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An ADMM Algorithm for Constrained Material Decomposition in Spectral CT

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Abstract—Thanks to photon-counting detectors, spectral computerized tomography records energy-resolved data from which the chemical composition of a sample can be recovered. This problem, referred to as material decomposition, can be formulated as a nonlinear inverse problem. In previous work, we proposed to decompose the projection images using a regularized Gauss-Newton algorithm. To reduce further the ill-posedness of the problem, we propose here to consider equality and inequality constraints that are based on physical priors. In particular, we impose the positivity of the solutions as well the total mass in each projection image. In practice, we first decompose the projection images for each projection angle independently. Then, we reconstruct the sample slices from the decomposed projection images using a standard filtered-back projection algorithm. The constrained material decomposition problem is solved by the alternating direction method of multipliers (ADMM). We compare the proposed ADMM algorithm to the unconstrained Gauss-Newton algorithm in a numerical thorax phantom. Including constraints reduces the cross-talk between materials in both the decomposed projections and the reconstructed slices.

Index Terms—Alternating direction method of multipliers, spectral computed tomography, material decomposition, nonlinear inverse problem

I. INTRODUCTION

While standard computerized tomography (CT) integrates data over the X-ray spectrum, losing the energy signature of the materials, spectral CT (SPCT) keeps tracks of the energy of the detected photons. Therefore, the material composition of the sample can be recovered. There are various methods for acquiring energy-resolved data, which include the use of rapid kVp-switching, multiple source beams, multi-layer detectors [1], or a photon-counting detector [2]. The latter approach records multiple energy bins using one source beam only, which reduces the irradiation dose. SPCT is particularly interesting for imaging K-edge materials [3] (i.e., gold, iodine or gadolinium) used as contrast agents and has many potential medical applications such as neck and head cancer [4].

Material decomposition and tomographic reconstruction can be done jointly [5] or sequentially, i.e., decomposing the projection images first and performing the tomographic reconstruction afterward [6], [7]. Here, we consider material

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decomposition in the projection domain since it allows to decompose each projection in parallel. We propose to address material decomposition as a nonlinear inverse problem. In [7], we considered a Gauss-Newton algorithm to minimize a regularized cost function. This approach enjoys a fast convergence, but it does not ensure the solutions to be positive. Positivity constraints for material decomposition have been enforced in both the image [8] and projection [9] domains. However, these methods use first-order algorithm to minimize a cost function, thus with a low convergence rate. Our contribution here is to develop a fast constrained algorithm. In this work, we also consider equality constraints. Indeed, the quantity of injected contrast agent is known, which can improved material decomposition.

Our constrained algorithm uses the augmented Lagrangian formulation to incorporate inequality and equality constraints [10]–[14]. An alternating direction method of multipliers (ADMM) minimizes the Lagrangian function to recover the projected material maps. ADMM has been already used to postprocess volumes obtained after tomographic reconstruction [15] or for joint decomposition-tomographic reconstruction [16]. Both approaches considered a linearized forward model. In this work, we consider a nonlinear forward model and perform material decomposition of the projections. Our constrained algorithm is tested on realistic simulated projections of numerical thorax phantom and compared with an unconstrained Gauss-Newton algorithm.

The rest of the paper is organized as follows. First, we present the forward and inverse problems. Second, we describe our optimization algorithm. Then, we report and discuss some numerical experiments.

II. MATERIAL DECOMPOSITION IN SPECTRAL CT

A. Forward model

Considering a photon-counting detector with P pixels and I energy bins, the measured data is gathered in a vector $\mathbf{s} \in \mathbf{R}^{IP}$.

$$\mathbf{s} = [s_{1,1}, \dots, s_{I,1}, \dots, s_{I,P}]^T \quad (1)$$

The projected mass density describes the mass of M materials on the P pixels, thus $\mathbf{a} \in \mathbf{R}^{MP}$

$$\mathbf{a} = [a_{1,1}, \dots, a_{m,1}, \dots, a_{M,P}]^T \quad (2)$$

The standard forward model [6], [7] reads as:

$$\mathbf{s}_{i,p} = \int_{\mathbf{R}} n_i^0(E) \exp\left(-\sum_{m=1}^M a_{m,p} \tau_m(E)\right) dE \quad (3)$$

where $\mathbf{s}_{i,p}$ is the number of photons detected at the pixel p for the i th energy bin, $n_i^0(E)$ is the effective spectrum (accounting for the incident spectrum and the detector response) at the energy E for the i -th energy bin, $\tau_m(E)$ is a function representing the attenuation of the m -th material at the energy E and $a_{m,p}$ is the projection mass of the m -th material at pixel p , such as

$$a_{m,p} = \int_{\mathcal{L}_p} \rho_m(\mathbf{x}) d\mathbf{x} \quad (4)$$

with \mathcal{L}_p is the x-ray path and $\rho_m(\mathbf{x})$ is the material density at the voxel \mathbf{x} .

