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Optimizing Spectral CT Parameters for Material Classification Tasks

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Abstract

In this work, we propose a framework for optimizing spectral CT imaging parameters and hardware design with regard to material classification tasks. Compared with conventional CT, many more parameters must be considered when designing spectral CT systems and protocols. These choices will impact material classification performance in a non-obvious, task-dependent way with direct implications for radiation dose reduction.

In light of this, we adapt Hotelling Observer formalisms typically applied to signal detection tasks to the spectral CT, material-classification problem. The result is a rapidly computable metric that makes it possible to sweep out many system configurations, generating *parameter optimization curves* (POC's) that can be used to select optimal settings.

The proposed model avoids restrictive assumptions about the basis-material decomposition (e.g. linearity) and incorporates signal uncertainty with a stochastic object model. This technique is demonstrated on dual-kVp and photon-counting systems for two different, clinically motivated material classification tasks (kidney stone classification and plaque removal). We show that the POC's predicted with the proposed analytic model agree well with those derived from computationally intensive numerical simulation studies.

1 Introduction

Spectral computed tomography (SCT) refers to an imaging technique whereby multiple CT datasets are acquired, each with a unique energy spectrum. The term has been broadly used to describe several recent dual-energy systems as well as scanners with energy-discriminating, photon-counting detectors (PCDs).

SCT offers several key advantages over conventional, single-energy CT. Through a process called “basis-material decomposition”, one can reconstruct quantitative, material-density maps [1] (e.g. bone and soft-tissue) or virtual-monoenergetic (VM) images [2] that have the familiar appearance of ordinary CT images but without polychromatic, beam-hardening artifacts. Furthermore, material-classification algorithms can be applied to these decomposed images in order to differentiate contrast materials based on their elemental

composition. For example, calcium ($Z=20$) and iodine ($Z=53$) may be indistinguishable in ordinary CT but can be differentiated by SCT [3][4][5].

It turns out that many clinical applications of spectral CT involve material-classification tasks. Primak et al. showed that dual-source CT can reliably differentiate uric acid (UA) from non-UA kidney stones [6]. This distinction is important because the former can be treated with oral medication while the latter may require more invasive therapies. Similar algorithms have also been used to identify gout in the hands and feet directly from reconstructed images [7]. This image analysis could eventually replace the gold-standard test: a painful joint aspiration followed by optical analysis of the synovial fluid [8]. Additionally, Thomas et al. demonstrated that dual-energy, bone-and-plaque-removal algorithms can enhance CT angiography (CTA) by using the spectral information to identify calcium- and iodine-containing voxels [5]. This can improve the assessment of arterial stenoses and eliminate the need for extra precontrast scans. Thus, spectral-CT-enabled material-classification algorithms may lead to lower-dose imaging protocols and valuable, new diagnostic tests.

Despite many potential advantages of SCT, it has not yet been widely adopted into clinical use. Marin et al. speculate that this may be partially attributed to diverging opinions on how best to implement SCT, and a lack of robust validation methods [9].

Compared with conventional single-energy systems, there can be significantly more parameters to tune. For example, one of the earliest clinically available dual-energy CT (DECT) scanners is the dual-source configuration; two x-ray tubes, offset by 90 degrees, simultaneously acquire low- and high-kVp projection data in a single rotation [10]. Holding the dose to the patient fixed, one has freedom to adjust the kVp, fractional dose allocation, and beam filtration of each tube separately. A future generation of scanners is likely to use energy-resolving PCD's, which can have five or more energy thresholds that can be adjusted on a per-scan basis [11]. The impact of these parameters on material-classification performance is seldom obvious and always task-dependent. Criteria for determining “good” parameters are essential for achieving high diagnostic utility while minimizing radiation dose. Several prior works have interrogated the effect of imaging parameters on sinogram and image noise. Alvarez and Macovski's foundational work on dual-energy CT [2] describes a method to estimate the variance of the basis-material sinograms using the Cramer-Rao lower bound (CRLB). Roessl generalized this technique with a more general noise model and demonstrated its use for optimizing detector parameters to achieve minimal noise-variance in material density maps [12]. This analysis is useful for characterizing material *quantification* tasks but does not provide a mechanism for measuring material *classification* performance.

In [13], a linear cascaded systems model is presented for analyzing material-classification tasks. This model is powerful in that it can track task-performance metrics through a “cascade” of image processing and reconstruction steps¹; however, it relies upon several

¹Linear cascaded systems models implicitly assume that each step in the can be represented by a circulant linear operator. In practice this is never strictly true but may be approximately valid within a region-of-interest.

restrictive assumptions: (1) the basis-material decomposition is linear and performed post-reconstruction, (2) the mass-densities of the contrast materials are known exactly. On the contrary, the most accurate basis-material decomposition algorithms are necessarily nonlinear [2] and account for varying noise levels in projection space. The latter fact is especially important in photon-counting CT, where the number of spectral bins often exceeds the number of basis materials. Also, one usually seeks to classify many image pixels spanning a range of mass-densities (or concentrations), such as iodine-enhanced regions comprising a continuous range of water-iodine mixing.

The goal of this work is to provide a simple metric for determining how best to acquire spectral imaging data, independent of reconstruction technique. Specifically, we seek imaging parameters that maximize material-classification performance while minimizing radiation dose. We extend the classical signal detection theory to material-classification tasks and derive a figure-of-merit (FOM) based on the Hotelling Observer (HO) SNR. As in [14] the mathematical observer model is computed post basis-material decomposition, and noise properties of the basis-material decomposition are estimated via the Fisher information matrix. Signal variability, such as variations in the concentration of contrast media, are incorporated with a stochastic object model. This stands in contrast to the signal-known-exactly/background-known-exactly approach of [13]. Furthermore, the proposed model considers merely a single ray, which serves as a surrogate to the complete projection data yet captures the relevant physics for profiling the tasks of interest. The result is an analytic FOM that directly relates SCT imaging parameters to material classification performance. It can be computed very rapidly, making it possible optimize multiple system parameters efficiently.

