SUPPLEMENTARY MATERIAL
for
Multi-Material Decomposition Using Statistical Image Reconstruction for Spectral CT

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1 Generalized Sequential Minimization Algorithm (GSMO) for Optimization with Given Material Types

The Generalized Sequential Minimization Algorithm (GSMO) [1] was proposed originally for solving quadratic programming problems arising in support vector machines. The GSMO is derived using Karush-Kuhn-Tucker (KKT) conditions, guaranteed to converge and significantly faster than the original SMO [1].

For simplification of notation, we drop the notations on iteration (n), pixel index j and material triplet ω, and write the quadratic optimization problem with constraints in equation (47) of this paper as

$$\begin{aligned} \hat{\boldsymbol{x}} &= \arg\min_{\boldsymbol{x}} \phi(\boldsymbol{x}) \\ \phi(\boldsymbol{x}) &\equiv \frac{1}{2}\boldsymbol{x}'\boldsymbol{H}\boldsymbol{x} + \boldsymbol{p}'\boldsymbol{x} \\ \text{s.t.} &\quad \begin{cases} \sum_{l=1}^{L} x_l = 1, \\ a_l \le x_l \le b_l. \end{cases} \end{aligned} \tag{1}$$

Table 1 summarizes the pseudo-code of GSMO for solving (1). Please refer to the original GSMO publication [1] for details and derivations of this algorithm. The algorithm is available in the image reconstruction toolbox online [2].

2 Supplementary Figures

Fig. 1 shows the fraction images reconstructed by the ID method [3] without median filtering. Fig. 2, Fig. 3, Fig. 4 and Fig. 5 show profiles of reconstructed fat, blood, bone and air component fraction images by the filtered ID method and the PL method.

References

[1] S. S. Keerthi and E. G. Gilbert. Convergence of a generalized SMO algorithm for SVM classifier design. *Machine Learning*, 46(1-3):351–60, 2002.

1. Choose a tolerance parameter $\tau > 0$.
2. Initialize $k = 0$ and $\hat{\boldsymbol{x}}^{(0)} \in \mathcal{F}$ where $\mathcal{F}$ denotes the feasible set of (1).
3. **Repeat**

   (a) Compute derivatives of $\phi\big(\hat{\boldsymbol{x}}^{(k)}\big)$

   $$F_l^{(k)} = \left[\boldsymbol{H}\hat{\boldsymbol{x}}^{(k)} + \boldsymbol{p}\right]_l$$

   (b) Update the following index sets

   $$\mathcal{I}_0^{(k)} = \left\{l : a_l < \left[\hat{\boldsymbol{x}}^{(k)}\right]_l < b_l\right\}, \quad \mathcal{I}_1^{(k)} = \left\{l : a_l = \left[\hat{\boldsymbol{x}}^{(k)}\right]_l\right\}, \quad \mathcal{I}_2^{(k)} = \left\{l : b_l = \left[\hat{\boldsymbol{x}}^{(k)}\right]_l\right\}$$

   $$\mathcal{I}_{\text{up}}^{(k)} = \mathcal{I}_0^{(k)} \cup \mathcal{I}_1^{(k)}, \qquad \mathcal{I}_{\text{low}}^{(k)} = \mathcal{I}_0^{(k)} \cup \mathcal{I}_2^{(k)}$$

   (c) Find the most τ-violating index pair (m, n) as

   $$m = m^{(k)} = \underset{l \in \mathcal{I}_{\text{up}}^{(k)}}{\arg\min}\, F_l^{(k)}, \quad n = n^{(k)} = \underset{l \in \mathcal{I}_{\text{low}}^{(k)}}{\arg\max}\, F_l^{(k)}$$

   (d) Minimize $\phi(\hat{\boldsymbol{x}})$ on $\mathcal{F}$ while varying only (x_m, x_n) and update them with the minimizer.

