NON-LINEAR ITERATIVE PHASE RETRIEVAL BASED ON FRECHET DERIVATIVE AND PROJECTION OPERATORS

V. Davidoiu[⋆]*, B. Sixou*[⋆]*, M. Langer*[⋆†]*, F. Peyrin*[⋆†]

[⋆] CREATIS, CNRS UMR5220 ; Inserm U630 ; INSA-Lyon ; Université Lyon 1; Université de Lyon, F-69621 Villeurbanne Cedex, France,
† European Synchrotron Radiation Facility, 6 rue Jules Horowitz, F-38043 Grenoble Cedex, France

ABSTRACT

Phase retrieval from Fresnel diffraction patterns is a non-linear ill-posed inverse problem of paramount importance in various areas of applied physics. Recently a new non-linear iterative algorithm based on a Landweber method with an analytic calculation of the Frechet derivative adjoint has been proposed. In this work, we refine this scheme by introducing Fienup projectors in the algorithm. The new method was tested on noisy simulated data. Our method outperforms the approaches based on the linearization of the relation between the phase shift induced by the object and the diffracted intensity and the former non linear algorithm with no projectors.

Index Terms— Inverse Problems, Phase Retrieval, Phase Contrast, X-ray imaging, Nonlinear Optimization

1. INTRODUCTION

The phase retrieval problem is of paramount importance in various areas of applied physics and especially in in-line x-ray phase tomography [1]. The phase imaging methods improve significantly the sensitivity of conventional μCT. The phase shift cannot be detected directly, nevertheless several methods to achieve phase contrast in the hard x-ray range have been developped [2]. X-ray phase imaging of synchrotron radiation is based on interferometry, analyzer-based and propagation based imaging. The last technique requires a high degree of coherence of the x-ray beam and is based on the Fresnel diffraction patterns.

Until recently, the most efficient phase retrieval algorithms were all based on a linearized relation between the phase and the intensity. These are the transport of intensity equation (TIE) [3], which is valid for short propagation distance, the contrast transfer function (CTF) [4], which gives good results for weak absorption and slowly varying phase, and the mixed approach based on the two former methods [4], which is valid for slowly varying objects. A new iterative method based on the minimization of a non-linear regularized functional with the Frechet derivative of $\mathcal{I}(\varphi)$ has been recently proposed in [5, 6]. It was shown that the iterative scheme proposed improves the results obtained in a linear framework, yet stagnation away from the true phase is observed [5, 6].

The aim of this work is to introduce Fienup like projection operators in the former non-linear phase retrieval approach. Classical algorithms based on projections and designed for solving phase retrieval problems have been discussed in the mathematical context of multi-valued projection operators and convex optimization [7]. The connection has been established between the widely used phase retrieval methods like Error Reduction Fienup approaches [8] and the standard convex optimization algorithms. The error reduction algorithm is identified with a non-convex alternating projection algorithm [7] and it is shown that the Fienup's basic input-output, and hybrid input-output algorithms corresponds to Dykstra and Douglas-Rachford algorithm. This work provides a theoretical framework to better understand and improve the new phase recovery scheme presented in [5, 6] by means of projection operators designed to satisfy convex or non-convex constraints.

This paper is organized as follows. The direct problem and the linear approaches used in the previous works are introduced first. In Sec. 3, we describe the non linear approach based on Frechet derivative, Landweber iterative algorithm and the projection operators used to refine this scheme. In Sec. 4 some results obtained on noisy-data to validate the proposed solution and finally we conclude in Sec. 5.

2. THE DIRECT PROBLEM OF IMAGE FORMATION

The interaction between a x-ray beam of wavelength λ and the object can be described by the 3D complex refractive index distribution [9]:

$$n(x,y,z) = 1 - \delta_r(x,y,z) + i\beta(x,y,z) \qquad (1)$$

where δ_r is the refractive index decrement and β is the absorption index for the spatial coordinate (x,y,z). The propagation direction of the x-rays is denoted by z. Considering a thin object, the propagation path of the x-ray with the object can be presumed straight, so the interaction of x-rays with

matter can be described by a transmittance function T [9]:

$$T(\mathbf{x}) = \exp[-B(\mathbf{x}) + i\varphi(\mathbf{x})] = a(\mathbf{x})\exp[i\varphi(\mathbf{x})] \quad (2)$$

where $a(\mathbf{x})$ is the amplitude modulation and $\varphi(\mathbf{x})$ is the phase shift induced by the object, with $B(\mathbf{x}) = \frac{2\pi}{\lambda}\int \beta(x,y,z)dz$ and $\varphi(\mathbf{x}) = -\frac{2\pi}{\lambda}\int \delta_r(x,y,z)dz$. In this formula, the coordinates $\mathbf{x} = (x,y)$ are perpendicular to the propagation direction z. The intensity detected at a distance D can be expressed as a Fresnel transform:

$$\mathcal{I}_D(\mathbf{x}) = |T(\mathbf{x}) * P_D(\mathbf{x})|^2 \quad (3)$$

where $*$ denotes the 2D convolution of the transmittance with the Fresnel propagator,

$$P_D(\mathbf{x}) = \frac{1}{i\lambda D}\exp\left(i\frac{\pi}{\lambda D}|\mathbf{x}|^2\right). \quad (4)$$