2 Theory and Methods

2.1 Material discrimination in dual-energy CT

Due to varying photoelectric and Compton cross-sections, as well as element-specific k-edges, different materials have unique spectral signatures related to their effective atomic numbers (Z_{eff}).

Figure 1 illustrates this principle with a disk phantom containing calcium and iodine inserts of varying concentration. The Hounsfield Unit (HU) values of the disks overlap significantly at a single-energy, so simple thresholding cannot successfully distinguish these two elements. On the other hand, if HU values at different energies (e.g. 53 keV and 71 keV) are plotted simultaneously in two dimensions, the calcium and iodine pixels cluster along unique rays in the resulting 2D vector space, making classification possible. However, due to image noise and the small angle of separation, some misclassifications are inevitable.

One can attempt to improve the separation between these material clusters by altering parameters of the x-ray source(s) or detectors (e.g. kVp, filtration, energy-thresholds), but there is a complex trade off between spectral separation and image noise that makes the optimal choices non-obvious. Some metric of material classification performance that can be related back to spectral parameters is needed. The schematic in Figure 2 illustrates this general concept for tuning a single imaging parameter. We will refer to this type of plot as a

parameter optimization curve (POC). In general a POC is an N -dimensional function relating spectral CT hardware/acquisition parameters to some metric of material classification performance. The optimal configuration corresponds to a global maximum of the POC.

In the following section, we present our single-ray Hotelling Observer (SRHO) model for computing analytic POC's.

2.2 Single-ray Hotelling Observer Model (SRHO)

The model we develop for characterizing material-classification performance is based on classical signal-detection theory, which has been applied to numerous medical imaging tasks [15, 16, 17]. Typically, a mathematical observer, privy to certain knowledge of the object and imaging physics, must decide whether a signal (e.g. cancer) is present or not [18]. The same notion can be applied to material classification by redefining the hypotheses: signal is material 1 (hypothesis 1), signal is material 2 (hypothesis 2).

In the same spirit as [12] and [19], we use a single ray as a surrogate to the complete projection data, leading to a one-dimensional model specified by the mass-thicknesses of the background and contrast materials. The path lengths used in the 1D model correspond a ray passing through the center of a circularly symmetric object. The diameters should be chosen to reflect the imaging task, e.g. based on the size of the patient and contrast objects.

2.2.1 SKE/BKE—First, we describe a common model-observer paradigm referred to as a “signal-known-exactly/background-known-exactly” (SKE/BKE) task [20], which serves as a natural segue into our signal-known-statistically/background-known-exactly (SKS/BKE) model. For SKE/BKE it is assumed that the contribution of the background (e.g. water) is known exactly. Additionally, the shape and size of the signals are presumed known; the only unknown parameter is whether the contrast object is made of material 1 or 2. This is illustrated in Figure 3.

The task of the mathematical observer is to make this determination based on the projection data $\mathbf{g} = [g_1, g_2, \dots, g_N]$, where $\mathbf{g}$ are line-integrals of the object's total attenuation along a single ray at energies $E_1, E_2, \dots, E_N$. The two hypotheses are explicitly 3 defined by the following equations:

$$E\{g_i|H_1\} = a_b f_b(E_i) + a_1 f_1(E_i) \quad (1)$$

$$E\{g_i|H_2\} = a_b f_b(E_i) + a_2 f_2(E_i), \quad (2)$$

where $E\{g_i|H_{1,2}\}$ represents the expected value of g_i under H_1 or H_2 . The density of the background material is denoted by ρ_b . The quantities $a_b \equiv \int_L \rho_b d\ell$ and $f_b(E) \equiv \mu_b(E)/\rho_b$ are its “mass-thickness” and “mass-attenuation coefficient (MAC),” respectively. Similar definitions hold for contrast materials 1 and 2, indicated by the subscripts.

We assume that the data, $\mathbf{g}$, are mono-energetic with known mean and covariance. This appears to be a very restrictive assumption, since real spectral CT systems use polychromatic illumination. However, virtual monoenergetic (VM) data can be synthesized from arbitrary spectral CT measurements, via nonlinear, basis-material decomposition algorithms. In this case, the VM data are considered to be the input to the HO, and the first- and second-order statistics of $\mathbf{g}$ are estimated via the Fisher information matrix. The details of these computations are given in Appendix A.

In this work, we specifically consider the Hotelling Observer (HO), which is the optimal *linear* observer; i.e. the HO constructs a test statistic, t , by performing linear operations on the data,

$$t = \mathbf{w}^T \mathbf{g}. \quad (3)$$

The weight-vector $\mathbf{w}$ is chosen to maximize

$$\text{SNR}_{\text{HO}}^2 \equiv \frac{[\text{E}\{t|H_1\} - \text{E}\{t|H_2\}]^2}{\frac{1}{2}\text{var}\{t|H_1\} + \frac{1}{2}\text{var}\{t|H_2\}}, \quad (4)$$

and the quantity, SNR_{HO} , describes how easily separable are the conditional distributions $\text{Pr}(t|H_1)$ and $\text{Pr}(t|H_2)$. The maximizer of (4), $\mathbf{w}_{\text{HO}}$, is given by

$$\mathbf{w}_{\text{HO}} \equiv K_g^{-1} \Delta \bar{\mathbf{g}}, \quad (5)$$

where $\bar{\mathbf{g}}$ is shorthand for

$$\Delta \bar{\mathbf{g}} \equiv \text{E}\{\mathbf{g}|H_1\} - \text{E}\{\mathbf{g}|H_2\}, \quad (6)$$

and K_g is the covariance of $\mathbf{g}$, averaged over each hypothesis:

$$K_g \equiv \frac{1}{2} (K_{g|H_1} + K_{g|H_2}). \quad (7)$$

Furthermore, it can be shown that

$$\text{SNR}_{\text{HO}}^2 = \mathbf{w}_{\text{HO}}^T \Delta \bar{\mathbf{g}}. \quad (8)$$

These relationships are all derived in [21].