   $$\hat{x}_m^{(k+1)} = \hat{x}_m^{(k)} + t, \quad \hat{x}_n^{(k+1)} = \hat{x}_n^{(k)} - t,$$

   where

   $$t = \min\left(\max\left(\frac{F_m^{(k)} - F_n^{(k)}}{[\boldsymbol{H}]_{mm} + [\boldsymbol{H}]_{nn} - 2\,[\boldsymbol{H}]_{mn}}, t_1\right), t_2\right),$$

   $$t_1 = \max\left(a_m - \hat{x}_m^{(k)}, \hat{x}_n^{(k)} - b_n\right), \quad t_2 = \min\left(b_m - \hat{x}_m^{(k)}, \hat{x}_n^{(k)} - a_n\right)$$

   (e) $k = k + 1$

   Until $\hat{\boldsymbol{x}}_j^{(k)}(\omega)$ satisfies the KKT condition

   $$\min_{l \in \mathcal{I}_{\text{up}}^{(k)}} F_l^{(k)} \geq \max_{l \in \mathcal{I}_{\text{low}}^{(k)}} F_l^{(k)} - \tau$$

4. Minimizer $\hat{\boldsymbol{x}} = \hat{\boldsymbol{x}}^{(k)}$

Table 1: Pseudo-code of GSMO for solving the quadratic optimization problem with constraints in (1).

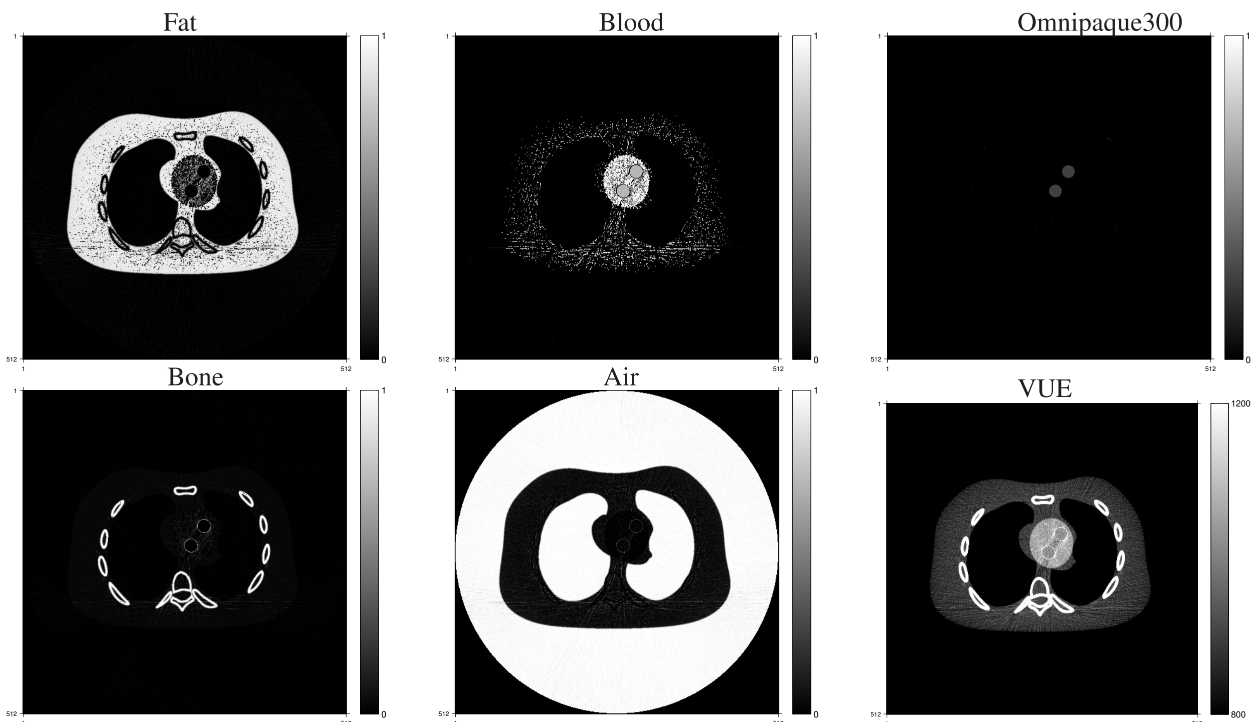

Figure 1: Reconstructed volume fractions of five component images and VUE image at 70 keV by the ID method. The volume fractions are in the range of [0, 1] and the monoenergetic image is displayed over [800, 1200] with the shifted Hounsfield unit (HU) scale where air is 0 HU and water is 1000 HU.

