Stabilizing dual-energy x-ray computed tomography reconstructions using patch-based regularization

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Abstract

Recent years have seen growing interest in exploiting dual- and multi-energy measurements in computed tomography (CT) in order to characterize material properties as well as object shape. Materials characterization is performed by decomposing the scene into constitutive basis functions, such as Compton scatter and photoelectric absorption functions. While well motivated physically, the joint recovery of the spatial distribution of photoelectric and Compton properties is severely complicated by the fact that the data are several orders of magnitude more sensitive to Compton scatter coefficients than to photoelectric absorption, so small errors in Compton estimates can create large artifacts in the photoelectric estimate. To address these issues, we propose a model-based iterative approach which uses patch-based regularization terms to stabilize inversion of photoelectric coefficients, and solve the resulting problem through use of computationally attractive alternating direction method of multipliers (ADMM) solution techniques. Using simulations and experimental data acquired on a commercial scanner, we demonstrate that the proposed processing can lead to more stable material property estimates which should aid materials characterization in future dual- and multi-energy CT systems.

Keywords: dual-energy, computed tomography, regularization, non-local means

1. Introduction

Typical computed tomography (CT) systems provide an image of the spatially varying x-ray absorption within the object being imaged. While CT is a key imaging modality in medical,
security, and non-destructive testing applications, this approach provides minimal information
on material properties. In recent years there has been substantial interest in dual- or multi-
energy CT systems, in which measurements are made either with differing x-ray energy
spectra [1, 2], or using energy-resolving detectors [3]. By exploiting the energy-dependence
of x-ray attenuation, these systems can provide additional, valuable information regarding
object material properties [4, 5].

For dual-energy CT processing, an important first question is the choice of basis func-
tions used to represent the energy dependence of materials. For medical imaging, attenuation
profiles of constituent materials provide useful basis functions [6–8]. Here we are concerned
with airport luggage screening, where the materials being scanned vary more widely. Thus it
is more natural to employ Compton and photoelectric coefficient basis functions, which
capture the dominant x-ray scattering mechanisms in this energy range [1]. In one approach, a
polynomial fit is used to decompose the two collected high- and low-energy sinograms into
separate Compton and photoelectric sinograms [9]. Compton and photoelectric coefficient
images are then recovered via filtered back projection (FBP) reconstructions for each sin-
ogram. This approach was extended by Ying, Naidu and Crawford (YNC) [1], who also per-
form a pre-reconstruction decomposition of the data into Compton and photoelectric
sinograms, followed by FBP reconstruction. YNC obtained improved decompositions by
solving a constrained optimization problem for each point in the sinogram, with non-nega-
tivity constraints applied to all coefficients. A key challenge in any Compton/photoelectric-
based approach is that the data are inherently less sensitive to the photoelectric coefficient (see
[10] for a sensitivity analysis). Thus, YNC applies preprocessing to suppress noise in the
estimated photoelectric sinogram. The YNC method is regarded as state-of-the-art in dual
energy luggage imaging [10].

Several authors have demonstrated that dual-energy imaging performance can be
improved by applying iterative reconstruction [11–13]. Iterative methods offer greater flex-
ibility in system and noise modeling, and incorporate prior information in the form of reg-
ularization terms [14]. Regularization terms may include, for example, L1-type penalties that
encourage sparse solutions or total variation (TV) penalties that encourage piecewise constant
solutions. The TV penalty has been shown to reduce artifacts, especially for sparsely sampled
CT data, in both monoenergetic CT [15–18] and in dual-energy CT [19–21], with the caution
that TV can lead to overly smoothed or ‘patchy’ images for low-SNR data [15]. In addition,
TV penalties must clearly be used with care during reconstruction of textured objects. Thus
there is a need for regularization approaches that can better adapt to the spatial structure of the
scene being reconstructed.

Such an alternative is potentially provided by patch-based regularization [22]. The
concept in [22] is that in some applications, a reference image is available which can be used
to guide the inversion of a less stably estimated image that has similar geometry. Patch
similarities calculated from the reference image capture the location of objects and edges
within the image. These patch similarities are then used in an edge-preserving denosing
algorithm such as non-local means (NLM) [23], thus stabilizing recovery by reducing the
effects of noise on inversion. In most applications, a reference image is not available. Thus in
[22], the reference image was taken to be the estimate from the previous iteration of the image
restoration. This concept has been applied to mono-energetic iterative CT reconstruction [24]
and PET imaging [25]. The method has also been applied to multi-modal reconstruction
problems in CT-SPECT imaging [26], with the CT image used as a reference image whose
geometry can be used to stabilize the SPECT. Because the CT and SPECT images may not be
sensitive to the same features in the image, [26] includes a parameter which indicates how
tightly the two images should be coupled.
Our dual-energy iterative reconstruction approach seeks to use images of stably estimated quantities to guide reconstruction of the photoelectric image. The stably-estimated Compton image is one candidate reference; attenuation estimates provide another. Because materials in luggage have both a Compton and a photoelectric signature, edges or objects present in one image should also be present in the other. Thus unlike with the CT-SPECT problem [26], where there was a need to consider objects that might be visible in one modality but essentially invisible in the other, the dual-energy physics allows us to more tightly couple the two solutions. Our group explored a similar regularization concept in [10], in which we developed a regularization penalty that correlated edge maps of the Compton and photoelectric images. Moving from edge map correlation to a patch-based regularization has two key advantages. First, we are moving from a non-convex regularization to a one that (under conditions discussed below) is convex, which lets us exploit methods such as the alternating direction methods of multipliers (ADMM) solvers. These methods were introduced in the 1970s [27, 28], but have recently become widely used [29] with applications in CT [30] and other inverse problems [31]. Second, we observe a reduction in photoelectric artifacts with the patch-based approach. The previously-used edge correlation method encourages edges to align in Compton and photoelectric, so streak artifacts in the Compton image could be carried over into the photoelectric estimate. In contrast, the proposed patch-based method relies on edge-preserving smoothing. Simulation results below demonstrate that this leads to a reduction in photoelectric streak artifacts.