Hypothetically, one could construct non-linear observers that may outperform the HO. For example, the Ideal Observer (IO) utilizes complete knowledge of the statistics of $\mathbf{g}$ to minimize Bayes' risk. However, the HO is commonly used in place of the IO because it is far simpler to compute and requires knowledge of only the second-order statistics of the data [21]. Furthermore, the HO often serves as an excellent approximation of the IO and may be a better indicator of human performance [22].

2.3 SKS/BKE

A crucial component of spectral CT material-classification tasks that we have not yet modeled is signal variability. Note that in Figure 1, classifying the calcium and iodine disks is difficult because both types of inserts span a range of concentrations. It is this variability in mass-density that necessitates the use of multi-energy CT rather than conventional CT. If the task were merely to classify two different materials, each of known density, one could always select a single beam energy that would sufficiently separate the two signals. In fact, for an SKE/BKE material classification task, there may be no benefit at all to a multi-energy imaging technique over single-energy imaging [23, 24]. We will demonstrate this effect later in the context of optimizing a dual-kVp CT system.

In the SKS/BKE model, signal variability is incorporated via a stochastic object model, where the mass-thicknesses, a_1 and a_2 are presumed to follow known distributions, $\Pr(a_1)$ and $\Pr(a_2)$. In this work, we assume that a_1 and a_2 are uniformly distributed on intervals $(a_1^{\min}, a_1^{\max})$ and $(a_2^{\min}, a_2^{\max})$, but any other probability distribution function can be used just as easily. In practice, the distribution functions characterizing the object variability would have to be obtained from prior knowledge. For example, if the task of interest is a kidney stone classification task, then population statistics can be used to determine the range or distribution of possible stone sizes.

In the SKS formalism, we start by expressing the hypotheses, conditional on a_1 and a_2 :

$$E\{g_i|H_1, a_1\} = a_b f_b(E_i) + a_1 f_1(E_i) \quad (9)$$

$$E\{g_i|H_2, a_2\} = a_b f_b(E_i) + a_2 f_2(E_i) \quad (10)$$

Computing the Mean Signal—To compute $E\{g|H_1\}$ we simply average equation 9 and over all possible objects, yielding

$$E\{g_i|H_1\} = a_b f_b(E_i) + \bar{a}_1 f_1(E_i) \quad (11)$$

where

$$\begin{aligned}\bar{a}_1 &\equiv \int \Pr(a_1) a_1 da_1 \\ &= \frac{1}{2} (a_1^{\min} + a_1^{\max}),\end{aligned}\quad (12)$$

for the uniform distribution. The computation of $E\{g|H_2\}$ is completely analogous, and the quantity $\bar{g}$ is given by equation 6.

Computing the Total Covariance—To compute $K_{g|H_1}$ we invoke the “law of total covariance” [21]. This matrix comprises two terms,

$$K_{g|H_1} = \bar{K}_{g|H_1}^{\text{noise}} + K_{\bar{g}|H_1}^{\text{obj}}, \quad (13)$$

where $\bar{K}_{g|H_1}^{\text{noise}}$ represents the noise-covariance averaged over all possible objects, and $K_{\bar{g}|H_1}^{\text{obj}}$ represents the variation in the conditional means. For a given mass-thickness a_1 , the covariance of g , under H_1 is denoted by $K_{g|H_1, a_1}$. The steps for computing $K_{g|H_1, a_1}$ for arbitrary spectral CT systems are detailed in appendix A. Then the noise covariance term is given by

$$\bar{K}_{g|H_1}^{\text{noise}} = \int \Pr(a_1) K_{g|H_1, a_1} da_1. \quad (14)$$

Likewise, the expected measurement, $\bar{g}$, for a given mass-thickness, a_1 , is denoted by $E\{g|H_1, a_1\}$. If we define $g'_i \equiv E\{g_i|H_1, a_1\} - E\{g_i|H_1\}$, then the second covariance term is given by

$$K_{\bar{g}|H_1}^{\text{obj}} = \int \Pr(a_1) \cdot \mathbf{g}' \mathbf{g}'^T da_1. \quad (15)$$

After computing $K_{g|H_2}$ in a similar fashion, the total covariance matrix K_g is given by equation 7. Finally, equations 5 and 8 are used to calculate the HO SNR, our figure-of-merit for classification tasks. By sweeping out different system parameters and recalculating the HO SNR, a curve like figure 2 can be generated, in order to determine which settings result in the optimal classification performance.

3 Simulation Studies

The SRHO model provides a rapid method for discovering optimal spectral imaging parameters with respect to material-classification performance. In this section we present a method for validating its predictions by directly measuring material classification performance in simulation studies.

3.1 Kidney Stone Classification Task

We created a numerical kidney stone phantom consisting of a water background and 100 randomly located kidney-stone inserts (see figure 4). This phantom is motivated by a kidney stone classification task [6] where the goal is to distinguish uric acid (UA) stones from non-UA stones in a known background (e.g. urine). The stone objects are a mixture of water and varying densities of either uric acid or calcium oxalate. Physiologically, the observed differences in stone density are due to the varying porosity of different calculi.

In figure 4 the stone materials are indicated in red (uric acid) and blue (calcium oxalate), and each stone's opacity is proportional to its physical density. In our simulations, the contrast objects are selected randomly from a uniform distribution to match the signal variability condition of our SRHO model. The size and composition of the contrast inserts can be modified to simulate other material classification tasks as well.

3.2 Plaque Removal Task

The second task is motivated by plaque-removal classification algorithms that have been developed for dual-energy CT (DECT) [5]. Occasionally, arteries can become occluded by calcified plaques that are indistinguishable from flowing contrast agent on conventional CT scans. Dual-energy measurements can be leveraged to identify and remove the pixels that are made of calcium, rather than iodine, resulting in a clean depiction of the arterial tree. To measure calcium vs. iodine classification performance, we use the same phantom as in the kidney-stone task, now with calcium and iodine as the insert materials.