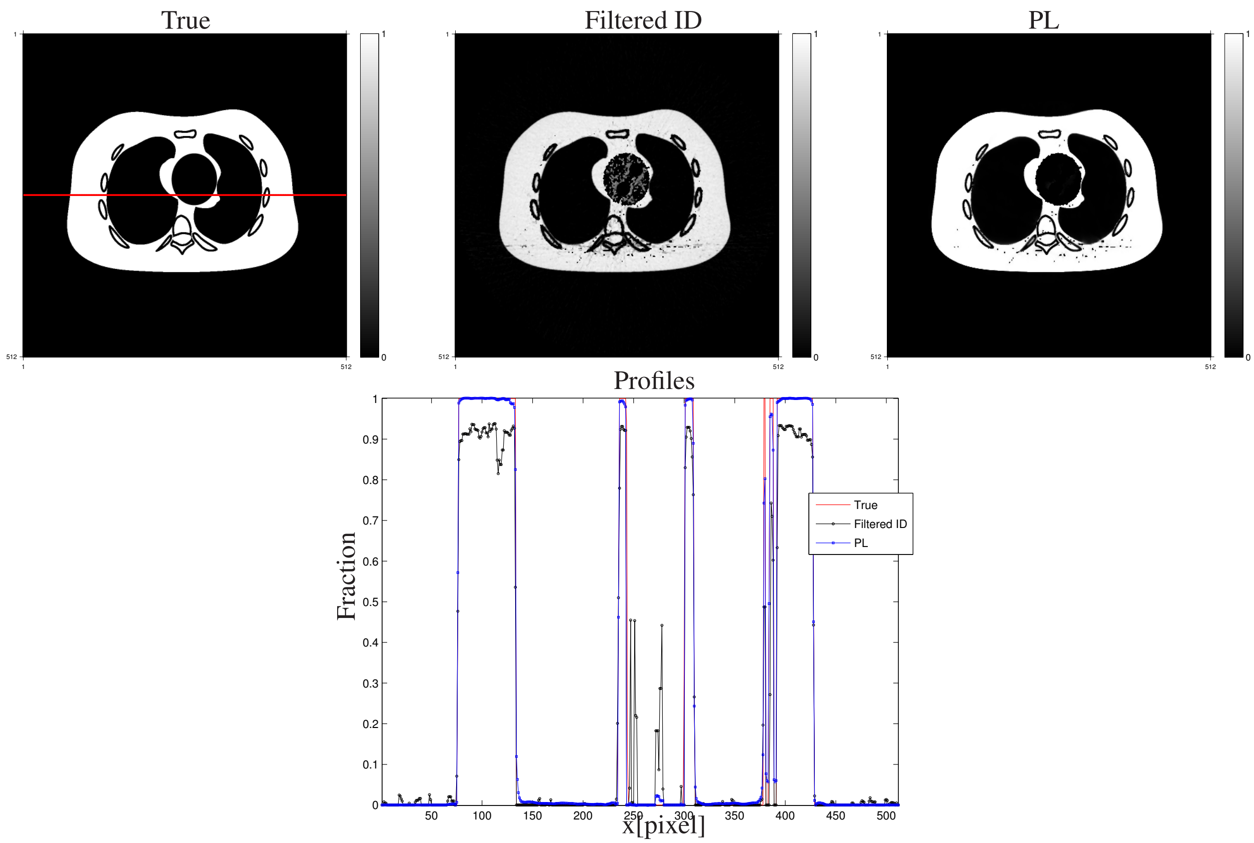

Figure 2: Fat component fraction images reconstructed by the filtered ID method (*upper center*) and the PL method (*upper right*). The upper left image is the down-sampled true image. The lower image shows the horizontal profiles through the red line in the down-sampled true image.

