Comparison of Optimization Techniques for Regularized Statistical Reconstruction in X-Ray Tomography

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Abstract—Numerical efficiency and convergence are matters of importance for regularized statistical reconstruction in X-ray tomography. We propose a performance comparison of four numerical methods that fall into two categories: first, variants of the SPS framework, a modern take on expectation-maximization-type algorithms, that benefit from acceleration through ordered subset strategies and were developed specifically for tomographic reconstruction; second, Hessian-free general-purpose nonlinear solvers with bound constraints, used to minimize directly the regularized objective function.

The comparison is established on a common target for the noise-to-resolution trade-off of the reconstructed images. The experiments show that while the ordered-subsets separable paraboloidal surrogate iteration variant is the fastest to reach the target, its nonconvergent nature precludes the use of a rigorous stopping rule. Conversely, the other three methods are convergent and can be stopped using a common criterion related to the noise-to-resolution target. Among convergent techniques, general purpose solvers achieve the highest efficiency.

Keywords—X-ray tomography, regularized statistical reconstruction, nonlinear optimization, numerical methods, expectation-maximization, ordered subsets.

I. INTRODUCTION

In X-ray computed tomography (CT), regularized statistical reconstruction methods have proved very useful when the quality of results provided by conventional, analytical methods is insufficient. However, X-ray CT statistical reconstruction is a very large nonlinear optimization problem, generally with bound constraints because of the positiveness of the attenuation coefficients, that needs to be solved efficiently in order for the approach to be attractive. For this reason, development of numerical methods specifically tailored to X-ray CT statistical reconstruction has been actively undertaken by the medical imaging community, and interesting trade-offs between memory footprint, convergence speed and quality of the results have been obtained with techniques such as iterated coordinate descent [1], order subsets expectation-maximization (OS-EM) [2] and extensions thereof.

The nonlinear optimization community has also proposed several methods capable of handling large-scale problems with bound constraints. These methods have been largely disregarded in X-ray CT reconstruction, either because of a high computational burden or because of an awkward and inefficient handling of bound constraints. However, recent advances in nonlinear optimization may make such criticisms less relevant. In addition, to our knowledge, no thorough performance comparison of solvers belonging the above families has been performed in the context of X-ray CT reconstruction. Therefore, the question of the choice of an appropriate optimization method adapted to this problem remains largely open.

The goal of the present study is to provide a partial answer to this question by comparing the behavior and performance of four recent optimization methods suitable for X-ray CT reconstruction. Among those four methods, two were specifically developed for CT reconstruction while the other two are general purpose solvers. Even though the significance of such a study is in essence limited by the number of the methods included in the comparison, it nonetheless provides useful information on the advantages and drawbacks of important families of optimization methods, as well as hints for the selection of an efficient solver in X-ray CT reconstruction.

II. PROBLEM FORMULATION

A. Regularized statistical reconstruction

This study was conducted in a bi-dimensional (2D) framework, under the assumptions that the attenuation coefficients of the object are independent from the energy of the X-ray source, and that the photon counts at the detectors are high. In this case, the data formation process takes the form of the following linear equation:

\[ y = A\mu + n \]  

(1)

where \( y \in \mathbb{R}^N \), \( \mu \in \mathbb{R}^M \) and \( n \in \mathbb{R}^N \) respectively denote the logarithm of the sinogram, the 2D object represented as a map of attenuation coefficients, and additive noise representing the various sources of modeling and measurement errors. \( A \) is the projection matrix that is a discrete approximation of the line integrals over each ray-path.

The inversion was carried out through minimization of the penalized least-squares objective function \( F(\mu) \) defined as:

\[ F(\mu) = \frac{1}{2} \| y - A\mu \|^2_{\Sigma} + \lambda R(\mu) \]  

(2)

where the elements of diagonal matrix \( \Sigma \) are computed as indicated in [1]. The corresponding least-squares term has been shown to be a valid quadratic approximation of the likelihood of \( \mu \) under the assumption of a Poisson distribution of the...
sinogram. $R(\mu)$ denotes a penalty term chosen so as to enforce desirable properties of the solution, and $\lambda$ weighs the two terms of the objective function. Here, in order to preserve the discontinuities present in $\mu$, we selected a differentiable total-variation penalty function acting on $\mu$ and its first differences; therefore, $R(\mu)$ takes the following expression:

$$R(\mu) = \sum_{k=0}^{4} \nu_k \psi[D^{(k)} \mu]$$

with $\psi(u) = \sqrt{u^2 + \eta^2}$

where $D^{(k)}$; $0 \leq k \leq 4$ respectively denote the identity matrix and the first difference operators along the horizontal, vertical and diagonal directions. For any size-$I$ vector $u$, $\psi[u]$ is a shorthand notation for $\sum_{i=1}^{I} \psi(u_i)$; parameters $\nu_k$; $0 \leq k \leq 4$ weigh the five components of the penalty term.