3.3 Simulation study processing chain

Using these phantoms, we can simulate various spectral CT system configurations and measure their material classification performance. First, raw transmission data are generated using an ellipse-based projector and realistic x-ray tube spectra [25]. Noise is added using a Poisson model for counting detectors and a Gaussian model for energy-integrating detectors [12]. A maximum-likelihood basis-material decomposition is performed, using calcium and water as the basis materials, and a pair of VM images, at energies E_1 and E_2 , is reconstructed using FBP. The pixels belonging to the contrast inserts are plotted in the same fashion as in figure 1, resulting in the scatter plot shown in figure 5. Each point represents a pixel in the reconstructed image pair, and the colors indicate either contrast material 1 (red) or contrast material 2 (blue).

As expected, the two different materials naturally cluster along straight lines, with some dispersion due to noise. We characterize the class separability by defining

$$\text{SNR}_{\text{LDA}}^2 = \max_w 2 \frac{(\mathbf{w}^T \bar{\mathbf{x}}_1 - \mathbf{w}^T \bar{\mathbf{x}}_2)^2}{\mathbf{w}^T (\Sigma_1 + \Sigma_2) \mathbf{w}}. \quad (16)$$

This ratio is known as Fisher's linear discriminant [21] (FLD) and is maximized at

$$\mathbf{w} = (\sum_1 + \sum_2)^{-1} (\bar{\mathbf{x}}_1 - \bar{\mathbf{x}}_2). \quad (17)$$

FLD can be thought of as an analog to the HO SNR, replacing the population means and covariances with sample statistics. The quantities $\bar{\mathbf{x}}_j$ and Σ_j represent the sample mean and covariance, respectively, of material class j , and the quantity $\mathbf{w}$ is the normal vector to the best separating hyperplane.

The quantity, SNR_{LDA} , provides a measure of how well the two contrast materials in the stone phantom can be separated. We can simply repeat this entire process while iterating through different imaging parameters in order to generate an empirical parameter-optimization curve, as in figure 2. This procedure is summarized by the chart in figure 6. In this work, we also repeated each simulation 100 times to reduce uncertainty in the measured POC's, so each point constitutes a considerable amount of computational effort.

Though computationally intensive, the POC's we generate from simulations provide an accurate reference with which to validate our SRHO model and further demonstrate the need for fast, analytic methods.

4 SRHO Model Validation

In this section we directly compare the POC's generated by the SRHO model to those derived from numerical simulations. As a proof of concept, we will optimize a dual-kVp system and a photon-counting system with respect to the kidney stone classification task and the plaque removal task. The parameters used for each are given in table 1. By sweeping out different spectral CT parameters and computing both SNR_{HO} and SNR_{LDA} we generate parameter-optimization curves (POC) that reveal which system configurations are optimal for each task.

4.1 Geometric Scale Factor

In order to compare POCs between the SRHO model and the simulation studies, we need to introduce a correction factor to account for the acquisition and phantom geometries used in the simulation studies.

The SRHO model is inherently one-dimensional, so a scaling factor is required to account for the geometry of the acquisition and the resolution of the reconstructed image. The mean number of transmitted photons along a given ray is

$$\bar{y}_i = I_0 \int s_i(E) e^{-\int_L \mu(\mathbf{r}, E) d\ell} dE, \quad (18)$$

where we have explicitly indicated the number of incident photons I_0 by defining the normalized spectrum $s_i(E) = S_i(E) / \int S_i(E) dE$. In the simulations, the classification performance is sensitive to the total number of views, N_θ , and the reconstructed pixel-size,

x . Specifically, increasing N_θ or x results in less noise per pixel and, thus, better classification performance.

One might think that these factors would only impact the overall scale of the POC and not the shape. However, both the absolute performance and the shape of the POC are impacted because the task is limited by both the measurement noise and the stochastic object model. Increasing N_θ or x can only help to reduce the measurement noise, thus altering the trade-off between these two sources of uncertainty. We introduce the scaling factor Ω in the SRHO model, such that

$$I'_0 \leftarrow \Omega I_0 \quad (19)$$

and

$$\Omega \equiv \frac{N_\theta}{A} I_0, \quad (20)$$

where N_θ is the number of projection views and A is the area of the contrast object (e.g. kidney stone) in # of pixels.

4.2 Case Study 1: Dual kVp dose allocation

First, we consider the task of optimizing the flux balance in a dual kVp system, operating at peak tube voltages of 80 and 140 kV. The goal is to determine what fraction of the total flux should come from the 80 kVp tube to maximize material classification performance. Specifically, we enforce that along each line integral through our object, a total of 10^6 photons are incident on the phantom:

$$\int r S_{80}(E) + (1-r) S_{140}(E) dE = 10^6. \quad (21)$$

We assume that $0 < r < 1$. The spectra used in our simulations are shown in figure 7.

Parameter optimization curves are computed for a range of r values between 0 and 1 using both the SRHO model and via simulations with the numerical phantom; this is shown in figure 8. Since SNR_{LDA} is based on image realizations, 100 averages were taken for each r value. The error bars from the simulation studies correspond to two standard deviations.

The POC curves derived from the SRHO model cannot be compared to those from the simulations in terms of absolute scale, since they correspond to fundamentally different things: one is based on a one-dimensional, data-domain model, and the other is measured from reconstructed images. However, since the goal of the SRHO model is to select optimal parameters, we are only interested in the shape of these curves, so we can rank order different spectral CT configurations. Therefore, we quantify their agreement with the

Pearson product-moment correlation coefficient [26] (PPMCC) because it is insensitive to these absolute scale differences. Note that the analytic model and simulations yield very similar curves, indicating that the SRHO model can accurately predict good operating parameters. For the kidney-stone task, the PPMCC is 0.994. Figure 9 shows an identical comparison for the plaque removal (Ca vs. I) task (PPMCC = 0.998).

4.3 Case Study 2: PC detector threshold optimization

In the second case study, we consider optimizing a 3-bin photon counting detector. For simplicity, we model an ideal detector with perfect energy resolution, as shown in figure 10.