The most common approaches for the phase retrieval problem are based on the linearization of Eq. 3 valid under the assumptions that the absorption is slowly varying. In this conditions the Fourier transforms of the intensity is the solution of an elliptic linear partial differential equation [4]. Regularization techniques allow stable solutions and increase the quality of the solution. Regularization methods like classical quadratic Tikhonov regularization and wavelet shrinkage have been tested in [10].

3. THE NON LINEAR INVERSE PROBLEM

3.1. Initialization

In order to improve the phase retrieved with this linear approach, an iterative Landweber type method based on the Frechet derivative of the non linear operator $\mathcal{I}_D$ has been proposed. The phase retrieval problem is an ill-posed problem and prior informations on the phase and regularization techniques are required. In view of Eq. 3, the operator $\mathcal{I}_D(\varphi)$ can be considered as a non-linear operator acting on the phase φ, which is Frechet differentiable in its domain. It is assumed that the phase has a Lipschitz bounded support Ω and that the domain $\mathcal{D}[\mathcal{I}_D(\varphi)]$ of the operator $\mathcal{I}_D(\varphi)$ belongs to the functional Sobolev space $H^{2,2}_{\diamond}(\Omega)$ [11]:

$$H^{2,2}_{\diamond}(\Omega) = \{\varphi \in H^{2,2}(\Omega), \quad \frac{\partial\varphi}{\partial\vec{n}} = 0\} \quad (5)$$

where $\frac{\partial\varphi}{\partial\vec{n}}$ is the normal derivative of the phase.

In order to regularize the problem, we introduce a Tikhonov's functional of the following form:

$$J_\alpha(\varphi) = \frac{1}{2}\|\mathcal{I}_D(\varphi) - \mathcal{I}_\delta\|^2_{L_2(\Omega)} + \frac{\alpha}{2}\|\nabla\varphi\|^2_{L_2(\Omega)} \quad (6)$$

where $\|.\|_{L_2(\Omega)}$ denotes the $L_2(\Omega)$ norm, $\mathcal{I}_\delta$ approximates the exact data $\mathcal{I}_D$ with the accuracy δ

$$\|\mathcal{I}_D - \mathcal{I}_\delta\|_{L_2(\Omega)} \leq \delta. \quad (7)$$

The stabilizing norm is thus a Sobolev type regularizing term based on the gradient of the phase to be retrieved.

The optimality condition can be written $\mathcal{I}'_D(\varphi)^*[\mathcal{I}_D(\varphi) - \mathcal{I}_\delta] - \alpha\nabla\cdot(\nabla\varphi) = 0$, where $\mathcal{I}'(\varphi)^*$ is the adjoint of the Frechet derivative of the intensity [6].

3.2. The Analytic Expressions Of The Frechet Derivative

In the algorithm proposed in [6], starting from the current phase estimate φ_k at the iteration k, a linear search procedure is introduced with a variable step τ_k yielding the following modification of the standard Landweber method :

$$\varphi_{k+1/2} = \varphi_k - \tau_k\{\mathcal{I}'_D(\varphi_k)^*[\mathcal{I}_D(\varphi_k) - \mathcal{I}_\delta] - \alpha\triangle\varphi_k\}. \quad (8)$$

The Frechet derivative $\mathcal{I}'_D(\varphi_k)(\varepsilon) = G_k(\varepsilon)$ can be calculated explicitly as [6]:

$$G_k(\varepsilon) = 2\mathtt{Real}\big(\{-[ia\varepsilon\exp(-i\varphi_k)] * P_D\} \{[a\exp(i\varphi_k)] * \overline{P_D}\}\big). \quad (9)$$

The adjoint operator G^*_k can also be calculated:

$$G^*_k(\varepsilon) = 2\mathtt{Real}\big[\big(\{\varepsilon[a\exp(-i\varphi_k)^* P_D]\}^* \overline{P_D}\big) \{ia\exp(i\varphi_k)\}\big]. \quad (10)$$

In order to obtain the best decrease of $J(\varphi)$ the regularizing parameter α is chosen by trial-and-error. This type of method has been used in several works on non-linear ill-posed problems [12]. This approach improves the results obtained with the linear approaches but some stagnation away from the solution is observed and the phase error should be further decreased.