**B. Optimization methods**

The scope of the study was limited to the comparison of two general purpose solvers and two methods developed specifically for CT reconstruction. In addition, in order to make the comparisons meaningful, the algorithms had to lend themselves to simultaneous update of the elements of $\mu$ in accordance with the computer representation and storage chosen for matrix $A$. This rules out schemes of the ICD family [1] in which $\mu$ is updated componentwise. For these reasons, the selected “specific” methods were taken from the SPS family, a recently proposed [3] set of methods based on a preconditioned gradient descent derived from the convexity of $F(\mu)$. Two members of this family are considered here. The first one is OS-SPS, a variant of SPS accelerated by an ordered-subset scheme that also makes the method nonconvergent. The second is TRIOT [4], a convergent extension to OS-SPS that updates the image using a full gradient approximation aggregated from single-subset gradients, which were obtained in previous iterations. As in [4], the implementation of TRIOT considered here is warm-started by running OS-SPS iterations, with TRIOT taking over once OS-SPS enters its limit cycle.

Regarding the general purpose solvers, the choice was guided by the trade-off between the ability of processing large-scale data, the robustness and the appropriate handling of bound constraints. The selected solvers were L-BFGSB [5], a limited-memory quasi-newton method that handle constraints by an active-set method, and IPOPT, an interior point technique that was set up to compute a limited-memory quasi-Newton representation of second-order derivatives.

**C. Implementation**

In order to ensure fairness of the comparisons, all four methods were implemented using the following common scheme: the reconstruction launched from Matlab, with a core loop written in C language. More importantly, the most costly memory and computational operations, i.e., storage of projection matrix $A$ and computation of reprojections and backprojections, were performed using common routines, which were also written in C.

**III. COMPARISON METHODOLOGY**

**A. Numerical phantom design**

The quality of a reconstructed image depends upon several factors such as resolution, residual “noise” present in the reconstruction, ability to render low contrast regions, etc. In order to account for this variety of factors, we designed a numerical phantom with the following structure\(^1\): the background consists of a large ball of water, whose attenuation coefficient is close to that of most soft tissues, in which three concentric rings of circular objects are placed. The inner ring is made up of very small inserts with very-high contrast ($\approx 150\%$) and varying radii; it allows one to assess the response of the reconstruction methods to very small objects that nonetheless have a significant impact on the measurements. The middle ring consists of small inserts with high contrast ($\approx 150\%$) and varying radii; it may be used to assess the resolution of the reconstructed image. The outer ring is made up of large inserts with constant radii and varying low contrasts (0.5% to 10%); it can be used as a contrast response gauge. The phantom is depicted in Figure 1.

\(^1\) Even though the phantom is numerical, it is described in terms of physical materials because the simulation process accounts for the variation of attenuation coefficients with respect to X-ray energy levels.
the object was discretized on a grid at least four times thinner than the one used for the reconstructions. Second, a polyenergetic X-ray source model was selected and discretized at 100 energy levels. Third, for each energy level, the attenuation map of the numeric phantom was computed and projections were performed. The noiseless sinogram was then obtained as the summation of the projections at all energy levels. Finally, a mix of Poisson and Gaussian pseudo-random noise was added to the noiseless sinogram in order to model the various sources of uncertainty that affect actual measurements (e.g., random propagation and detection phenomena, electronic noise, modeling errors).

C. Tuning and stopping rules for reconstruction methods

When the objective function and the experimental conditions are set, each reconstruction method yields a specific sequence of reconstructed images. Thus arises the question as to which image to select in each sequence in order to perform the comparison. Here, we propose an answer based on the following observations:

1) A major characteristic of a reconstructed image is its trade-off between residual noise (i.e., estimation variance) and resolution. Images with similar trade-offs should be selected to perform the comparisons.

2) The distance between a reconstructed image and the true image, i.e., the estimation mean square error (MSE), expresses the variance-resolution trade-off. Therefore, a common stopping rule tied to the estimation MSE should provide reconstructed images suitable for comparison of the reconstruction methods.

3) In [7], we derived a majorization of the MSE of a reconstructed image \( \mu^k \) as a function of the MSE of the global minimum of the objective function. We also showed that, if the following condition is fulfilled:

\[
\| \nabla O F(\mu^k) \|_2 \leq \tau \sqrt{\frac{\alpha \sigma^2}{\| Q^{-1} \|_2} \left( 1 + \frac{M - 1}{\kappa(Q)} \right)}
\]

with \( \nabla O F(\mu) \) the projected gradient of (2), \( Q = \nabla^2 F(\mu^k) \) the Hessian of (2) computed at some early iterate, \( \kappa(Q) = \| Q \|_2 \| Q^{-1} \| \) the condition number of \( Q \) and \( M \) the number of pixels of \( \mu^k \), then the MSE of \( \mu^k \) falls below \((1 + \alpha)\) times the MSE of the global minimum.

