Fast iterative reconstruction for multi-spectral CT by a Schmidt orthogonal modification algorithm (SOMA)

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Abstract
Multi-spectral CT (MSCT) is increasingly used in industrial non-destructive testing and medical diagnosis because of its outstanding performance like material distinguishability. The process of obtaining MSCT data can be modeled as a nonlinear system and the basis material decomposition comes down to the inverse problem of the nonlinear system. For different spectra data, geometric inconsistent parameters cause geometrical inconsistent rays, which will lead to the mismatched nonlinear system. How to solve the mismatched nonlinear equations accurately and quickly is a hot issue. This paper proposes a general iterative method (SOMA) to invert the mismatched nonlinear equations. The SOMA method gives different equations different confidence and searches along the more accurate hyperplane by Schmidt orthogonalization, which can get the optimal solution quickly. The validity of the SOMA method is verified by MSCT basis material decomposition experiments. The results show that the SOMA method can decompose the basis material images accurately and improve the convergence speed greatly.

Keywords: multi-spectral computed tomography, basis material decomposition, iterative reconstruction, Schmidt orthogonal modification, nonlinear equations, inverse problem

(Some figures may appear in colour only in the online journal)
1. Introduction

Computed tomography (CT) can show the internal details without destroying or damaging the objects and has been widely used in many fields such as medicine [1–3], materials [4, 5], geological engineering [6] and so on [7, 8]. Multi-spectral CT (MSCT) takes photon energy into account [9] and obtains more information about the objects [10]. Compared with conventional CT, MSCT has better artifact-removing performances [11, 12], quantitative detectability [13, 14], and material distinguishability [15–17]. So MSCT is increasingly used in industry [18] and medicine [19], especially in medical diagnosis [20–22].

Various scan configurations have been developed to get MSCT polychromatic projections [23–25]. Figure 1 shows some schematic drawings of common ways, including multiple full scans configuration (shown in figure 1(a)) [26], dual-detector configuration (shown in figure 1(b)) [27, 28], fast kVp switching configuration (shown in figure 1(c)) [29, 30], dual-source configuration (shown in figure 1(d)) [31], photon-counting detector configuration (shown in figure 1(e)) [32–34] and primary modulation configuration (shown in figure 1(f)) [35, 36]. Among the mentioned scan configurations, the data obtained by dual-detector configuration and photon-counting detector configuration are geometrically consistent and the data obtained by other methods are geometrically inconsistent. Geometrically inconsistent means that, on the one hand, using each projection set to reconstruct can show the same object, but, on the other hand, the paths of x-rays taken between different spectra are different because of the geometric inconsistent parameters [37].

Researchers usually model the process of obtaining MSCT data as nonlinear equations [26, 38]. Omitting scattered photons and taking MSCT basis material decomposition as an example, the discrete nonlinear model of obtaining polychromatic projections is

\[ p_{k,L} = -\ln \sum_{\omega=1}^{M} s_{k,\omega} \delta e^{-\sum_{m=1}^{K} \theta_{m,\omega} q_{m,L}}, \quad q_{m,L} = R_{L} f_{m}, \quad (1) \]

where \( p_{k,L} \) denotes the polychromatic projection of the \( k \)th spectrum under the x-ray path \( L \), \( L \in \zeta_k \). \( \zeta_k \) represents the x-ray path set of the \( k \)th spectrum, \( k = 1, 2, \ldots, K \) and \( K \) is the total number of spectra. The valid energy range of \( k \)th normalized effective spectrum is equally divided into \( \Omega_k \) intervals and the length of each interval is \( \delta \). \( s_{k,\omega} \) describes the sampling value of the \( k \)th normalized effective spectrum at \( \omega \) keV and \( \sum_{\omega=1}^{M} s_{k,\omega} = 1 \). \( \theta_{m,\omega} \) represents the sampling value of the mass attenuation coefficient (MAC) of the \( m \)th basis material in \( \omega \) keV interval, \( m = 1, 2, \ldots, M \) and \( M \) is the total number of basis materials. \( q_{m,L} \), i.e. the so-called basis material projection, is line integral of the \( m \)th basis material along the x-ray path \( L \). \( f_{m} = (f_{m,1}f_{m,2}\ldots f_{m,K})^{T} \) denotes the discrete form of the \( m \)th basis material density image, where \( f_{m,j} \) is the sampling value of \( f_{m} \) at the \( j \)th pixel. \((\cdot)^{T}\) represents transpose and \( J \) is the total number of image pixels. \( R_{L} = (r_{L,1}, r_{L,2}, \ldots, r_{L,J}) \) is called the projection operator corresponding to the x-ray path \( L \), where \( r_{L,j} \) represents the contribution of the \( j \)th pixel to the x-ray path \( L \). In this paper, \( s_{k,\omega} \) and \( \theta_{m,\omega} \) are assumed to be known. The estimation of \( s_{k,\omega} \) and the measurement of \( \theta_{m,\omega} \) can be referred to [39–42].

Dual spectral CT (DSCT) data two basis material decomposition is a typical case of MSCT basis material decomposition. The process to get DSCT polychromatic projection is
In the case of geometric consistency, $L_1$ and $L_2$ coincide. At this time, the nonlinear system (2) contains two unknowns, and solving the system is a well-posed problem. However, the great majority of measured data are geometrically inconsistent. Figure 2 shows the so-called geometrically inconsistent rays. $L_1$ and $L_2$ pass through the same pixel $f_{m,j}$, but $q_{m,L_1} \neq q_{m,L_2}$ ($m = 1, 2$). In this case, the nonlinear equations (2) contain four unknowns and solving the system is an underdetermined problem, which is called mismatched nonlinear equations in this paper.

MSCT basis material decomposition can be summarized as reconstructing basis material density image $f_{m}$ from measured data $p_k$ by inversion of the nonlinear system (1). Works exist on investigating mapping methods, deep learning methods, or iterative methods for the inversion of the nonlinear equations. The mapping methods [43–49] establish the mapping relationship in advance between the polychromatic projections and the basis material images. High precision mapping relationship means high solution complexity and high noise sensitivity, thus the decomposition accuracy is usually limited. CT reconstruction based on deep learning
is a hot issue [50]. Deep learning methods [51–54] have been used in MSCT reconstruction and basis material decomposition. However, in many cases, CT training data are difficult to obtain, especially industrial CT data. The iterative methods are most commonly used to solve the nonlinear system. Researchers use statistical models or algebraic models to construct different iterative schemes and obtain high-precision solutions by gradual correction. The iterative methods based on the statistical model take the noise distribution into account and can obtain high signal-to-noise ratio results in the case of high noise [55–57]. The iterative methods based on the algebraic model either invert the nonlinear model directly [26, 58] or convert the nonlinear model into the linear model and then solve it by linear methods [59–62]. On the foundation of the statistical model or the algebraic model, some researchers introduce prior information and propose optimization models to further improve the accuracy of the solution [63–68].

Only focusing on the solution of the nonlinear equations, this paper summarizes most iterative methods into three steps:

**Step1 Decomposition** In this step, the nonlinear equations are inverted to get the basis material projection $q^{(n+1)}_m$.

**Step2 Reconstruction** In this step, traditional reconstruction methods, such as ART, FBP, etc., are performed to reconstruct the basis material image $f^{(n+1)}_m$ from $q^{(n+1)}_m$.

**Step3 Update** In this step, the new $f^{(n+1)}_m$ is used to update polychromatic projection $p^{(n+1)}_k$ and get new nonlinear equations.