This is a two-parameter optimization problem, as we must select two thresholds given by t_1 and t_2 . Figure 11 depicts the SNR values for the kidney stone classification task from both the SRHO model (left) and the simulation studies (right) over a wide range of possible threshold values (PPMCC = 0.999). The results from the plaque removal task are shown in figure 12 (PPMCC = 0.981). Again, 100 averages are taken at each combination of (t_1, t_2) when computing SNR_{LDA} . For this task, we also find that HO model accurately predicts the trends in material classification performance for varying threshold values.

In Figure 12, agreement is not as good as for the kidney stone classification task. One possible explanation is that the simulation study utilized a two-material decomposition (calcium and water), despite the presence of three materials in the phantom (water, calcium and iodine). We relied on the approximation that attenuation is dominated by Compton scatter and photo-electric absorption, since very few photons are detected below the k-edge of iodine. For configurations where $t_1 \approx t_2$ it should technically be possible to perform a three-material decomposition, but we only used two because the three material-decomposition was numerically unstable. However, we also point out that the SNR tends to vary slowly around the optimum. Even if the HO model does not exactly predict the optimal operating point, it is still very likely to provide a configuration that achieves nearly optimal performance.

4.4 Impact of signal variability

One important component of the aforementioned SRHO model is the inclusion of signal variability. Physically, this may arise due to the mixing of contrast agents during uptake and perfusion (e.g. iodine and blood) or natural variations in tissue composition (e.g. bone density). Mathematically, this enters the SRHO model by specifying a stochastic object model; the density of objects being classified are presumed to follow a known distribution function. In [13], the objects are, instead, presumed to be of a fixed density, corresponding to the signal-known-exactly/background-known-exactly (SKE/BKE) task.

In our experience, the SKE/BKE model is too simple to guide the selection of imaging parameters, which is the goal of this work. In fact, we find that in many situations, conventional, single-energy CT performs no worse than spectral CT in material classification tasks with low signal uncertainty. We can illustrate this phenomenon by, again, considering the dual-kVp, flux-balancing problem while shrinking the amount of signal variability toward zero.

In the previous results, we modeled the density of the contrast objects (calcium, iodine, uric acid, or calcium-oxalate) with a uniform distribution,

$$\rho \in \mathcal{U}(\rho_{\min}, \rho_{\max}), \quad (22)$$

where the particular values of $\rho_{\min}$ and $\rho_{\max}$ are specified in table 1. In order to investigate the impact of the *amount* of signal variability, we define

$$\begin{aligned} \rho'_{\min} &= \bar{\rho} - k\Delta\rho \\ \rho'_{\max} &= \bar{\rho} + k\Delta\rho \end{aligned} \quad (23)$$

where $\bar{\rho} = (\rho_{\min} + \rho_{\max})/2$, $\rho = (\rho_{\max} - \rho_{\min})/2$, and $k \in (0, 1)$.

The amount of signal variability is controlled by the fraction k , where $k = 0$ corresponds to *no* variability (SKE/BKE), $k = 1$ yields the same distributions as in the previous studies, and $0 < k < 1$ specifies a range of intermediate scenarios.

Figure 13 demonstrates what happens to material classification performance as k varies. The top row illustrates that when k is small enough, the POCs are monotonic, indicating the optimal classification performance is achieved when all of the flux is allocated to a single kVp.

This has two important consequences: (1) For SKE/BKE material classification tasks, dual-energy CT may actually perform *worse* than single-energy CT, and (2) any reasonable material classification model must account for signal variability if it is to be used for parameter tuning or hardware optimization. Figure 13 also shows that these observations are confirmed by both the SRHO model and the numerical simulations.

4.5 Impact of background shape

Another concern that arises when comparing the SRHO model to numerical simulations is how to handle asymmetric backgrounds. For example, cross-sections of the human body may span a wide range of apparent diameters, depending upon the projection view angle.

Since the SRHO is inherently one-dimensional, we need a procedure for extracting a single *effective diameter* that allows for a reasonably fair comparison to our 2D simulations. For this reason, we have considered both circular and elliptical kidney stone phantoms. In particular, we considered an elliptical phantom with major and minor axis lengths of 40cm and 24cm, respectively, shown in Figure 14. For an elliptical phantom, the intersection length of a line passing through its center is given by

$$d(\theta) = 2 \sqrt{a^2 \cos^2 \theta + b^2 \sin^2 \theta}. \quad (24)$$

Next, we define the quantities

$$V_{\text{ellipse}}(\theta) \equiv \left(\int S(E) e^{-\mu_b(E)d\theta} dE \right)^{-1} \quad (25)$$

and

$$V_{\text{circ}} \equiv \int S(E) e^{-\mu_b(E)d_{\text{eff}}} dE. \quad (26)$$

The desired quantity d_{eff} is found numerically by equating

$$\langle V_{\text{ellipse}}(\theta) \rangle_{\theta} = V_{\text{circ}} \quad (27)$$

where $\langle V_{\text{ellipse}}(\theta) \rangle_{\theta}$ is an average of V_{ellipse} over a discrete set of projection angles, $0 \leq \theta < 2\pi$. In this work, we used 1200 equally spaced angles matching those of our simulation geometry and apply the bisection method to find a value d_{eff} that lies somewhere in between the minor and major axis lengths of the ellipse phantom. More details on the effective diameter computation are found in Appendix B.

Once d_{eff} is computed, the SRHO model can be applied to elliptical backgrounds. Figures 15–18 demonstrate this, with comparisons to POC's derived from numerical simulations. The agreement between the 1D SRHO model and the simulations is slightly worse than with the circular phantom (see Figure 15) but still quite good. Most importantly, we can see that the model still accurately predicts near-optimal imaging parameters for these material classification tasks.

5 Discussion

In this work, we have presented a simple, analytic model for characterizing spectral CT, material-classification tasks that is suitable for optimizing image acquisition parameters and hardware design. Specifically, we have adapted the Hotelling Observer formalism in order to derive an unambiguous, task-specific metric that is independent of the reconstruction method.

