems having individual model uncertainty estimates like above.

To handle the model uncertainty issue for multiple problems simultaneously, we use the RESESOP-Kaczmarz procedure presented by Blanke et al in [7]. They extended the RESESOP method, developed by Schoepfer and Schuster [41] for exact forward operator but noisy data, to inexact forward operators and combined it with Kaczmarz’ method [22]. In section 3.1 below we give a recap on their RESESOP-Kaczmarz procedure for general systems of inverse problems. RESESOP is a regularization of SESOP method, which has originally been introduced by Narkiss and Zibulevski [30] and generalized to Banach spaces by Schöpfer et al [41]. We hence start the recall by presenting the SESOP-Kaczmarz procedure in section 3.1.1 for general Hilbert spaces. In section 3.1.2 we then state the functionality and regularization properties of RESESOP-Kaczmarz derived in [7].

In order to regularize inverse problems with RESESOP, the forward operators must be continuous and their adjoints should be computable. As we have already pointed out in the previous sections, the semi-discrete operators $L_\mu^\mu_1, L_\mu^{\mu^*}_1$ are continuous with respect to the Sobolev norm, but in this case the adjoint operators have not analytically been derived, yet. On the other hand, when considering the $L^2$-norm they are no longer continuous. As a way out, we restricted them to a finite dimensional subspace $X_j$ and by that obtained fully discrete operators $(L_\mu^\mu_1)_j, (L_\mu^{\mu^*}_1)_j$, see section 2.3. The RESESOP-Kaczmarz method is then able to regularize the inverse problem corresponding to these fully discrete operators, according to the theory from [7].

Since we want to apply RESESOP-Kaczmarz to the restriction of semi-discrete operators $\mathcal{X} \to \mathcal{Y}$ to a subspace domain $\mathcal{X}_j \subset \mathcal{X}$, we will inspect in section 3.2, whether there is in general some relation between RESESOP applied to the restricted (fully discrete) and the non-restricted (semi-discrete) case. In order to distinguish between the restricted and non-restricted problem, we hence start in section 3.2.1 by establishing some notation for the restricted problem and rewrite the theory from section 3.1 in the light of the restricted setting, see corollary 3.10. A natural question is whether the RESESOP reconstructions for the restricted problem are stable with respect to the chosen subspace $\mathcal{X}_j$. More precisely, we need to answer what happens if $\mathcal{X}_j \not\subseteq \mathcal{X}$, i.e. $\mathcal{X}_j$ approaches the full domain $\mathcal{X}$. At this end, we provide an extension of the RESESOP theory in section 3.2.2 by proving in theorem 3.13 that the RESESOP reconstructions of the restricted problem converge to the SESOP reconstructions of the semi-discrete case, as soon as $\mathcal{X}_j$ approaches $\mathcal{X}$ and the noise level and model uncertainty goes to zero. Finally, in section 3.3 we carefully explain how the RESESOP-Kaczmarz framework can be applied to CST.

### 3.1. RESESOP-Kaczmarz for a system of linear inverse problems

Consider finitely many linear bounded operators $\mathcal{A}_k : (\mathcal{X}, \| \cdot \|_\mathcal{X}) \to (\mathcal{Y}_k, \| \cdot \|_{\mathcal{Y}_k})$ between Hilbert spaces $\mathcal{X}, \mathcal{Y}_k$, where $k \in \{0, 1, 2, \ldots, K - 1\}$ for some $K \in \mathbb{N}$. We assume that only
approximate versions of $A_k$ in the form of other linear bounded operators $A^\eta_k : \mathcal{X} \rightarrow \mathcal{Y}_k$ are available, satisfying
\[
\|A^\eta_k - A_k\|_{\mathcal{X} \rightarrow \mathcal{Y}_k} \leq \eta_k,
\]  
where $\| \cdot \|_{\mathcal{X} \rightarrow \mathcal{Y}_k}$ denotes the operator norm of linear bounded functions between $\mathcal{X}$ and $\mathcal{Y}_k$.

In what follows, we abbreviate all norms by $\| \cdot \|$ when there is no ambiguity. For the sake of readability, we avoid writing $\eta_k$ in the superscript of the inexact forward operators. Further, the following notation will be useful:
\[
[n] := n \mod K.
\]

Thereupon the RESESOP-Kaczmarz procedure, presented in [7], will be twofold: First, in case that all $A_k$ are known and exact data $g_k$ in the range of $A_k$, noted $\text{Ran}(A_k)$, are available, we illustrate the concept of SESOP-Kaczmarz for solving this system of inverse problems. Second, we recall how this method can be extended if only inexact forward operators and noisy data is available.

Beforehand, we give an important definition.

**Definition 3.1.** Let $u \in \mathcal{X}$ and $\alpha \in \mathbb{R}$. Define the corresponding hyperplane via
\[
H(u, \alpha) := \{ x \in \mathcal{X} : \langle u, x \rangle = \alpha \},
\]
and upper halfspace via
\[
H_\alpha(u, \alpha) := \{ x \in \mathcal{X} : \langle u, x \rangle \geq \alpha \}.
\]
In addition, for $\xi \geq 0$ we define the corresponding stripe as
\[
H(u, \alpha, \xi) := \{ x \in \mathcal{X} : |\langle u, x \rangle - \alpha| \leq \xi \}.
\]
Note that $H(u, \alpha) \subset H(u, \alpha, \xi)$ for all $\xi$.

### 3.1.1 SESOP-Kaczmarz for exact forward operators and data.

We start with the observation that for any $w \in \mathcal{Y}_k$ the hyperplane
\[
H(A^*_k w, \langle w, g_k \rangle) = \{ z \in \mathcal{X} : \langle A_k z, w \rangle = \langle w, g_k \rangle \}
\]
contains the solution set
\[
M_A(g) := \{ z \in \mathcal{X} : A_k z = g \text{ for all } j \}
\]
of the system of inverse problems. Moreover, it follows from Riesz’ Representation theorem [25, theorem 3.8.1] that
\[
\bigcap_{k=0}^{K-1} \bigcap_{w \in \mathcal{Y}_k} H(A^*_k w, \langle w, g_k \rangle) = M_A(g).
\]
Therefore, the idea of SESOP is to choose $w_n \in \mathcal{Y}_n$ and iteratively project onto the corresponding hyperplanes
\[
H_n := H(A^*_n w_n, \langle w_n, g_n \rangle).
\]
That is, given a start iterate $f_0 \in \mathcal{X}$, we set $f_n := \mathcal{P}_H(f_{n-1})$, where $\mathcal{P}_H$ denotes the orthogonal projection onto the closed convex set $H_n$, see figure 2(a). The projection onto a single hyperplane can be computed by the following formula
**Lemma 3.2.** Let $u \in X \setminus \{0\}$ and $\alpha \in \mathbb{R}$. Then the projection onto $H(u, \alpha)$ can be computed via
\[ P_H(u, \alpha)x = x - \frac{\langle u, x \rangle - \alpha}{\|u\|^2}u \]
for any $x \in X$.

Instead of projecting onto a single hyperplane at each iteration, projecting onto the intersection of multiple hyperplanes may significantly increase the convergence rate, see [41], and leads to multiple search directions, see [7]. This effect is also illustrated in figure 2. However, we did not observe empirically a significant benefit in the convergence rate in our CST example. This is the reason why we consider only one search direction in the following.

### 3.1.2. RESESOP-Kaczmarz for inexact forward operator.

Let us now assume that only noisy data $g_k^\delta$ with noise levels $\delta_k \geq \|g_k - g_k^\delta\|$ and inexact forward operators $A_k^\eta$ are available, for $k \in \{0, 1, \ldots, K-1\}$. At this point, we also set some convenient notation
\[ \eta := (\eta_0, \ldots, \eta_{K-1})^T \in \mathbb{R}^K, \]
\[ \delta := (\delta_0, \ldots, \delta_{K-1})^T \in \mathbb{R}^K. \]

We further make the assumption that for some constant $\rho > 0$ the restricted solution set
\[ M'_\rho A(g) := M_A(g) \cap B_\rho(0) \]
is non-empty, that means there is a solution whose norm is smaller than $\rho$.

The main issue is that for $w \in \chi_k$ the preceding hyperplanes $H((A_k^\eta)^* w, \langle w, g_k^\delta \rangle)$ may no longer contain the restricted solution set of the respective subproblem and hence, neither $M'_\rho A(g)$. This problem is tackled by projecting onto stripes instead of hyperplanes whose thickness is chosen in accordance with the level of noise $\delta$ and the model inexactness $\eta$, see figure 3. This approach combined with the discrepancy principle is summarized in the following algorithm.

**Algorithm 3.3** (Similar to algorithm 2.7. in [7]). Choose an initial value $f_0 := f_{0,\eta,\delta}^0 \in B_\rho(0) \subset X$ and a constant $\tau > 1$. If the current iterate $f_n^{\eta,\delta}$ fulfills the discrepancy principle for the current subproblem, i.e.
\[ \|A_{\lceil n \rceil}^\eta f_{n,\eta,\delta}^\delta - g_{\lceil n \rceil}^\delta\| \leq \tau (\rho_{\lceil n \rceil} + \delta_{\lceil n \rceil}), \]
set $f_{n+1}^{\eta,\delta} := f_n^{\eta,\delta}$. Otherwise set $w_{n+1}^{\eta,\delta} := A_{\lceil n \rceil}^\eta f_{n,\eta,\delta}^\delta - g_{\lceil n \rceil}^\delta$ and compute the next iterate via
\[ f_{n+1}^{\eta,\delta} := P_{H_{\lceil n \rceil,\delta}^\eta} w_{n+1}^{\eta,\delta}, \]
Figure 3. Increasing the thickness of the hyperplane so that the resulting stripe contains the restricted solution set.

i.e. by projecting onto the stripe
\[ H^\eta,\delta_n := H\left( (\mathcal{A}^\eta_n)^* w_n, (\mathcal{A}^\eta_n)^* \right), \]
where
\[ u^\eta,\delta_n := (\mathcal{A}^\eta_n)^* w^\eta,\delta_n, \]
\[ \alpha^\eta,\delta_n := \left( w^\eta,\delta_n, \delta^\eta_n \right), \]
\[ \xi^\eta,\delta_n := (\rho^\eta_n + \delta^\eta_n) \left\| w^\eta,\delta_n \right\|. \]

Stop iterating as soon as \( f^\eta,\delta_n + k = f^\eta,\delta_n \) for all \( k \geq 1 \).