For most iterative methods, the latter two steps, i.e. the reconstruction and update step, are the same. The difference appears in the decomposition step, which is the inversion of the nonlinear equations. Alvarez uses the Newton–Raphson method to solve nonlinear equations [9]. The Alvarez method can get accurate solutions and have a fast convergence speed for noise-free and geometrically consistent data. However, it has poor noise resistance and cannot apply to geometrically inconsistent data [37]. Our team extended the classic ART method (E-ART) to solve the nonlinear system [59] and high-precision basis material images can be reconstructed. Chen proposed the ASD-NC-POCS method in 2017 [26]. The ASD-NC-POCS method combines the spectrum and the attenuation coefficient to obtain the linear part of the
nonlinear model and uses POCS to solve it. In 2021, Chen modified the intercept of the ASD-NC-POCS method and developed a non-convex primal-dual (NCPD) method to solve a non-convex optimization model based on the nonlinear system [58]. The above three methods can deal with data collected with non-standard configurations and obtain high-quality basis material images, but they have slow convergence speeds.

How to solve the nonlinear system accurately and quickly is still a hot issue. This paper proposes a general iterative method (SOMA) to invert the nonlinear system. The SOMA method gives different equations different confidence and searches along the more accurate hyperplane by Schmidt orthogonalization, which can get the optimal solution quickly.

The remainder of the article is organized as follows. In section 2, the principle and detailed implementation of the SOMA method will be shown. In section 3, the simulation MSCT data and real MSCT data experiments are used to study some characteristics of the SOMA method. The discussion will be given in section 4. For the convenience of expression, the mark of x-ray path \( L \) and the length of interval \( \delta \) in (1) are omitted in the rest of this article.

2. Method

This section introduces the main idea firstly, and then, gives the iteration scheme in the case of the mismatched nonlinear system. Next, the SOMA method in the case of noise and the corresponding iteration scheme are given in section 2.3. Finally, section 2.4 shows the pseudo-code and the detailed implementation of applying the SOMA method to MSCT basis material decomposition.

2.1. Main idea

Assuming that the matched nonlinear system is

\[
\begin{aligned}
G_1(x) &= p_1 \\
&\vdots \\
G_K(x) &= p_K,
\end{aligned}
\]

where \( G_k \) represents the \( k \)th nonlinear equation and \( x = (x_1, x_2, \ldots, x_M)^T \) are the unknowns. Performing the first-order Taylor expansion at the \( n \)th iteration point \( x^{(n)} \), then

\[
\begin{pmatrix}
\frac{\partial G_1}{\partial x_1} \big| x^{(n)} & \frac{\partial G_1}{\partial x_2} \big| x^{(n)} & \cdots & \frac{\partial G_1}{\partial x_M} \big| x^{(n)} \\
\vdots & \vdots & \ddots & \vdots \\
\frac{\partial G_K}{\partial x_1} \big| x^{(n)} & \frac{\partial G_K}{\partial x_2} \big| x^{(n)} & \cdots & \frac{\partial G_K}{\partial x_M} \big| x^{(n)}
\end{pmatrix}
\begin{pmatrix}
x_1 - x_1^{(n)} \\
\vdots \\
x_M - x_M^{(n)}
\end{pmatrix}
= \begin{pmatrix}
p_1 - G_1(x^{(n)}) \\
\vdots \\
p_K - G_K(x^{(n)})
\end{pmatrix},
\]

which can be denoted as a linear system \( Ax = b \). Obviously, the \( k \)th tangent plane \( H_k \) can be represented as \( A_k x = b_k \) and the normal direction is \( g_k = A_k^T \).

The algebraic reconstruction technique (ART) method [69] takes projections alternately on the hyperplanes, i.e. alternating \( g_k \) as the search direction. For ill-conditioned equations, there is a small angle between the hyperplanes. Thus, the search path will be zigzag, which leads to a slow convergence speed [62]. A simplified geometric illustration is shown in figure 3.

The SOMA method let the search directions as orthogonal as possible, which can reduce ‘redundancy’ and ‘repeat’ between \( g_k \). The orthogonal direction \( d_k \) can be obtained by the Schmidt orthogonalization

\[
d_k = P_k g_k,
\]

(5)
Figure 3. Simplified geometric illustration in the case of the matched nonlinear system. The true solution \( x^* \) is represented by the yellow pentagram. \( G_k \) \((k = 1, 2)\) is the hyperplane of nonlinear equation, and \( H_k \) is the corresponding tangent plane obtained by the first-order Taylor expansion. \( g_k \) is the corresponding normal direction. The SOMA method gets the orthogonal directions \( d_k \) by Schmidt orthogonalization and searches the next iteration point along \( d_k \).

where \( P_k \) is the orthogonal modification matrix and the initial \( P_1 \) is set as the identity matrix. The update formula of \( P_k \) can be obtained by recursion

\[
P_{k+1} = P_k - \frac{d_k d_k^T}{d_k^T d_k + \epsilon},
\]

where \( \epsilon \) is generally set to a small value to ensure that the denominator is not zero. As the detailed derivation of the recursion process can be found in appendix A.

Let \( x^{(n,k-1)} \) is the solution that satisfied the first \( k-1 \) equations and \( d_k \) is \( k \)th search direction. \( x^{(n,k)} \) is the minimum of a linear manifold \( \{x | x = x^{(n,k-1)} + \alpha_k d_k \} \) spanned at \( x^{(n,k-1)} \) by \( H_k \) and \( d_1, \ldots, d_k \), where \( \alpha_k \) is the optimal step size. The problem on the linear manifold is transformed into finding \( \alpha_k \) satisfied

\[
\alpha_k = \min_\alpha \|A_k x - b_k\|_2^2 \quad \text{s.t.} \quad x = x^{(n,k-1)} + \alpha_k d_k.
\]

Let the partial derivative with respect to \( \alpha \) be equal to 0 and it is easy to calculate the solution

\[
\alpha_k = \frac{d_k^T g_k (b_k - A_k x^{(n,k-1)}))}{d_k^T g_k d_k} = \frac{b_k - A_k x^{(n,k-1)}}{g_k^T d_k}.
\]

A simple convergence proof of the SOMA method is given in appendix B.

2.2. In the case of mismatched nonlinear system

In the case of mismatched nonlinear system, as shown in figure 2, there is only one equation can be obtained. At this time, the SOMA method can search for the next iteration point along the hyperplane of the accurate equation by the one-dimensional search method.

Or, there is another simple way. There are many methods to estimate the desired consistent projections from the collected inconsistent projections, such as [70–73]. However, the estimated intercepts are inaccurate. Figure 4 shows the simplified geometric illustration.
Figure 4. The simplified geometric illustration in the case of mismatched nonlinear system. The black dotted lines $H_k$ are the accurate tangent planes. The blue dotted line $\tilde{H}_2$ represents the tangent plane with the estimated inaccurate intercept. The curves $G_k$ are omitted for showing clearly.

Algorithm 1. The iteration scheme of the SOMA method.