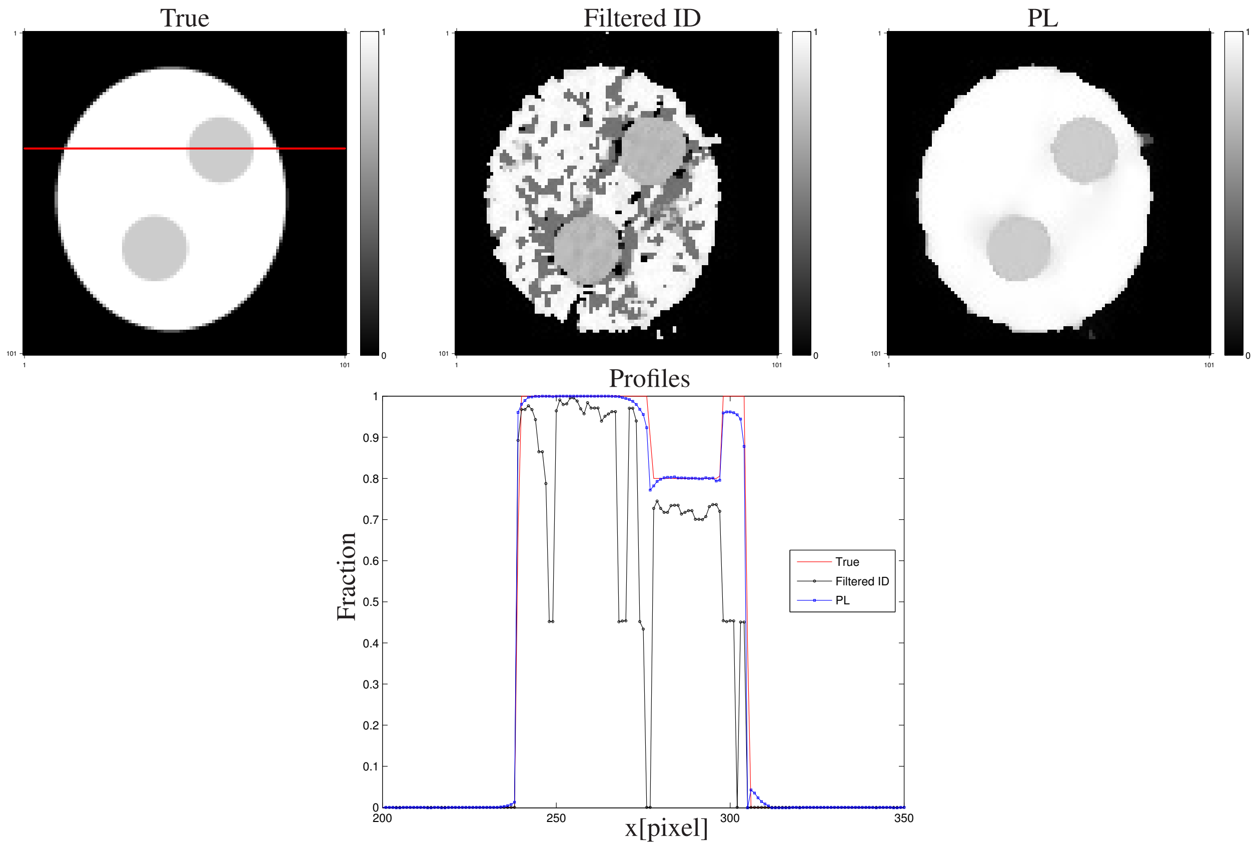

Figure 3: Zoom-in blood component fraction images reconstructed by the filtered ID method (*upper center*) and the PL method (*upper right*). The upper left image is the down-sampled true image. The lower image shows the horizontal profiles through the red line in the down-sampled true image.