B. Constrained Inverse problem

For each projection angle, we propose to recover the material map \mathbf{a} from the data \mathbf{s} by solving the constrained optimization problem

$$\min_{\mathbf{a}} \mathcal{C}(\mathbf{a}, \mathbf{s}) \quad \text{s.t.} \quad \begin{cases} \mathbf{a} \geq \mathbf{0} \\ \sum_p a_{m,p} = c_m \end{cases}, \quad (5)$$

where \mathcal{C} is the cost function and c_m represents the total mass of the m -th material. Here, we assume that materials maps are positive and that the total mass of each material c_m is known and constant across angles, which is a valid hypothesis when the detector field-of-view is wide enough.

To stabilize the minimization in the presence of noise, we consider

$$\mathcal{C}(\mathbf{a}, \mathbf{s}) = \mathcal{D}(\mathbf{a}, \mathbf{s}) + \alpha_{\mathbf{R}} \mathcal{R}(\mathbf{a}) \quad (6)$$

where \mathcal{D} is the data fidelity term, \mathcal{R} the regularization term, and $\alpha_{\mathbf{R}}$ the regularization parameter. Following [7], we choose

$$\mathcal{D}(\mathbf{a}, \mathbf{s}) = \|\mathbf{s} - \mathcal{F}(\mathbf{a})\|_{\mathbf{W}}^2 \quad (7)$$

where \mathcal{F} represents the forward model of Eq. (3) and \mathbf{W} is a diagonal weighting matrix with elements $1/\sqrt{s}$. Assuming that only three materials (soft tissues, bones and gadolinium as a marker) are present in the sample, we choose

$$\mathcal{R}(\mathbf{a}) = \|\Delta \mathbf{a}_{\text{soft}}\|_2^2 + \|\nabla \mathbf{a}_{\text{bone}}\|_1 + \|\nabla \mathbf{a}_{\text{Gd}}\|_1 \quad (8)$$

where ∇ and Δ are first- and second-order differential operator and $\|\cdot\|_2$ and $\|\cdot\|_1$ are the ℓ_2 - and ℓ_1 -norm, respectively.

III. CONSTRAINED MATERIAL DECOMPOSITION ADMM ALGORITHM

We propose an ADMM algorithm to solve the minimization problem described above. To this aim, we minimize the augmented Lagrangian functional

$$\begin{aligned} \mathcal{L}(\mathbf{a}, \mathbf{b}, \boldsymbol{\alpha}_{\mathbf{I}}, \alpha_{\mathbf{E}}, \mathbf{s}) &= \mathcal{D}(\mathbf{a}, \mathbf{s}) + \alpha_{\mathbf{R}} \mathcal{R}(\mathbf{a}) \\ &+ \mathcal{H}_{\mathbf{E}}(\mathbf{a}, \alpha_{\mathbf{E}}) + \mathcal{G}_{\mathbf{E}}(\mathbf{a}) \\ &+ \mathcal{H}_{\mathbf{I}}(\mathbf{a}, \mathbf{b}, \boldsymbol{\alpha}_{\mathbf{I}}) + \mathcal{G}_{\mathbf{I}}(\mathbf{a}, \mathbf{b}) + \mathbf{1}(\mathbf{b}) \end{aligned} \quad (9)$$

where $\mathcal{H}_{\mathbf{E}}$ and $\mathcal{H}_{\mathbf{I}}$ are the Lagrangian terms associated to the equality and inequality constraints, respectively, $\mathcal{G}_{\mathbf{E}}$ and $\mathcal{G}_{\mathbf{I}}$ are the augmented Lagrangian terms, $\mathbf{1}$ denotes the indicator function of the positive orthant, $\alpha_{\mathbf{E}} \in \mathbf{R}$ and $\boldsymbol{\alpha}_{\mathbf{I}} \in \mathbf{R}^{MP}$ are the Lagrangian multipliers, and $\mathbf{b} \in \mathbf{R}^{MP}$ is an auxiliary variable.