Furthermore, the proposed model does not make restrictive assumptions about the basis-material decomposition being linear or the contrast objects having an exactly known density/concentration. We demonstrated that modeling the variability of the contrast objects, e.g. due to uptake and perfusion of contrast agents or natural variations in tissue composition, is essential to material classification tasks. For dual-kVp scans, our model even showed that for low signal variability, the spectral information is not needed, and it is better to deliver all of the dose at a single optimized kVp. This trend was confirmed by our simulations, and echoes a similar sentiment to that expressed in [24] about CNR limited tasks; specifically, they

report that for tasks that do not require material classification or quantification, it is better to deliver all of the radiation dose at a single, optimized tube potential, rather than performing a dual-energy scan. Based on this work, we find that *trivial* material classification tasks, where the density of each material is precisely known, also do not benefit from multi-energy scanning.

The proposed model could be especially useful for exploring large parameter spaces because it is analytic and rapidly computable. For example, a photon counting detector with five adjustable thresholds [11] can realize millions of different configurations, making it immensely impractical to explore them all experimentally.

Although this work only considers binary classification tasks, the Hotelling Observer can be easily extended to the L -class problem, where $L > 2$. A detailed discussion of the L -class HO can be found in Chapter 13 of [21]. The linear discriminant analysis applied in our simulation studies can also be generalized in similar manner [27]. This makes it possible to address classification tasks involving more than two different materials with minimal modification to the methods presented here.

One potential weakness of the proposed approach is the inability to compensate for highly inhomogeneous backgrounds. The SRHO reduces the classification task to a one-dimensional model, where the background and signal are represented by a single path length through each material. This may not pose significant problems in relatively homogeneous slices, such as kidney stone classification in the abdomen, since few bony structures exist. On the other hand, in slices where different projection views may see vastly different attenuation, e.g. due to the skull, shoulders, or hip bones, it is unclear if this simple 1D model would still predict useful operating parameters.

One possible solution to this problem would be to consider multiple rays in the Hotelling Observer model. In principle, one could use the complete sinogram data to derive the HO SNR, but this would significantly increase the computational cost. To balance this trade off, a small subset of rays (e.g. 10) could be used as a surrogate to the entire projection data, in order to capture some of the heterogeneities. However, one typically does not have much a priori knowledge of the object anyway. For these reasons, we have focused on developing a simple metric that is rapidly computable that can be used to guide the search for optimal imaging parameters. Extending the proposed model to include multiple projection rays and prior knowledge about heterogeneous background anatomy is an interesting subject for a future investigation, but it is beyond the scope of this work.

We believe that the simulation studies presented here do demonstrate some robustness to heterogeneities; however, since the projection data comprises rays passing through many different path lengths of water and contrast materials (see Figure 4), yet the 1D SRHO model still accurately predicted parameter optimization curves. Furthermore, we showed that even an elliptical phantom, which has a highly view-dependent attenuation profile, could be characterized well with the proposed metric.

In this study, the parameter-optimization curves inherently frame the problem as one of achieving maximal material-classification performance at a fixed dose. An alternative,

equally valid viewpoint is one of achieving clinically acceptable material-classification performance at the lowest possible radiation dose. Therefore, as new spectral CT imaging protocols and hardware become available, it is of increasing importance that careful consideration is given to parameter selection.

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A Statistical Properties of Virtual Monoenergetic Data

A.1 Maximum Likelihood Material Decomposition

For a general spectral CT system we denote a measurement along a ray $\mathcal{L}$ in the i^{th} spectral channel by

$$\bar{y}_i = \int S_i(E) e^{-\int_{\mathcal{L}} \mu(\mathbf{r}, E) d\ell} dE. \quad (28)$$

The quantity $S_i(E)$ encompasses the energy-dependence of the incident beam and the detector response. A key insight of spectral CT is that the attenuation can be parametrized by a finite number of basis functions:

$$\mu(\mathbf{r}, E) = \sum_{j=1}^M \rho_j(\mathbf{r}) f_j(E) \quad (29)$$

where the $f_j(E)$ may correspond to physical interaction cross-sections or to the mass-attenuation functions of basis-materials [28]. In the latter case, the spatially varying coefficient, $\rho_j(\mathbf{r})$, corresponds to the density distribution of material j . This parametrization allows us to write the transmission measurements as

$$\bar{y}_i(\mathbf{a}) = \int S_i(E) e^{-\mathbf{a}^T \mathbf{f}(E)} dE, \quad (30)$$

where $\mathbf{a} = (a_1, \dots, a_M)^T$, $\mathbf{f}(E) = (f_1, \dots, f_M(E))^T$, and a_j is the line integral of $\rho(\mathbf{r})$:

$$a_j \equiv \int_{\mathcal{L}} \rho(\mathbf{r}) d\ell. \quad (31)$$

When the number of spectral measurements, $N = M$, we can estimate $\mathbf{a}$ from $\bar{\mathbf{y}}$. Specifically, the maximum likelihood estimate of $\mathbf{a}$ is given by

$$\hat{\mathbf{a}} = \underset{\mathbf{a}}{\operatorname{argmax}} L(\mathbf{a}), \quad (32)$$

where $L(\mathbf{a})$ is the log-likelihood function. For Poisson data,

$$L(\mathbf{a}) = \sum_i -\bar{y}_i(\mathbf{a}) + y_i \log(\bar{y}_i(\mathbf{a})). \quad (33)$$

Given an estimate of $\mathbf{a}$, virtual monoenergetic (VM) projections can be synthesized at any energy:

$$g(E) = \hat{\mathbf{a}}^T \mathbf{f}(E). \quad (34)$$

Therefore, basis decomposition can be used to transform any arbitrary spectral CT measurements into virtual-monoenergetic (VM) data. By defining $\mathbf{g} = (g_1, g_2, \dots, g_M)^T$ and $F_{ij} = f_j(E_i)$, we get

$$\hat{\mathbf{g}} = F \hat{\mathbf{a}}. \quad (35)$$

Typically, material classification is performed on VM images, since unique materials naturally cluster along straight lines in this space. Since the VM data vector, $\hat{\mathbf{g}}$, is related to $\hat{\mathbf{a}}$ by a linear transformation, we know that the covariance matrices are related by

$$K_{\hat{g}} = F K_{\hat{a}} F^T. \quad (36)$$

Therefore, the HO SNR will depend upon how noise is propagated through the basis-material decomposition.