As photoelectric reconstruction is much more difficult than Compton reconstruction, different regularization strategies may be appropriate. Thus, we propose a framework which applies TV regularization to the Compton image to reduce artifacts, while using patch-based regularization to stabilize the photoelectric image.

Our contributions in this paper are: (1) we describe in detail the regularization strategy described in the previous paragraph, which combines TV and patch-based regularization; (2) we apply the ADMM techniques to the regularized dual-energy reconstruction problem, and (3) we demonstrate the above techniques on both simulated and experimental data, comparing against previous methods [1, 10]. To obtain quantitative results from experimental data (where ground truth is not known), we tabulate the estimated material properties for a set of CT slices with varying clutter but with a set of objects (water, rubber sheets, etc) which are known to be homogeneous and to have identical material properties. Our method leads to material estimates with improved repeatability across slices as well as improved homogeneity within objects.

The structure of this paper is as follows. In section 2, we review the physical model used for polyenergetic, dual-energy CT image formation, and describe the inverse problem being solved. We then describe the unique features of the solution method, namely (a) use of NLM methods to regularize the photoelectric image and (b) an ADMM-based solution technique. Results of applying these methods to data are shown in section 3, and we conclude in section 4.

2. Methods

Typical x-ray sources used in CT applications generate an energy spectrum roughly between 20 KeV and 140 KeV [32]. In this energy range, x-ray attenuation is dominated by Compton scatter and photoelectric absorption effects. We model these phenomena as a product of energy- and material-dependent terms [2] as follows
\[
\mu(x, y, E) = c(x, y)f_{\text{KN}}(E) + p(x, y)f_p(E)
\]  

where \(\mu(x, y, E)\) is the total attenuation and \(c(x, y)\) and \(p(x, y)\) are the material dependent Compton scatter and photoelectric absorption coefficients respectively. The quantity \(f_{\text{KN}}\) is the well-known Klein–Nishina cross section for Compton scattering [10] while \(f_p\) approximates the energy dependency of the photoelectric absorption as \(f_p = E^{-3}\). The units of \(\mu(x, y, E)\) and \(c(x, x)\) are \(\text{cm}^{-1}\) while \(p(x, y)\) has units of \(\text{Kev}^3\text{cm}^{-1}\). For reconstruction, we will discretize the spatial region to be reconstructed. Thus below, \(c\) will represent a discretized version of the Compton coefficient image which is lexicographically unwrapped into a vector, and \(p\) will represent a similarly discretized and lexicographically unwrapped photoelectric image.

The measured quantities for CT are normalized logarithmic projections captured for each of \(M\) different x-ray paths. In dual-energy CT, measurements are repeated for two energy levels (different source settings or different detector filters, depending on the system), so that on the \(i\)th x-ray path we have the measurements:

\[
\begin{align*}
[m_L]_{i} &= -\ln \left[ \frac{Y_L}{Y_{0,L}} \right], \\
[m_H]_{i} &= -\ln \left[ \frac{Y_H}{Y_{0,H}} \right],
\end{align*}
\]

where \(Y_{0,L}\) and \(Y_{0,H}\) are values obtained from a background scan. Measurements for low and high energy source spectra are stacked to create a measurement vector \(m = [m_L^T, m_H^T]^T\) consisting of \(2M\) elements. The data \(Y_L\) and \(Y_H\) are modeled as being Poisson-distributed with Gaussian noise added to represent detector electronics noise [10]. The expected value of the low-energy scan on path \(i\) is modeled as

\[
[\bar{Y}_L]_{i} = \int S_L(E) \exp \left( -f_{\text{KN}}(E)A_{i\ast}c - f_p(E)A_{i\ast}p \right) dE,
\]

where \(S_L(E) > 0\) is the low-energy spectrum at energy \(E\), \(A_{i\ast}\) is the \(i\)th row of the system matrix \(A\) which maps from \(N\) image pixels to \(M\) ray paths (capturing the path length through each pixel corresponding to each raypath), and other quantities are as defined above. For our analysis \(A\) was found using a ray trace approach similar to [33], for a parallel ray path geometry connecting all sources and receivers at every angle, but \(A\) could be calculated for arbitrary source/receiver geometries. The calibration scan is assumed to be constant for all raypaths and is given as

\[
Y_{0,L} = \int S_L(E) dE.
\]

The expected value of the high-energy measurements is found similarly to (2.3) and (2.4) but with an integration over the high-energy spectrum \(S_H(E)\). Note that the data will also include scatter contributions not captured above. However, we neglect scatter here, assuming scatter corrections are applied to measured data in pre-processing [34].

We seek to estimate the Compton and photoelectric coefficients. We can collect these unknowns as:

\[
\theta = [c^T p^T]^T.
\]

Next, we define forward models for the low- and high-energy measurements and collect them as \(K(\theta) = [K_L(\theta)^T, K_H(\theta)^T]^T\). For the \(i\)th raypath, the low-energy model is
where we have replaced the integral over energy in (2.3) by a sum highlighting the fact that for processing, the energy spectrum is discretized into \( N_e \) different values (so \( \Delta E = (E_{\text{max}} - E_{\text{min}})/N_e \), where \( E_{\text{min}} \) and \( E_{\text{max}} \) are the lowest and highest energies in the spectrum). \( \mathbf{K}(\theta) \) is found similarly but involves a summation over \( S_i(E) \). Since the log of a sum of exponentials is a convex function, and the exponents here are affine functions of \( \mathbf{c} \) and \( \mathbf{p} \), we can conclude that \( -\mathbf{K}(\theta) \) is jointly convex in both \( \mathbf{c} \) and \( \mathbf{p} \) [35]. Next, we define a weighted least squares data fidelity term, derived by Sauer and Bouman [36] as a quadratic approximation to the Poisson log-likelihood function:

\[
F_{\text{DF}}(\theta) = \frac{1}{2} (\mathbf{m} - \mathbf{K}(\theta))^T \Sigma (\mathbf{m} - \mathbf{K}(\theta))^T
\]

\[
\equiv \frac{1}{2} \mathbf{e} \Sigma \mathbf{e}^T
\]  

