Stochastic level set evolution for nonlinear phase contrast tomography

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Abstract. A stochastic perturbation of a level-set regularization method to find stable inverses for the nonlinear reconstruction of the complex refractive index in in-line phase tomography is presented under the assumption that the index is piecewise constant. The stochastic algorithm is tested on a multi-material object. It is useful to escape the local minima with decrease of the reconstruction errors localized on the boundaries.

1. Introduction

In-line phase tomography is based on a coupling of tomography and phase retrieval. Its aim is to reconstruct the real part of the refractive index [1]. The experimental set-up of Figure 1 shows that the phase contrast can be obtained for several projection angles by letting the X-rays propagate after the object and by recording the Fresnel intensity for one or several propagation distances [2, 3]. Several linear inversion methods have been already studied [4, 5, 6, 7, 8]. The simultaneous nonlinear reconstruction of the real and of the imaginary part of the index has been studied with a Tikhonov regularization [9]. We investigate here a level-set regularization assuming that the ratio of the imaginary to the real part of the complex refractive index is piecewise constant. The nonlinear phase tomography problem is non-convex and the reconstructed solution is a local minimum. We use here stochastic level-set methods to improve the reconstruction obtained with a deterministic level-set scheme. We first summarize the direct problem of the image formation. Then we detail the level-set regularization method and the stochastic approach. The numerical results obtained on noisy simulated data are presented and discussed in the next section before the conclusion.

2. The direct problem

We assume that the real and imaginary parts of the complex refractive index to reconstruct from the Fresnel intensity measurements, denoted as $\delta$ and $\beta$ are defined on a 3D bounded domain ($\Sigma$) with spatial coordinates $(x, y, z)$. We denote $(x_\theta, y_\theta, z)$ be the rotated spatial coordinate system for an angle $\theta$ around the z axis (Figure 1). We consider a monochromatic, parallel X-ray beam propagating in the $y_\theta$ direction. For a fixed projection angle $\theta$, the interaction can be described by a transmittance function $T_\theta$ of the coordinates $X_\theta = (x_\theta, z)$:

$$T_\theta(X_\theta) = \exp[-B_\theta(X_\theta) + i\phi_\theta(X_\theta)] = a_\theta(X_\theta) \exp[i\phi_\theta(X_\theta)]$$

(1)
The direct nonlinear operator

where \( a(\theta) \) is the absorption and \( \varphi(\theta) \) the phase shift induced by the object \[1\]. The phase and the negative logarithm of the absorption, \( B(\theta) = -\log(a(\theta)) \), are the projections of the absorption index and refraction index respectively:

\[
B(\theta) = \frac{2\pi}{\lambda} \int \beta(y_\theta, X_\theta) dy_\theta \quad \varphi(\theta) = \frac{2\pi}{\lambda} \int (1 - \delta(y_\theta, X_\theta)) dy_\theta
\]

For parallel beam projection, with a beam parallel to the \( x = (x, y) \) plane and \( f \in L^1(\Sigma) \), the Radon transform is the line integral:

\[
Rf(\theta, p, z) = R_\theta f(p, z) = \int_{\vec{t} \in L(\theta, p, z) \cap \Sigma} f(\vec{t}) d\vec{t}
\]

where \( L(\theta, p, z) \) the line at height \( z \) defined by \( L(\theta, p, z) = \{ \tau \theta^* + p \theta^* : \tau \in \mathbb{R} \} \), with \( \theta = (\cos(\theta), \sin(\theta)) \) and \( \theta^* = (-\sin(\theta), \cos(\theta)) \).

\[1\] With the Radon projection operator, the phase and the absorption can be rewritten \( B(\theta) = \frac{2\pi}{\lambda} R_\theta[\beta](X_\theta) \) and \( \varphi(\theta) = \frac{2\pi}{\lambda} R_\theta[\delta](X_\theta) \). The Fresnel intensity detected at a distance \( D \) after the sample is the 2D convolution, \( I_D(\theta)(X_\theta) = |T_\theta(\theta) * P_D(\theta)X_\theta) |^2 \) where the Fresnel propagator is \( P_D(\theta) = \frac{1}{\pi D} \exp(i \frac{\pi D}{\lambda} |X_\theta|^2) \) \[1\]. The direct nonlinear operator \( I_D[\delta, \beta](\theta, X_\theta) = I_D[\delta, \beta](X_\theta) \) is thus the composition of the Fresnel intensity operator and of the Radon projection operator \[9\].

3. Level-set regularization of in-line phase tomography

3.1. The level-set approach

The phase contrast tomography inverse problem can be regularized with Tikhonov \[9\] or level-set regularization. Level-set methods have been designed to reconstruct piecewise constant solutions of inverse problems \[12, 13\]. We assume that \( \delta \) and \( \beta \) are piecewise constant and that they can take two values \( \delta_1 \), \( \delta_2 \) and \( \beta_1 \), \( \beta_2 \) on disjoint measurable subsets \( \Sigma_1 \), \( \Sigma_2 \) such that \( \Sigma = \Sigma_1 \cup \Sigma_2 \).

