F3-A2/F3-A3: Tensor-based Formulation for Spectral Computed Tomography (CT) with Novel Regularization Techniques

Abstract—Spectral computed tomography (CT) has become increasingly of interest with the development of photon counting X-ray detector technology. The energy selective measurement capabilities of these devices open the doors to many exciting directions in CT research across a number of fields including security applications. Over the past year our work under ALERT support has been directed at the continued development of tensor-based, iterative algorithms that simultaneously reconstruct the X-ray attenuation distribution in space across a range of energies. This approach has allowed for the design of a number of regularization methods built on low rank assumptions on the multi-spectral unknown. The first approach we developed was based on the use of a nuclear norm penalty in each of the three so-called unfoldings of the tensor. The second method, developed in the past year, makes use of the tensor singular value decomposition (tSVD) developed in [1]. In all cases, reconstruction requires the solution of a convex optimization problem the solution of which is obtained using alternating direction method of multipliers (ADMM) techniques. Simulation results shows that both generalized tensor nuclear norm methods can be used as stand-alone regularization techniques for the energy selective (spectral) computed tomography problem and when combined with total variation regularization both enhance the reconstruction accuracy especially at low energy images where the effects of noise are most prominent. In all cases, our methods clearly outperform the current state of the art techniques based on energy-by-energy filtered backprojection reconstruction.

I. PARTICIPANTS

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<tr>
<td>Name</td>
<td>Title</td>
<td>Institution</td>
<td>Email</td>
<td>Phone</td>
<td></td>
</tr>
<tr>
<td>Eric Miller</td>
<td>Professor</td>
<td>Tufts University</td>
<td><a href="mailto:eric.miller@tufts.edu">eric.miller@tufts.edu</a></td>
<td>617.627.0835</td>
<td></td>
</tr>
<tr>
<td>Brian Tracey</td>
<td>Research Assistant Professor</td>
<td>Tufts University</td>
<td><a href="mailto:btracey@eecs.tufts.edu">btracey@eecs.tufts.edu</a></td>
<td>617.627.6424</td>
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<tr>
<td>Name</td>
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<td>Email</td>
<td>Intended Year of Graduation</td>
<td></td>
</tr>
<tr>
<td>Oguz Semerci</td>
<td>PhD</td>
<td>Tufts University</td>
<td><a href="mailto:oguz.semerci@gmail.com">oguz.semerci@gmail.com</a></td>
<td>Oct. 2012</td>
<td></td>
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II. PROJECT OVERVIEW AND SIGNIFICANCE

Preventing the access of explosive materials to aviation facilities is the first step of airport security. Therefore, automatic detection of explosives is crucial. This aim of this project is to design X-ray CT image formation methods with potential application for luggage screening in airports. Our work introduces a novel iterative
algorithm for the spectral CT problem. Accurate identification of the spectral characteristics of the medium under investigation is required as the first step to material characterization.

III. RESEARCH AND EDUCATION ACTIVITY

A. State-of-the-Art and Technical Approach

A conventional computed tomography (CT) imaging system utilizes energy integrating detector technology [2] and provides a monochromatic reconstruction of the linear attenuation coefficient distribution of an object under investigation. The polychromatic nature of the X-ray spectra is either neglected [3,4], or incorporated into the model in an iterative reconstruction method to achieve more accurate results [5,6]. Energy resolving (photon counting) detector technology [7], on the other hand, provides the possibility of energy selective measurement and opens the door to spectral CT technology. Spectral CT promises improved diagnostic imaging [8,9] and applicability to the security domain [10] due to the contrast enhancement and material characterization capabilities.

In this work, we have developed iterative reconstruction methods for the spectral CT problem where we model the multi-spectral unknown as a low rank 3rd order tensor. Recently, there has been considerable work on recovering corrupted matrices or tensors based on low-rank and sparse decomposition [11] or solely on low-rank assumptions [12-15]. Our goal here is to adopt the generalized tensor rank formulation [16] to regularize the spectral CT problem. Similar studies where the multi-spectral unknown is modeled as a superposition of low rank and sparse matrices had been conducted for 4D cone beam CT [16] and spectral tomography [18]. In these approaches, the multi-spectral unknown is represented as a matrix with row dimension in space and column dimension in energy. Applying the low rank prior to the multi-spectral matrix is a special case of our tensor model where only the unfolding in the energy dimension is considered. However, more powerful regularization can be achieved, especially when the number of energy bins is limited, if the redundancy in the spatial dimensions is also exploited [15].