3.3. Projector Operator

In this work, we use projectors in order enforce some constraints on the retrieved phase and to improve the former phase recovery algorithm. Common approaches for solving the classical phase retrieval problem is to enforce alternatively object domain and Fourier constraints. In this work, we have considered an image modulus constraint in the object domain.

For each distance D and diffracted intensity $\mathcal{I}_D$, we consider the set $\mathcal{M}_D = \{u \in L_2, |u| = \sqrt{I_D}\}$. This set is closed but not convex and this lack of convexity is related to the difficulty of the phase retrieval problem. For a given transmission T_k at the iteration k, obtained with the former iterative method, defined by:

$$T_k(\mathbf{x}) = a(\mathbf{x})\exp[i\varphi_k(\mathbf{x})] \quad (11)$$

we consider the projection of $T_k * P_D$ on the set $\mathcal{M}_D$. The set $\mathcal{M}_D$ defines a non-convex constraint, the associated projector

is multi-valued and a particular selection must be picked. We have thus defined the projection $P_{\mathcal{M}_D}$ by:

$$P_{\mathcal{M}_D}(T_k * P_D) = \begin{cases} \sqrt{\mathcal{I}_D} \cdot \frac{T_k * P_D}{|T_k * P_D|} & \text{if } T_k * P_D \neq 0 \\ T_k * P_D & \text{otherwise.} \end{cases} \tag{12}$$

The new transmission T'_k is calculated with successive Fourier and inverse Fourier transforms:

$$T'_k = \mathcal{F}^{-1}\left\{\mathcal{F}\left[P_{\mathcal{M}_D}\left(T_k * P_D\right)\right] / \mathcal{F}\left(P_D\right)\right\} \tag{13}$$

and projected phase is defined by :

$$P_D(\varphi(\mathbf{x})) = \operatorname{argmin}\left\{\left|T'_k(\mathbf{x}) - a(\mathbf{x}) \exp\left[i\varphi(\mathbf{x})\right]\right|\right\} \tag{14}$$

where P_D is an additional projector. We have also considered a support constraint and a projection $P_{\mathcal{S}}$ on the support $\mathcal{S}$ of the phase $P_{\mathcal{S}} = \varphi.1_{\mathcal{S}}$.

At each iteration the projectors $P_{\mathcal{M}_D}$ and $P_{\mathcal{S}}$ are applied successively as in the Error Reduction algorithm (ER) [8]. The iterate φ_{k+1} is obtained from $\varphi_{k+1/2}$ using Eq. 8 :

$$\varphi_{k+1} = P_{\mathcal{S}} P_D(\varphi_{k+1/2}). \tag{15}$$

This additional projection step leads to an alternative phase retrieval scheme. It should be noted that the term $\|\mathcal{I}_D - \mathcal{I}_\delta\|_{L_2}$ is not a convex function of φ and that the convergence is local. The distances are stepped through randomly.

4. SIMULATIONS

In this work, this algorithm was tested on noisy-data. Following [13], the imaging system was simulated in a deterministic fashion. Two phantoms were defined, one for the absorption coefficient and one for the refractive index decrement. The corresponding pixel size was 1.5μm. Theoretical values for δ and β at 24 keV were used ($\lambda = 0.5166\mathring{A}$) for the phantom. Propagation in free-space was simulated using Eq. 3 for the distances $D = \{0.2, 0.4, 0.6, 0.8, 1.0, 1.2, 1.4, 1.6\}$m. The original phase map to be retrieved is displayed in Fig. 1(a), together with the corresponding Fresnel diffraction pattern for $D = 1.4$ m with 24dB in Fig. 1(b). The convolution product was calculated by Fourier transforms and the intensity has been obtained as the squared modulus in the spatial domain of this convolution.

The intensity and phase values were discretized on a regular grid and they are considered as vectors of a $N = 75 \times 75$ dimensional real space $\mathbb{R}^{75\times75}$. A Gaussian white noise well adapted to our synchrotron imaging system with a peak-to-peak signal to noise ratio (PPSNR) of 24dB was added to the image. In our simulations the distances were considered in a random way. The phase support $\mathcal{S}$ is assumed to be restricted to the 70×70 inner pixels. Two different starting points have been used to test our algorithm. Fig. 1(c) displays the difference maps between the phase obtained with the algorithm and the true phase to be retrieved with the initial phase obtained from the mixed method proposed in [13]. Fig. 1(d) displays the difference map between the true phase and the phase obtained with the new algorithm for an initialization far from the solution.