(2.7)

where \( \mathbf{e} = \mathbf{m} - \mathbf{K}(\theta) \) is the data-model error and \( \Sigma \) is a positive definite diagonal matrix whose diagonal entries are the normalized number of detected counts (i.e. the arguments to the log functions from (2.2)). This preferentially weights measurements with high counts, corresponding to ray paths where attenuation is low and therefore signal-to-noise ratio is high. We note here that, like (2.6), \( F_{\text{DF}} \) in (2.7) remains convex in \( \theta \). As (2.7) is a quadratic form with a positive definite weighting, it is convex in \( \mathbf{e} \). Further, as the weighting matrix \( \Sigma \) is both diagonal and non-negative, (2.7) is also non-decreasing in \( \mathbf{e} \). Since \( \mathbf{e} \) is an affine transformation of \( -\mathbf{K} \) and hence is jointly convex in \( \mathbf{c} \) and \( \mathbf{p} \), according to the composition rule [35], the overall data fidelity term is jointly convex in \( \mathbf{c} \) and \( \mathbf{p} \). This form of data fidelity term was previously used in dual energy CT [11]. Finally, the overall inverse problem combines the data fidelity term with regularization terms:

\[
\arg \min_{\theta} F(\theta) = F_{\text{DF}}(\theta) + \lambda \| \mathbf{D} \mathbf{c} \|_1 + R_{\text{NLM}}(\| \mathbf{p} \|_{\text{ref}})
\]

subject to \( \mathbf{c} \geq 0 \)  

(2.8)

where the second and third terms are regularization terms, whose convexity is discussed below. The non-negativity constraint is imposed on the Compton image, as we rely on patch-based regularization for stabilizing the photoelectric coefficients.

The second term in (2.8) imposes a TV penalty on the Compton coefficient image, encouraging solutions that are piece-wise constant. \( \mathbf{D} \) is an \( 2N \times N \) difference matrix which computes derivatives in the x and y directions (so \( \mathbf{D} = [\mathbf{D}_x; \mathbf{D}_y] \), where \( \mathbf{D}_x \) and \( \mathbf{D}_y \) are difference matrices in the x and y directions respectively). As noted above, TV regularization has been widely applied to CT inversion problems and is a convex regularization [35].

Finally, the \( R_{\text{NLM}} \) term in (2.8) conditions the photoelectric estimate on a reference image \( \mathbf{I}_{\text{ref}} \), which may be either a FBP reconstruction or the previous iteration’s Compton estimate. \( R_{\text{NLM}} \) and its convexity are further discussed in the next section. The overall model also

\[1\] See example 3.14 of [35]. Because \( \ln(\sum_{i=1}^{N_e} e^x) \) is convex and nondecreasing in each argument, \( \ln(\sum_{i=1}^{N_e} e^x) \) is convex by vector composition when the \( R_i \) are convex, which is the case here.
depends on knowledge of the source spectrum and system matrix, although these are assumed
known and therefore are not shown explicitly.

2.1. Patch-based regularization of photoelectric image

Our group’s previous work used an edge-correlation regularization term to stabilize the
photoelectric image. This term, written using a pixel-wise representation of the image, is
given as [10]

$$R_{\text{edge}}(c, p) = \lambda_{\text{edge}} \left[ \left( \frac{Dc \cdot Dp}{(Dc^T Dp)^{1/2}} - 1 \right)^2 \right]$$  (2.9)

This penalty term has the desirable property that it decreases as the correlation of the gradients
increases in negative or positive direction and vanishes when they are perfectly correlated or
anti-correlated. However, it is not convex in \(c, p\).

Instead, here we apply a NLM regularization approach, which helps to reduce noise
artifacts in the recovered image by building a denoising step into the inversion. Preliminary
work on patch-based regularization was presented in a conference [37], but did not include
TV regularization or the ADMM formulation outlined below. Similar to [22], we define a
discrete form of the regularization term \(R_{\text{NLM}}\) by summing over pixels \(k\):

$$R_{\text{NLM}} = \lambda_{\text{NLM}} \sum_k (p_k - \text{NLM}^{\text{Ref}}(p_k))^2 \equiv \lambda_{\text{NLM}} \sum_k \delta_k^2$$  (2.10)

where \(\text{NLM}^{\text{Ref}}(p)\) represents NLM averaging of the photoelectric image. The superscript ‘Ref’
denotes that smoothing weights are calculated from a reference image \(I^{\text{ref}}\) (and below, the \(k\)th
pixel of this image is denoted as \(I_k^{\text{ref}}\)). This regularization encourages the photoelectric
estimate to converge towards a smoothed version of itself, but with smoothing done in an
edge-preserving manner so that important image details are retained. For later convenience, \(\delta_k\)
has been defined as a ‘difference image’, i.e. the difference between the smoothed and
unsmoothed solutions.