1) *Inequality constraint*: To enforce the inequality constraints, we introduce an auxiliary variable \mathbf{b} and rewrite the constraint as

$$\mathbf{a} = \mathbf{b} \quad (10)$$

$$\mathbf{b} \geq \mathbf{0} \quad (11)$$

The constraints (10) and (11) translate into

$$\mathcal{H}_{\mathbf{I}}(\mathbf{a}, \mathbf{b}, \boldsymbol{\alpha}_{\mathbf{I}}) = \boldsymbol{\alpha}_{\mathbf{I}}^{\mathbf{T}} (\mathbf{b} - \mathbf{a}) \quad (12)$$

$$\mathcal{G}_{\mathbf{I}}(\mathbf{a}, \mathbf{b}) = \frac{\beta_{\mathbf{I}}}{2} \|\mathbf{b} - \mathbf{a}\|_2^2 \quad (13)$$

whereas Eq. (11) is formulated with the term

$$\mathbf{1}(\mathbf{b}) = \begin{cases} 0, & \text{if } \mathbf{b} \geq \mathbf{0} \\ \infty, & \text{otherwise} \end{cases} \quad (14)$$

Where $\beta_{\mathbf{I}} \in \mathbf{R}$ is an augmented Lagrangian parameter.

2) *Equality constraint*: The equality constraints lead to

$$\mathcal{H}_{\mathbf{E}}(\mathbf{a}, \alpha_{\mathbf{E}}) = \alpha_{\mathbf{E}} \left(\sum_{p=1}^P \frac{a_{\text{gd},p}}{c_{\text{gd}}} - 1 \right) \quad (15)$$

$$\mathcal{G}_{\mathbf{E}}(\mathbf{a}) = \frac{\beta_{\mathbf{E}}}{2} \left(\sum_{p=1}^P \frac{a_{\text{gd},p}}{c_{\text{gd}}} - 1 \right)^2 \quad (16)$$

where $\beta_{\mathbf{E}} \in \mathbf{R}$ is an augmented Lagrangian parameter. Note that the constraint applies to the gadolinium material only.

3) *Minimization scheme*: According to the ADMM framework, a saddle point of the augmented Lagrangian functional is obtained alternating the update of the primal variables and the Lagrangian multipliers [10]:

$$\mathbf{a}^{\ell+1} \in \underset{\mathbf{a}}{\text{argmin}} \mathcal{L}(\mathbf{a}, \mathbf{b}^{\ell}, \alpha_{\mathbf{E}}^{\ell}, \boldsymbol{\alpha}_{\mathbf{I}}^{\ell}) \quad (17)$$

$$\mathbf{b}^{\ell+1} \in \underset{\mathbf{b}}{\text{argmin}} \mathcal{L}(\mathbf{a}^{\ell+1}, \mathbf{b}, \alpha_{\mathbf{E}}^{\ell}, \boldsymbol{\alpha}_{\mathbf{I}}^{\ell}) \quad (18)$$

$$\alpha_{\mathbf{E}}^{\ell+1} \in \underset{\alpha_{\mathbf{E}}}{\text{argmax}} \mathcal{L}(\mathbf{a}^{\ell+1}, \mathbf{b}^{\ell+1}, \alpha_{\mathbf{E}}, \boldsymbol{\alpha}_{\mathbf{I}}^{\ell}) \quad (19)$$

$$\boldsymbol{\alpha}_{\mathbf{I}}^{\ell+1} \in \underset{\boldsymbol{\alpha}_{\mathbf{I}}}{\text{argmax}} \mathcal{L}(\mathbf{a}^{\ell+1}, \mathbf{b}^{\ell+1}, \alpha_{\mathbf{E}}^{\ell+1}, \boldsymbol{\alpha}_{\mathbf{I}}) \quad (20)$$