A.2 Noise in the basis-material decomposition

In general, the ML basis decomposition is an implicit, nonlinear operation, so we cannot write down a closed form expression for the covariance of the basis coefficients, $K_{\hat{a}}$. However, we can derive a useful lower-bound from the Fisher Information matrix, as in [2] and [12].

A general lower bound on the variance of any estimator is

$$\text{var}(\hat{\theta}_i) \geq \mathcal{F}_{ii}^{-1}, \quad (37)$$

where $\mathcal{F}$ is known as the Fisher information matrix and is related to the curvature of the log-likelihood function. Specifically, it is given by

$$\mathcal{F} = -\text{E}\{\nabla^2 L(\theta)\}. \quad (38)$$

This inequality is widely known as the Cramér-Rao lower bound (CRLB). A slightly more general form of the CRLB is

$$K_{\hat{\theta}} \succeq \mathcal{F}^{-1}, \quad (39)$$

where the notation $A \succeq B$ means $(A - B)$ is positive semidefinite. When the above holds with equality, the estimator $\hat{\theta}$ is said to saturate the CRLB. All maximum-likelihood estimators (MLE) asymptotically saturate the CRLB, and under many circumstances, it is an excellent approximation to assume

$$K_{\hat{\theta}} \approx \mathcal{F}^{-1}. \quad (40)$$

Likewise, if $\hat{a}$ is an MLE, it is asymptotically unbiased, so with a sufficient number of counts, $\text{E}\{\hat{a}\} \approx a$. For the Poisson case, it can be shown that the Fisher information matrix is given by

$$\mathcal{F}_{\alpha\beta} = \sum_{i=1}^N \frac{1}{\bar{y}_i} \frac{\partial \bar{y}_i}{\partial a_\alpha} \frac{\partial \bar{y}_i}{\partial a_\beta}. \quad (41)$$

For CT systems with energy-integrating detectors, a Gaussian noise model may be more appropriate, due to energy-dependent detector gain. The detector response is approximately linear with x-ray energy, so the mean and variance are sometimes approximated by

$$\begin{aligned} \bar{y}_i &= \int E S_i(E) e^{-\mathbf{a}^T \mathbf{f}(E)} dE \\ v_i &= \int E^2 S_i(E) e^{-\mathbf{a}^T \mathbf{f}(E)} dE, \end{aligned} \quad (42)$$

and the resulting Fisher information matrix is given by the following equation [12]:

$$\mathcal{F}_{\alpha\beta} = \sum_i \frac{1}{v_i} \frac{\partial \bar{y}_i}{\partial a_\alpha} \frac{\partial \bar{y}_i}{\partial a_\beta} + \frac{1}{v_i^2} \frac{\partial v_i}{\partial a_\alpha} \frac{\partial v_i}{\partial a_\beta}. \quad (43)$$

Using these formulas we can compute an accurate approximation of $K_{\hat{a}}$ for arbitrary spectral CT systems. Combined with equation 36, one can compute the covariance of synthetic VM data. Therefore, we have all of the inputs we need for the SRHO model.

For the SRHO model, the Fisher information matrix is used to compute the conditional covariance matrices under each hypothesis (see equation 14). In the Poisson case, the mean transmission measurements can be expressed in terms of the known background and possible contrast materials,

$$\bar{y}_i(a_1, a_2) = \int S_i(E) e^{-a_b f_b(E) - a_1 f_1(E) - a_2 f_2(E)} dE, \quad (44)$$

Then using equations 35 and 41, we have

$$K_{g|H_1, a_1} = F [\mathcal{F}(a_1, 0)]^{-1} F^T \quad (45)$$

$$K_{g|H_2, a_2} = F [\mathcal{F}(0, a_2)]^{-1} F^T \quad (46)$$

where partial derivatives of $\bar{y}_i$ are only taken with respect to a_1 and a_2 (and not a_b) since the background is presumed to be exactly known. For the gaussian case, the same process is carried out with equations 42 and 43. The specific energies used to compute VM projections are unimportant, since the HO is invariant to invertible linear transformations.

B Effective Diameter Computation for Elliptical Phantoms

One limitation of the SRHO model is that it is inherently one-dimensional, so it is not clear how to choose the appropriate lengths for the background and contrast materials. In reality, the projection data will consist of many different path lengths through both signal and background objects.

When comparing the SRHO to simulation studies, we simply used the diameters of the circular phantom and contrast inserts as the path length for the 1D model. This choice resulted in excellent agreement between the predicted and observed POC curves. However, a modification is required if the aspect ratio of the object is not nearly circular, such as an ellipse with eccentricity $e \neq 0$. For these cases, we introduce a method for computing an *effective* diameter.

Consider an elliptical phantom with background attenuation $\mu_b(E)$, defined parametrically by

$$\begin{aligned} x(\theta) &= a \cos \theta \\ y(\theta) &= b \sin \theta. \end{aligned} \quad (47)$$

The intersection length of a ray passing through its centroid (see Figure 19) is defined by

$$d(\theta) = 2 \sqrt{a^2 \cos^2 \theta + b^2 \sin^2 \theta}. \quad (48)$$

If the attenuation of the signal is small compared to the background, then we can approximate the number of transmitted photons along angle θ by

$$I(\theta) = \int S(E) e^{-\mu_b(E) d(\theta)} dE, \quad (49)$$

where $S(E)$ is the incident x-ray spectrum. If $I(\theta)$ is approximately Poisson, then the logged data, $g(\theta) \equiv -\log (I(\theta) / \int S(E) dE)$ has variance

$$V(\theta) \approx \left[\int S(E) e^{-\mu_b(E) d(\theta)} dE \right]^{-1}. \quad (50)$$

If we consider the summation of N independent measurements along different angles, the total variance is

$$\sum_{k=1}^N V(\theta_k) \quad (51)$$

For a circular phantom, with diameter $d = d_{\text{eff}}$, the variance along any ray is given by

$$V_{\text{circ}} \approx \left[\int S(E) e^{-\mu_b(E) d_{\text{eff}}} dE \right]^{-1}, \quad (52)$$

and the total variance of N independent measurements is

$$N \cdot V_{\text{circ}} \quad (53)$$

The effective diameter, d_{eff} is found by equating equations 53 and 51, which results in

$$\langle V(\theta_k) \rangle_{\theta} = V_{\text{circ}}, \quad (54)$$

where $\langle . \rangle_{\theta}$ indicates a discrete average over $\theta_1, \dots, \theta_N$.