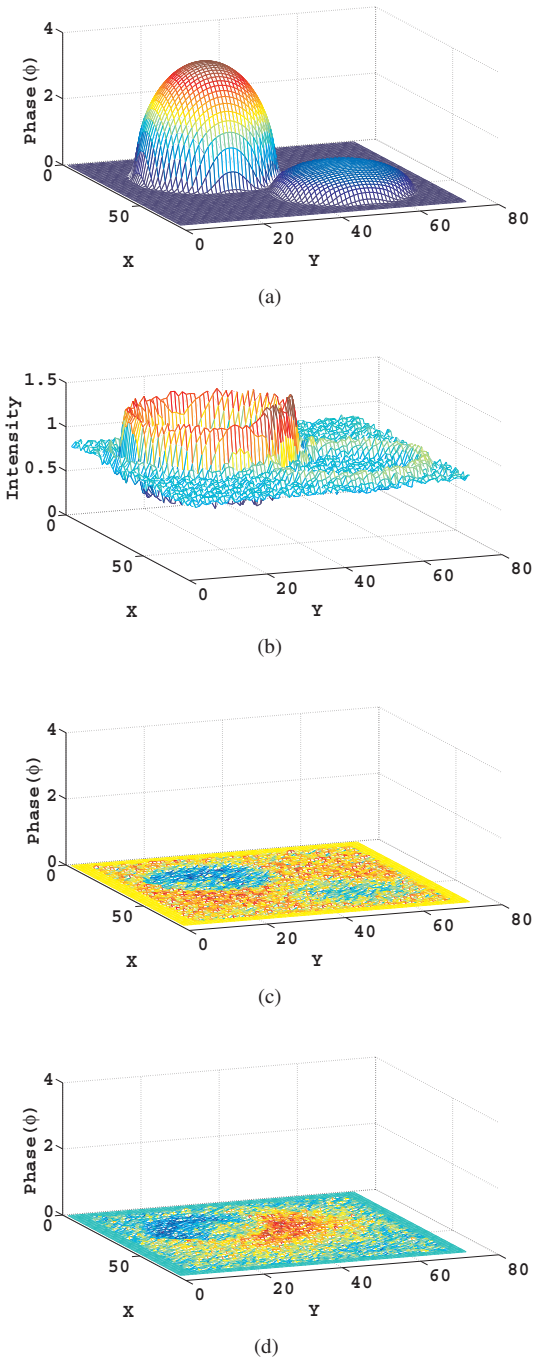
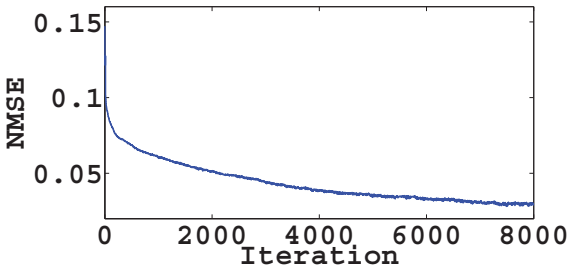


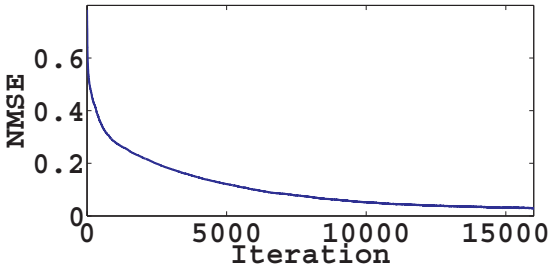
Fig. 1: (a)Original phase map to be retrieved, (b) Fresnel diffraction pattern at propagation distance $D = 1$ m with 24dB, Error map for the phase retrieved with the new algorithm initialized with (c) the mixed approach and (d) an arbitrary solution.

The method works well with a weak smoothing regularization ($\alpha = 0.5$) when the initialization is performed far from the solution. For a starting point obtained with the mixed approach, the regularization does not improve the phase recovery and one may choose $\alpha = 0$.

The evolution of the mean square error obtained for noisy-data with 24dB (PPSNR) is displayed in Fig. 2(a) Fig. 2(b) as a function of the number of iterations. The normalized mean square error on the phase decreases from 0.1471 to 0.0268 and 0.8121 to 0.0234 respectively. It should be noted that for a smooth regularization ($\alpha = 0.01$) with additive white Gaussian noise (PPNSR=24 dB) without projectors the final errors are 0.359 and 0.095 [6]. The use of the projectors improves the convergence properties of the non linear iterative method presented in [6].



(a)



(b)

Fig. 2: Normalized mean square error for the phase versus iteration number for noisy-data (PPSNR 24dB): (a) initialized with the mixed solution ($\alpha = 0$), (b) initialized with the arbitrary solution ($\alpha = 0.5$).

5. CONCLUSION

To conclude, the proposed non-linear iterative method uses the Frechet derivative of the intensity recorded at small number of propagation distances and projection method on convex or non-convex sets as in the Fienup algorithms. It outperforms the linear methods and our former non linear approach for simulated noisy-data. In future work, the method will be tested on more complex phantoms and experimental data. The method is expected to open new perspective for the examination of biological samples.

6. REFERENCES

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