1. **initialize:** assign $x^{(0)}$, $\beta$ and $\epsilon$ with some initial values
2. **while** not satisfying the stopping criterion **do**
   3. Perform the first-order Taylor expansion at $x^{(n)}$ and get the linear equations
   4. $P_1 = I$
   5. $g_k = A_k^\top$
   6. $x^{(n,0)} = x^{(n)}$
   7. **for** $k = 1$ to $K$ **do**
   8. $d_k = P_k g_k$
   9. $\alpha_k = \frac{b_k - A_k x^{(n,k-1)}}{d_k^\top d_k}$
   10. $x^{(n,k)} = x^{(n,k-1)} + \beta \alpha_k d_k$
   11. $P_{k+1} = P_k - \frac{dd^\top}{d_k^\top d_k + \epsilon}$
   **end**
13. $x^{(n+1)} = x^{(n,K)}$
14. **end**

In the case of geometric inconsistency, only $H_1$ and $\tilde{H}_2$ can be obtained. The search direction $d_2$ is correct and the optimal step size has error. So a rough step size $\alpha_k$ can be calculated by the formula (8) using the estimated inaccurate intercepts $\tilde{b}_k$. Then, the step size relaxation factor $\beta$ can be added to reduce the estimation error when updating $x$

$$x = x^{(n,k-1)} + \beta \alpha_k d_k.$$ (9)

Note that only inaccurate equations (i.e. $k \neq 1$) need relaxation factor. That means the SOMA method gives the accurate equation highest confidence. The general iteration scheme of the SOMA method is shown in algorithm 1.
Figure 5. The simplified geometric illustration of the SOMA method in the case of noise. The true solution $\mathbf{x}^*$ is represented by the yellow pentagram. $G_k$ is the hyperplane of nonlinear equation and $H_k$ is the corresponding tangent plane obtained by the first-order Taylor expansion.

2.3. In the case of noise

In the case of real situations, all equations contain noise, i.e. all equations are inaccurate. For consistent data, low-energy data contains a larger proportion of noise than high-energy data [74]. For inconsistent data, the influence of estimation error is generally higher than noise. The above cases can boil down to inverting a noisy mismatched nonlinear system, in which one equation is more accurate than others.

At this time, the weighting coefficient $\kappa (\in [0, 1])$ is applied to the SOMA method and get the convex combination $\kappa \mathbf{d}_k + (1-\kappa) \mathbf{g}_k$ of the normal direction and the orthogonal direction. The geometric illustration is shown in figure 5. At this time, the equation (7) becomes

$$\alpha_k = \min_{\alpha} \| \mathbf{A}_k \mathbf{x} - \mathbf{b}_k \|_2^2 \quad \text{s.t.} \quad \mathbf{x} = \mathbf{x}^{(n,k-1)} + \alpha_k (\kappa \mathbf{d}_k + (1-\kappa) \mathbf{g}_k),$$

and the solution is

$$\alpha_k = \frac{\mathbf{b}_k - \mathbf{A}_k \mathbf{x}^{(n,k-1)}}{\mathbf{g}_k^T (\kappa \mathbf{d}_k + (1-\kappa) \mathbf{g}_k)}.$$

Algorithm 2 shows the iteration scheme in the case of noise and the convergence proof of algorithm 2 can refer to [38].

At last, a brief summary is given next. The tangent method [59] and the secant method [58] can solve the mismatched nonlinear system but they have slow convergence speeds when solving the ill-conditioned mismatched nonlinear system. The Newton–Raphson method [9] has fast convergence speeds but it will amplify noise [65] and is not available for the mismatched nonlinear system. The core of the SOMA method is giving different equations different confidence by the weighting coefficient $\kappa$. Apply the SOMA method to different cases are as follows.
Algorithm 2. The general iteration scheme of the SOMA method.

1.  \textbf{initialize:} assign \( x^{(0)} \), \( \beta \) and \( \epsilon \) with some initial values
2.  \textbf{while} not satisfying the stopping criterion \textbf{do}
3.      Perform the first-order Taylor expansion at \( x^{(n)} \) and get the linear equations
4.      \( P_1 = I \)
5.      \( g_k = A_k^T \)
6.      \( x^{(n,0)} = x^{(n)} \)
7.      \textbf{for} \( k = 1 \) to \( K \) \textbf{do}
8.          \( d_k = P_k g_k \)
9.          \( \alpha_k = \frac{\alpha_k - \alpha_{k-1}}{\epsilon} \)
10.         \( x^{(n,k)} = x^{(n,k-1)} + \beta \alpha_k (\epsilon d_k + (1 - \epsilon) g_k) \)
11.         \( P_{k+1} = P_k - \frac{d_k d_k^T}{d_k^T d_k + \epsilon} \)
12. \textbf{end}
13. \textbf{end}
14. \( x^{(n+1)} = x^{(n,K)} \)

1. In the case of the noise-free and matched nonlinear system, all equations are accurate. At this time, the SOMA method lets the search directions as orthogonal as possible by the Schmidt orthogonalization, which improves convergence speed greatly.
2. In the case of the mismatched nonlinear system, there is only one accurate equation. The SOMA method searches for the solution along the accurate hyperplane by the one-dimensional search method, or by a small step size to reduce the impact of estimation errors.
3. In the case of noise, all equations are inaccurate, but there is still one equation with higher confidence. The SOMA method gives the more accurate equation higher confidence by the weighting coefficient, so it gets more accurate solutions than comparative methods.

2.4. Implementation in MSCT basis material decomposition

In section 1, this paper summarizes the most iterative methods into three steps

\textbf{Step1 Decomposition} Inverting the nonlinear system to get the basis material projection \( q_m^{(n+1)} \).

\textbf{Step2 Reconstruction} Applying the traditional reconstruction methods, such as ART, FBP, etc., to reconstruct the basis material image \( f_m^{(n+1)} \) from \( q_m^{(n+1)} \).

\textbf{Step3 Update} Updating the new polychromatic projection \( p_k^{(n+1)} \) and getting the new nonlinear equations.

For MSCT basis material decomposition, the SOMA method is applied to the decomposition step, i.e., solve \( q_m^{(n+1)} \) from \( p_k \). The pseudo-code is shown in algorithm 3. To avoid adjusting parameters, an adaptive step size strategy is proposed. The detailed implementation is explained after the pseudo-code.
Algorithm 3. Pseudo-code of applying the SOMA method to MSCT basis material decomposition.

1. **initialize**: set \( f_{kn}^{(0)} = 0 \), \( \lambda = 0.95 \), \( \epsilon = 10^{-5} \), \( T = 1.5 \), \( \kappa = 0.99 \), \( \beta = 0.9 \) and \( \beta_{\text{red}} = 0.9 \)

2. **while not satisfying the stopping criterion**
   3. **if** the polychromatic projections are inconsistent **then**
      4. estimate the unknown projection \( \hat{p}_k \) and set \( p_k = \hat{p}_k \)
   5. **end**

6. \( x^{(n)} = (q_1 - q_1^{(n)}, q_2 - q_2^{(n)}, \ldots, q_M - q_M^{(n)})^{-T} \)

7. Perform the first-order Taylor expansion at \( x^{(n)} \) and get the linear equations \( A_k x = b_k \)

8. \( P_1 = I \)

9. \( g_k = A_k^+ \)

10. \( q_{(n,0)} = q^{(n)} \)

11. **for** \( k = 0 \) to \( K - 1 \) **do**

12. \( d_k = P_k g_k \)

13. \( \alpha_k = \frac{g_k^T (p_k - A_k x^{(n,k-1)})}{g_k^T (p_k - A_k x^{(n,k)})} \)

14. \( x^{(n,k)} = x^{(n,k-1)} + \beta \alpha_k (p_k - A_k x^{(n,k)}) \)

15. \( P_{k+1} = P_k - \frac{d_k d_k^T}{d_k^T d_k + \epsilon} \)

16. **end**

17. \( q_{(n,1)} = x^{(n,1)} + q^{(n)} \)

18. \( q^{(n,K)} = x^{(n,K)} + q^{(n)} \)

19. \( dp = \frac{||p_k - p_k^{(n,K)}||}{||p_k - p_k^{(n,1)}||} \)

20. \( df_m = \frac{||f_m^{(n,K)} - R^{-1}(q_m^{(n,K)})||}{||f_m^{(n,1)} - R^{-1}(q_m^{(n,1)})||} \)

21. **if** \( dp > 1 \) or \( df_m > T \) **then**

22. \( \beta = \beta \cdot \beta_{\text{red}} \)

23. **end**

24. \( q_m^{(n+1)} = q_m^{(n,1)} \)

25. \( f_m^{(n+1)} = f_m^{(n)} + \lambda \cdot R^{-1}(q_m^{(n+1)} - q_m^{(n)}) \)

26. **end**

Line 1 gives the initial values of parameters and basis material images. Lines 2–27 form the loop part can be divided into three modules, using the SOMA method to perform MSCT basis material decomposition (lines 6–16), the adaptive step size strategy (lines 17–24), and updating the estimated values of basis material images (lines 25–26). Each module is described in detail below.