Note that for \((\eta, \delta) = (0, 0)\), the previous algorithm is just the SESOP-Kaczmarz procedure from the previous section. In this case we will omit all superindices and write for example \( f_n \) instead of \( f^\eta,\delta_n \).

As shown in [7], by the construction of the stripe \( H^\eta,\delta_n \), it contains the restricted solution set \( M^\rho_{\mathcal{A}(g)} := M^\rho_{\mathcal{A}(g)} \setminus B_{\rho}(0) \).

Furthermore, it might happen that \( \left\| u^\eta,\delta_n \right\| = 0 \) although the discrepancy principle (16) is not fulfilled. In that case the stripe \( H^\eta,\delta_n \) may be the empty set and hence the iteration step not well-defined. This leads to the following definition:

**Definition 3.4.** We call a start iterate \( f^\eta,\delta_n \) of algorithm 3.3 to be feasible if \( u^\eta,\delta_n \neq 0 \), whenever the discrepancy principle (16) is not fulfilled.

However, it is to be noted here that if \((\mathcal{A}^\eta_n)^* \) is injective, or equivalently \( \mathcal{A}^\eta_n \) is surjective, all start iterates are feasible.

Regarding the computation of the projection onto the stripe \( H(u^\eta,\delta_n, \alpha^\eta,\delta_n + \xi^\eta,\delta_n) \) we have the following result.

**Lemma 3.5.** If the iterate \( f^\eta,\delta_n \) of algorithm 3.3 does not fulfill the discrepancy principle (16), then it holds that
\[ f^\eta,\delta_{n+1} = f^\eta,\delta_n - t^\eta,\delta_n u^\eta,\delta_n \quad \text{with} \quad t^\eta,\delta_n := \frac{\left\langle u^\eta,\delta_n, f^\eta,\delta_n \right\rangle - \left( \alpha^\eta,\delta_n + \xi^\eta,\delta_n \right)}{\left\| u^\eta,\delta_n \right\|^2}. \]

**Proof.** Due to proposition 3.5 in [7] we have \( f^\eta,\delta_{n+1} \in H_{\rho}(u^\eta,\delta_n, \alpha^\eta,\delta_n + \xi^\eta,\delta_n) \). Hence, the claim follows from lemma 3.2.

**Remark 3.6.** Due to the form of \( f^\eta,\delta_{n+1} \), the \( u^\eta,\delta_n \) are also called search directions.

Next we state two theorems from [7], which will be important in the next section. The first one is about the convergence of the SESOP-Kaczmarz iteration.
Theorem 3.7 ([7, theorem 3.3]). For \((\eta, \delta) = 0\) let \(\{f_n\}_{n \in \mathbb{N}}\) be the sequence generated by algorithm 3.3 for a feasible initial value \(f_0 \in \mathcal{X}\). If the parameters \(t_n\) from lemma 3.5 are bounded, then it holds that
\[
\lim_{n \to \infty} f_n = \mathcal{P}_{M_A(\delta)}(f_0),
\]
i.e. \(\{f_n\}_{n \in \mathbb{N}}\) strongly converges to the projection of \(f_0\) onto the solution set \(M_A(\delta)\).

Before we state that the RESESOP-Kaczmarz method is indeed a regularization of the inverse problems \(A_k f = g_\delta\), it is to be noted here that whenever \((\eta, \delta) \neq 0\) algorithm 3.3 terminates after a finite number of iterations according to [7, lemma 3.7.], that is
\[
n^*_n(\eta, \delta) : = \min \left\{ n \in \mathbb{N} : \| A^\eta g_{\delta} - g_{\delta} \| \leq \tau \right\}, \forall n \]
is finite. It is called finite stopping index, but note that it is called auxiliary stopping index in [7].

Theorem 3.8 ([7, theorem 3.9]). Let \((\{(\eta, \delta)\}_{l \in \mathbb{N}})\) be a null-sequence and \((\eta, \delta)_l \neq 0\) for all \(l\). Given a feasible start iterate \(f_0 \in B_{\rho}(0)\), let \(f_n^{(\eta, \delta)_l}\) be the outcome of algorithm 3.3. Assume that the parameters \(t_n^{(\eta, \delta)_l}\) from lemma 3.5 are bounded with respect to \(n, l \in \mathbb{N}\). Then it holds that
\[
\lim_{l \to \infty} f_n^{(\eta, \delta)_l} = \mathcal{P}_{M_{A^\eta}(\delta)}(f_0).
\]

3.2. Restriction of the domain space

As mentioned in section 2 and in the introduction of this section, we aim for an approximate solution of a semi-discrete inverse problem by considering a fully-discrete version of it. Therefore, in this section we assume \(\mathcal{Y}\) to be finite dimensional and inspect what happens if we restrict the domain space \(\mathcal{X}\) to some closed subspace \(\mathcal{X}_j\). To simplify the notation, we consider only a single forward operator \(A, A^\eta : \mathcal{X} \to \mathcal{Y}\) in the following and denote the exact data by \(g \in \text{Ran}(A)\). However, note that together with ideas from [7] it might be possible to adapt the results in this section to the case of multiple forward operators. The restrictions of \(A\) and \(A^\eta\) to \(\mathcal{X}_j\) are denoted by \(A_j, A^\eta_j : \mathcal{X}_j \to \mathcal{Y}\), respectively. These are also linear and bounded operators between Hilbert spaces \(\mathcal{X}_j\) and \(\mathcal{Y}\).

In the first part of this section, we want to apply the RESESOP-Kaczmarz method to the restricted operators and settle down some notation, in order to distinguish between the restricted and non-restricted case. In particular, we apply the preceding theory from section 3.1 and immediately observe in corollary 3.10 that for fixed subspace \(\mathcal{X}_j\), RESESOP yields a regularized solution of the semi-discrete inverse problem \(A f = g^\delta\). In the second part, we further inspect the connection between the restricted and non-restricted case and prove stability with respect to the chosen subspace in theorem 3.13.

3.2.1. RESESOP-Kaczmarz applied to a restricted forward operator. Throughout this section we make the assumption that
\[
g \in \text{Ran}(A^j),
\]

(18)
which seems to be restrictive at first, but as $\mathcal{Y}$ is finite dimensional, the restricted operator $\mathcal{A}$ has even a high chance of being surjective if the dimension of $\mathcal{X}$ is sufficiently large. The assumption (18) implies that there exists some $\rho > 0$ such that

$$M^\rho_{\mathcal{A}}(g) := M_{\mathcal{A}}(g) \cap B_{\rho}(0) \neq \emptyset,$$

i.e. the (restricted) solution set is non-empty.

For start iterates $f^0_n := f^0_n(\delta_j) \in \mathcal{X}_j$, we apply the RESESOP algorithm 3.3 to the operator $\mathcal{A}^{\eta,j}$ and extend the notation in algorithm 3.3 by an additional superindex $j$, that is, we denote the iterates by $f^{\eta,j}_n$ and further set

$$w^{\eta,j}_n = A^j f^{\eta,j}_n - g^\delta,$$
$$u^{\eta,j}_n = (A^j)^* w^{\eta,j}_n,$$
$$\alpha^{\eta,j}_n = \langle w^{\eta,j}_n, g^\delta \rangle,$$
$$\xi^{\eta,j}_n = \|w^{\eta,j}_n\| \|\eta\rho + \delta\|.$$

Also, we replace $\rho$ by $\rho_j$ so that the stripes $H^{\rho,j}_n$ will contain the restricted solution set $M^\rho_{\mathcal{A}}(g)$. Again, if $\eta = 0$, we omit them in the superindex, for example, we then write $f^{j}_n$ instead of $f^{\eta,j}_n$. The theory presented in section 3.1 is also applicable to the restricted operators $\mathcal{A}$ and $\mathcal{A}^{\eta,j}$, which also means that for $(\eta, \delta) \neq 0$ there is a finite stopping index

$$n_*(\eta, \delta, j) := \min \left\{ n : \|A^j f^{\eta,j}_n - g^\delta\| \leq \tau(\rho_j \eta + \delta) \right\} \in \mathbb{N}.$$

(19)

and for $n \geq n_*(\eta, \delta, j)$ it holds that $f^{\eta,j}_n = f^{j}_n$. Moreover, from theorems 3.7 and 3.8 we immediately obtain the following result:

**Corollary 3.9 ([7], theorem 3.3).** For $(\eta, \delta) = 0$ let $(f^0_n)_{n \in \mathbb{N}}$ be the sequence generated by algorithm 3.3 for a feasible initial value $f^0_0 \in \mathcal{X}$. If the parameters $t_n$ from lemma 3.5 are bounded, then it holds that

$$\lim_{n \to \infty} f^0_n = P_{M_{\mathcal{A}}(g)}(f^0_0) \in M_{\mathcal{A}}(g),$$

i.e. $(f^0_n)_{n \in \mathbb{N}}$ strongly converges to the projection of $f^0_0$ onto the solution set $M_{\mathcal{A}}(g)$.

This means that in case of $(\eta, \delta) = 0$, the application of the SESOP algorithm to the restricted operator $\mathcal{A}$ indeed converges to a solution of $\mathcal{A}f = g$. Further, in case of model uncertainty or noisy data, applying RESESOP to $\mathcal{A}^{\eta,j}$ regularizes the inverse problem regarding $\mathcal{A}$ in the following way.

**Corollary 3.10 ([7], theorem 3.9).** Let $((\eta, \delta)_l)_{l \in \mathbb{N}}$ be a null sequence and $(\eta, \delta)_l \neq 0$ for all $l$. Further, for some feasible start iterate $f^0_0 \in B_{\rho}(0)$ let $f^{\eta,j}_n$ be the outcome of algorithm 3.3. Assume that the parameters $(t^0_n)_{n \in \mathbb{N}}$ from lemma 3.5 are bounded with respect to $n, l \in \mathbb{N}$. Then it holds that

$$\lim_{n \to \infty} f^{\eta,j}_n = P_{M_{\mathcal{A}}(g)}(f^0_0) \in M_{\mathcal{A}}(g).$$

However, at this point it is not clear, whether the RESESOP reconstruction is stable with respect to the chosen subspace $\mathcal{X}_j$. This is analyzed in the next subsection.

We recall now a descent property for the RESESOP iterates as from [7], which will be helpful for the analysis in the next subsection.