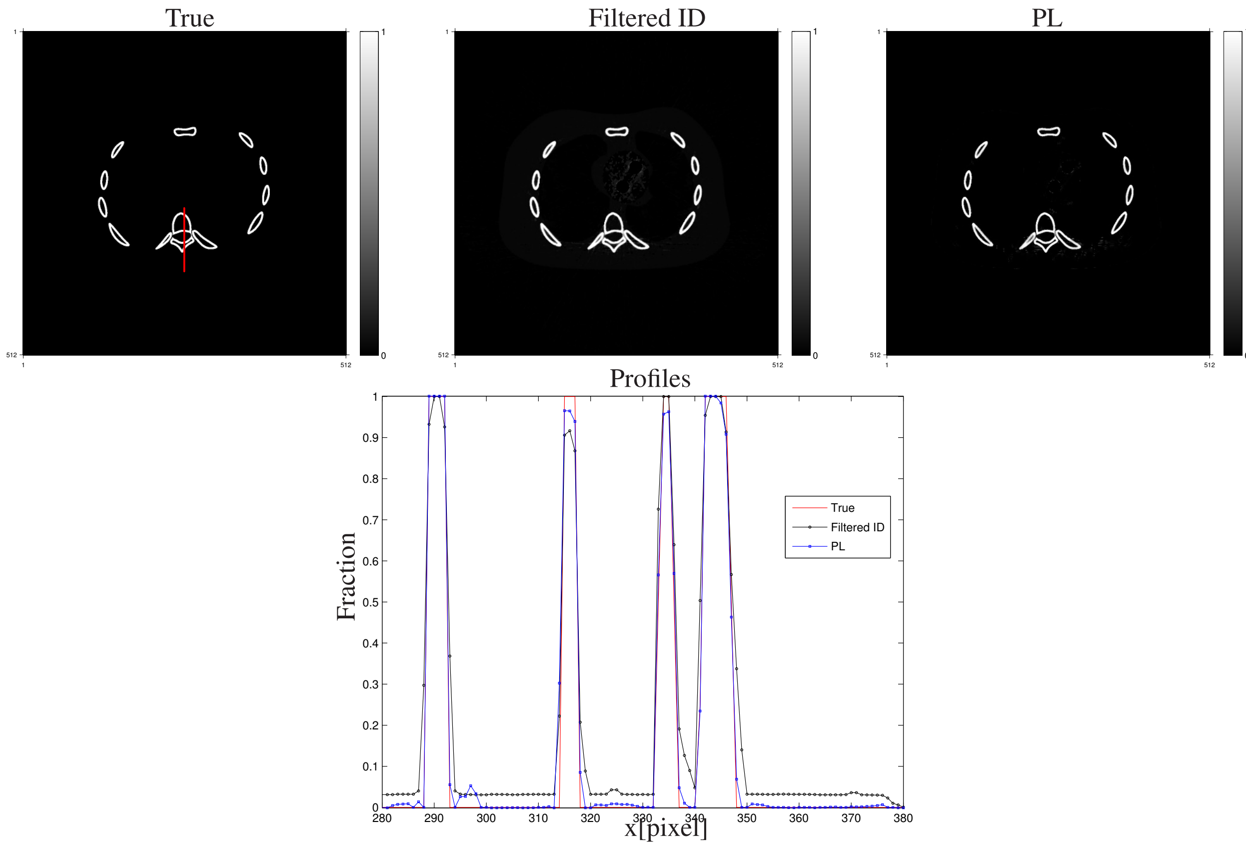

Figure 4: Cortical bone component fraction images reconstructed by the filtered ID method (*upper center*) and the PL method (*upper right*). The upper left image is the down-sampled true image. The lower image shows the vertical profiles through the red line in the down-sampled true image.