Lines 3–5 are only performed when the polychromatic projections are geometrically inconsistent. The way to estimate the projections can be referred to [70–73].

Lines 6–16 are using the SOMA method to solve the nonlinear equations (correspond to algorithm 2). Line 7 is performing the first-order Taylor expansion of (1) at \( x^{(n)} \), where

\[
A_k = \begin{pmatrix}
\Theta_k^{(n,1)} & \Theta_k^{(n,2)} & \cdots & \Theta_k^{(n,M)} \\
\Phi_k^{(n)} & \Phi_k^{(n)} & \cdots & \Phi_k^{(n)}
\end{pmatrix},
\]

\[
b_k = p_k - p_k^{(n)} \quad ,
\]

\[
\Theta_k^{(n,m)} = \sum_{\omega=1}^{C_k} s_{k,\omega} \theta_{m,\omega} - \sum_{\omega=1}^{M} \theta_{m,\omega} q_{(n,\omega)} \quad ,
\]

and get the linear equations \( A_k x = b_k \).
\[ \Phi_k^{(n)} = \sum_{\omega=1}^{\Omega_k} s_{k,\omega} e^{-\sum_{m=1}^{M} \theta_{m,\omega} q^{(n)}}, \]  
(15) 

\[ p_k^{(n)} = -\ln \sum_{\omega=1}^{\Omega_k} s_{k,\omega} e^{-\sum_{m=1}^{M} \theta_{m,\omega} q^{(n)}}. \]  
(16) 

The adaptive step size strategy is shown in lines 17–24 and the step size is adjusted by changing the step size relaxation factor \( \beta \). The adjustment conditions are \( dp \) and \( df_m \), which are calculated in line 19 and line 20 respectively. \( dp \) is the ratio of the polychromatic projection changes between \( k = 1 \) and \( k = K \), and \( df_m \) is the ratio of the basis material images changes. On the one hand, the residual of \( k = K \) should be smaller than the residual of \( k = 1 \), that is \( dp < 1 \). On the other hand, the images should not change too much, that is \( df_m < T \) (where \( T \) is the threshold set in advance and its value can be referred to [75]). If above conditions are not met, it means the step size may be large at this time and should to be reduced. In lines 21–24, the step size is adjusted adaptively according to \( dp \) and \( df_m \). Line 22 shows that the results obtained by the old step size are not credible, so using the results at \( k = 1 \) as final result. In line 23, \( \beta_{\text{red}} \) is used to reduce the step relaxation factor and its value should be chosen in the interval \((0,1)\) [75]. 

Line 25 is obtaining the new basis material projection values and line 26 updates the basis material images by the projection residuals. \( \lambda \) is reconstruction relaxation factor and generally speaking, \( \lambda = 1 \) is enough. When higher-precision reconstruction results are required, \( \lambda \) can be attenuated as the iterations increasing [60].

3. Experiment

In this section, three MSCT basis material decomposition experiments are carried out. Firstly, the DSCT numerical experiment shows that the SOMA method can greatly improve the convergence speed and is robust to noise. Then, the triple material data experiment studies the feasibility of multiple basis material decomposition. Finally, a real data experiment illustrates its practical value.

3.1. DSCT numerical experiments

3.1.1. Phantom. This section uses two phantom. One is a slice of the commonly used 3D FORBILD thorax phantom with resolution \( 512 \times 512 \), and its geometric information and the reference density value are detailed on the website [76]. Assuming that the phantom is composed of water and bone, whose densities are \( 1.00 \text{ g cm}^{-3} \) and \( 1.92 \text{ g cm}^{-3} \) respectively. Figures 6(a) and (b) shows two basis material images respectively. The mass attenuation coefficients of water and bone can be obtained from the National Institute of Standard Technology (NIST) website [77], which is shown in figure 7(a).

The other one is the breast phantom used in 2022 AAPM DL-spectral CT challenge, which contains adipose and fibroglandular [78] shown in figures 6(c) and (d). The mass attenuation coefficients of adipose and fibroglandular can be obtained from the DL-spectral CT challenge website [78], which is shown in figure 7(b).

3.1.2. Experiment design. The spectra used in the thorax experiment are generated by the open-source software Spectrum GUI [79], the x-ray source is GE Maxiray 125 x-ray tube, the tube voltage is set to 80 kVp and 140 kVp, and the latter is filtered by 1 mm copper. The
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Figure 6. Phantoms used in the DSCT numerical experiments. (a), (b) Water and bone basis material image (display windows are set to [0, 1.20] and [0, 1.92] respectively) [76]. (c), (d) Adipose and fibroglandular basis material image (display windows are both set to [0, 1.00]) [78].

Figure 7. MAC used in the DSCT numerical experiments. (a) MAC of bone and water [77]. (b) MAC of adipose and fibroglandular [78].

normalized x-ray spectra are shown in figure 8(a). The sampling intervals of the x-ray energy spectra and the mass attenuation coefficients are both 1 keV. The spectra used in the breast experiment are provided by the DL-spectral CT challenge website [78], the tube voltage is set to 50 kVp and 80 kVp, and the normalized x-ray spectra are shown in figure 8(b). The sampling intervals of the x-ray energy spectra and the mass attenuation coefficients are both 0.5 keV. The scanning configurations are shown in table 1.

Simulate the polychromatic projections according to formula (1). Use multiple full scans and when generating geometrically inconsistent data, the initial angle of the single full scanning differs by 0.25°. Noisy polychromatic projections are simulated by adding Poisson noise with an initial number of $10^6$ photons.

The computer used in the experiment is equipped with a 2.40 GHz Intel Xeon E5-2620 six-core CPU and an NVIDIA Quadro K2200 graphics card. The reconstruction size is $512 \times 512$, and each pixel of the initial estimated image is set to 0.

The Alvarez method [9], the E-ART method [59] and the NCPD method [58] are selected as the comparison methods. The Alvarez method is the first DSCT reconstruction technique but it only can be applied to geometrically consistent data. Its result is a benchmark. The latter two methods, not only can they invert the mismatched system and get high-quality reconstruction
results, but also can deal with data collected with non-standard configurations. The parameters of the SOMA method are as follows: for thorax data, $\epsilon = 10^{-8}$, $T = 1.5$, $\kappa = 0.99$, $\beta = 0.3$ and $\beta_{\text{red}} = 0.9$. For breast data, $\epsilon = 10^{-8}$, $T = 1.5$, $\kappa = 0.99$, $\beta = 0.03$ and $\beta_{\text{red}} = 0.1$. The parameters of the NCPD method are referred to [58]. In order to be more fairly, $\lambda$ of all methods are set to 0.95 in all experiments below.

3.1.3. Experiment results. Figure 9 shows the reconstruction results of the DSCT numerical experiments. The first two columns are the results of the thorax phantom after 50 iterations and the last two columns are the results of the breast phantom after 100 iterations.

The Alvarez method can reconstruct structure of the basis material, but it amplifies the noise. For the breast phantom, the MAC of adipose and fibroglandular are closer, which leads the DSCT decomposition problem to be more ill-conditioned. So, the breast results reconstructed by the Alvarez method are more affected by noise amplification.