**Proposition 3.11 ([7], proposition 3.5).** If $\|A^j f^{\eta,j}_n - g^\delta\| > \tau(\rho_j \eta + \delta)$, then it holds that

(a) $f^{\eta,j}_n$ is contained in the half-space $H^{\rho,j}_n(u^{\eta,j}_n, \alpha^{\eta,j}_n + \xi^{\eta,j}_n).$
(b) For all \( z \in H(u_n^{\eta,\delta_j}, \alpha_n^{\eta,\delta_j}, \xi_n^{\eta,\delta_j}) \) it holds that
\[
\| z - f_{n+1}^{\eta,\delta_j} \| \leq \| z - f_n^{\eta,\delta_j} \| - \left( \frac{\| w_n^{\eta,\delta_j} \| (\| w_n^{\eta,\delta_j} \| - (\rho \eta + \delta))}{\| u_n^{\eta,\delta_j} \|} \right)^2.
\]

In particular, (b) holds for all elements \( z \) of the restricted solution set \( M_A^0(g) \).

The following lemma addresses the computation of the adjoint of the restricted forward operator.

**Lemma 3.12.** For all \( y \in \mathcal{Y} \) it holds that \((A^j)^* y = P_{X_j} A^* y\) and similarly for \((A^{\eta,\delta})^*\).

**Proof.** Let \( y \in \mathcal{Y} \). For all \( v \in X_j \) it holds that
\[
\langle (A^j)^* y - A^* y, v \rangle = \langle y, A^j v - Av \rangle = \langle y, Av - Av \rangle = 0.
\]
Therefore, \((A^j)^* y - A^* y\) is orthogonal to \( X_j \). As \((A^j)^* y \in X_j\), we conclude
\[
0 = P_{X_j}((A^j)^* y - A^* y) = P_{X_j}(A^* y) - (A^j)^* y.
\]

\[\Box\]

### 3.2.2. Stability with respect to the chosen subspace.

In this section we consider a nested sequence of closed subspaces \( X_j \) of \( X \), i.e.
\[
X_j \subset X_{j+1} \quad \text{for all } j \in \mathbb{N}.
\]  
(20)

Further, we assume that
\[
N(A)^\perp \subseteq \bigcup_j X_j
\]  
(21)

and make the stronger assumption, compared to section 3.2.1 that there exists some \( J \in \mathbb{N} \) such that the restriction \( A^J \) of \( A \) to \( X_J \) is surjective. Due to the nestedness (20), it follows that \((A^j)\) is surjective for \( j \geq J \). Therefore, without loss of generality we assume all \( A^j \) to be surjective. Furthermore, it is to be noted here that for closed subspaces \( V \subseteq X \) the expression \( V^\perp \) stands for the orthogonal complement in \( X \). The orthogonal complement in \( X_j \) is denoted by \( V_j^\perp \).

The main goal of this section is to prove the following result:

**Theorem 3.13.** Let \( f_0^j := f_0^{\eta,\delta_j} \in N(A^j)^\perp \cap B_{\rho_j}(0), j \in \mathbb{N}, \) be start iterates for the RESESOP method applied to \( A^{\eta,\delta} \) and assume that \( f_0^j \) converges to some start iterate \( f_0 \in N(A)^\perp \cap B_{\rho}(0) \) for the SESOP method applied to \( A \). Given some sequence \((\eta_j, \delta_j)_{j \in \mathbb{N}}\) converging to \((0,0,\infty) \) we assume that the parameters \( l_n^j(\eta, \delta) \) and \( t_n \) from lemma 3.5 are bounded with respect to \( n, l \in \mathbb{N} \). Then it holds that
\[
\lim_{l \to \infty} f_{n(l)}^{\eta_j(\eta, \delta_j)_l} = P_{M_A(g)} f_0,
\]
where \( n_s(l) := n_s((\eta_j, \delta_j)_l) \) is the finite stopping index from (19).

**Remark 3.14.** We say that a sequence \((\eta_j, \delta_j)_l\) is convergent to \((0,0,\infty) \), if for all \( \varepsilon > 0 \) and \( N > 0 \) there exists some \( L \in \mathbb{N} \) such that for all \( l \geq L \)
\[
|\eta_j| < \varepsilon, |\delta_j| < \varepsilon \quad \text{and} \quad f_{l(L)} > N.
\]
Moreover, we want to emphasize again that the assumption of $\mathcal{A}^!$ being surjective implies that all start iterates $f_0^j := f_{0,\mathcal{A}^!}^j \in X_j$ and $f_0 \in \mathcal{X}$, respectively, are feasible. Therefore, we omitted these conditions in theorem 3.13.

In order to prove this theorem, some preparations are required. First, we inspect the projections onto solution sets.

**Lemma 3.15.** Let $f_0 \in N(\mathcal{A})^\perp$. Then it holds that
\[
\mathcal{P}_{M_\mathcal{A}(g)}f_0 = \mathcal{A}^+ g,
\]
where $\mathcal{A}^+$ denotes the generalized inverse of $\mathcal{A}$, see for example \cite[definition 2.1.5.]{36}. By analogy, it holds that
\[
\mathcal{P}_{M_\mathcal{A}(g)}f_0^j = (\mathcal{A}^!)^+ g,
\]
for any $f_0^j \in N(\mathcal{A})^\perp$.

**Proof.** Let $f \in M_\mathcal{A}(g)$. As the solution set is an affine set, namely $M_\mathcal{A}(g) = f + N(\mathcal{A})$, the corresponding orthogonal projection can be computed via
\[
\mathcal{P}_{M_\mathcal{A}(g)} f_0 = f + \mathcal{P}_{N(\mathcal{A})} (f_0 - f).
\]
Due to $f_0 \in N(\mathcal{A})^\perp$ we conclude
\[
\|\mathcal{P}_{M_\mathcal{A}(g)} f_0\| = \|f - \mathcal{P}_{N(\mathcal{A})} f\| = \|\mathcal{P}_{N(\mathcal{A})} f\| \leq \|f\|.
\]
This means that $\mathcal{P}_{M_\mathcal{A}(g)} f_0$ is the minimum-norm solution of $\mathcal{A} f = g$. \hfill $\Box$

At this point it is to be noted here that, as $\mathcal{A}$ and $\mathcal{A}^!$ both map into a finite dimensional space $\mathcal{Y}$, their generalized inverses are bounded operators defined on the whole space $\mathcal{Y}$, see \cite[satz 2.1.8]{36}. The next step is to show that $(\mathcal{A}^!)^+ g$ converges to $\mathcal{A}^+ g$. For that purpose we need some results on orthogonal projections:

**Lemma 3.16.** Let $(V_j)_{j \in \mathbb{N}}$ be a sequence of nested subspaces of $\mathcal{X}$. For all $f \in \mathcal{X}$ it holds that
\[
\lim_{j \to \infty} \mathcal{P}_{V_j} f = \mathcal{P}_{\bigcup_{j \in \mathbb{N}} V_j} f,
\]
where $V := \bigcup_{j \in \mathbb{N}} V_j$.

In particular, for all $f \in \mathcal{X}$ it holds that
\[
\lim_{j \to \infty} \mathcal{P}_{M_\mathcal{A}(g)} f = \mathcal{P}_{\bigcup_{j \in \mathbb{N}} M_\mathcal{A}(g)} f \quad \text{as well as} \quad \lim_{j \to \infty} \mathcal{P}_{N(\mathcal{A})} f = \mathcal{P}_{\bigcup_{j \in \mathbb{N}} N(\mathcal{A})} f.
\]

**Proof.** Let $f \in V$ and $\varepsilon > 0$. By definition of $V$, there exists some $N \in \mathbb{N}$ and $f_N \in V_N$ such that $\|f - f_N\| < \varepsilon$. Due to the nestedness of the $V_j$ we conclude that $f_N$ belongs to all $V_j$ for $n \geq N$. Thus,
\[
\|\mathcal{P}_V f - \mathcal{P}_{V_j} f\| \leq \|f - f_N\| + \|\mathcal{P}_V f_N - \mathcal{P}_{V_j} f_N\| \\
\leq (1 + \|\mathcal{P}_{V_j}\|) \varepsilon \leq 2\varepsilon.
\]
Therefore $\mathcal{P}_V f$ converges to $\mathcal{P}_V f$. Due to the nestedness, the general case $f \in \mathcal{X}$ follows analogously by rewriting $f = f_V + f_{V^\perp}$ for $f_V \in V$ and $f_{V^\perp} \in V^\perp$. \hfill $\Box$

**Corollary 3.17.** Let $(x_n)_{n \in \mathbb{N}}$ be a sequence in $\mathcal{X}$ converging to some $x \in \mathcal{X}$. It holds that
\[
\lim_{j \to \infty} \mathcal{P}_{M_\mathcal{A}(g)} x_j = \mathcal{P}_V x, \quad \text{where} \quad V := \bigcup_{f} M_\mathcal{A}(g).
\]
As we set enables us to derive another important result, which is a special case of (3.16). It holds that for all \( f \in \mathcal{A} \),
\[
M_{\mathcal{A}}(g) = x' + N(\mathcal{A}).
\]

Hence, we conclude by lemma 3.16 that
\[
\lim_{j \to \infty} \mathcal{P}_{M_{\mathcal{A}}}(x) = x' + \lim_{j \to \infty} \mathcal{P}_{N(\mathcal{A})}(x' - x) = x' + \mathcal{P}_{\bigcup N(\mathcal{A})}(x' - x) = \mathcal{P}_{x'} + \mathcal{P}_{\bigcup N(\mathcal{A})}x = \mathcal{P}_{x'}.\]

Therefore, for \( \varepsilon > 0 \) there exists a \( J \in \mathbb{N} \) such that
\[
\|\mathcal{P}_{M_{\mathcal{A}}}(x) - \mathcal{P}_{x'}\| \leq \frac{\varepsilon}{2} \quad \forall j \geq J.
\]
As \( (x_k) \) converges to \( x \) there is some \( J' \geq J \) such that \( \|x_j - x\| \leq \frac{\varepsilon}{2} \) for all \( j \geq J' \). Altogether, for \( j \geq J' \) it follows
\[
\|\mathcal{P}_{x'} - \mathcal{P}_{M_{\mathcal{A}}}(x)\| = \|\mathcal{P}_{x'} - \mathcal{P}_{M_{\mathcal{A}}}(x)_j\| \\
\leq \|\mathcal{P}_{x'} - \mathcal{P}_{M_{\mathcal{A}}}(x)\| + \|\mathcal{P}_{M_{\mathcal{A}}}(x) - \mathcal{P}_{M_{\mathcal{A}}}(x)_j\| \\
\leq \varepsilon/2 + \|\mathcal{P}_{M_{\mathcal{A}}}(x)\| \cdot \|x - x_j\| \leq \varepsilon
\]
which ends the proof. \( \square \)

Lemma 3.16 enables us to derive another important result, which is a special case of [36, lemma 6.1.5].