Therefore, for all convergent methods, using the common stopping rule (3) will ensure that the corresponding reconstructions present similar noise-to-resolution trade-offs. For nonconvergent methods, stopping rule (3) cannot be used since it may never be fulfilled. Therefore, one must revert to some heuristic assessment of variance and resolution, one of which is described in Section IV-B.

D. Comparison criterion

The main goal of the study is to compare the numerical performance of each of the selected reconstruction methods. Visual examination of reconstructed images, in

<table>
<thead>
<tr>
<th>Penalty Value</th>
<th>Stopping test Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>( \lambda )</td>
<td>0.003 ( \kappa(Q) ) 24.8</td>
</tr>
<tr>
<td>( \eta )</td>
<td>0.002 ( Q^{-1} ) 4170.2</td>
</tr>
<tr>
<td>( \nu_0 )</td>
<td>0.01 ( \sigma^2 ) 0.0024</td>
</tr>
<tr>
<td>( \nu_1, \nu_2 )</td>
<td>1 ( \alpha ) 0.05</td>
</tr>
<tr>
<td>( \nu_3, \nu_4 )</td>
<td>0.707 ( \tau ) 0.017</td>
</tr>
</tbody>
</table>

Once images with similar noise-to-resolution trade-offs are obtained, either through the use of stopping rule (3) or in a heuristic manner, the residual noise (estimated from the uniform water region of the image) and the resolution (assessed through evaluation of the modulation transfer function [8]) are computed independently in order to make sure that they are similar in all reconstructed images. The MTF corresponds to the spectrum of an average 1D projection of the point-spread function (PSF) of the reconstruction process, modeled as a linear degradation of the original image. Assuming that the PSF has compact support and knowing the true phantom image, the PSF is computed by least squares deconvolution of the reconstructed image. The MTF is then obtained by taking the Fourier transform of the average 1D projection of the PSF.

Finally, numerical performance is assessed from the number of reprojection and backprojections that were performed in order to achieve convergence. This alleviates differences in performance appreciation that may arise from implementation issues, as for all considered methods, reprojection and back-projection operations account for more than 80 % of the total runtime.

IV. RESULTS AND DISCUSSION

All experiments were performed on the same workstation (Intel Core 2 Duo 2.83 GHz, 4 GB main memory, GNU/Linux operating system), under minimal load from other processes. Projection matrix \( A \) was built in accordance with the geometry of an actual X-ray CT scanner (fan-beam geometry, 672 detectors, 1160 projections per rotation, angular flying focal spot, 20 cm field-of-view). The entries of \( A \) were computed using a thin, ray-driven assumption and were stored in a parsimonious manner as proposed in [9]. The image size was equal to 512 \times 512, and the signal-to-noise ratio on the sinogram was set to 30 dB. In order to control the parameters of the penalty function and of the stopping rule (3), initial reconstructions were carried out so as to obtain visually satisfying image with respect to both resolution and contrast response. The selected parameter values are reported in Table 1. Then, in a first stage, comparison of convergent methods was performed. The nonconvergent algorithm was included in a second stage, as explained below.

A. Convergent methods

First, we present results that validate performance comparison. The left part of Table 2 reports the variance measured from a uniform water region of the image obtained from each method. Visual examination of reconstructed images, in
(a) L-BFGS-B, showing resolution.

(b) IPOPT, showing resolution.

(c) OS-SPS, showing resolution.

(d) TRIOT, showing resolution.

(e) L-BFGS-B, showing contrast.

(f) IPOPT, showing contrast.

(g) OS-SPS, showing contrast.

(h) TRIOT, showing contrast.

Fig. 2. Images reconstructed from each method under consideration. Images on the left exhibit resolution in the central region, on a [-1000,2850] Hounsfield unit scale. Images on the right show contrast response on a [25,180] Hounsfield unit scale. To the naked eye, these images do not present any significant variations in resolution nor in noise structure.

Table 2. Number of product operations and total runtime for each considered reconstruction method. Among the convergent methods, L-BFGS-B emerges as the fastest, although some nondefault barrier penalty update sequence could make IPOPT more efficient. Nonconvergent OS-SPS was truncated after 116 iterations. While this makes OS-SPS appear as the fastest method overall, the comparison is not fair, since the manual stopping condition asserts convergence differently from the criterion used with convergent methods.