The projected mass map \mathbf{a} is updated using a Gauss-Newton algorithm (SPRAY toolbox [17]), the auxiliary variable \mathbf{b} is updated using a proximal algorithm, and the Lagrangian multipliers $\alpha_{\mathbf{E}}$ and $\boldsymbol{\alpha}_{\mathbf{I}}$ are updated with an ascent gradient algorithm [10]. The parameters $\beta_{\mathbf{E}}$ and $\beta_{\mathbf{I}}$ are increased every outer iteration ℓ with a multiplicative update:

$$\beta_{\mathbf{E}}^{\ell+1} = \omega \beta_{\mathbf{E}}^{\ell} \quad (21)$$

$$\beta_{\mathbf{I}}^{\ell+1} = \omega \beta_{\mathbf{I}}^{\ell} \quad (22)$$

with a positive constant $\omega > 1$. This update rule for the Lagrangian parameter allows the algorithm to minimize in

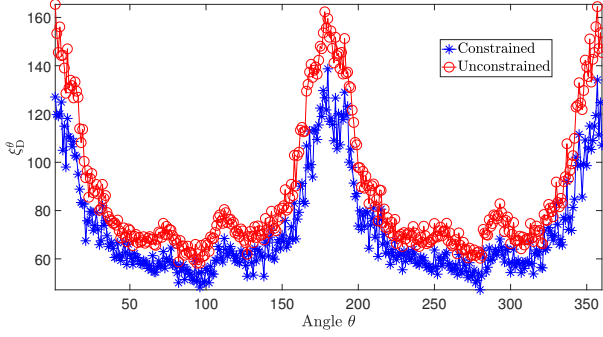


Fig. 1. Euclidean decomposition error ξ_D^θ over all projections for the constrained algorithm (in blue) and the unconstrained algorithm (in red)

the first iterations the function $\mathcal{C}(\mathbf{a}, \mathbf{s})$, and then after a few outer iterations the constraints since they become the predominant contribution to the Lagrangian. Denoting Π the projector operation onto the positive orthant and considering elements-wise operations, the constrained algorithm is given in Algorithm 1.

Algorithm 1: ADMM algorithm

```

while Stopping criteria aren't met for the outer loop do
  while Stopping criteria aren't met for the inner loop
  do
    solve ( $\mathbf{H}^k \delta \mathbf{a}^k = -\mathbf{g}^k$ )
     $\mathbf{a}^{k+1} = \mathbf{a}^k + \lambda^k \delta \mathbf{a}^k$ 
     $k = k + 1$ 
  end
   $\mathbf{a}^{\ell+1} = \mathbf{a}^{k-1}$ 
   $\mathbf{b}^{\ell+1} = \Pi(\mathbf{a}^{\ell+1} - \frac{\alpha_E^\ell}{\beta_I})$ 
   $\alpha_E^{\ell+1} = \alpha_E^\ell + \beta_E \frac{\mathcal{H}_E(\mathbf{a}_m^{\ell+1})}{\alpha_E^\ell}$ 
   $\alpha_I^{\ell+1} = \alpha_I^\ell + \beta_I(\mathbf{b}^{\ell+1} - \mathbf{a}^{\ell+1})$ 
   $\beta_E^{\ell+1} = \omega \beta_E^\ell$ 
   $\beta_I^{\ell+1} = \omega \beta_I^\ell$ 
  if  $\beta_E^{\ell+1} > \beta_{\max}^\ell$  then
     $\beta_E^{\ell+1} = \beta_{\max}^\ell$ 
  end
  if  $\beta_I^{\ell+1} > \beta_{\max}^\ell$  then
     $\beta_I^{\ell+1} = \beta_{\max}^\ell$ 
  end
   $\ell = \ell + 1$ 
end

```

IV. NUMERICAL EXPERIMENTS

A. Phantom, simulation and decomposition parameters

In this work, a numerical phantom of a thorax is considered ($240 \times 185 \times 84$ voxels) [18]. The phantom is composed of $M = 3$ materials, namely soft tissues, bones and gadolinium (in the portal vein). Projections are created using the radon function of Matlab, providing 84×306 images.