**Lemma 3.18.** For all \( f \in N(\mathcal{A})^\perp \) it holds that \( \mathcal{P}_{N(\mathcal{A})}f \xrightarrow{j \to \infty} 0 \).

**Proof.** Let \( \varepsilon > 0 \) and set \( V := \bigcup_{i=1}^n X_i \). As \( \mathcal{A}^* \) maps \( \text{Ran}(\mathcal{A}) \) into a dense subset of \( N(\mathcal{A})^\perp \), there exists an element \( y \in \text{Ran}(\mathcal{A}) \) such that \( \|x - \mathcal{A}^*y\| < \varepsilon/2 \). It follows from lemma 3.16 that
\[
\mathcal{P}_{X} \mathcal{A}^* y \xrightarrow{j \to \infty} \mathcal{P}_{V} \mathcal{A}^* y = \mathcal{A}^* y,
\]
as \( \mathcal{A}^* y \in N(\mathcal{A})^\perp \subseteq V \) by assumption (21). Therefore, there exists \( J \in \mathbb{N} \) such that \( \|\mathcal{P}_{X} \mathcal{A}^* y - \mathcal{A}^* y\| \leq \varepsilon/2 \) for all \( j \geq J \). Using lemma 3.12, the desired result follows since for all \( j \geq J \) we have
\[
\|\mathcal{P}_{N(\mathcal{A})}y\| \leq \|\mathcal{P}_{N(\mathcal{A})}(f - \mathcal{A}^* y)\| + \|\mathcal{P}_{N(\mathcal{A})}(\mathcal{A}^*) y\| + \|\mathcal{P}_{N(\mathcal{A})}(\mathcal{A}^* - (\mathcal{A}^*)) y\| \\
\leq \varepsilon/2 + \|\mathcal{A}^* y - (\mathcal{A}^*) y\| = \varepsilon/2 + \|\mathcal{A}^* y - \mathcal{A}^* y\| \leq \varepsilon.
\]
\( \square \)

Now we are able to prove the convergence of the sequence of the generalized solutions \( (\mathcal{A}^*)^+ \). Regarding the proof, we follow the ideas in [36, section 6.1.2].

**Theorem 3.19.** It holds that \( (\mathcal{A}^*)^+ \) converges to \( \mathcal{A}^+ \).

**Proof.** We set \( f^+ := \mathcal{A}^+ g \) and \( f_j^+ := (\mathcal{A}^j)^+ g \). We recall the notation \( N(\mathcal{A})^\perp \) for the orthogonal complement of \( N(\mathcal{A}) \) in \( \mathcal{X} \). We start with the consideration
\[
f^+ - f_j^+ = f^+ - (\mathcal{A}^j)^+ g \\
= (I - (\mathcal{A}^j)^+ A)f^+ \\
= (I - (\mathcal{A}^*)^+ A)(f^+ - \mathcal{P}_{X} f^+) - (I - (\mathcal{A}^*)^+ A)\mathcal{P}_{X} f^+,
\]
which allows us to define a new sequence \( (f_j^+) \).
where $I$ denotes the identity on $\mathcal{X}$. Regarding the second term we apply \cite[theorem 2.1.9]{36} to derive
\[
(I - (A^\dagger)^+ A)P_{X_j} f^+ = P_{X_j} f^+ - (A^\dagger)^+ A P_{X_j} f^+ \\
= P_{X_j} f^+ - (A^\dagger)^+ A P_{X_j} f^+ \\
= P_{X_j} f^+ - P_{N(A^\dagger)^+} f^+ \\
= P_{X_j} f^+ - P_{N(A^\dagger)^+} f^+ = P_{N(A^\dagger)^+} f^+,
\]
which converges to 0, according to lemma 3.16, as $f^+ \in N(A)^\perp$.

It remains to show that also the first term above converges to zero. We start by mentioning that the generalized solutions of $A^\dagger$ and $A$ are bounded operators. By the surjectivity of the $A^\dagger$ we conclude for arbitrary $y \in \mathcal{Y}$ that $(A^\dagger)^+ y$ solves the inverse problem $Af = y$. It is due to the nestedness (20) of the $\mathcal{X}_i$ that it solves also $A^\dagger f = y$. Thus, by definition of the generalized inverse we obtain
\[
\|(A^\dagger)^+ y\| \leq \|(A^\dagger) y\| \text{ for all } j \in \mathbb{N}.
\]
As a consequence, there is a $C > 0$ such that
\[
\|(A^\dagger)^+\| \leq C \text{ for all } j \in \mathbb{N}. \tag{22}
\]
Therefore, we are able to estimate
\[
\|(I - (A^\dagger)^+ A)(f^+ - P_{X_j} f^+)\| \leq (1 + C)\|f^+ - P_{X_j} f^+\|.
\]
As $f^+ \in N(A)^\perp \subseteq \bigcup_j \mathcal{X}_j$, the right-hand-side of the inequality converges to 0, according to lemma 3.16. Finally, we have shown that $(f^+_j)_j$ indeed converges to $f^+$. 

\begin{remark}
If we had not assumed the surjectivity of $A^\dagger$, then the estimate $\|(A^\dagger)^+ y\| \leq \|(A^\dagger) y\|$ in the proof of the previous theorem might not hold in general.
\end{remark}

\begin{corollary}
For any $f \in N(A)^\perp$ it holds that
\[
P_v f = P_{M_{\mathcal{A}^\perp}(g)} f, \quad \text{where} \quad V := \bigcup_{j \in \mathbb{N}} M_{\mathcal{A}^\perp}(g).
\]
\end{corollary}

\begin{proof}
According to lemma 3.15 we have that $P_{M_{\mathcal{A}^\perp}(g)} f = A^\dagger g$. Since $N(A)^\perp \subseteq N(A)^\perp$, it follows that $P_{M_{\mathcal{A}^\perp}(g)} f = (A^\dagger)^+ g$. Therefore, applying corollary 3.17 and lemma 3.15 and theorem 3.19 yields
\[
P_v f = \lim_{j \to \infty} P_{M_{\mathcal{A}^\perp}(g)} f = \lim_{j \to \infty} (A^\dagger)^+ g = A^\dagger g = P_{M_{\mathcal{A}^\perp}(g)} f.
\]
\end{proof}

We recall our assumption that $Af = g$ has a solution in $B_{\rho}(0)$ and $Af = g$ has a solution in $B_{\rho}(0) \cap \mathcal{X}_j$. Note that due to the nestedness of the $\mathcal{X}_j$ we may assume that $\rho_{j+1} \leq \rho_j$ for all $j$.

In all what follows, we consider for the application of RESESOP to $A^{\theta_j}$ and for the application of SESOP to $A$ a uniform
\[
\rho' := \max_j \{\rho_j, \rho_j\} = \max_j \{\rho, \rho_j\}. \tag{23}
\]
This guarantees that the restricted solution sets $M_{\mathcal{A}^\perp}(g) \cap B_{\rho'}(0)$ are non-empty for all $j$ and are contained in the respective stripes $H_{\mathcal{A}^\perp}^{\rho, \delta_j}$ from algorithm 3.3.
In order to prove theorem 3.13, we follow the same strategy as in [7] for proving theorem 3.8 for the case $\mathcal{X} = \mathcal{X}_j$. For that, we first show that the iterates $f_n^{\eta,\delta,j}$ from the application of RESESOP to $A^{\eta,j}$ converges to $f_\eta$, the iterates from the application of SESOP to $A$. To simplify the notation, we denote by $x^{\eta,\delta,j} \to x$ the following

$$\lim_{(\eta,\delta,j) \to (0, 0, \infty)} x^{\eta,\delta,j} = x$$

and state a useful result.

**Lemma 3.22.** Let $n \in \mathbb{N}$ and consider a sequence $(\eta, \delta, j)$ converging to $(0, 0, \infty)$. If $f_n^{\eta,\delta,j}$ converges to $f_\eta$, then

$$w_n^{\eta,\delta,j} \to w_\eta, \quad u_n^{\eta,\delta,j} \to u_\eta, \quad \alpha_n^{\eta,\delta,j} \to \alpha_\eta, \quad \xi_n^{\eta,\delta,j} \to \xi_\eta.$$  

**Proof.** First, note that for $x \in \mathcal{X}_j$ it holds that $A^j x = Ax$ and $A^\eta x = A^\eta x$. Consider

$$\|w_n^{\eta,\delta,j} - w_\eta\| = \|A^{\eta,j} f_n^{\eta,\delta,j} - g - (A f_\eta - g)\|
\leq \delta + \|A^{\eta,j} f_n^{\eta,\delta,j} - A f_\eta\|
\leq \delta + \|A^{\eta,j} f_n^{\eta,\delta,j} - A f_\eta\| + \|A f_\eta - A f_\eta\|
\leq \delta + \|A\| \cdot \|f_n^{\eta,\delta,j} - f_\eta\| + \eta \|f_\eta\|.$$  

Note that $\|A\|$ is bounded, as $A^\eta$ converges to $A$. Moreover, $f_n^{\eta,\delta,j}$ converges to $f_\eta$ by assumption, so that we conclude from the estimation above that $w_n^{\eta,\delta,j} \to w_\eta$ if $(\eta, \delta, j)$ converges to $(0, 0, \infty)$.

Using lemma 3.12, we obtain

$$\|u_n^{\eta,\delta,j} - u_\eta\| = \|(A^{\eta,j})^* w_n^{\eta,\delta,j} - A^* w_\eta\|
\leq \|\mathcal{P}_{\mathcal{X}_j} (A^\eta) w_n^{\eta,\delta,j} - \mathcal{P}_{\mathcal{X}_j} (A^\eta)^* w_\eta\| + \|\mathcal{P}_{\mathcal{X}_j} (A^\eta)^* w_n^{\eta,\delta,j} - A^* w_\eta\|
\leq \|A^\eta\|^\star \cdot \|w_n^{\eta,\delta,j} - w_\eta\| + \|\mathcal{P}_{\mathcal{X}_j} (A^\eta)^* w_n^{\eta,\delta,j} - A^* w_\eta\|.$$  

Therefore, it follows that

$$\|\mathcal{P}_{\mathcal{X}_j} (A^\eta)^* w_n - A^* w_\eta\| \leq \|\mathcal{P}_{\mathcal{X}_j} (A^\eta)^* w_n - \mathcal{P}_{\mathcal{X}_j} A^* w_\eta\| + \|\mathcal{P}_{\mathcal{X}_j} A^* w_n - A^* w_\eta\|
\leq \|A^\eta\|^\star \cdot \|w_n^{\eta,\delta,j} - w_\eta\| + \|\mathcal{P}_{\mathcal{X}_j} A^* w_n - A^* w_\eta\|.$$  

Since $A^* w_\eta \in N(A)^\perp \subseteq \bigcup_{j=1}^J \mathcal{X}_j$, the second term on the right-hand side converges to 0 by lemma 3.16. Therefore, it follows by the estimations above and the convergence of the $w_n^{\eta,\delta,j}$ that $u_n^{\eta,\delta,j}$ converges to $u_\eta$. It is now straightforward to see that also $\alpha_n^{\eta,\delta,j}, \xi_n^{\eta,\delta,j}$ converge to $\alpha_\eta, \xi_\eta$, respectively.