The denoised image \(\text{NLM}^{\text{Ref}}(p)\) is found using the NLM method developed in the image
denoising literature [22, 38]. In this approach, each pixel location \(k\) is associated with a patch,
typically a square region centered on the pixel. The NLM kernel calculates the weights based
on measures of similarity between patches. The most common similarity measure is mean-
squared difference [39], for which the NLM kernel is:

$$K_{\text{NLM}}(k, l, I^{\text{ref}}) = \exp \left( -\frac{\sum_{\delta \in \Delta} \left( I^{\text{ref}}_{\Delta(k+\delta)} - I^{\text{ref}}_{\Delta(l+\delta)} \right)^2}{2L^2 \beta^2} \right)$$  (2.11)

(note [40] defined the denominator above as \(h^2\)). In (2.11), \(\beta\) is a bandwidth parameter, while
\(\Delta\) represents a local patch of pixels surrounding \(k\), containing \(L\) pixels; a patch of the same
shape also surrounds \(l\), and \(\delta\) indicates the offset from each patch center. While the results are
most sensitive to the bandwidth parameter \(\beta\), it is also important that the patch size be
comparable to the smallest features of interest. Parameter selection for dual-energy CT is
discussed below.

The NLM kernel, calculated from a reference image \(I^{\text{ref}}\), is then used to compute the
regularization term. In dual-energy CT, several choices for \(I^{\text{ref}}\) are possible. FBP recon-
structions of single-energy scans provide computationally cheap reconstructions of image
geometry, so one choice is to take \(I^{\text{ref}} = I^{\text{FBP}}\), where the FBP reconstruction \(I^{\text{FBP}}\) can be
computed from either the high- or low-energy scan. With this choice, the smoothed photo-
electric image in (2.10) is explicitly given as

$$N_{\text{FNP}}(p_k) = \frac{1}{Z_k} \sum_{l \in N_{\text{FNP}}(k)} K_{\text{NLM}}(k, l, p_{\text{FNP}}) p_l$$

(2.12)

where $Z_k = \sum_{l \in N_{\text{FNP}}(k)} K_{\text{NLM}}(k, l, p_{\text{FNP}})$ is a normalizing term. Thus, (2.12) represents a weighted average of $p$ and is convex in $p$. Here, $N_{\text{FNP}}$ is the neighborhood of pixels over which averaging should be done. If similar patches can be found throughout the image, then ideally $N_{\text{FNP}}$ is the entire image, so the averaging is fully non-local. In practice, $N_{\text{FNP}}$ is usually limited to reduced computational load [23].

We have also explored using the Compton image from the previous iteration as a reference. Empirically, we observe that the Compton image converges within a few iterations to a solution which closely mirrors the geometry of FBP. While the approach of taking the previous iteration’s estimate as a reference for non-local regularization has been used previously [41–44], convergence proofs have not been established [25]. Thus we use an attenuation image from FBP as reference for most of our solutions, and discuss use of a Compton reference in section 4.

### 2.2. ADMM reformulation

We apply an ADMM approach to dual energy-reconstruction, that is similar to previous approaches for monoenergetic CT [30] but has been expanded by introducing separate equations solving for Compton and photoelectric coefficients, and by introducing non-negativity constraints. Details of the modified solution method are shown in the appendix. Briefly, the problem in (2.8) can be reformulated as follows: we define $z = [t^T u^T v^T s^T]^T$ as a vector of auxiliary constrained variables. These are related to the original parameter vector $\theta$ (from (2.5)) as $z = C \theta$, where $C = [I_N \ 0_N; \ 0_N \ I_N; \ D \ 0_N; \ I_N \ 0_N]$, where $I_N$ is an $N \times N$ identity matrix and $0_N$ is an $N \times N$ matrix of zeros, $D$ is the TV difference matrix, and $0_N$ is a vector of zeros of the dimension of $D$. Thus, $t$ and $u$ are auxiliary variables for the Compton and photoelectric images respectively, $v$ is related to the TV constraint, and $s$ captures non-negativity constraints on the Compton image. Using an FBP reference image for NLM, the overall problem can be written as:

$$\arg \min_z f(z) = \frac{1}{2} \left\| m - K(t, u) \right\|_W^2$$

$$+ \lambda_{\text{TV}} \sum_{k=1}^N |v_k| + \Psi_{\text{NLM}}(u|p_{\text{FNP}}) + g(s)$$

(2.13)

subject to

$$z = C \theta. \quad (2.14)$$

where $g(s)$ is an indicator function for the non-negative orthant. Because $C$ is full column rank and $f(z)$ is convex, Theorem 1 of [30] states that the solution to (2.13)–(2.14) will converge to the solution of (2.8). Solution details are in the appendix.

### 3. Results

Here we present processing results for both simulated and experimental data for the Imatron C300 CT scanner. We first briefly discuss the Imatron system geometry and energy spectra.
used, then discuss parameter selection and comparison. Extensive documentation on the scanner measurement campaign is available at [45]. We then demonstrate qualitative improvements in image quality and quantitative improvements in image metrics.

3.1. Description of Imatron C300 system

Data were acquired from a set of dual-energy scans performed on the Imatron C300 CT scanner. This commercial single-energy scanner (developed for the cardiology market) was re-purposed for dual-energy scans by performing sequential scans of each object, with x-ray source voltage adjusted between scans. In all cases here, the registration between the sequential scans appears excellent. The Imatron scanner performs helical scans, with the source scanning through 2588 source positions covering 210 degrees, with measurements made on 864 detector channels. The Imatron system software can be used to output a wide variety of intermediate results, ranging from raw data to single-energy FBP reconstructions. While the regularization methods we present are applicable to general geometries, we chose to work with sinograms where data was rebinned into a parallel beam geometry, with scatter corrections applied to the data.

One disadvantage of re-purposing a standard scanner to acquire dual-energy data is that the x-ray source energies cannot be tuned over as wide a range as would be typical for a dedicated dual-energy system. Figure 1 shows the estimated high- and low-energy spectra for our data, modeled based on detector settings. The significant overlap between the spectra makes the decomposition problem more ill-posed than it would be if scan energies were better separated.