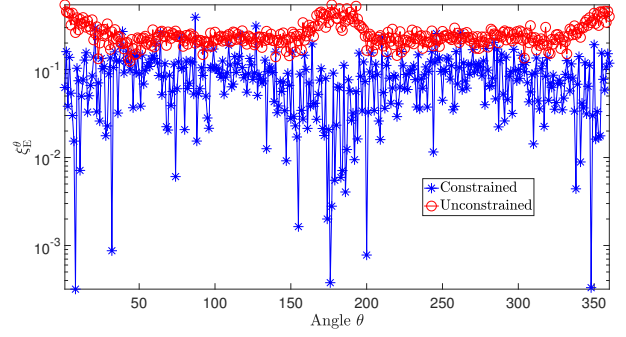


Fig. 2. Quantification error ξ_E^θ over all projections for the constrained algorithm (in blue) and the unconstrained algorithm (in red)

We consider a 120 kV X-Ray source, generated by the spekCalc software [19]. The photon-counting detector detect photons in $I = 4$ energy bins. For each pixel, 10^7 photons are send.

For both algorithms (unconstrained and constrained), the initialization is the same, with uniform materials maps $\mathbf{a}_m^0 = 0$ g.cm^{-2} for all materials. The regularization parameter is the same as well, set at $\alpha_R = 1$. For the unconstrained algorithm, the algorithm stops after 100 iterations to ensure the optimal solution, for a better comparison. For the ADMM algorithm the Lagrangian multipliers are initialized $\alpha_E^0 = 0$ and $\alpha_I^0 = \mathbf{0}$. The following initialisation parameters are used: $\beta_E^0 = 10^0$ and $\beta_I^0 = 10^{-2}$, with a maximum at $\beta_{\max}^\ell = 10^{10}$ and an evolution parameter $\omega = 1.5$. The algorithm stops the inner loop (update of \mathbf{a} , Eq. (17)) if the relative decrease of \mathcal{L} is small ($< 10^{-3}$) or if there is more than 30 iterations. The outer loop stops if the constraints are satisfied: $\|\mathbf{a}^\ell - \mathbf{b}^\ell\| < 10^{-3}$ and $|\left(\sum_p^P \frac{a_{\text{gd},p}^\ell}{c_{\text{gd}}} - 1\right)| < 10^{-3}$ for the index $m =$ corresponding to gadolinium.

The decomposition are made for every degree in the range $\theta = [0^\circ, 359^\circ]$. We denote \mathbf{a}^θ the decomposition for the angle θ and ρ^z the decomposed material at a given slice z .

B. Evaluation of the methods

The constraints are evaluated by looking at the percentage of negative values, the smallest value in the projections: $\min(\mathbf{a}_m^\theta) \forall m, \theta$ and by computing the relative distance between the sum of the gadolinium projections and the constraint c_{gd} :

$$\xi_E^\theta = \frac{|\sum_{p=1}^P a_{\text{gd},p}^\theta - c_{\text{gd}}|}{c_{\text{gd}}} \quad (23)$$

The decomposed projections are also evaluated by computing the ℓ_2 distance between the decomposition and the ground truth:

$$\xi_D^\theta = \sum_m^M \|\mathbf{a}_m^\theta - \mathbf{a}_m^{\text{truth},\theta}\|_2 \quad (24)$$

In the image domain (after the tomographic reconstruction), the ℓ_2 distance is also computed to evaluate the decomposed