<table>
<thead>
<tr>
<th>Method</th>
<th>Variance (×10^-5)</th>
<th>Proj.</th>
<th>Back.</th>
<th>Total</th>
</tr>
</thead>
<tbody>
<tr>
<td>L-BFGS-B</td>
<td>5.85</td>
<td>193</td>
<td>193</td>
<td>386</td>
</tr>
<tr>
<td>IPOPT</td>
<td>5.56</td>
<td>1005</td>
<td>261</td>
<td>1266</td>
</tr>
<tr>
<td>TRIOT</td>
<td>5.23</td>
<td>833</td>
<td>833</td>
<td>1666</td>
</tr>
<tr>
<td>OS-SPS</td>
<td>5.56</td>
<td>116</td>
<td>116</td>
<td>232</td>
</tr>
</tbody>
</table>

Figure 2, ascertains that noise and artifact structure are similar for each reconstruction method. Also, Figure 3 presents the MTF computed for each image. Differences among computed variance are correlated to differences among MTF curves: lower variance entails lower resolution and reciprocally. Observed differences are negligible, so the noise-to-resolution trade-off for each method is considered equivalent.

The right part of Table 2 shows the breakdown of the product operations that were performed during each reconstruction. The L-BFGS-B is clearly the fastest method, achieving convergence in less than 25% the runtime cost of the other methods. The runtime dominance of general purpose solvers over tailor-made algorithms for CT reconstruction is striking.

However, among matrix-free solvers, limited-memory quasi-Newton algorithms are known to perform consistently well, and more often than not, better than gradient descent methods. It appears to be the case as well for this study.

The large difference in numerical performance between L-BFGS-B and IPOPT is more surprising, since both methods
use limited-memory quasi-Newton updates for the representation of second-order derivatives. Closer inspection of the progress of IPOPT shows that early barrier subproblems are solved at a rather high runtime cost. It is likely that nondefault adjustments of the barrier parameter sequence and subproblem resolution accuracy with IPOPT could yield faster convergence for CT reconstruction, and thus operation counts closer to those of L-BFGS-B.

B. OS-SPS termination and analysis

As mentioned in Section III-C, method OS-SPS does not meet the stopping criterion (3), since it asymptotically cycles between suboptimal iterates that surround the global minimum. However, initial reconstruction experiments suggested that it could yield images of quality equivalent to convergent methods, making its investigation compelling.

It is well known that the cycling behavior of OS methods is composed of interleaved converging subsequences of images (each of which corresponds to the accumulation point of the reconstruction problem formulated with one data subset). We tracked the variance of the images of one of these subsequences over 200 OS-SPS iterations. We observed that, after the tenth iteration, the sequence of variances increased monotonically and converged. We then “stopped” OS-SPS retrospectively at iteration 116, where the variance approached that of the 200th image to within 1%. As observed in Table 2 and Figure 3, the noise-to-resolution trade-off for this image is equivalent to that of the convergent methods.

At first glance, OS-SPS appears as the overall fastest method. However, this conclusion would not result of a fair comparison. Indeed, convergent methods were not closely monitored to stop at the exact iteration where they reach their optimal noise-to-resolution trade-off. Stopping criterion (3) guarantees bounds on the trade-off as measured from the MSE, but not necessarily tight bounds. In other words, convergent methods could have reached a variance within 1% of that reported by Table 2 long before stopping according to (3). Hence, while the computational cost of “convergence” of OS-SPS is precisely accounted, that of the convergent methods is likely overshot.

In addition, even though ordered-subset methods are known to progress quickly to images that are found useful in CT applications, derivation of a useful stopping rule remains an open problem. In practice, heuristics that do not relate iterates to sound optimality conditions or to expected statistical properties are use. Therefore, in spite of their practical advantages, OS methods cannot guarantee that a prespecified noise-to-resolution trade-off target is reached.

V. CONCLUSION

This study addressed the question of the choice of efficient solvers suitable for regularized statistical reconstruction in X-ray CT. The comparison encompassed techniques developed specifically for this application, as well as general purpose methods. Our results indicate that, among the selected algorithms, even though accurate results are quickly obtained with OS-SPS, the lack of convergence of this method which makes it extremely difficult to determine when a specific quality target for the reconstructed image is reached. The other three tested solvers are convergent and a common stopping rule tied to the quality of the reconstruction could be derived. The fastest convergence was achieved by the general purpose L-BFGS-B solver, which proved significantly more efficient than the remaining two methods. These results are confirmed by preliminary results obtained on real tomographic data.

In order to gain in significance, this study should be extended so as to encompass other commonly encountered reconstruction algorithms, such as those of the ICD family or other, modern general purpose descent algorithms such as the one presented in [10]. Inclusion of real data experiments should also provide additional information on the relevance of these optimization technique for statistical CT reconstruction.

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REFERENCES