3.2. Parameter selection and legacy method comparison

The regularization approach outlined above requires selection of the weights for TV and NLM penalties ($\lambda_{TV}$ and $\lambda_{NLM}$) and denoising parameters for NLM (bandwidth $\beta$, patch size, and search neighborhood). Methods for optimizing regularization parameter selection exist, including L-curve and generalized cross-validation, as discussed in [10]. NLM denoising parameter selection can be approached by minimizing Stein’s unbiased risk estimate [39], potentially in combination with additional constraints [46]. However, the above-discussed methods are not straightforward to apply. Because our present goal is a proof of concept that

Figure 1. Normalized x-ray energy spectra for high- and low-energy scans.
our approach offers potential benefits, we instead manually tuned parameters based on visual inspection of the results. NLM parameters were selected to give good denoising of typical Compton images from our dataset (i.e., results that were visually judged to reduce noise without smearing small object details). The motivation for this approach is that parameters which create weights that lead to good Compton denoising should successfully capture image structure, and are therefore also appropriate for photoelectric regularization. We found $\beta = 0.5e^{-4}$, 7 pixel $\times$ 7 pixel patches, and 19 pixel $\times$ 19 pixel search neighborhoods to be a good choice across the images examined. In addition, because many objects in our experimental dataset have texture, we set the TV penalty weight to be low ($\lambda_{TV} = 0.01$). We used these values across all images instead of re-tuning to optimize individual images.

We compare our results against an implementation of the YNC dual-energy method [1]. Our implementation of YNC includes the photoelectric denoising step proposed in [1], but does not apply the calibration steps discussed in [1]. Our proposed dual-energy results also are uncalibrated, which aids side-by-side comparison. YNC solves a constrained least-squares problem for each point in the sinogram and applies non-negativity constraints. This constraint is applied by first solving an unconstrained problem, then zeroing out one of the coefficients if negative results are obtained. The presence of zeros in the sinogram can produce substantial reconstruction artifacts. To address this, we applied an inpainting algorithm [47] to interpolate across zeroed points in the sinogram. We note that these artifacts are greater in our system than in systems designed specifically for dual-energy, because the relatively low energy separation between the two scan energies.

### 3.3. Simulation results

Dual-energy data were simulated for a suitcase phantom scanned with the Imatron C300 scanner, assuming the spectra in figure 1. Gaussian noise was added to the Poisson-distributed simulated data to achieve 70 dB signal-to-noise ratio for electronics noise. The phantom suitcase consists of a polyethylene outer case surrounding an aluminum block (center of image), a C-shaped neoprene rubber sheet, and water in a container (upper right). Table 1 describes the materials used in simulation in more detail.

Table 1. Compton and photoelectric coefficients of objects in suitcase phantom.

| Object | Material | Compton cm$^{-1}$ | Photoelectric, KeV$^3$ cm$^{-1}$ |
|--------|----------|-------------------|----------------------------------|
| Case   | Polyethylene | 0.16 | 1765               |
| Block  | Al       | 0.37 | 72435              |
| Water  | H$_2$O   | 0.16 | 5275               |
| Sheet  | Neoprene | 0.21 | 30717              |

Figure 2 shows Compton (left) and photoelectric (right) coefficient images for a series of reconstruction approaches. Compton images are plotted on the range 0–0.7 cm$^{-1}$, while photoelectric images are plotted for the range 0–8 $\times 10^4$ KeV$^3$ cm$^{-1}$. The upper row in figure 2 shows the ground truth, while the second row shows YNC results. While the Compton image is partially recovered by YNC, there is essentially no structure in the recovered photoelectric image. The third row shows the edge-correlation approach of (2.9), proposed in [10]. The photoelectric image is greatly improved, but there is noticeable noise in the image and the outline of the object to the upper right (simulated water bottle) is obscured.

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Figure 2. Compton images (left) and photoelectric images (right) for suitcase phantom. Top row (a), (b) is ground truth; 2nd row is the YNC result; 3rd row is Levenberg–Marquardt solution, using the edge-based regularization of [10]; 4th row is the proposed ADMM solver with patch-based regularization of photoelectric; and bottom row is the proposed method but additionally applying total variation regularization to the Compton image.
Using our proposed patch-based regularizer in the ADMM framework we obtain the fourth row in figure 2. The NLM regularizer leads to a much smoother photoelectric estimate while the Compton image is little changed. In this result we apply non-negativity constraints to the Compton image but do not apply the TV penalty. Because the edge-based regularizer encourages photoelectric solutions with similar edges to the Compton image, any streak artifacts in the Compton image will tend to appear in the photoelectric image (subfigure (f)). The NLM regularizer, by contrast, encourages averaging during the photoelectric reconstruction of patches that are similar in the reference image, but is less likely to map streak artifacts from Compton to photoelectric (subfigure (h)). Finally, the last row in figure 2 shows our proposed method which additionally includes TV regularization of the Compton image. The TV penalty leads to a more homogeneous Compton image for the aluminum block.

Figure 2 shows all iterative methods over-estimate the photoelectric coefficient of the outer case. The overall solution accuracy is dominated by objects such as the aluminum block, which is large and has high coefficient values, so estimation of small, low-coefficient objects such as the outer case is challenging. To understand this, we examined the photoelectric estimate for ADMM with no regularization. Visually similar to figure 2(f), this estimate showed that the high coefficient values of the aluminum block were smeared across the image. Adding NLM regularization reduces estimated values for the case by roughly fourfold, reducing but not eliminating the overestimate.