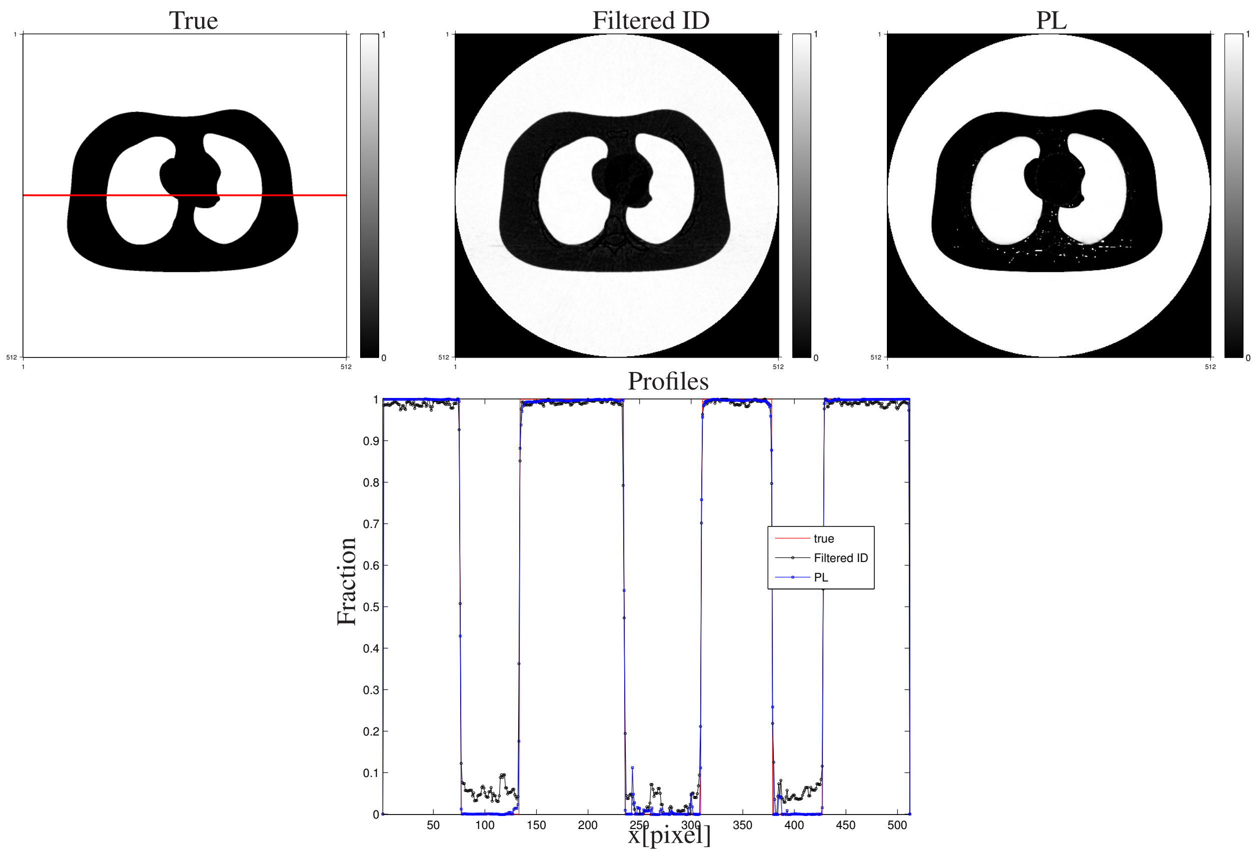

Figure 5: Air component fraction images reconstructed by the filtered ID method (*upper center*) and the PL method (*upper right*). The upper left image is the down-sampled true image. The lower image shows the horizontal profiles through the red line in the down-sampled true image.

[2] J. A. Fessler. Matlab tomography toolbox, 2004. Available from http://www.eecs.umich.edu/∼fessler.

[3] P. R. S. Mendonca, P. Lamb, and D. Sahani. A flexible method for multi-material decomposition of dual-energy CT images. *IEEE Trans. Med. Imag.*, 33(1):99–116, January 2014.