After 50 iterations, the E-ART method and the NCPD method can get high-quality bone basis material images and reconstruct most of water basis material structures. But the SOMA method can get more accurate results after the same iterations. For details of water basis material images, all methods can reconstruct the low-contrast areas (marked with blue). However, the spine structures (marked with red) reconstructed by the E-ART method and NCPD method are blurred, but the spine structure reconstructed by the SOMA method is visually the same as the phantom.
Figure 9. Reconstruction results of the DSCT numerical experiments.
For breast phantom, the closer MAC lead to the smaller angle between the polychromatic projection curves and there is more overlapping information between the normal directions. Thus, the E-ART method and the NCPD method need more iterations for decomposition. After 100 iterations, the two methods cannot decompose into adipose and fibroglandular. However, the SOMA method can decompose accurately using the orthogonal direction and improve the convergence speed greatly.

Figure 10 shows PSNR, SSIM and RMSE of the results. It can be observed that all quantitative indicators of the SOMA method are better than the E-ART method and the NCPD method except the SSIM of the water basis material images. However, it does not mean the results of the SOMA method are worse. Figure 9 shows clearly that the water basis material structures obtained by the SOMA method are visually closer to the phantom than the other methods.

Table 2 shows the mean values of the region marked with blue and yellow in the breast phantom. It can be observed that whether the data is consistent or not, the mean values of the SOMA method are closer to the true value after the same iterations.

Refer to the 2022 AAPM DL-spectral CT challenge, the mean RMSE is calculated and the output of the Alvarez method is used as the termination threshold, i.e. when the mean RMSE is less than termination threshold, the iterative process is stopped. Table 3 shows the required iterations. It can be observed that the convergence speed of the SOMA method is about 94%–98% faster than the E-ART method and the NCPD method.

3.2. Triple material data experiment

The experiment simulates an oral model including a copper teeth with resolution 512 × 512, and the phantom is composed of water, bone, and copper, with densities are 1.0 g cm\(^{-3}\), 1.92 g cm\(^{-3}\), and 8.96 g cm\(^{-3}\) respectively. Figures 11(a)–(c) shows the basis material images. Using Spectrum GUI [79] to simulate the spectra, the x-ray source is GE Maxiray 125 x-ray tube, the tube voltage is set to 40 kVp, 80 kVp, and 140 kVp, a 1 mm copper filter is added in front of the x-ray source at 140 kVp, and the normalized x-ray spectra are shown in figure 11(d). The mass attenuation coefficients of water, bone, and copper can be obtained from the NIST website [77]. The scan configurations are the same as the thorax phantom in section 3.1.2.

Figure 12 shows the reconstruction results after 200 iterations. Three methods can get correct copper basis material images and reconstruct most of water basis material structure. However, the bone basis material images reconstructed by the E-ART and the NCPD method has errors. It takes thousands of iterations for the E-ART method and the NCPD method to get the correct images, because the spectra overlap more, which leads to the ill-condition of the nonlinear model being stronger. The SOMA method to find the optimal solution along the orthogonal direction, which can obtain high-precision reconstruction results with fewer iterations.

Figure 13 shows quantitative indicators and profiles of the reconstruction results. Observing figures 13(a)–(c), the quantitative indicators of the SOMA method are higher than the E-ART method and the NCPD method, while the RMSE is lower than the two methods. Observing figures 13(d)–(f), the profiles of the reconstructed results show that the value of the basis material images reconstructed by the SOMA method is closer to the phantom.

3.3. Real data experiment

In this section, the SOMA method is performed on real data with complex structures. The equipment, phantom, and spectra are shown in figures 14(a)–(c), the mass attenuation
coefficients of water and bone can be obtained from the NIST website \[\cite{77}\], and the scan configurations are shown in table 4.

Figure 15 shows the reconstruction results of the E-ART method, the NCPD method and the SOMA method after five iterations. When the iterations are the same, the three methods can get acceptable bone density images. The trabecular structures (marked with red) in water
Table 2. Mean values of the region of the breast phantom results.

| Phantom | Consistent data | Inconsistent data |
|---------|-----------------|-------------------|
|         | Alvarez | EART | NCPD | SOMA | EART | NCPD | SOMA |
| Blue    | 1.000000 | 0.788875 | 0.952555 | 0.917477 | **0.990913** | 0.953291 | 0.917217 | **0.995075** |
| Yellow  | 1.000000 | 0.768347 | 0.980053 | 0.988373 | **0.991384** | 0.979992 | 0.991743 | **0.994825** |

Note: The bold values represent the best results of these results.

Table 3. Required iterations when the mean RMSE is less than the termination threshold.

| Consistent data | Inconsistent data |
|-----------------|-------------------|
| EART | NCPD | SOMA | EART | NCPD | SOMA |
| Thorax phantom  | 108 | 75 | 3 | 117 | 77 | 6 |
| Breast phantom  | 54 | 122 | 1 | 54 | 132 | 2 |

Figure 11. Phantom and spectra used in triple material data experiment. (a) The water basis material image (display window: [0, 1.0]). (b) The bone basis material image ([0, 1.0]). (c) The copper basis material image ([0, 1.0]). (d) Simulated spectra [79].

basis material images reconstructed by the E-ART method and the NCPD method are unclear. On the contrary, the structures are clearly visible in the results reconstructed by the SOMA method. The upper left part of the bone trabecula in the water density image has an obvious edge, and the other two methods will get similar results if they continue to iterate. Thus, the edge is speculated empirically to be caused by the movement of the object during the scanning...
Figure 12. Reconstruction results of triple material data after 200 iterations.

Figure 13. Quantitative indicators and profiles of the triple material data experiment results. (a) PSNR. (b) SSIM. (c) RMSE. (d) Profiles of the water basis material images (marked with red line in figure 11). (e) Profiles of the bone basis material images. (f) Profiles of the copper basis material images. For the convenience of the display, the RMSE of the gold basis material images are enlarged by ten times.
Figure 14. CT system, phantom, and spectra for the real data experiment. (a) Photograph of the industrial CT system in our laboratory. (b) Bone-water phantom. (c) The estimated spectra.

Table 4. Scan configuration for the real data experiment.

|                  | Scan 1          | Scan 2          |
|------------------|-----------------|-----------------|
| Voltage          | 80 kVp          | 140 kVp         |
| Current          | 240 μA          | 120 μA          |
| Filter           | 1.5 mm Al       | 0.5 mm Cu       |
| Exposure time per projection | 0.5 s          | 0.6 s           |
| SOD              | 355.61 mm       | 355.61 mm       |
| SDD              | 673.96 mm       | 673.96 mm       |
| Projections      | 1440            | 1440            |

Figure 15. Reconstruction results of real data after five iterations.
process but not caused by solution error. The results illustrate that the SOMA method can process real data and has practical value.

4. Discussion

This paper proposed a general iterative method, the so-called SOMA method, to invert the nonlinear equations. The SOMA method gives different equations different confidence and the convergence speed can be improved by the Schmidt orthogonalization when solving ill-conditioned system.

In section 3, the validity of the SOMA method is verified by MSCT basis material decomposition experiments. Three simulation data experiments verify the acceleration of convergence speed, the robustness to noise, and the feasibility of the multiple basis material decomposition. A real data experiment illustrates the practical value of the SOMA method. The above experiment results show that the SOMA method has a comparative convergence speed with the Alvarez method and can get more high-precision solutions than the compared methods.

The SOMA method is not sensitive to most of the parameters. In order to make parameter selection easier, an adaptive step size strategy is given in section 2.4. It should be emphasized that the adaptive step size strategy is not necessary. The fixed step size can satisfy the need under usual conditions. Besides the adaptive step size strategy, other strategies such as linear method or piecewise linear method can also be used.