Because ground truth is known in simulation, the reconstructions methods can be compared using metrics such as peak signal-to-noise ratio (PSNR) and the structural similarity index (SSIM) [48]. PSNR compares image $I$ to reference image $I^{ref}$ as

$$
\text{PSNR} = 10 \log_{10} \frac{L^2}{\frac{1}{N} \sum_k (I_k - I_k^{ref})^2}
$$

where $L$ is the expected maximum value in the image, taken here $L$ to be 0.7 for Compton images and $1.2 \times 10^5$ for photoelectric images, values chosen as they exceed the maximum values in any of the estimated images. Table 2 shows the PSNR AND SSIM metrics corresponding to figure 2. The two patch-based regularization solutions are similar and outperform the other options, with the greatest gain seen versus YNC as expected.

3.4. Experimental data

A series of test suitcases were assembled and scanned on the Imatron scanner, as described in [45]. The bags included clothing and consumer items as well as liquids, bottles, and rubber sheets. The experts also identified a set of homogeneous objects (water, doped water, and rubber sheets) which are seen in multiple scans and have identical material properties. These materials allow quantitative comparison of various methods, as reconstructions ideally should produce material parameter estimates for these objects which are homogeneous within a scan and repeatable between scans.

3.4.1. Individual slices. Figures 3, 4, and 5 show processing results for three slices taken from different bags. In each figure, Compton estimates are on the top row while photoelectric estimates are on the bottom. Each column in the figure (Compton/photoelectric pair) demonstrates results from a different processing method. Because each data case highlights a different issue, the processing methods used may vary between figures (thus for example, the left-most columns in figures 3 and 4 were generated from different methods). For all results, the NLM parameter $\beta$ was tuned as discussed above. TV and NLM penalties were assigned
values of $\lambda_{TV} = 0.001$ and $\lambda_{NLM} = 50$ based on visual inspection of a number of slices in the dataset (not just those shown here).

Figure 3 shows a fairly typical comparison between the legacy YNC method (left column) and the proposed method (middle column). YNC provides a good-quality Compton reconstruction, but the YNC photoelectric reconstruction is extremely corrupted by noise so that significant features (for example, the circular water bottle in the lower right of figure 3) are obscured. By contrast, the proposed method provides a much stabler photoelectric reconstruction, which is important as materials characterization is based on both Compton and photoelectric estimates [1].

Because YNC provides a high-resolution although noisy reconstruction, one valid question is whether or not the two methods are being compared at different operating points. To address this question, we filtered the legacy YNC result with an edge-preserving bilateral filter [49, 50], tuning the filter parameters to minimize the mean-squared error between Compton images for our proposed approach and the filtered YNC result. The resulting filter parameters were then used to produce the filtered YNC images shown in the right-most column in figure 3. As can be seen, while the resulting Compton image in (c) more closely
Figure 4. Packed suitcase including metal cooking pots, sinogram angles subsampled by factor of 10. Compton images are on top row, photoelectric on bottom. Left column (a), (d) has very low regularization; middle column (b), (e) includes regularization on photoelectric image ($\lambda_{TV} = 0$, $\lambda_{NLM} = 50$); right column (c), (f) additionally includes TV regularization on Compton coefficients ($\lambda_{TV} = 0.01$, $\lambda_{NLM} = 50$).

Figure 5. Packed suitcase including rubber sheet and metal objects. Compton images are on top row, photoelectric on bottom. Left (a), (d) are legacy; middle (b), (e) are iterative results with proposed regularization; right (c), (f) are the proposed method but with very low regularization. Streaks due to metal artifacts are apparent but appear not to be caused by regularization.
resembles the result in (b), the photoelectric estimate in (f) is still extremely corrupted by noise.

We next highlight the relative impact of the regularization terms by constructing a sparse-view scenario where there is a greater need for regularization. We subsampled the Imatron sinograms by selecting every 10th angle, reducing the sinogram from 720 angles to 72. The system model was similarly decimated, and the reconstruction code was otherwise unchanged. Reconstructions using the ADMM solver are plotted in figure 4, for three parameter settings: no regularization (left), patch-based regularization of the photoelectric image but no TV (middle), and the proposed method with both forms of regularization (right). In this case we apply a higher TV penalty to make the impact of TV more visually apparent. Applying the patch-based regularization reduces small ripples in the estimated photoelectric image, but also smears structure across the image. Addition of TV regularization cleans up the Compton image and further improves the photoelectric image, which is sensitive to the Compton solution.

Finally, figure 5 shows a challenging case where metal artifacts are significant. As before, the proposed photoelectric reconstruction is much more stable than the YNC result. However, the proposed Compton reconstruction exhibits higher metal artifacts than the YNC method. To investigate whether this is a result of our proposed regularization methods, we reprocessed this case but reduced the regularization constants by a factor of 100 (so $\lambda_{TV} = 10^{-4}$, $\lambda_{NLM} = 0.5$). The resulting images, in the rightmost column, show that the metal artifacts are basically unchanged, indicating they do not appear to be a result of the regularization. Instead, the artifacts appear to result from metal-generated inconsistencies in the data which affect the both Compton and photoelectric reconstructions, which are coupled in the proposed method. Metal artifact reduction (MAR) is discussed further in the next section.

3.4.2. Uncertainty clouds for material estimates. To provide quantitative measures of image improvement, manual segmentations of homogeneous test objects were created for water, doped water, and rubber (neoprene sheets) objects; examples of each type of material were pulled from separate scans. Examples of these objects include the rubber sheets and water containers shown in figures 3 and 5.
For both the legacy YNC and our proposed method, the estimated Compton and photoelectric coefficients were extracted for all pixels within each of the manually segmented objects, and the mean and standard deviation were calculated. Ideally, the mean values should be repeatable for all objects made of the same material, and the standard deviation should approach zero as objects are homogeneous. The calculated mean and standard deviations were used to generate parameter ‘clouds’ for Compton and photoelectric estimates, as shown in figure 6. Results are shown for legacy results (a) and the approach developed here (b). Here, each ellipse corresponds to one segmented object. The object centroid is set by the mean Compton and photoelectric values in the object, while the ellipses extend to mean ±1 standard deviation. The material type is coded by color (water, doped water, and rubber).