The unknown functions \( \delta \) and \( \beta \) are associated with a level-set function of the first order Sobolev space \( \eta \in H_1(\Sigma) \), \( \beta = \beta_1 + H(\eta)(\beta_2 - \beta_1) \) and \( \delta = \delta_1 + H(\eta)(\delta_2 - \delta_1) \). \( H(\eta) \) is the Heaviside distribution, \( H(\eta) = 1 \) if \( \eta > 0 \) and 0 otherwise.

A variational approach is followed and the following \( TV - H_1 \) regularization functional is minimized:

\[
F(\eta) = \| I_D[\eta] - I_{\delta_n} \|^2 + \alpha_1 |H[\eta]|_{TV} + \alpha_2 |\eta|_{H_1}^2
\]

where \( I_{\delta_n} \) are the noisy intensity data, \( \alpha_1 \), \( \alpha_2 \) are regularization parameters. To obtain the minimizers, the following smooth approximations of the Heaviside function \( H \) has been used,

\[
H_\epsilon(x) = \frac{1+2\epsilon}{\pi}(erf(x/\epsilon) + 1) - \epsilon.
\]

The length of the boundary between the sets \( \Sigma_1 \) and \( \Sigma_2 \) is penalized with the TV term.
3.2. Implementation of the nonlinear regularization approach

The TV term is dominated by the Sobolev term and can be ignored in a first approximation. For one projection angle $\theta$, the first order optimality condition obtained with the variation of the regularization functional with respect to $\eta$ can be then written:

$$\delta F[\eta] = I_{D,\theta}^\ast[\eta][I_{D,\theta}[\eta] - I_{\delta u}] + \alpha_2(I - \Delta)[\eta] = 0$$

where $I_{D,\theta}^\ast$ denotes the adjoint of the forward operator with respect to $L_2$ spaces, $I$ the identity and $\Delta$ the Laplacian operators. The update is calculated with a Gauss-Newton by $\eta_{k+1} = \eta_k + \delta \eta$ and $\delta \eta$ is the solution of the linear system:

$$([I_{D,\theta}^\ast[\eta] I_{D,\theta}[\eta]]) \delta \eta + \alpha_2(I - \Delta)\delta \eta = -\delta F[\eta_k]$$

An explicit formula can be derived for the Fréchet derivative of the intensity $I_D[\delta, \beta]$ and its adjoint based on the results obtained for the Tikhonov regularization [9]. Let $T_k = \exp(-B[\beta_k] - i \varphi[\delta_k])$, $U_k = [T_k \ast P_D]$, $\Delta \beta = \beta_2 - \beta_1$, $\Delta \delta = \delta_2 - \delta_1$, the Fréchet derivative of the operator $I_D[\eta_k]$ at the point $\eta_k$ is the operator $I_{D,\theta}^\ast[\eta_k] : L^2(\Sigma) \rightarrow L^2([0, \pi] \times \mathbb{R}^2)$ defined by:

$$I_{D,\theta}^\ast[\eta_k](e) = 2\text{Real} \{(-R_\theta H'_e[\eta_k]\beta + i \Delta \delta \epsilon T_k) \ast P_D]U_k\}$$

where $H'_e$ is the derivative of the smoothed Heaviside function. The adjoint $I_{D,\theta}^\ast[\eta_k] : L^2([0, \pi] \times \mathbb{R}^2) \rightarrow L^2(\Sigma)$ is defined by $I_{D,\theta}^\ast[\eta_k]^\ast(u) = 2\text{Real}(v_1 + v_2)$ with:

$$v_1 = (\beta_2 - \beta_1)H'_e[\eta_k]R_\theta^\ast \{[-u(T_k \ast P_D) \ast P_D]T_k\}$$

$$v_2 = (\delta_2 - \delta_1)H'_e[\eta_k]R_\theta^\ast \{[u(T_k \ast P_D) \ast P_D]T_k\}$$

3.3. Stochastic level-set evolution

The deterministic level-set minimization algorithm may be trapped in local minima. The aim of this work is to obtain a stochastic evolution of the boundary curve to improve the reconstruction image obtained with the deterministic level-set evolution. The evolution of the boundary curve is independent of the level-set function used for its representation with the Stratanovich integral formalism [10]. We thus propose to improve the reconstruction image obtained with the deterministic level-set approach by:

$$d\eta(r, t) = \delta \eta(r, t) + \rho(t)|\nabla \eta(r, t)|o dW(t)$$

where $o$ denotes the Stratonovich convention [19] and $\delta \eta$ is the deterministic change calculated as explained in Section 3.2. We obtain the following Itô stochastic differential equation with the definition of the Stratanovich integral [10, 19]:

$$d\eta(r, t) = \delta \eta + \rho(t)|\nabla \eta(r, t)|dW(t) + \frac{1}{2} \rho(t)(\Delta \eta(r, t) - |\nabla \eta(r, t)|)$$

$$\frac{\nabla \eta(r, t)}{\nabla \eta(r, t)}$$

(9)
In this study, the deterministic level-set and stochastic level-set schemes are applied successively on random time intervals with an intermittent diffusion [17]. For the stochastic evolution, the time interval lengths and the diffusion strengths $\mu$ are chosen at random in the range $[0, T_{max}]$ and $[0, \mu_{max}]$ where $\mu_{max}$ is the scale for the diffusion strength and $T_{max}$ is the scale for the diffusion time.