In practical applications, the optimization model combined with the assumption of minimizing the total variation can be proposed. We have tested a variety of optimization models, and the SOMA method combines well with the ASD-NC-POCS method [26]. Refer to the ASD-NC-POCS method, an optimization model can be constructed as

\[
f^* = \text{arg} \min \sum_{m=1}^{M} \| f_m \|_{TV} \quad \text{s.t.} \quad \sqrt{\frac{\sum_{k=1}^{K} \| p_k - p_k^* \|_2^2}{\sum_{k=1}^{K} \| p_k \|_2^2}} < \tau, \tag{17}
\]

where \( \tau \) is the threshold of the data term and \( p_k^* \) is the measured polychromatic projection of the \( k \)th spectrum. For solving the above optimization model, a natural but non-strict method can be given. First, use the SOMA method to solve the data term (or non-linear model), then perform the POCS method, and at last solve the total variation minimization by the steepest descent method. (17) is not the only model that can be combined with the SOMA method and the given method is not the only method to solve (17). Other optimization models and solutions are worthy of in-depth study but are not discussed further here.

In this paper, the influence of scattered photons is ignored when modeling the MSCT reconstruction problem, however, the scattered photons have a great influence on the actual scanning. MSCT model containing scattered photons and its solution is the focus of the next step.

Data availability statement

The data generated and/or analysed during the current study are not publicly available for legal/ethical reasons but are available from the corresponding author on reasonable request. The data that support the findings of this study are available upon reasonable request from the authors.
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Appendix A

In this section, the recursion process of the Schmidt orthogonalization is shown. The initial vectors are $g_1, g_2, \ldots, g_K$ and the orthogonal vectors are $d_1, d_2, \ldots, d_K$.

Firstly, let $d_1 = g_1 = P_1 g_1$ and $P_1$ is set as the identity matrix. Then, the orthogonal vectors $d_2$ can be obtained by the Schmidt orthogonalization

$$d_2 = g_2 - d_1 \frac{<g_2, d_1>}{<d_1, d_1>}$$

$$= g_2 - d_1 \frac{d_1^T g_2}{d_1^T d_1}$$

$$= \left( I - \frac{d_1 d_1^T}{d_1^T d_1} \right) g_2$$

$$= \left( P_1 - \frac{d_1 d_1^T}{d_1^T d_1} \right) g_2$$

$$= P_2 g_2,$$

where $<a, b>$ represents the dot product of $a$ and $b$.

Next, the third orthogonal vectors $d_3$ can be calculated in the same way

$$d_3 = g_3 - d_1 \frac{<g_3, d_1>}{<d_1, d_1>} - d_2 \frac{<g_3, d_2>}{<d_2, d_2>}$$

$$= g_3 - d_1 \frac{d_1^T g_3}{d_1^T d_1} - d_2 \frac{d_2^T g_3}{d_2^T d_2}$$

$$= \left( I - \frac{d_1 d_1^T}{d_1^T d_1} - \frac{d_2 d_2^T}{d_2^T d_2} \right) g_3$$

$$= \left( P_2 - \frac{d_1 d_1^T}{d_1^T d_1} - \frac{d_2 d_2^T}{d_2^T d_2} \right) g_3$$

$$= P_3 g_3,$$

Similarly, it can be obtained by recursion

$$d_k = g_k - d_1 \frac{<g_k, d_1>}{<d_1, d_1>} - \cdots - d_{k-1} \frac{<g_k, d_{k-1}>}{<d_{k-1}, d_{k-1}>}$$

$$= \left( I - \frac{d_1 d_1^T}{d_1^T d_1} - \cdots - \frac{d_{k-1} d_{k-1}^T}{d_{k-1}^T d_{k-1}} \right) g_k$$

$$= \left( P_{k-1} - \frac{d_{k-1} d_{k-1}^T}{d_{k-1}^T d_{k-1}} \right) g_k$$

$$= P_k g_k.$$
So, the formula to get the orthogonal direction is

\[ d_k = P_k g_k, \]  

(A.4)

and the update process of the orthogonal correction matrix is

\[ P_k = P_{k-1} - \frac{d_{k-1}^\top d_{k-1}}{d_{k-1}^\top d_{k-1}}, \]  

(A.5)

In order to avoid the zero denominator, a small value \( \epsilon \) is added in the denominator as the correction term. As a result, the final update formula is

\[ P_k = P_{k-1} - \frac{d_{k-1}^\top d_{k-1}}{d_{k-1}^\top d_{k-1} + \epsilon}. \]  

(A.6)

**Appendix B**

This section gives a simple brief convergence proof of the SOMA method.

The convergence proof is equivalent to proving that the sequence \( \{x_k\} \) generated by \( x_k = x_{k-1} + \alpha_k d_k \) converges to the solution \( x^* \) of the linear system \( Ax = b \).

There are a series of linearly independent vectors \( d_1, d_2, \ldots, d_K \) and they span the solution space. The difference between \( x^* \) and \( x_0 \) can be written as

\[ x^* - x_0 = a_1 d_1 + a_2 d_2 + \cdots + a_K d_K, \]  

(B.1)

where \( a_k \) is a scalar. Multiply both sides of the formula by \( d_k^\top A \) and use the property of orthogonality, then

\[ d_k^\top A (x^* - x_0) = d_k^\top A (a_1 d_1 + a_2 d_2 + \cdots + a_K d_K) = d_k^\top A a_k d_k. \]

So the coefficient can be obtained

\[ a_k = \frac{d_k^\top A (x^* - x_0)}{d_k^\top A d_k}. \]  

(B.2)

Assume \( x_k \) is generated by the iterative scheme, then

\[ x_{k-1} = x_0 + \alpha_1 d_1 + \cdots + \alpha_{k-1} d_{k-1}. \]

Similarly, multiplying both sides of the formula by \( d_k^\top A \), there is

\[ d_k^\top A (x_{k-1} - x_0) = 0. \]  

(B.3)

Therefore,

\[ d_k^\top A (x^* - x_0) = d_k^\top A (x^* - x_{k-1}) = d_k^\top (Ax^* - Ax_{k-1}) = d_k^\top (b - Ax_{k-1}). \]  

(B.4)
It has been mentioned in section 2.1 that
\[
\alpha_k = \frac{b_k - A_xk_{k-1}}{A_id_i}.
\]
Thus \(b_k - A_xk_{k-1} = \alpha_k A_id_i\) and substituting it into (B.4), then
\[
d^\top_k A(x^* - x_0) = d^\top_k (b - A_xk_{k-1})
\]
\[
= d^\top_k \alpha_k A_id_i
\]
\[
= d^\top_k Aa_kd_i.
\]
That means \(a_k = \alpha_k\), giving the result.