In last year’s report, we detailed one approach to capturing the notion of low tensor rank based through the use of a nuclear norm concept involving a superposition of the matrix nuclear norms of the three unfoldings of our tensor. This gives a weak upper bound on the rank of a tensor [19]. However, the approach does not make use of the correlations among all the dimensions simultaneously. With this motivation, over the past year we have developed a new tensor nuclear norm based on the tensor singular value decomposition (t-SVD), introduced by Kilmer and Martin [1] and has been proved to be useful for applications such as facial recognition and image deblurring [20]. The t-SVD employs a new tensor multiplication scheme and has similar structure to the matrix SVD which allows optimal low-rank representation (in terms of the Frobenius norm) of a tensor by the sum of outer product of matrices [1].

We start with a discussion of the physical model underlying our methods. At the photon counting detectors the photons in the polychromatic spectrum are classified into energy bins. If we assume perfect energy resolution (i.e., infinitesimal bin width) the polychromatic X-ray CT problem reduces to NE linear monochromatic problems:

$$Ax_i = y_i + n_i, \quad i = 1, ..., N_E.$$  

where $A$ is the CT system matrix discretizing the Radon transform, $x_i$ is the vectorized 2D linear attenuation coefficient image, $n_i$ is the noise vector and $y_i$ is the measurement vector for the $i^{th}$ energy bin.

Let us define the 3rd order tensor $\chi \in \mathbb{R}^{N_1 \times N_2 \times N_e}$ where $N_1$ and $N_2$ are the number of pixels in spatial dimensions. Note that $x_i \in \mathbb{R}^{N_1 N_2}$ can be obtained by lexicographical ordering of the $N_1 \times N_2$ attenuation distribution
at the $i^{th}$ energy. A depiction of a multi-spectral phantom along with the corresponding attenuation curves are given in Figure 1. With this notation we can define the forward operator $K$ in a block diagonal form as follows:

$$K(\chi) := \begin{bmatrix} A & 0 & \cdots & 0 \\ 0 & A & \cdots & 0 \\ \vdots & \ddots & \ddots & \vdots \\ 0 & \cdots & 0 & A \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ \vdots \\ x_{N_E} \end{bmatrix}$$

The tensor singular value decomposition [1] allows any $\chi \in \mathbb{R}^{N_1 \times N_2 \times N_3}$ to be written as the finite sum of outer products:

$$\chi = \sum_{i} U(:,i,:) \circ S(i,i,:) \circ V^T(:,i,:).$$

where $U$, $S$, and $V$ are all three-tensors, the $\circ$ operator is defined in [1], and the indexing (e.g., $(:,i,:)$ and $(i, i,:)$) follow Matlab convention. While the details concerning the tSVD can be found in [1], most relevant to the work here is that we can define a meaningful norm (measure of size) for the tensor in terms of the fast Fourier transform of the “vectors” $S(i,i,:)$. Denoting this norm as $|\chi|_\circ$, our work this past year has demonstrated that this norm plays a role similar to that of the traditional SVD in the compressive sensing literature. Specifically, for tensors that are in a sense sparse, this norm should be small. Across a range of scenarios relevant to the problem of CT inspection for security, we have seen that the absorption tensors are in fact sparse. Thus, we have employed $|\chi|_\circ$ as a sparsity-enhancing regularization method for the tensor-based CT reconstruction problem.

$$\text{minimize}_{\chi} \frac{1}{2} \| K(\chi) - y \|^2 + \lambda_1 |\chi|_\circ + \lambda_2 \sum_i \alpha_i TV(\chi(:,i,:))$$ (1.1)

Given the models developed above, mathematically, we seek a solution for the spectral CT problem via the convex optimization problem:

Where $\lambda_1$ and $\lambda_2$ are regularization parameters and the third term in the above cost function represents the sum of the total variations for the spatial images at the $i$-th energy. As discussed in [21], the energy-dependent nature of the noise (higher noise at low energies) associated with the underlying Poisson statistics of the X-ray data made it necessary to apply a quadratically decreasing factor to $\lambda_2$, represented by $\alpha_i$ so that more regularization was applied to the lower energies. It is the case that (1.1) is a convex function of $\chi$. Thus we developed an efficient iterative method scheme to solve (1.1) based on alternative direction, method-of-multipliers (ADMM) technology [21].
RECONSTRUCTION EXAMPLES

We compared the following methods in our simulations:

1. Filtered back projection (FBP) [22] algorithm applied to each energy bin separately. A RamLak filter multiplied with a Hamming window was used in the FBP inversion [22].