4. Results and Discussion

4.1. Simulation details

The deterministic and intermittent stochastic level-set algorithms for the refraction index recovery are compared on a multi-material object, with an Al homogeneous cylinder of 20 $\mu$m in diameter and 110 $\mu$m in height embedded in PMMA. Let $\mu = \frac{4\pi\beta}{\lambda}$, the $\delta$ and $\mu$ values used for PMMA and Al for 24 keV X-rays are $4.628 \times 10^{-7}$, $9.396 \times 10^{-7}$ and $41.2$ $m^{-1}$, $502.6$ $m^{-1}$ respectively. The $\beta$ and $\delta$ values were discretized on a regular grid with a pixel size of 1.5 $\mu$m. The cylinder is included in a rectangular volume of size $N_1 \times N_1 \times N_2$ with $N_1 = 74$ and $N_2 = 109$. Horizontal sections of the original maps to be retrieved $\delta^*$ and $\beta^*$ are displayed in Fig.2.

Figure 2. True beta and delta map.

Figure 3. Evolution of the data term $\|I_{D,\phi[\eta]} - I_{\delta_n}\|$ with the iterations for the deterministic (plain line) and intermittent stochastic algorithms (dotted line).

The discrete approximation of the Radon transform is the projection operator implemented in the Matlab Toolbox. The reconstruction was performed with 400 projection angles, the X-ray wavelength $\lambda = 0.5166 \ A$ (24keV) and the distance $D = 100$ mm. The intensity data were corrupted with additive Gaussian white noise with a peak-to-peak signal to noise ratio (PPSNR) of 18 dB. To obtain a good accuracy, the $\epsilon$ parameter was fixed to $\epsilon = 0.03$. The initial level-set function chosen is $\theta_0 = 0$. The regularization parameters were chosen to obtain
Figure 4. Evolution of the normalized mean square error for $\beta$ and $\delta$ with the iterations for the deterministic (plain line) and stochastic algorithms (dotted line).

Figure 5. Reconstructed $\beta$ and $\delta$ maps.

the best decrease of the data term. A first reconstruction is performed with the deterministic algorithm. Then the intermittent diffusion is applied with projection angles chosen at random. For a fixed projection angle, the deterministic and stochastic steps are thus applied successively. The numbers of iterations are chosen randomly with a uniform distribution in $[1, 50]$ and the noise strength in the range $[1, 10^{-3}]$. For the simulation of Eq.(9), we use an explicit scheme with finite differences, the WENO scheme [20] with $\Delta x = 0.1$ and $\Delta t = 0.01$. The level-set function is periodically reinitialized. For comparison, the deterministic level-set algorithm is applied iteratively with projection angles also chosen at random and periodic reinitializations of $\eta$.

4.2. Results
The evolutions of the the relative data term $\|I_{D,\theta}[\eta] - I_{\delta_n}\|/\|I_{\delta_n}\|$ are displayed on Figure 3 for the deterministic and intermittent stochastic algorithms starting from the initial reconstruction. The deterministic minimization can not escape the local minimum corresponding to the initial reconstructed $\delta$ and $\beta$ volumes. A larger decrease is obtained for the deviation between the discrepancy term and the noise level with the stochastic scheme. In order to have a more quantitative information about the efficiency of the method, the evolution of the normalized mean square error using the $L_2(\Sigma)$ norm, $\|\delta^* - \delta\|_2/\|\delta^*\|_2$ and $\|\beta^* - \beta\|_2/\|\beta^*\|_2$, are displayed as a function of the number of iterations for the deterministic and stochastic algorithms on Figure 4. The deterministic algorithm is not efficient to achieve lower reconstruction errors.
On the contrary, the reconstruction errors for $\beta$ and $\delta$ are much reduced with the intermittent stochastic diffusion. Figure 5 displays some horizontal section of the real and imaginary part of the reconstructed index map obtained for the minimum of the discrepancy term. These figures show that the reconstruction errors have been significantly reduced.

5. Conclusion
In this work, we have investigated the nonlinear inverse problem associated to the reconstruction of the real and complex part of the refractive index in phase contrast tomography. The a priori information that the real and imaginary parts $\delta$ and $\beta$ are piecewise constant is introduced and the regularization is performed on the level-set function. The main contribution of this work is to compare the reconstruction results obtained for a deterministic and stochastic evolution of the level-set function on an homogeneous cylinder phantom. The stochastic algorithm is useful to escape the local minimum obtained with the level-set regularization and it leads to a larger decrease of the reconstruction errors localized on the boundaries.

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