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**References**

[1] Ai T, Yang Z, Hou H, Zhan C, Chen C, Lv W, Tao Q, Sun Z and Xia L 2020 Correlation of chest CT and RT-PCR testing for coronavirus disease 2019 (COVID-19) in China: a report of 1014 cases Radiology 296 32–40

[2] Ye Z, Zhang Y, Wang Y, Huang Z and Song B 2020 Chest CT manifestations of new coronavirus disease 2019 (COVID-19): a pictorial review Eur. Radiol. 30 4381–9

[3] Shaik N K and Cherukuri T K 2022 Transfer learning based novel ensemble classifier for COVID-19 detection from chest CT-scans Comput. Biol. Med. 141 105127

[4] Kim J, Silva A B, Hsu J C, Maidment P S N, Shapira N, Noël P B and Cormode D P 2020 Radioprotective garment-inspired biodegradable polymeric nanoparticles for enhanced CT contrast production Chem. Mater. 32 381–91

[5] Zhao S, Zhang W, Sheng W and Zhao X 2018 A frame of 3D printing data generation method extracted from CT data Sens. Imaging 19 13

[6] Xu J, Haque A, Gong W, Gamage R P, Dai G, Zhang Q and Xu F 2020 Experimental study on the bearing mechanisms of rock-socketed piles in soft rock based on micro x-ray CT analysis Rock Mech. Rock Eng. 53 3395–416

[7] Du F, Wang K, Zhang G, Zhang Y, Zhang G and Wang G 2022 Damage characteristics of coal under different loading modes based on CT three-dimensional reconstruction Fuel 310 122304

[8] Bossema F G, Coban S B, Kostenko A, van Duin P, Dorscheid J, Garachon I, Hermens E, van Lier R and Batenburg K J 2021 Integrating expert feedback on the spot in a time-efficient explorative CT scanning workflow for cultural heritage objects J. Cult. Herit. 49 38–47

[9] Alvarez R and Macovski A 1976 Energy-selective reconstructions in x-ray computerised tomography Phys. Med. Biol. 21 733–44

[10] Alvarez R and Seppi E 1979 Comparison of noise and dose in conventional and energy selective computed-tomography IEEE Trans. Nucl. Sci. 26 2653–6

[11] Wang G, Gao Q, Wang Z, Lu X, Yu S and Jin Z 2021 Reduction of microwave ablation needle related metallic artifacts using virtual monenergetic images from dual-layer detector spectral CT in a rabbit model with VX2 tumor Sci. Rep. 11 9295

[12] Agostini A, Floridi C, Borgheresi A, Badaloni M, Esposto Pirani P, Terilli F, Ottaviani L and Giovagnoni A 2020 Proposal of a low-dose, long-pitch, dual-source chest CT protocol on third-generation dual-source CT using a tin filter for spectral shaping at 100 kVp for CoronaVirus Disease 2019 (COVID-19) patients: a feasibility study Radiol. Med. 125 365–73

[13] Roski F et al 2019 Bone mineral density measurements derived from dual-layer spectral CT enable opportunistic screening for osteoporosis Eur. Radiol. 29 6355–63

[14] Sauter A P, Kopp F K, Münzel D, Dangelmaier J, Renz M, Renger B, Braren R, Fingerle A A, Rummeny E J and Noël P B 2018 Accuracy of iodine quantification in dual-layer spectral
CT: influence of iterative reconstruction, patient habitus and tube parameters Eur. J. Radiol. 102 83–88

[15] Kalender W A, Perman W H, Vetter J R and Klotz E 1986 Evaluation of a prototype dual-energy computed tomographic apparatus. I. Phantom studies Med. Phys. 13 334–9

[16] Vetter J R, Kalender W A, Mazess R B and Holden J E 1986 Evaluation of a prototype dual-energy computed tomographic apparatus: II. Determination of vertebral bone mineral content Med. Phys. 13 340–3

[17] Doniyou J, Koo J, Poulsen H F, Olsen U L and Iovea M 2021 The significance of the spectral correction of photon counting detector response in material classification from spectral x-ray CT Proc. SPIE 11771 1177103

[18] Xu X, Xing Y, Wang S and Zhang L 2018 Systematic implementation of spectral CT with a photon counting detector for liquid security inspection Nucl. Instrum. Methods Phys. Res. A 893 99–108

[19] Broeke L V, Grillon M, Yeung A W L, Wu W, Tanaka R Vardhanabhuti V 2021 Feasibility of photon-counting spectral CT in dental applications—a comparative qualitative analysis BDJ Open 7 4

[20] Rotzinger D C et al 2021 Performance of spectral photon-counting coronary CT angiography and comparison with energy-integrating-detector CT: objective assessment with model observer Diagnostics 11 2376

[21] Nagayama Y, Inoue T, Oda S, Tanoue S, Nakaura T, Ikeda O and Yamashita Y 2020 Adrenal adenomas versus metastases: diagnostic performance of dual-energy spectral CT virtual non-contrast imaging and iodine maps Radiology 296 324–32

[22] Si-Mohamed S A, Miaihes J, Rodesch P, Boccalini S, Lacombe H, Leitman V, Cottin V, Boussel L and Douek P 2021 Spectral photon-counting CT technology in chest imaging J. Clin. Med. 10 5757

[23] Szczykutowicz T P and Chen G H 2010 Dual energy CT using slow kVp switching acquisition and prior image constrained compressed sensing Phys. Med. Biol. 55 6411–29

[24] Fang C, Xu G and Zhu L 2020 Single scan dual energy cone beam CT using a rotating filter Proc. SPIE 11312 113123S

[25] Jiang X, Fang C, Hu P, Cui H, Zhu L and Yang Y 2021 Fast and effective single-scan dual-energy cone-beam CT reconstruction and decomposition denoising based on dual-energy vectorization Med. Phys. 48 4843–56

[26] Chen B, Zhang Z, Sidky E Y, Xia D and Pan X 2017 Image reconstruction and scan configurations enabled by optimization-based algorithms in multispectral CT Phys. Med. Biol. 62 8763–93

[27] Rassouli N, Etesami M, Dhanantwari A and Rajiah P 2017 Detector-based spectral CT with a novel dual-layer technology: principles and applications Insights Imaging 8 589–98

[28] Altman A and Carmi R 2009 A double-layer detector, dual-energy CT - principles, advantages and applications Med. Phys. 36 2750–2750

[29] Zou Y and Silver M 2008 Analysis of fast kV-switching in dual energy CT using a pre-reconstruction decomposition technique Proc. SPIE 6913 691313

[30] Xu D, Langan D, Wu X, Pack J D, Benson T M, Eric Tkaczky J and Schmitz A M 2009 Dual energy CT via fast kVp switching spectrum estimation Proc. SPIE 7258 72583T

[31] Flohr T G et al 2006 First performance evaluation of a dual-source CT (DSCT) system Eur. Radiol. 16 256–68

[32] Llopart X, Campbell M, Dinapoli R, San Segundo D and Pernigotti E 2002 Medipix2: a 64-k pixel readout chip with 55 µm square elements working in single photon counting mode IEEE Trans. Nucl. Sci. 49 2279–83

[33] Llopart X, Ballabriga R, Campbell M, Tlustoš L and Wong W 2007 Timexip, a 65k programmable pixel readout chip for arrival time, energy and/or photon counting measurements Nucl. Instrum. Methods Phys. Res. A 581 485–94

[34] Steadman R, Herrmann C and Livne A 2017 ChromAIX2: a large area, high count-rate energy-resolving photon counting ASIC for a Spectral CT Prototype Nucl. Instrum. Methods Phys. Res. A 862 18–24

[35] Wang T and Zhu L 2015 Dual energy CT with one full scan and a second sparse-view scan using structure preserving iterative reconstruction (SPIR) Med. Phys. 42 3682

[36] Petrongolo M and Zhu L 2018 Single-scan dual-energy CT using primary modulation IEEE Trans. Med. Imaging 37 1799–808