With this result we are able to prove the following.

**Corollary 3.23 ([7, lemma 3.8]).** Assume that the RESESOP start iterates $f_0^{\eta,\delta,j} \in B^{\eta,j}(0) \cap \mathcal{X}_j$ converge to the SESOP start iterate $f_0 \in N(A)^\perp \cap B^{\eta,j}(0)$. Then it holds that

$$f_n^{\eta,\delta,j} \to f_\eta \quad \forall \ n \in \mathbb{N}.$$  

**Proof.** We prove this statement by induction. The base case for $n = 0$ is fulfilled just by assumption. Assume that $f_n^{\eta,\delta,j}$ converges to $f_\eta$. From algorithm 3.3 and proposition 3.11, we observe that
First, consider sequences in

\[ I_1 := \{ (\eta, \delta) : \|w_n^{\eta, \delta}\| \leq \tau(\rho' \eta + \delta) \} \]

This means, that for those \((\eta, \delta, j)\) the discrepancy principle (16) is fulfilled at iteration index \(n\), which means \(f_n^{\eta, \delta} = f_n^{\eta, \delta} \). In this case, we conclude by the induction hypothesis and the previous lemma 3.22

\[ \|w_n\| = \lim \|w_n^{\eta, \delta}\| = 0, \]

which implies \(A_n - g = w_n = 0\) and hence \(f_{n+1} = f_n = \lim f_n^{\eta, \delta} = \lim f_{n+1}^{\eta, \delta} \).

Second, consider sequences in

\[ I_2 := \{ (\eta, \delta) : \|w_n^{\eta, \delta}\| > \tau(\rho' \eta + \delta) \} \]

If \(w_n \neq 0\), it follows by the feasibility of \(f_0\) that \(w_n = 0\). Therefore, we conclude by the induction hypothesis, lemma 3.22 and proposition 3.11 (a) that

\[ f_n^{\eta, \delta} = f_n^{\eta, \delta} \]

\[ = f_n^{\eta, \delta} - \frac{(w^{\eta, \delta} - f_n^{\eta, \delta}) - (\alpha_n \eta \delta + \xi_n \eta \delta)}{\|u_n^{\eta, \delta}\|^2} u_n^{\eta, \delta} \]

\[ \to f_n - \frac{(\alpha_n + \xi_n)}{\|u_n\|^2} u_n = f_{n+1}. \]

Let now \(w_n = 0\), which means that \(f_n\) is the outcome of the SESOP algorithm. Due to theorem 3.7, we conclude \(f_{n+1} = f_n = \mathcal{P}_{M_A(\varepsilon)} f_0\). Let \(\varepsilon > 0\). We insert \(z := \mathcal{P}_{M_A(\varepsilon)} f_0\) into proposition 3.11 (b) and obtain

\[ \left\| \frac{(w^{\eta, \delta} - f_n^{\eta, \delta}) - (\alpha_n \eta \delta + \xi_n \eta \delta)}{\|u_n^{\eta, \delta}\|^2} u_n^{\eta, \delta} \right\| \leq \left( \frac{\|w_n^{\eta, \delta}\|}{\|u_n^{\eta, \delta}\|} \right)^2 \leq \|\mathcal{P}_{M_A(\varepsilon)} f_0 - f_n^{\eta, \delta}\| \leq \|\mathcal{P}_{M_A(\varepsilon)} f_0 - \mathcal{P}_{M_A(\varepsilon)} f_0\| + \|\mathcal{P}_{M_A(\varepsilon)} f_0 - f_n^{\eta, \delta}\|. \]

The first term on the right-hand side converges to zero according to corollaries 3.21 and 3.17, whereas the second term converges to zero by the induction hypothesis. Finally, this means that

\[ f_n^{\eta, \delta} = f_n^{\eta, \delta} \]

\[ = f_n^{\eta, \delta} \]

\[ \to f_n = f_{n+1}. \]

Altogether we conclude that \(f_n^{\eta, \delta}\) converges to \(f_{n+1}\).

\[ \square \]

Now we are able to prove the main result of this section.

**Proof of theorem 3.13.** First, each subsequence of \(n_s(\ell)\) has a bounded or a monotonically increasing, unbounded subsequence. Therefore, it suffices to consider these two cases—namely \(n_s(\ell)\) to be bounded or unbounded but monotonically increasing—and show that in both cases \(f_{n_s(\ell)}^{\eta, \delta}\) converges to the same element \(\mathcal{P}_{M_A(\varepsilon)} f_0\).
(a) Assume \( n_\star(l) \) to be bounded and set
\[
N := \max_l n_\star(l) \in \mathbb{N}.
\]
We observe by the definition of the finite stopping index that
\[
f(\eta, \delta, j)_n = f(\eta, \delta, j)_N, \quad \text{for all } n \geq N.
\]
As a consequence, for those \( n \geq N \) the discrepancy principle is satisfied which yields
\[
kA(\eta)_n \leq kA(\eta)_N \leq (\rho' \eta_l + \delta_l)^{l \to \infty} ! 0.
\]
On the other hand, we have
\[
kA(\eta)_n \leq n kA(\eta)_n = 0,
\]
according to corollary 3.23 and lemma 3.22. This implies \( w_n = 0 \), which means that \( f_n \) is the output of the SESOP algorithm. By theorem 3.7 we conclude
\[
f_n = P_{M_A} f_0 \quad \text{for all } n \geq N,
\]
which together with corollary 3.23 leads to
\[
f_n(\eta, \delta, j)_N \to P_{M_A} f_0.
\]

(b) Now assume that \( n_\star(l) \) is monotonically increasing and unbounded.
On the one hand, the SESOP iterates \( (f_n)_n \) converge to \( P_{M_A} f_0 \). On the other hand, by corollaries 3.21 and 3.17 we have that
\[
P_{M_A} f_0 \to P_{M_A} f_0.
\]
Therefore, let \( \varepsilon > 0 \) and choose an \( N \in \mathbb{N} \) such that
\[
\|f_n - P_{M_A} f_0\| < \frac{\varepsilon}{4}, \quad (24)
\]
\[
\|P_{M_A} f_0 - P_{M_A} f_0\| < \frac{\varepsilon}{4}, \quad (25)
\]
for all \( n, j \geq N \). According to corollary 3.23 there exists some \( l' \in \mathbb{N} \) with \( l' \geq N \) such that
\[
\|f_n(\eta, \delta, j) - f_n\| < \frac{\varepsilon}{4}, \quad (26)
\]
for all \( l \geq l' \). As \( n_\star(l) \) is unbounded and monotonically increasing we can choose \( l'' \geq l' \) such that \( n_\star(l) \geq N \) for all \( l \geq l'' \). For those \( l \) we derive
\[ \|f^{(\eta, \delta, j)}_{n,l(t)} - P_{A(f)}f_0\| \leq \|f^{(\eta, \delta, j)}_{n,l(t)} - P_{M^\rho_{A^\mu}(g)}f^N_0\| + \|P_{M^\rho_{A^\mu}(g)}f^N_0 - P_{A(f)}f_0\| \]
\[ \leq \frac{\varepsilon}{4} + \|f^{(\eta, \delta, j)}_{n,l(t)} - P_{M^\rho_{A^\mu}(g)}f^N_0\| \]
where the last step follows from proposition \ref{prop:continuity} (b), which is applicable as \(P_{M^\rho_{A^\mu}(g)}f^\mu_0\) belongs to the restricted solution set \(M^\rho_{A^\mu}(g)\), which is a subset of \(M^\rho_{A^\mu}(g)\). We further estimate
\[ \|f^{(\eta, \delta, j)}_{n,l(t)} - P_{M^\rho_{A^\mu}(g)}f^N_0\| \leq \|f^{(\eta, \delta, j)}_{n,l(t)} - f^N_0\| + \|f^N_0 - P_{M^\rho_{A^\mu}(g)}f^N_0\| \]
\[ \leq \frac{\varepsilon}{4} + \|f^N_0 - P_{M^\rho_{A^\mu}(g)}f^N_0\| \]
\[ \leq \frac{3}{4} \varepsilon, \]
due to (24) and (25). Altogether, we have shown that for all \(l \geq l'\)
\[ \|f^{(\eta, \delta, j)}_{n,l(t)} - P_{M^\rho_{A^\mu}(g)}f_0\| < \varepsilon. \]
Finally, we have shown convergence of \(f^{(\eta, \delta, j)}_{n,l(t)}\) to \(P_{M^\rho_{A^\mu}(g)}f_0\) in both cases and hence, by our introductory discussion, in all cases.

We have shown in the last theorem that the RESESOP iterates for \(A^{\eta, \delta}\) converge to the SESOP outcome for \(A\), namely \(P_{M^\rho_{A^\mu}(g)}f_0\). By the choice of \(f_0 \in N(A)^\perp \cap B^\rho_0\) we have seen in lemma \ref{lemma:continuity} that \(P_{M^\rho_{A^\mu}(g)}f_0\) must be the minimum-norm solution of \(Af = g\). As we assumed that \(f\) has a solution in \(B^\rho_0\) we conclude that \(P_{M^\rho_{A^\mu}(g)}f_0\) must also be in \(B^\rho_0\) and not only in \(B^\rho_0\) for \(\rho' = \max\{\rho, k\}\).