2. Only TV regularization at each energy bin separately (i.e., \( \lambda_1 = 0 \) in (1.1)).

3. 3D-TV regularization in which the total variation function was applied to all three dimensions of the absorption tensor.

4. The tensor nuclear norm method developed in Year 4, here called TNN-1.

5. The t-SVD tensor nuclear norm regularization discussed in this report, here called TNN-2.

6. TNN-1 and TV regularization.

7. TNN-2 and TV regularization.

We simulated multi-spectral data for 12 energies between 25 and 85 keV for 16 uniformly distributed angles between 0 and 180 degrees. We assumed the X-ray spectra are uniform with 10^6 photons at each energy. We have used two different phantoms in our experiments. One was a synthetic phantom comprised of piecewise textures embedded in a slowly varying background. The absorption maps at 25 keV and 85 keV for this phantom are shown in Figure 2. For the second phantom, we used a DICOM image obtained from a CT scan of a duffel bag and artificially assigned attenuation values that are in the same range as Phantom-1 (see Fig. 3). The simulations are performed in MATLAB except for the 3D-TV implementation we have used the code available at http://www2.imm.dtu.dk/ pcha/TVReg/, which is written in C. The linear attenuation values for the materials in Phantom-1 are taken from the XCOM database [23].

In all examples we tuned the regularization parameters manually and used the same set of parameters for both phantoms, as they gave the best error performance. We emphasize that systematic selection of regularization parameters is an important problem, which continues to be an active area of research, especially for non-quadratic regularization techniques such as TV and nuclear norm regularization.

The results of the various reconstruction methods for both phantoms are displayed in Figures 4, 5, 6, and 7 on the following page for the lowest and highest energies. As a measure of quantitative accuracy, the relative error in each reconstruction for these phantoms at 25 and 85 keV are provided in Table 1 on the following page. From these results we see that pure FBP fails to provide reasonable reconstructions at low energies due to limited number of views and noise. Second, when TNN-1 or TNN-2 is used as the only regularizer, each provides considerable noise reduction while preserving much of the detail. Additionally, they allow rapid processing relative to the other methods considered here with computation times over an order of magnitude smaller than when TV is also used. When combined with TV, TNN-1 and TNN-2 regularizers enhance the detail preserving capabilities of TV and increase the reconstruction quality of low energy at the price of increased computational burden, which can be observed especially in the case of the first phantom. Although 3D-TV provides marginally improved performance compared to energy-by-energy TV, TNN-1 and TNN-2 combined with TV gives superior results.
B. Major Contributions

Years 4 and 5:

Development of a new approach to multi-energy CT reconstruction based on (a) the tensor singular value decomposition and (b) minimizing weighted sum of nuclear norms of tensor unfoldings. This work allows for the recovery of spatial-spectral maps of X-ray absorption that are far more accurate with far less data than competing techniques based on e.g., filtered back projection ideas. The impact is especially significant at lower energies where noise can be a problem. The approach is designed to function well for problems where only limited view data is available.

Year 4:

Development of a new approach to edge-preserving image formation based on adaptive and iterative reweighting of image gradient energy. The approach has performance comparable to the state of the art total variation but is more computationally efficient requiring the solution of a sequence of least squares problem each of which can be solved using well-established linear solvers.

Year 3:

Development of a simulation tool for the generation of realistic energy-resolved X-ray

![Table 1: Reconstruction errors (ratio of energy in the difference between truth and estimate to the energy in the true object) for phantoms in Figures 2 and 5 using seven different approaches to image formation. Bold font indicates lowest error.](image)
data. We built an initial version of a software tool which offers educators and researchers user-friendly access to the Monte Carlo Nuclear Particle transport (MCNP) software. Our program allows users to select important parameters for testing arbitrary or problem specific scan geometries and specifications. Such a tool enables further research into reconstruction techniques, as well as a better understanding of the benefits of multi-spectrum CT.

**Years 1-3:**

Over this period, we focused on the development of a novel polychromatic dual energy computed tomography (CT) image formation algorithm for the detection of explosives whose chemical properties are assumed to be known with some level of uncertainty and which are located in a cluttered background. We determine the shape, number (perhaps zero) and material properties of these regions along with low-resolution images of the background, non-explosive areas. A parametric level-set method was used to model the boundary of the object. Due to a severe mismatch in the sensitivity of the data to the two physical parameters of interest (photoelectric and Compton coefficients), we introduce a new gradient-based similarity regularizer to obtain accurate reconstruction of the background properties. The reconstructed Compton and photoelectric coefficient images uniquely identify the chemical properties of the region of interest.