In the legacy results (subfigure (a)), Compton is observed to have much lower variation about the mean than PE, as the standard deviations in estimated PE are very large. The proposed method (subfigure (b)) stabilizes the PE image, reflected in lower PE standard deviations. Material separation between rubber and water is relatively good, with the two outliers being the rubber and water objects labeled as Slice 281. Inspection of this slice, previously shown in figure 5, shows that streaking artifacts generated by metal are present, affecting material estimates. These effects could be mitigated by explicitly incorporating MAR [51, 52] into the processing.

4. Discussion and conclusions

This paper has outlined an iterative image formation approach for dual-energy CT data. In this work, we used patch-based regularization to stabilize the poorly estimated photoelectric image based on the much more stably estimated Compton image, and demonstrated improvements on both simulated and actual data. We further demonstrated that using this approach in conjunction with TV denoising of the Compton image leads to additional image improvements. We extended previous work using the ADMM method to dual-energy CT. An important advantage of ADMM is that can be used to create parallelizable implementations [29]. Finally, we compared our method to a state-of-the-art sinogram decomposition method and show improved homogeneity and reduced noise, particularly in recovered photoelectric images.

As noted above, several choices of reference image exist. The results above used the FBP attenuation image estimate to give a convex regularization term. Empirically, we have found good results by using NLM weights estimated from the previous iteration’s Compton estimate. While we were not able to prove convergence for this approach, we note that it differs from other methods [41–44] which use a previous iteration’s estimate as a reference image. In those approaches, a single image is being estimated, so there is a strong coupling between solution estimates at each iteration. In our case, we base our reference on the Compton image, which is relatively insensitive to the photoelectric estimate and converges more rapidly. This more rapid convergence is shown in figure 7(a), with differences between each Compton iteration being roughly an order of magnitude smaller than changes in the photoelectric estimates. We also found that NLM weights computed from Compton become essentially constant within 3–4 iterations (not shown here). For our data set, use of the Compton estimate leads to improved separability of material estimates, shown in figure 7(b), primarily because the combination of dual-energy processing and TV regularization for Compton helps to mitigate metal artifacts. Thus if possible, a valuable future contribution could be establishing a convergence proof for problems of this type.
We see several promising additional areas for future research. First, we did not include MAR steps in our processing, and the effects of metal can be noticeable, for example in figure 5. Our approach to regularizing the photoelectric image depends on good structural information being available, which is not a good assumption when metal artifacts are large. Thus it would clearly be beneficial to combine methods previously developed for MAR \cite{51, 52} with the reconstruction approaches outlined above. Second, patch-based regularization may help to improve performance of pre-reconstruction decomposition methods such as Ying et al \cite{1}, by reducing the effects of noise. Finally, it should be possible to extend these concepts to multi-energy CT data collected using energy-discriminating detectors.

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Appendix: ADMM solution details

Continuing from (2.13) and following \cite{30}, we form the augmented Lagrangian (AL)

$$\mathcal{L}(\theta, z, \gamma, \mu) \triangleq f(z) + \gamma^T \Lambda(z - C\theta) + \frac{\mu}{2} \| z - C\theta \|_N^2$$  \hspace{1cm} (A.16)
where the second term is the Lagrangian term, and the last term is an augmented term which is known to improve the convergence of the problem. One difference of the equation above from the standard AL discussed in [29] is the introduction of $\Lambda$. This matrix is introduced by Ramani and Fessler [30] to balance the sub-matrices in $C$, because the terms $D$ may be orders of magnitude different from unity. In our case this term would be $\Lambda = [I_N 0_N 0_N; 0_N I_N 0_N; 0_N 0_N \sqrt{\nu_0} I_N]$ where $\nu$ is a scaling constant. $\nu$ and also $\gamma$ affect only the convergence rate, not the final answer, and guidelines for choosing them exist [30]. $\Lambda$ can be absorbed into the quadratic penalty by defining $\eta = \frac{1}{\lambda} \Lambda^{-1} \gamma$. As shown previously in [30], the AL becomes (dropping constant terms that do not affect the solution)

$$L(\theta, z, \gamma, \mu) = f(z) + \frac{\mu}{2} \| z - C\theta - \eta \|^2_{\mathbb{R}^N}$$ \hspace{1cm} (A.17)

For convenience, the vector $\eta$ can be written as $\eta = [\eta^T, \eta^T, \eta^T, \eta^T]^T$ to emphasize the terms associated with each auxiliary variable. Finally, we use the ADMM setup to solve the problem using an alternating minimization scheme:

$$t^{(j+1)} = \arg \min_t L(\theta^{(j)}, t^{(j)}, u^{(j)}, v^{(j)}, s^{(j)}, \gamma^{(j)}, \mu)$$ \hspace{1cm} (A.18)

$$v^{(j+1)} = \arg \min_v L(\theta^{(j)}, t^{(j+1)}, u^{(j)}, v^{(j)}, s^{(j)}, \gamma^{(j)}, \mu)$$ \hspace{1cm} (A.19)

$$s^{(j+1)} = \arg \min_s L(\theta^{(j)}, t^{(j+1)}, u^{(j)}, v^{(j+1)}, s^{(j+1)}, \gamma^{(j)}, \mu)$$ \hspace{1cm} (A.20)

$$u^{(j+1)} = \arg \min_u L(\theta^{(j)}, t^{(j+1)}, u^{(j+1)}, v^{(j+1)}, s^{(j+1)}, \gamma^{(j)}, \mu)$$ \hspace{1cm} (A.21)

$$\theta^{(j+1)} = \arg \min_\theta L(\theta^{(j)}, t^{(j+1)}, u^{(j+1)}, v^{(j+1)}, s^{(j+1)}, \gamma^{(j)}, \mu)$$ \hspace{1cm} (A.22)

$$\eta^{(j+1)} = \eta^{(j)} + (z^{(j+1)} - C\theta^{(j+1)})$$ \hspace{1cm} (A.23)