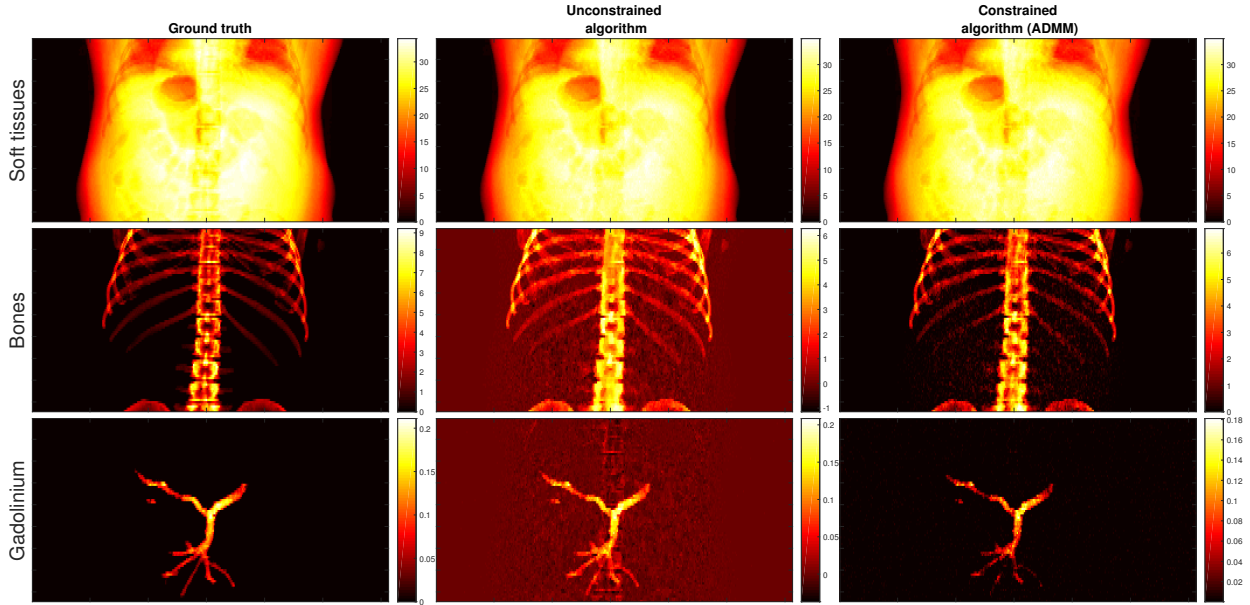


Fig. 3. Decomposition of the thorax for $\theta = 90^\circ$. Ground truth (first column), unconstrained algorithm (second column) and constrained (ADMM) algorithm (third column) for the 3 different materials: soft tissues (top row), bones (middle row) and gadolinium (bottom row).

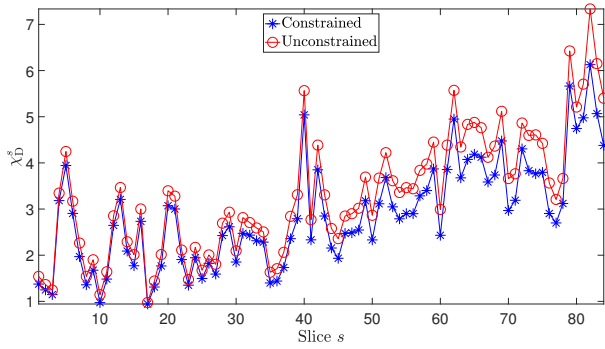


Fig. 4. Euclidean decomposition error χ_D^s over all slices for the constrained algorithm (in blue) and the unconstrained algorithm (in red)

slices, as:

$$\chi_D^z = \sum_m^M \|\rho_m^z - \rho_m^{\text{truth},z}\|_2 \quad (25)$$

where $\rho_m^{\text{truth},z}$ is the reconstructed slice from the ground truth sinogram.

V. RESULTS AND DISCUSSION

A. Projection domain

Table I presents the percentage of negative values, the smallest projection value, and the smallest and highest values for ξ_E for all the angles θ . The error ξ_D^θ and ξ_E^θ are displayed in Fig. 1 and Fig. 2, respectively, for all angles θ . These metrics show that the constrained algorithm gives better decomposition than the unconstrained one (by looking at the error ξ_D), and that the constraints are well satisfied for the constrained algorithm. The decomposition images are displayed in Fig. 3 for $\theta = 90^\circ$. The first column displays the ground truth, the

	Constrained algorithm	Unconstrained algorithm
% of negative value	2.08%	27.7%
Smallest value	-0.02	-3.78
Smallest ξ_E	3.19×10^{-4}	0.12
Biggest ξ_E	0.39	0.54

TABLE I

PERCENTAGE OF NEGATIVE VALUES, SMALLEST VALUE, SMALLEST AND LARGEST ξ_E , CONSIDERING ALL PROJECTIONS FOR BOTH ALGORITHMS.

second one the reconstruction obtained with the unconstrained algorithm and the third one the image obtained with the constrained algorithm (ADMM). We can see that the proposed algorithm gives visually better decomposition. Moreover, there is less bones in the gadolinium image, i.e., less cross-talk.

B. Image domain

The evolution of the error χ_D is displayed on Fig. 4 as a function of the slice number z . As in the projection domain, a better decomposition is obtained with the proposed constrained algorithm. Fig. 5 displays two slices: $z = 1$ and $z = 40$. The first column shows the ground truth, the second one the slice reconstructed with unconstrained algorithm and the third one the reconstruction obtained with the constrained algorithm. The left picture, for $z = 1$, is a slice where there is no marker. The constrained algorithm leads to very small values whereas the unconstrained one shows some bone regions. The effect of the constrained algorithm is more clear at slice $z = 40$ where there is a lot of cross-talk with the unconstrained algorithm that disappears with our algorithm.