### 3.3. Application to CST

In this section we specify how the previous framework can be applied to the semi-discrete and fully discrete operators of CST. We assume that the chosen subspace \(X_\nu\) of \(H^1_0(\Omega)\) ensures surjectivity of the fully discrete operator \((A^{\mu^*}_1)_j : X_\nu \rightarrow \mathbb{R}^{p \times K}\) from section 2.3. We then set
\[ A' := (A^{\mu^*}_1)_j \quad \text{and} \quad A^{\eta, \delta} := (A^{\mu^*}_1)_j, \]
as well as
\[ A := A^{\mu}_1 \quad \text{and} \quad A^{\eta, \delta} := A^{\mu^*}_1, \]
for a chosen prior \(\mu^*\) to the ground truth \(\mu\). If we equip the domain spaces with the Sobolev norm, all operators above are continuous so that the theory in both sections 3.2.1 and 3.2.2 is applicable. That means that applying RESESOP to \((A^{\mu^*}_1)_j\) does not only regularize \(A^{\mu}_1 f = g\), see corollary 3.10, but is also stable with respect to the chosen subspace in the sense of theorem 3.13. However, as mentioned before, we do not have access to the adjoint operators regarding
the Sobolev norm, so that for our numerical experiments we need to equip $X_j$ with the $L_2$-norm. In this case, it still holds that RESESOP applied to $(\mathcal{L}_1^{\mu^*})_j$ converges to a solution of $\mathcal{L}_1^{\mu} f = g$ as soon as the model uncertainty $\eta$ and the noise-level $\delta$ go to zero. However, this reconstruction may not be stable with respect to the chosen $X_j$, as the semi-discrete forward operator $\mathcal{L}_1^{\mu}$ is no longer continuous.

Since the model uncertainty highly depends on the respective source, detector positions and energies of incoming photons, we split the operators up by $A_{\eta,j}$:

$$A_{\eta,j} \colon ((\mathcal{L}_1^{\mu^*})_j f)_{p,k} \in \mathbb{R}, \text{ for } p \in \{1, \ldots, P\} \text{ and } k \in \{1, \ldots, K\}$$

and analogously for the other operators. Therefore, in our simulations in section 5, we apply the RESESOP-Kaczmaz algorithm 3.3 to $A_{\eta,j}$.

4. A DIP approach for CST

Solving the inverse problem in CST using standard learning techniques would require large databases obtained from energy-resolved detectors with sufficient energy resolution and $\gamma$-ray sources. Unfortunately, such datasets do not exist preventing the training of a neural network for the CST problem. Alternatively, it is possible to use unsupervised techniques such as DIP, see [28]. Therefore, in this section we inspect how the DIP approach can be applied and adapted to the model inexactness in CST.

In this section, we use the same notation as in section 3.3. For the sake of readability, we denote the fully discrete inexact forward operator $(\mathcal{L}_1^{\mu^*})_j f$ by $A_{\eta,j}$ and the exact operator $(\mathcal{L}_1^{\mu})_j f$ by $A_j$.

In order to apply a DIP approach to these operators, we consider a suitable (neural network) mapping $\varphi_{\theta} : Z \to X_j$, where $\theta$ belongs to some parameter space $\Theta$. Given a single data point $\mathbf{g}^\delta \in \mathbb{R}^{P \times K}$ and some random input $z \in Z$, the DIP approach seeks for finding parameters $\theta_{\text{opt}} \in \Theta$ that minimizes some loss function $\ell$, i.e.

$$\theta_{\text{opt}} \in \arg\min_{\theta \in \Theta} \ell \left( (A_{\eta,j} \varphi_{\theta}(z), \mathbf{g}^\delta_{p,k})_{p,k} \right).$$

The DIP reconstruction is then obtained by evaluating $\varphi_{\theta_{\text{opt}}}(z)$.

Usually, the construction and efficiency of such an approach requires:

(a) a suitable network architecture must be chosen, which should capture information about the ‘nature’ of images we are looking for, see also [12];

(b) a stopping criterion in order to avoid noise over-fitting, and

(c) a proper loss function $\ell$, which, as we will see, should also contain information about the model uncertainty between $A_{\eta,j}$ and $A_j$. In our experiments we focus on inspecting the effect of including model uncertainty estimates to the loss function.

4.1. Network architecture

Motivated by the similarities between the model of the first-order scattered and the standard Radon transform, we consider the U-Net provided by J. Leuschner on GitHub, which was also successfully used in [5] for CT reconstructions. In our simulation settings, see section 5.

3 https://github.com/jleuschn/dival/tree/master/dival/reconstructors/networks.
we obtained the best results for seven layers with (32, 32, 64, 64, 128, 128, 256) channels. For this, we needed to slightly adapt the code, as it was designed for at most six layers. Moreover, we used six skip connections and a sigmoid function as a final step of the neural network. For the details of the down and up sampling parts of the U-Net we refer directly to the code mentioned above. However, it is reasonable to think that a more optimal network architecture for CST could be constructed in the future, in particular to address the complexity of the model and the multiple-order scattering.

### 4.2. Loss functions

As a first and standard approach—in case of an exact forward operator, see also [12]—we consider the mean squared error loss function

$$\ell_1(\theta) := \frac{1}{PK} \sum_{p,k} \left\| A_{p,k}^\theta \varphi_\theta(z) - g_{p,k}^\delta \right\|^2,$$

for $\theta \in \Theta$. This means that no information on the model uncertainty is explicitly included. By this, we want to inspect, whether the network itself is capable of reducing artifacts caused by considering the inexact forward operators $A_{p,k}^\theta$. As we will see in the next section, this is not the case.

Hence, we want to include information on the model uncertainty to the loss function. Motivated by the approach in [7] to include the model uncertainty to the RESESOP-Kaczmarz procedure, we propose to include the model uncertainty to a loss function via

$$\ell_2(\theta) := \frac{1}{PK} \sum_{p,k} \left\| A_{p,k}^\theta \varphi_\theta(z) - g_{p,k}^\delta \right\|^2 - \left( \frac{c_{p,k}}{\epsilon_{p,k}} \right)^2,$$

where $c_{p,k} := \tau(\rho' \eta_{p,k} + \tilde{\delta}_{p,k})$ is a model correction term inspired from the RESESOP method studied in the previous section. The connection to RESESOP-Kaczmarz is revealed by the following observation: If we assume that one of the summands in (27) is zero, then it is not difficult to see that $\varphi_\theta(z)$ belongs to the boundary of the restricted stripe $B_{\rho'}(0) \cap H(u_{p,k}^{\eta,\delta,j}, \alpha_{p,k}, \xi_{p,k})$, where

$$u_{p,k}^{\eta,\delta,j} := (A_{p,k}^\theta)^* (A_{p,k}^\theta \varphi_\theta(z) - g_{p,k}^\delta),$$

$$\alpha_{p,k} := (A_{p,k}^\theta \varphi_\theta(z) - g_{p,k}^\delta),$$

$$\xi_{p,k}^{\eta,\delta,j} := c_{p,k} \| A_{p,k}^\theta \varphi_\theta(z) - g_{p,k}^\delta \|$$

are analogously defined as in algorithm 3.3. Hence, if $\theta_{opt}$ is a minimizer of $\ell_2$, then $\varphi_{\theta_{opt}}(z)$ is expected to be close to the boundary of all those stripes. As illustrated in figure 3, the solution of $Af = g$ is expected to be close to the stripe boundaries. Further note that $\ell_2$ is also differentiable with respect to $\theta$, given that $\varphi_\theta$ is differentiable, which enables backpropagation.

**Remark 4.1.** It would also be an option to include $c_{p,k}$ from (27) to the parameter space $\Theta$. However, it is then important to restrict the $c_{p,k}$ to an interval determined by an estimation of the model uncertainty. This could be achieved in the following way: Include $\theta_{\text{opt}}(c) \in \mathbb{R}^{\rho' \times K}$ to the parameter space $\Theta$ and choose $c_{p,k}(\theta_{\text{opt}}(c))$ as a differentiable function of $\theta_{\text{opt}}(c)$, whose range is contained in the desired interval. This way, the network could learn a better estimation of the model uncertainty and be less vulnerable to bad model uncertainty estimates. This idea might be valuable for further research. Moreover, the advantage of considering loss functions like $\ell_2$ is that they probably do not require a stopping criterion.
We end this section by describing the general training process. For minimizing the loss functions we used the stochastic optimizer Adam from Pytorch\(^4\), where the name Adam stands for *adaptive moment estimation*. We observed that in the beginning of the training process \(\ell_2\) seems to be more sensitive than \(\ell_1\) to the choice of the learning rate in the ADAM optimizer. More precisely, if the learning rate does not decrease quickly enough during the training, it sometimes happened that the current reconstruction completely changes from one training step to another. This might be explained by inspecting the gradients of the loss functions with respect to \(\theta\): For simplicity, we consider instead the following functions and their gradients

\[
 f_1(x) := \sum_{k=1}^{N} |x_k|^2 \quad \text{with} \quad (\nabla f_1(x))_k = 2x_k,
\]

\[
 f_2(x) := \sum_{k=1}^{N} |x_k^2 - c_k^2|^2 \quad \text{with} \quad (\nabla f_2(x))_k = 2x_k \cdot 2(x_k^2 - c_k^2).
\]

Thus, if \(x\) is not close to \(c\)—which is the case in the beginning of the optimization—the gradients of \(f_2\) have a larger dynamic than those of \(f_1\). So, if the learning rate is not small enough, the gradient descent step for \(\ell_2\) is more likely to be too large. In order to stabilize the minimization of \(\ell_2\) the following strategies turned out to be efficient: first, starting with \(\ell_1\) and later changing the loss function to \(\ell_2\) is more robust to the choice of the learning rate. Second, clipping the gradients during the backpropagation turned out to be another good option to stabilize the loss function \(\ell_2\), i.e. rescaling the current gradient as soon as its norm is larger than a chosen threshold. This threshold can iteratively be reduced during the training process. In our simulations we combined both approaches.

The training procedure, as well as our choice of the algorithmic parameters are visualized in algorithm 4.2).

**Algorithm 4.2** (Training of the DIP-network)

Let \(\varepsilon > 0\) be some tolerance for the second loop below.

**While \(\ell_1(\theta) > 0.2\|g^i\|_{\infty}\) do:**

- Train network \(\varphi_{\theta}(z)\) with \(\ell_1\)-loss.
- Learning rate of ADAM-optimizer: 0.001
- Gradient clipping if \(\left\| \frac{d\varphi_{\theta}(z)}{d\theta} \right\|_2 > 2.5\|g^i\|_2\) via

  \[
  \text{torch.nn.utils.clip_grad_norm_\(_(network.parameters(),2.5\|g^i\|_2)),}
  \]

  see https://pytorch.org/docs/stable/generated/torch.nn.utils.clip_grad_norm_.html.