[37] Maas C, Meyer E and Kachelrieß M 2011 Exact dual energy material decomposition from inconsistent rays (MDIR) Med. Phys. 38 691–700
[38] Zhao S, Pan H, Zhang W, Xia D and Zhao X 2021 An oblique projection modification technique (OPMT) for fast multispectral CT reconstruction Phys. Med. Biol. 66 065003
[39] Sidky E Y, Yu L, Pan X, Zou Y and Vannier M 2005 A robust method of x-ray source spectrum estimation from transmission measurements: demonstrated on computer simulated, scatter-free transmission data J. Appl. Phys. 97 124701
[40] Zhang L, Zhang G, Chen Z, Xing Y, Cheng J and Xiao Y 2007 X-ray spectrum estimation from transmission measurements using the expectation maximization method IEEE Nuclear Science Symp. Conf. Record pp 3089–93
[41] Ha W, Sidky E Y, Barber R F, Schmidt T G and Pan X 2019 Estimating the spectrum in computed tomography via Kullback-Leibler divergence constrained optimization Med. Phys. 46 81–92
[42] Liu B, Yang H, Lv H, Li L, Gao X, Zhu J and Jing F 2020 A method of x-ray source spectrum estimation from transmission measurements based on compressed sensing Nucl. Eng. Technol. 52 1495–502
[43] Brooks R A 1977 A quantitative theory of the Hounsfield unit and its application to dual energy scanning J. Comput. Assist. Tomogr. 1 487–93
[44] Kachelrieß M, Berkus T and Stenner P 2007 Empirical dual energy calibration (EDEC) for cone-beam computed tomography Med. Phys. 34 3630–41
[45] Maaß C, Baer M and Kachelrieß M 2009 Image-based dual energy CT using optimized precorrection functions: a practical new approach of material decomposition in image domain Med. Phys. 36 3818–29
[46] Maaß C, Stefan S, Michael K and Kachelrieß M 2011 Empirical multiple energy calibration (EMEC) for material-selective CT IEEE Nuclear Science Symp. and Medical Imaging Conf. vol 4222
[47] Feng C, Shen Q, Kang K and Xing Y 2016 An empirical material decomposition method (EMDM) for spectral CT IEEE Nuclear Science Symp., Medical Imaging Conf. and Room-Temperature Semiconductor Detector Workshop
[48] Chuang K S and Huang H K 1987 A fast dual-energy computational method using isotransmission lines and table lookup Med. Phys. 14 186–92
[49] Zhao X, Hu J, Zhao Y and Zhang H 2014 A novel iterative reconstruction method for dual-energy computed tomography based on polychromatic forward-projection calibration Insight 56 541–8
[50] He J, Wang Y and Ma J 2020 Radon inversion via deep learning IEEE Trans. Med. Imaging 39 2076–87
[51] Zhang W, Zhang H, Wang L, Wang X, Hu X, Cai A, Li L, Niu T and Yan B 2019 Image domain dual material decomposition for dual-energy CT using butterfly network Med. Phys. 46 2037–51
[52] Xu Y, Yan B, Chen J, Zeng L and Li L 2018 Projection decomposition algorithm for dual-energy computed tomography via deep neural network J. X-Ray Sci. Technol. 26 361–77
[53] Touch M, Clark D P, Barber W and Badea C T 2016 A neural network-based method for spectral distortion correction in photon counting x-ray CT Phys. Med. Biol. 61 6132
[54] Wu X et al 2019 Multi-material decomposition of spectral CT images via fully convolutional dense-nets J. X-Ray Sci. Technol. 27 461–71
[55] Zhang R, Thibault J-B, Bouman C A, Sauer K D and Hsieh J 2014 Model-based iterative reconstruction for dual-energy x-ray CT using a joint quadratic likelihood model IEEE Trans. Med. Imaging 33 117–34
[56] Xue Y, Ruan R, Hu X, Kuang Y, Wang J, Long Y and Niu T 2017 Statistical image-domain multi-material decomposition for dual-energy CT Med. Phys. 44 886–901
[57] Long Y and Fessler J A 2014 Multi-material decomposition using statistical image reconstruction for spectral CT IEEE Trans. Med. Imaging 33 1614–26
[58] Chen B, Zhang Z, Xia D, Sidky E Y and Pan X 2021 Non-convex primal-dual algorithm for image reconstruction in spectral CT Comput. Med. Imaging Grap. 87 101821
[59] Zhao Y, Zhao X and Zhang P 2015 An extended algebraic reconstruction technique (E-Art) for spectral CT IEEE Trans. Med. Imaging 34 761–8
[60] Hu J, Zhao X and Wang F 2016 An extended simultaneous algebraic reconstruction technique (E-SART) for x-ray dual spectral computed tomography Scanning 38 599–611
[61] Li M, Zhao Y and Zhang P 2019 Accurate iterative FBP reconstruction method for material decomposition of dual energy CT IEEE Trans. Med. Imaging 38 802–12
[62] Zhang W, Zhao S, Pan H, Zhao Y and Zhao X 2021 An iterative reconstruction method based on monochromatic images for dual energy CT Med. Phys. 48 6437–52
[63] Xue Y et al 2021 Multi-material decomposition for single energy CT using material sparsity constraint IEEE Trans. Med. Imaging 40 1303–18
[64] Dong X, Niu T and Zhu L 2014 Combined iterative reconstruction and image-domain decomposition for dual energy CT using total-variation regularization Med. Phys. 41 051909
[65] Niu T, Dong X, Petrongolo M and Zhu L 2014 Iterative image-domain decomposition for dual-energy CT Med. Phys. 41 475–6
[66] Harms J, Wang T, Petrongolo M, Niu T and Zhu L 2016 Noise suppression for dual-energy CT via penalized weighted least-square optimization with similarity-based regularization Med. Phys. 43 2676–86
[67] Wang Q, Zhu Y and Yu H 2017 Locally linear constraint based optimization model for material decomposition Phys. Med. Biol. 62 8314–40
[68] Ding Q, Niu T, Zhang X and Long Y 2018 Image-domain multimaterial decomposition for dual-energy CT based on prior information of material images Med. Phys. 45 3614–26
[69] Gordon R, Bender R and Herman G T 1971 Algebraic reconstruction technique (ART) for three-dimensional electron microscopy and x-ray photography J. Theor. Biol. 29 471–81
[70] Stayman J W and Fessler J A 2004 Compensation for nonuniform resolution using penalized-likelihood reconstruction in space-variant imaging systems IEEE Trans. Med. Imaging 23 269–84
[71] Knaup M, Stenner P and Kachelrieß M 2007 Rawdata-based dual energy CT (DECT) from inconsistent scans IEEE Nuclear Science Symp. Conf. Record pp 4457–9
[72] Zhao X, Hu J, Zhao Y, Zhang H-T and Zhang P 2014 Iterative dual energy material decomposition from spatial mismatched raw data sets J. X-Ray Sci. Technol. 22 745–6
[73] Hu J and Zhao X 2016 A practical material decomposition method for x-ray dual spectral computed tomography J. X-Ray Sci. Technol. 24 407–25
[74] Fu L, Lee T, Kim S M, Alessio A M, Kinahan P E, Chang Z, Sauer K, Kalra M K and De Man B 2017 Comparison between pre-log and post-log statistical models in ultra-low-dose CT reconstruction IEEE Trans. Med. Imaging 36 707–20
[75] Sidky E Y and Pan X 2008 Image reconstruction in circular cone-beam computed tomography by constrained, total-variation minimization Phys. Med. Biol. 53 4777–807
[76] Sourbelle K 2014 FORBILD thorax phantom (available at: www.imp.uni-erlangen.de/phantoms/index.html)
[77] Hubbell J H and Seltzer S M 2004 X-ray mass attenuation coefficients table NIST (available at: https://physics.nist.gov/PhysRefData/XrayMassCoef/tab4.html) (https://doi.org/10.18434/T4D01F)
[78] Sidky E Y and Pan X 2023 Report on the AAPM deep-learning spectral CT grand challenge Med. Phy. (https://doi.org/10.1002/mp.16363)
[79] Spectrum GUI 2006 (available at: https://sourceforge.net/projects/spectrumgui/)