VI. CONCLUSION

We proposed an algorithm for material decomposition in SPCT. The non linear inverse ill-posed problem is solved by minimizing a cost function. Equality and inequality constraints

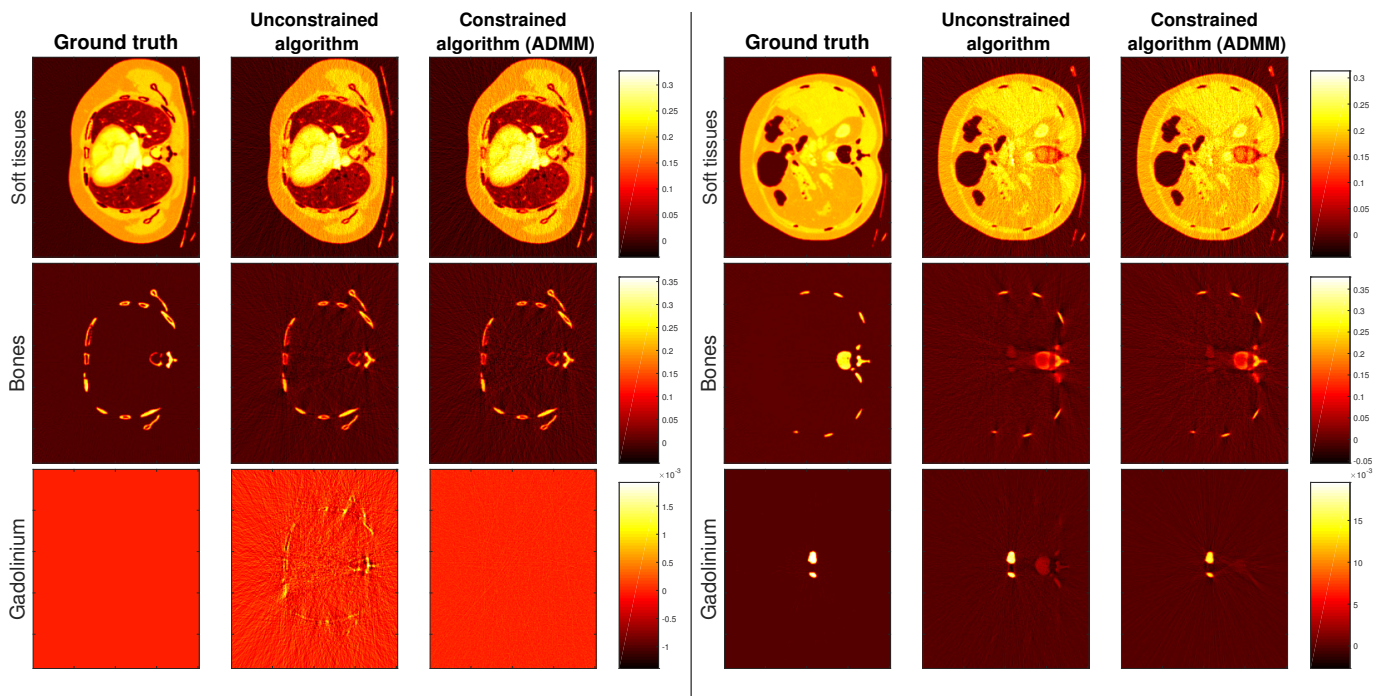


Fig. 5. Reconstructed slice of the thorax after tomographic reconstruction for $z = 1$ (left) and $z = 40$ (right). Ground truth (first column), unconstrained algorithm (second column) and constrained (ADMM) algorithm (third column) for the 3 different materials: soft tissues (top row), bones (middle row) and gadolinium (bottom row), for each slice.

were included in an augmented Lagrangian formulation. An ADMM algorithm was used to find its saddle point. Our new algorithm was compared with an unconstrained algorithm (a Gauss-Newton algorithm) on a numerical phantom of a thorax. Decomposition on the projections shows an improvement (qualitatively and quantitatively) of the material decomposition. Indeed, the cross-talk is reduced when the constraints are included. The improvement of the decomposition on the projection domain is maintained in the image domain after the tomographic reconstruction. Future work will address the decomposition of real data.

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