Let us consider these problems one at a time. (A.18) updates the Compton image coefficients. Solving this first is a natural choice, as the Compton image is the most stable. Dropping constant terms, we seek to minimize:

$$\arg \min_{t^{(j+1)}} \frac{1}{2} \| m - K(t^{(j+1)}, u^{(j)}) \|_W^2 + \frac{\mu}{2} \| t^{(j+1)} - c^{(j)} - \eta^{(j)} \|^2_{\mathbb{R}^N}$$ \hspace{1cm} (A.24)

where the constraint terms (2nd term) are simplified because the weights in $\Lambda$ are 1 for the terms in $t$, and we can use the fact that $c^{(j)} = \theta^{(j)}(1 : N_\theta))$. This problem is a weighted non-linear least-squares problem and can be solved using standard approaches [10], projecting the result into the non-negative orthant. In doing so, we need to calculate the derivative terms $\frac{\partial L}{\partial t}$.

This derivative is the derivative of the data fidelity terms (calculated in [10]) and the derivative of the AL. The AL derivative terms gives a contribution which is added to every element of $\frac{\partial L}{\partial t}$:

$$\mu \sum_k (t^{(j+1)}_k - c^{(j)}_k - \eta^{(j)}_{t,k})$$ \hspace{1cm} (A.25)

where $k$ is pixel number. Next, (A.19) seeks to minimize the sum of the TV term and the relevant terms in the $\|z\|_* \text{term in (A.17)}$. As shown in Boyd et al [29], it is solved by soft thresholding, on a term-by-term basis:
The argument of the softmax function $S_{\text{TV}/(\mu \phi)}$ is found by setting the constraint term $(z - C \theta - \eta)$ to zero and solving for $v$ (ignoring the other terms in $z$). A similarly simple solution is found for (A.20), which imposes the non-negativity constraint by projecting onto the non-negative orthant [29]:

$$s^{(j+1)} = \max \{ 0, c^{(j)} + \eta \}$$  \hspace{1cm} (A.27)

Next, (A.21) updates the photoelectric image coefficients. It solves a similar problem to that addressed when solving the Compton coefficients:

$$\arg \min_{\mathbf{u}^{(j+1)}} \frac{1}{2} \| \mathbf{m} - K (t^{(j+1)}, \mathbf{u}^{(j+1)}) \|_W^2 + \Psi_{\text{NLM}}(\mathbf{u}^{(j+1)}|t^{(j+1)}) + \frac{\mu}{2} \| \mathbf{u}^{(j+1)} - \mathbf{p}^{(j)} - r^{(j)} \|_2^2$$

(A.28)

The key difference is that this problem involves the NLM regularization term; here, the weights in NLM are calculated from the reference image. This term’s contribution to the Jacobian can be shown to be [37]

$$J_{\text{NLM}}(i) = \frac{\partial R_{\text{NLM}}}{\partial p_i} = 2 \left( \delta_i - \sum_k w^{(C)}_{ik} Z_k \right)$$

(A.29)

Here, note that the second term is equal to a NLM-smoothed version of the difference image $\delta_k$ (defined in (2.10)). Thus, it can easily be found by calling the NLM code twice, using the reference image from the previous iteration in both cases to calculate weights. Like (A.18), this can be solved using Levenberg–Marquart. Here, the AL adds a term to every element of $\partial J / \partial u_i$:

$$-\mu \sum_k \left( u_k^{(j+1)} - p_k^{(j)} - r_{ik}^{(j)} \right)$$

(A.30)

(A.22) applies the constraints to adjust $\theta$ into agreement with the auxiliary variables. This leads to a weighted least squares problem:

$$\arg \min_{\mathbf{z}^{(j+1)}} \| \mathbf{z}^{(j+1)} - C \theta^{(j+1)} - \eta \|_X^2$$

(A.31)

Finally, (A.23) updates the Lagrange multipliers. The solution continues until a preset number of iterations is exceeded, or residuals fall below a threshold [29].

We found the TV term to require many iterations to converge. However, a single iteration of the TV term is very cheap to calculate, as is a single iteration of the non-negativity term, whereas a single iteration of the Compton or photoelectric terms is very expensive. We therefore modify the approach above to complete many TV and non-negativity iterations after each Compton update. The terms involving $v$ and $s$ in (A.22) and (A.23) are updated while other parameters are held constant.

**Computation:** because of our problem sizes, explicit storage of $J$ and $J^T J$ is not possible. Similar to others [53], we instead compute $J^T J \theta$ in two steps (first, $y = J \theta$, then $J^T y$). We also reduce memory requirements by reformulating the Jacobian terms as products of stored vectors with the system matrix, then computing $J$ and $J^T$ on-the-fly as needed. Because we are computing in a Linux cluster environment, the run times for our solutions vary depending on the node used. However, typical run times for a single slice are between 6 and 9 hours. We note however that our implementation was optimized to reduce memory use, not run time,
and that commercial systems for iterative CT reconstruction are available. It is quite possible that overall run time could be reduced using alternative solvers such as Powell’s dogleg method [54] or approaches such as the ordered subset methods [13]. The computational cost of regularization (both TV and NLM-based regularization) is moderate (roughly 20% increase in run time). We use the integral image technique introduced in [55] to reduce computation of NLM weights.

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