Solving for d_{eff} , numerically, can be accomplished by applying any scalar, root-finding method to the function

$$f(d_{\text{eff}}) = V_{\text{circ}}(d_{\text{eff}}) - \langle V(\theta_k) \rangle_{\theta}. \quad (55)$$

Specifically, we are looking for a root of $f(d_{\text{eff}})$ on the interval $[2b, 2a]$, where we have assumed that $b < a$; d_{eff} must lie somewhere between the minor and major axes lengths of the ellipse. In this work, we have used the well-known bisection method.

Figure 1. Example of calcium vs. iodine classification with numerical disk phantom (left). Pixels of indicated ROI's are plotted in 2D vector space, with HU values at two different energies as x-y coordinates. One possible linear decision boundary is shown.

Figure 2. Example parameter optimization curve (POC). Optimal spectral parameters, with respect to material classification performance, are identified by the maximum value of the POC.

Figure 3.
The task is determining if the contrast object is material 1 or 2, and the background is presumed to be known.

Figure 4. “Material classification phantom” containing a water background with different concentrations of contrast material 1 (red) and contrast material 2 (blue). The color opacity is proportional to the concentration. The grayscale image (left) depicts the phantom at 65 keV. Note there is a significant amount of overlap in HU values. The display window is [0 – 400] HU.

Figure 5.

A sample scatter plot illustrating the vector space representation of the VM images created from the numerical material classification phantom. The two contrast materials are color coded red and blue, while the background pixels are shown in gray. Fisher's linear discriminant provides an SNR-like measure of how well separated these point clouds are.

Figure 6.

This chart describes the processing chain for measuring material classification performance from simulation data. Simulated spectral CT projection data are ultimately converted into VM images, and linear discriminant analysis (LDA) is used to derive a classification SNR based on *Fisher's Linear Discriminant*

Figure 7. Dual kVp spectra used for the simulation study and HO SNR computations are computed using Tucker's model [25].

Figure 8.

Kidney stone classification task: Comparison of classification SNRs derived from SRHO model and 2D simulations with numerical material classification phantom containing uric acid (UA) and calcium oxalate inserts. For the simulation study, 100 averages are used at each r value, and error bars represent two standard deviations. PPMCC = 0.994.

Figure 9.

Plaque removal task: Comparison of classification SNRs derived from SRHO model and 2D simulations with numerical material classification phantom containing iodine and calcium inserts. For the simulation study, 100 averages are used at each r value, and error bars represent two standard deviations. PPMCC = 0.998.

Figure 10.
Ideal photon counting detector with two adjustable energy thresholds, t_1 and t_2 .

Figure 11.

Kidney stone classification task: Comparison of classification SNRs derived from SRHO model (left) and 2D simulations (right) with numerical material classification phantom containing uric acid and calcium oxalate inserts. The upper diagonal is omitted because it is redundant with the lower diagonal. PPMCC = 0.999.

Figure 12.

Plaque removal task: Comparison of classification SNRs derived from SRHO model (left) and 2D simulations (right) with numerical material classification phantom containing Ca and I inserts. The upper diagonal is omitted because it is redundant with the lower diagonal. PPMCC = 0.981.

Figure 13.

The shape of the POC changes significantly with different amounts of signal uncertainty. The parameter k refers back to equation 23. For small values of k , the POC is monotonic, indicating that optimal performance is achieved when 100% of the radiation dose is allocated to a single kVp. Kidney stone classification task (from top to bottom): PPMCC = 0.999, 0.999, 0.995. Plaque removal task (from top to bottom): PPMCC = 0.999, 0.999, 0.998.

Figure 14.
An elliptical kidney stone phantom with major and minor axis lengths of 40cm and 24cm respectively. The display window is [0 – 400] HU.

Figure 15.

Kidney stone classification task with ellipse phantom: Comparison of classification SNRs derived from SRHO model and 2D simulations with elliptical material classification phantom containing uric acid (UA) and calcium oxalate inserts. PPMCC = 0.997.

Figure 16.

Plaque removal task with ellipse phantom: Comparison of classification SNRs derived from SRHO model and 2D simulations with elliptical material classification phantom containing Ca and I inserts. PPMCC = 0.999.

Figure 17.

Kidney stone classification task with ellipse phantom: Comparison of classification SNRs derived from SRHO model (left) and 2D simulations (right) with numerical material classification phantom containing uric acid and calcium oxalate inserts. The upper triangle is omitted because it is redundant with the lower triangle. PPMCC = 0.990.

Figure 18.

Plaque removal task with ellipse phantom: Comparison of classification SNRs derived from SRHO model (left) and 2D simulations (right) with numerical material classification phantom containing Ca and I inserts. The upper triangle is omitted because it is redundant with the lower triangle. PPMCC = 0.973.

Figure 19.

For elliptical phantoms, the apparent diameter depends upon the angle, θ , of the intersecting ray. Four different angles are shown here, for illustrative purposes.

Table 1

Phantom parameters used for kidney stone classification and plaque removal tasks

parameter	kidney stone classification	plaque removal
phantom diameter	30 cm	30 cm
background material	water	water
insert (stone) diameter	5mm	5mm
material 1	uric acid	Ca
material 1 concentration	200 to 550 mg · cm ⁻²	150 to 350 mg · cm ⁻²
material 2	calcium oxalate	iodine
material 1 concentration	75 to 950 mg · cm ⁻²	5 to 30 mg · cm ⁻²