**IV. FUTURE PLANS**

Over the coming year we are considering a number of possibilities for extending the work in multi-energy X-ray CT reconstruction including the following

1. Development of more sophisticated tensor nuclear norm regularization strategies: The methods we have considered to date make use of two ways of decomposing a tensor: unfolding and the t-SVD approach developed in [1]. The intent of both of these methods is to provide a convex approximation to the rank of a tensor. Given the need to move from 3D to 4D or perhaps even 5D (three space, one energy, and maybe time) reconstruction problems, there is motivation for developing new concepts of tensor nuclear norm. Here, based on the success of the t-SVD decomposition as the basis for regularization, we hypothesize that alternative approaches to tensor decomposition, specifically the Tucker and PARFAC/CANDECOMP methods will be of use for moving to higher dimensional problems.

2. Dictionary methods for tensor texture identification: In the image processing and analysis field, another area of recent activity has focused on the use of overcomplete dictionaries of image patch structure for efficiently representing texture. To the best of our knowledge, these concepts have not been carried over to the tensor problem where now both space and energy have structure. Given the potential of texture features for identification of modern explosive materials, we feel there is merit in considering this issue as we move forward on this project.

3. Compressive imaging: The results of our current tensor methods were demonstrated in a 2D imaging problem where only 16 projections were used. The promising performance suggests that one may be able to employ reduced, or compressed, data sets with limited reduction in performance opening up the possibility for simpler CT systems and faster reconstruction processing. While ideas in compressive sensing could be brought to bear here, these methods largely consider random sampling of the data. As there is significant prior information concerning characteristics of threat objects including texture and spectral signature we propose here to build tensor-based compressive sampling methods that are adapted to this information. We anticipate that the approach will be useful not only for reconstructing data but also for the design of next-generation CT systems by providing guidance concerning how much spectral information is require, geometric distribution of sources and detectors, etc.

4. Relaxation of physical model: To date we have assume perfect energy resolution for the detectors. In truth, there will be some band over which any real detector is sensitive. To avoid imaging artifacts, the correct model involves integration over energy of an exponential function of the absorption. It turns out
that this model though no longer linear is convex in the unknown absorption. We propose then to extend our algorithms to allow for the use of this more accurate model. Because this more general model is the same one used for dual energy reconstruction problems, we will immediately be able to explore the utility of our tensor-based ideas on this class of problems for which there are a number of existing systems produced by vendors such as Analogic and SureScan.

5. Implementation: Our current methods are implemented in Matlab and run on a cluster at Tufts. It is clear that a key task for the current project will be to move from this environment to a high performance embedded system based employing GPUs. Hence migration of the current codes and their implementation using e.g., CUDA will be a major focus of our work here.

V. RELEVANCE AND TRANSITION

The work we have done under this project is directly relevant to the DHS mission of explosives detection in checked luggage using X-ray data. We have developed new approaches to image formation aimed at enhancing the ability of X-ray methods to identify materials from severely limited data sets. Our dual energy work allows for direct identification of materials of interest as part of the image formation process (i.e., not requiring post-processing or segmentation). Our multi-energy approach is applicable to next generation scanners which will incorporate energy resolved detectors. Here we focus on recovery of the full spatial-spectral image cube where some form of post processing would be required to identify materials. Our method stabilizes the recovery of this information, especially at low energies. Moreover, the algorithms do not require data collected from all angles but offer the potential for high quality reconstructions from limited view data as is the case for a number of scanners currently under development. Both of these factors should allow for increased accuracy in materials identification relative to the use of techniques based on energy-by-energy filtered back projection processing. Moreover, the direct reconstruction of materials which was a feature of our dual energy work could, in the future, be adapted here as well.

VI. LEVERAGING OF RESOURCES

We have spoken with a number of vendors regarding the adoption of subsets of the ideas developed under this project including Analogic, AS&E, SureScan, and PDSI. We have also participated in a number of proposal efforts to DARPA (Methods for Explosive Detection at Standoff) as well as DHS (BAA 13-05: Advanced X-ray Materials Discrimination). In the case of DHS BAA 13-05 we continue to talk with PDSI concerning collaboration on their Task 5 effort and have been invited to work with the AS&E/Lawrence Livermore team on their full proposal for this task as well.

VII. PROJECT DOCUMENTATION AND DELIVERABLES

A. Other Publications


VIII. REFERENCES