  **While \(\ell_2(\theta) > \varepsilon \cdot \|g^i\|_{\infty}\) do:**

  - Train \(\varphi_{\theta}(z)\) with \(\ell_2\)-loss.
  - Learning rate of ADAM-optimizer: 0.0005
  - Decrease learning rate after every 1500 optimization steps by 0.00005.
  - Gradient clipping if \(\left\| \frac{d\varphi_{\theta}(z)}{d\theta} \right\|_2 > 1.5\|g^i\|_2\).

\(^4\) https://pytorch.org/docs/stable/generated/torch.optim.Adam.html.
In the next section we will illustrate in some simulations how the previous DIP algorithm and the RESESOP approach from section 3 are capable of dealing with model uncertainty in the CST problem.

5. Solving a CST problem

In this section, we consider only the two-dimensional case for CST for convenience as the three-dimensional case is significantly more expensive in terms of computations, as mentioned in section 2. However, there is no obstacle in the analysis of both forward models and reconstruction techniques for a direct application to 3D.

We start by presenting the setting of our numerical experiments and exhibit then how the first- and second-order scattering data \( g_1, g_2 \in \mathbb{R}^{P \times K} \) are simulated. Afterwards, we present the reconstruction results for the RESESOP and the DIP approach.

5.1. Experimental setup

5.1.1. Image domain. During our experiments the region \( \Omega \subset \mathbb{R}^2 \) to be scanned is a square of 30 cm side-length and center at zero.

5.1.2. Architecture of the CST scanner. The detector space \( \mathcal{D} \) is a sphere with radius 30 cm and center at zero. At one half of this sphere \( n_s = 10 \) sources are evenly positioned. For each source we evenly sample 80\% of the detector space at \( n_d \) locations for the detectors, which is illustrated in figure 4. 20\% are omitted because detectors close to the source will only receive a low signal. In total, we have \( K = n_s \cdot n_d = 200 \) source-detector tuples.

5.1.3. Sources and energy. The monochromatic sources are assumed to emit \( \gamma \)-rays at energy \( E_0 = 1173 \text{ keV} \), which corresponds to the maximal peak of Cobalt-60. Moreover, the total number of emitted photons per source is set to \( I_0 = 8 \times 10^8 \). Further research and simulations shall take into account the polychromacy of the source as in [27] but our proposed method can be adapted to this physical aspect. We also discard the backscattering, i.e. scattering angles \( \omega_2 \in (\pi/2, \pi) \), as the flux of this part of the spectrum is rather low, thus heavier affected by noise, and further delivers a poorer information for fixed energy resolution, see [37]. Therefore, accordingly with to the Compton formula (4), we equally sample the energy space \( \mathcal{E} \) at \( P = 80 \) energies in the interval \( (359.6, 1161.5) \text{ keV} \), so for scattering angles \( \omega \in (0, \pi/2) \).

5.1.4. A modified Shepp–Logan phantom. For the ground truth \( \mu \) we consider a bilinear interpolator of a modified Shepp–Logan Phantom defined on a grid twice as fine as \( \Omega_n \), so \( \mu \notin \mathcal{X}_f \). The original Shepp–Logan phantom has a very low contrast in the inner part which is not suited for the level of model inexactness we consider. In order to still provide a challenge for the algorithms, we increased the contrast but not as much as for the ‘Modified Shepp-Logan’ defined in MATLAB. The electron densities relative to water of \( \mu \) are in the interval \([1.36, 5.66]\), see figure 5(a). This means its maximal electron density corresponds to bone. Note that the electron density of water is \( 3.23 \times 10^{23} \) electrons per cm\(^3\). The horizontal and
vertical diameters of the phantom are 19.5 cm and 26 cm, respectively. Regarding the prior $\mu^*$, see figure 5(b), we choose the same shape as for $\mu$, but set the relative electron density of the interior constantly to 0.67. Both $\mu$ and $\mu^*$ are positioned in $\Omega$ such that their center are at zero.
5.1.5. Restricting the domain space. The finite dimensional subspace \( \mathcal{X}_j \) of \( H_0^1(\Omega) \) is constructed in the following way: On \( \Omega = (-15,15)^2 \), we consider a regular \( 100 \times 100 \) grid
\[
\Omega_h := \{(x_n,y_m) = (-15 + nh, 15 + mh)^T : n,m = 0, \ldots, 99 \}
\]
for \( h = 0.3 \). For each grid point, \((x_n,y_m) \in \Omega_h\) we define a gaussian function via
\[
e_{nm}(x,y) = c_{nm} \cdot \exp \left( \frac{1}{2} \left( \frac{x - x_n}{0.5h} \right)^2 + \frac{1}{2} \left( \frac{y - y_m}{0.5h} \right)^2 \right),
\]
where \( c_{nm} \) is chosen such that \( \|e_{nm}\|_{L^2(\Omega)} = 1 \). Each Gaussian is truncated to the set \( \Omega \cap B_r((x_n,y_m)) \), for \( r := 1.5h \). By setting \( \mathcal{X}_j \) as the linear span of the \( e_{nm} \) we obtain a 10000 dimensional space.

5.1.6. Forward models. For the implementation of the first-order CST operator \( \mathcal{R}_1 \), we used the trapezoidal rule for computing the involved integrals. The first-order scattering data \( g_1 \in \mathbb{R}^{p \times k} \) is then computed by evaluating the semi-discrete \( \mathcal{R}_1^\mu \) at \( \mu \) for the respective detector-source-energy triples described above. The second-order scattering data \( g_2 \in \mathbb{R}^{p \times k} \) was generated using Monte-Carlo simulations \([37]\). Since ‘only’ \( I_0 = 8 \times 10^8 \) photons were sent by the source, the second-order scattered radiation is subject to noise due to the stochastic nature of the emission of photons. The data \( g_1 \) and \( g_2 \) are flattened versions of the vectors \( \mathcal{R}_1^\mu(e_{nm}) \in \mathbb{R}^{p \times k} \). This allows a fast evaluation of the fully-discrete operator. For computing the matrix entries, we pre-computed the weight \( M_1(\mu^*) \) on a grid twice as fine as \( \Omega_h \) and used linear interpolation. Thereby, the computation time was reduced.

5.1.7 Inexact model. Regarding the inexact fully discrete operator \( (\mathcal{R}_1^\mu)^* : \mathcal{X}_j \to \mathbb{R}^{p \times k} \), we compute its matrix representation \( (P_1^\mu)^* \)—an 16000 \times 10000 matrix—with respect to the basis \( (e_{nm})_{n,m} \) and the standard basis of \( \mathbb{R}^{p \times k} \), that is, its columns are flattened versions of the vectors \( \mathcal{R}_1^\mu(e_{nm}) \in \mathbb{R}^{p \times k} \). This allows a fast evaluation of the fully-discrete operator. For computing the matrix entries, we pre-computed the weight \( M_1(\mu^*) \) on a grid twice as fine as \( \Omega_h \) and used linear interpolation. Thereby, the computation time was reduced.

5.1.8. Different scenarios. In our numerical experiments with RESESOP and DIP, we consider the following reconstruction problems and use the notation introduced in the previous sections.

(I) \( A_{p,k}^{\nu,f} = (g_1)_{p,k} \) for \( p = 1, \ldots, P, \ k = 1, \ldots, K \);

(II) \( A_{p,k}^{\nu,f} = (g_1^\delta)_{p,k} \), where \( g_1^\delta \) is \( g_1 \) disturbed by 2.4\% Poisson noise;

(III) \( A_{p,k}^{\nu,f} = (g_1 + g_2)_{p,k} \) where \( g_2 \) is corrupted by Poisson noise due to the Monte-Carlo process;

(IV) \( (\Psi A)p,k P^{\nu,f} = (\Psi(g_1 + g_2))_{p,k} \), where \( \Psi \) computes finite differences of the input vector.

For our reconstructions we need accurate estimates of the model uncertainty for every subproblem, i.e. sharp discrepancy terms \( \tau(\mu_{p,k} + \delta_{p,k}) \) in the RESESOP-Kaczmarz algorithm 3.3 and the \( \ell_2 \)-loss of the DIP approach. We computed them numerically by inspecting the discrepancy between data generated by the exact and inexact forward operators. Further, we use three different similarity measurements in tables 1 and 2 in the appendix for comparing the different reconstructions, namely: Peak signal-to-noise ratio (PSNR), structural self-similarity (SSIM) and normalized mean square error (NMSE).
5.2. Reconstruction results

In Scenario (I), that is dealing only with exact first-order scattering data $g_1$, we present the outcome of seven reconstruction methods. Three of them, Landweber with early stopping, Mollified TV (MTV)—see remark 5.1—and the DIP approach with loss function $\ell_1$ (denoted by DIP-$\ell_1$), do not take the model uncertainty into account and are depicted in figures 6(a), (b) and 8(a), respectively. We observe that the overall contours of different tissues are well recognizable, which is expectable according to the results in [37]. However, the contrast between different tissues is badly reconstructed.

In comparison to that, inspecting the RESESOP-Kaczmarz reconstruction in figure 6(c), the contrast between different tissues is much better retained, leading to significantly smaller error measurements in appendix table 1. But a certain noisy pattern is noticeable in this reconstruction, which might be caused by considering multiple inverse problems instead of one. To deal with this problem one could e.g. do some post-processing with a suitable denoiser. We applied denoising by TV as a post-processing step—see remark 5.2—and by that obtained satisfactory results, see figure 6(d). The combination of RESESOP with TV post-processing will be denoted by RESESOP+TV in the following.

Finally, the DIP reconstruction with loss function $\ell_2$ (denoted by DIP-$\ell_2$) as well as its combination with TV-denoising afterwards is depicted in figures 8(b) and (c), respectively.
They look pretty similar to the RESESOP(\(+\)TV) reconstructions, which is not very surprising, as the discrepancy term $c_{p,k}$ in $\ell_2$ was chosen as the discrepancy principle (16) in the RESESOP algorithm. Again, the quality of the DIP-$\ell_2$ reconstruction increased after some TV post-processing.

The reconstruction errors are listed in appendix table 1 and the best results were achieved by RESESOP+TV, so by the combination of RESESOP and TV denoising as a post-processing step.

Remark 5.1. We considered MTV introduced and analyzed by Acar and Vogel in [1], i.e. for solving an inverse problem $Bf = g^\delta$ we find a minimizer of

\[ \|Bf - g^\delta\|_{L^2(\Omega)}^2 + \lambda \int_\Omega \sqrt{\|\nabla f\|^2 + \beta}, \quad \beta > 0. \]

The objective function is differentiable, so gradient methods can be used for deriving a solution.

Remark 5.2. Introduced by Rudin et al [40], TV has become a standard for contrast-preserving image denoising. In the continuous case, given some noisy image $f^\delta$ it seeks for a minimizer $f$ of

\[ \|f - f^\delta\|_{L^2}^2 + \lambda \|\nabla f\|_{L^1}. \]

In the discrete case, this is typically solved by some primal-dual algorithm. For that we used the pylops-package in Python\(^5\).

In Scenario (II) for corrupted data $g^1$ we observe that RESESOP, RESESOP+TV, DIP-$\ell_2$ and DIP-$\ell_2$+TV are able to handle both the model uncertainty and noise if good approximations of the discrepancy terms $\tau(\rho_{p,k} + \delta_{p,k})$ are known, see figures 6(g), (h) and 8(e), (f), respectively. However, the corresponding reconstruction errors in appendix table 1 are a bit worse than in case of noise-free data in table 1. Except for DIP-$\ell_2$ and DIP-$\ell_2$+TV. Here the reconstructions get slightly better, which may be due to the stochastic nature of the ADAM optimizer. Further, in the Landweber and MTV reconstructions in figures 6(e) and (f) some details are gone.

Incorporating the second-order scattering data $g^2$ to $g^1$ in Scenario (III) leads to a huge additional uncertainty, as the flux of $g^2$ is almost as high as the flux of $g^1$, that is $\|g^2\|_1 \approx \|g^1\|_1$, where

\[ \|x\|_1 := \sum_{p,k} |x_{p,k}|, \quad \text{for } x \in \mathbb{R}^{P \times K}. \]

In this case, we see that RESESOP is no longer capable to handle it, see figure 7(b). Also MTV in figure 7(a) is no longer able to reconstruct the inner contours.

Therefore, we followed the approach in [37] and applied a finite difference operator $\mathcal{P}$ in Scenario (IV) to both sides of the problem $A^\delta f = (g^1 + g^2)$. This reduced the flux of both first- and second-order data, but more importantly, the latter decreased more: $\|\mathcal{P}g^2\| \leq 0.44 \cdot \|\mathcal{P}g^1\|$. This observation should also be seen in the light of theorem 2.4, which already suggests that $g^2$ is smoother than $g^1$, see also figure 5(c). Indeed, by this, both RESESOP and RESESOP+TV lead to good reconstructions which are slightly better than the reconstructions in Scenario (II), see figures 6(k) and (l), as well as the reconstruction errors in appendix table 1. However, the DIP-$\ell_2$(+TV) reconstructions in figures 8(h) and (i) are worse and have some

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\(^5\) https://pylops.readthedocs.io/en/latest/gallery/plot_tvreg.html.
Figure 7. Reconstructions for Scenario (III).

Figure 8. DIP reconstruction for Scenario (I) in the first, Scenario (II) in the second and Scenario (IV) in the third row, respectively.

artifacts in form of scratches. One reason for that could be that applying the pseudo differential operator creates additional local minima in the optimization landscape.

Remark 5.3. As also the DIP reconstructions in figure 8 include some noisy pattern, we tried to add a further denoising penalty to the loss function $\ell_2$ in the DIP approach. Unsurprisingly, thereby the influence of the model uncertainty gets more visible again. Therefore, we propose to gain improvements rather by some post-processing, for example by TV denoising, which we did in our reconstructions in figure 8.
Figure 9. Comparison of RESESOP reconstructions for Scenario (II) with accurate and too large model uncertainty estimates. The distance between accurate and inaccurate estimates in the Euclidean norm relative to the norm of $g^1$ is 2.8%.

Remark 5.4. The prior $\mu^*$ is very simple, so the model uncertainty is rather large. To decrease the model uncertainty, one could use one of the reconstructions as a new prior $\tilde{\mu}^*$ and consider $A^\eta \cdot \Sigma_{\mu^*}^\eta$, which probably is a better approximation of $\Sigma_{\mu^*}$. Furthermore, a prior $g^2$ could be included in the discrepancy term, both for RESESOP and DIP, in order to reduce the model uncertainty. We did not consider these improvements to stress the algorithms in terms of model uncertainty.

As mentioned above, for the RESESOP and DIP reconstructions we assumed to have accurate estimates of the model uncertainty for each subproblem on hand, i.e. sharp discrepancy terms (16) in the RESESOP algorithm 3.3 and model correction terms (27) in the loss function $\ell_2$ for the DIP approach, respectively. However, in practice such accurate estimates would be unreachable, which asks for the development of empiric ways to estimate the model uncertainty. One way would be to create a CST dataset and learn the mapping that maps some data $g^\delta$ and prior $\mu^*$ to the corresponding discrepancy terms $\tau(\rho_{p,k} + \delta_{p,k})$. We want to end this section by showing the effects of inaccurate model uncertainty estimates for the RESESOP method.

As a first example, for Scenario (II), we consider discrepancy terms which are an upper bound of the accurate terms, see figure 9. The difference between accurate and inaccurate estimates in the Euclidean norm relative to the norm of the data $g^1$ is 2.8%. The resulting RESESOP reconstruction is a bit smoother than for the case with accurate estimates, which is expectable due to the larger regularization parameters. On the other hand, some details like the tumors in the center and also the contrast between different tissues are less sharply reconstructed, see also the error measurements in appendix table 2. The reconstructions are better than for Landweber and Mollified TV, which do not involve information on the model uncertainty at all.

Second, we scale the previous inaccurate estimates, so that some of them are lower than the corresponding accurate terms, see figure 10. Although the gap between accurate and inaccurate terms is 2.2%, so smaller than in the first example, the reconstruction gets less accurate in terms of the reconstruction errors, see appendix table 2, and also noisier, which is reasonable since RESESOP loses its capability to regularize the problem for too small discrepancy terms, which are the regularization parameters. To conclude, it is recommended to use rather too large discrepancy terms than too small ones.

Last but not least, we consider the MTV reconstruction $f_p$ in Scenario (II) and consider an empiric estimate of the discrepancy terms via

$$\tau(\rho_{p,k} + \delta_{p,k}) \approx \|A^{\eta, f_p}_{p,k} - (g^1)_{p,k}\|.$$
Figure 10. Comparison of RESESOP reconstructions for Scenario (II) with accurate and inaccurate uncertainty estimates. Some estimates are too low. The distance between accurate and inaccurate estimates in the Euclidean norm relative to the norm of $g_1^\delta$ is 2.2%.

Figure 11. Comparison of RESESOP reconstructions for Scenario (II) with accurate and empiric model uncertainty estimates obtained from the MTV reconstruction. The distance between accurate and inaccurate estimates in the Euclidean norm relative to the norm of $g_1^\delta$ is 7.8%.

Here, the gap between inaccurate terms and accurate discrepancy terms is quite large with 7.2%. The RESESOP reconstruction with these discrepancy terms is depicted in figure 11 and is worse than the MTV reconstruction itself, see appendix table 2.

6. Conclusion

We have proposed two data-driven reconstruction strategies able to handle the model uncertainty occurring in imaging based on Compton scattering. The construction of these algorithms is based on the study of the properties of the forward models: nonlinearity, mapping properties and model uncertainty. The first approach considers the RESESOP method which is studied in terms of convergence and regularization for the fully discrete case in order to fit the restrictions of our spectral inverse problem. The second approach exploits the popular DIP method, suited for the treated problem since unsupervised, it does not require a dataset. We modified the learning loss function using the model uncertainty model used in the first approach. Simulation results on synthetic data for the first-order scattering and on Monte-Carlo data for the second-order scattering attest the efficiency of both approaches.

The performed simulations assumed an almost perfect estimation of the model uncertainty for every subproblems which is hard to achieve in practice and remains an open issue for the general RESESOP approach or here for our modified DIP method. A first possibility would be to learn the model uncertainty coefficients from a synthetic dataset or from real dataset in the future. Another more general approach would be to relax the uncertainty parameter in the
RESESOP method, for instance by incorporating a minimization problem at each iterate to find the best parameter. These questions will be the core of future research.

**Data availability statement**

The data that support the findings of this study are available upon reasonable request from the authors.

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**Appendix**

Below we list the reconstruction errors of all presented reconstructions. We use the following abbreviations: Landweber (LW), Mollified Total Variation (MTV), DIP with $\ell_n$-loss (DIP-$\ell_n$) for $n \in \{1, 2\}$, RESESOP-Kaczmarz (RES). If TV-denoising is used as a post-processing step we add ‘+TV’ to the notation.

**Table 1.** Error measures for the different reconstructions and methods to solve scenarios (I), (II) and (IV). The regularization parameter $\lambda$ in the MTV is 12, 45 and 26 respectively. The best reconstructions errors are highlighted in bold, respectively.

|       | LW   | MTV  | DIP-$\ell_1$ | RES  | RES+TV | DIP-$\ell_2$ | DIP-$\ell_2$+TV |
|-------|------|------|--------------|------|--------|--------------|-----------------|
| I     |      |      |              |      |        |              |                 |
| PSNR  | 24.297 | 24.807 | 24.644 | **33.657** | 30.710 | 32.825      |
| SSIM  | 0.968 | 0.970 | 0.962 | 0.992 | **0.996** | 0.989 | 0.994 | 0.071 | 0.115 | 0.084 |
| NMSE  | 0.196 | 0.190 | 0.213 | 0.099 | **0.071** | 0.115 | 0.084 | 0.071 | 0.115 | 0.084 |
| II    |      |      |              |      |        |              |                 |
| PSNR  | 24.040 | 24.007 | 29.211 | 31.373 | **32.682** | 35.014      |
| SSIM  | 0.961 | 0.960 | 0.988 | 0.993 | 0.994 | **0.997** |
| NMSE  | 0.217 | 0.216 | 0.124 | 0.091 | 0.089 | 0.064       |
| IV    |      |      |              |      |        |              |                 |
| PSNR  | 21.800 | 21.379 | 29.966 | 33.509 | **26.793** | 27.915      |
| SSIM  | 0.938 | 0.940 | 0.990 | **0.996** | 0.972 | 0.982       |
| NMSE  | 0.275 | 0.273 | 0.114 | **0.071** | 0.187 | 0.145       |

**Table 2.** Inaccurate model uncertainty estimates: RESESOP-Kaczmarz applied to Scenario (II), i.e. to solve $A^\theta f = \mathbf{g}^d$.

| Figure 9(a) | Figure 10(a) | Figure 11(a) |
|-------------|---------------|---------------|
| PSNR (dB)   | 24.772        | 23.735        | 23.252        |
| SSIM        | 0.968         | 0.960         | 0.950         |
| NMSE        | 0.196         | 0.221         | 0.227         |
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