Allowable Forward Model Misspecification for Accurate Basis Decomposition in a Silicon Detector Based Spectral CT

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Abstract—Material basis decomposition in the sinogram domain requires accurate knowledge of the forward model in spectral computed tomography (CT). Misspecifications over a certain limit will result in biased estimates and make quantum limited (where statistical noise dominates) quantitative CT difficult. We present a method whereby users can determine the degree of allowed misspecification error in a spectral CT forward model and still have quantification errors that are limited by the inherent statistical uncertainty. For a particular silicon detector based spectral CT system, we conclude that threshold determination is the most critical factor and that the bin edges need to be known to within 0.15 keV in order to be able to perform quantum limited material basis decomposition. The method as such is general to all multibin systems.

Index Terms—Accuracy, forward model, photon counting multibin computed tomography (CT), quantification, spectral CT.

I. INTRODUCTION

SPECTRAL computed tomography (CT) systems allows for, among other things, quantitative CT using basis decompositions methods [1], [2]

$$\mu(\mathbf{r}; E) = a_1(\mathbf{r})f_1(E) + a_2(\mathbf{r})f_2(E). \quad (1)$$

Equation (1) indicates that the entire energy dependence of the linear attenuation for each voxel can be determined and not just an energy weighted average. There are several ways in which such a decomposition can be carried out. If only two bases are used in (1) dual energy systems, with two independent measurements, give adequate energy resolving power to allow for basis decomposition. If more bases are desired, or higher precision of the basis coefficients needed, energy sensitive multibin systems can be applied. The decomposition could be performed in image space but this would not eliminate beam hardening artifacts. Therefore a projection based approach is desired [3].

There are two basic methods whereby such a decomposition in the projection domain can be carried out. One is by means of

calibration measurements where known combinations of calibration material thicknesses is used to obtain a set of detector responses against which actual measurements can be “compared” (polynomially fitted [4] or otherways interpolated [5]). A second approach is to directly determine the line integrals of $a_i(\mathbf{r})$ from the sinogram data using a maximum likelihood approach and then reconstruct a_i 's using the inverse Radon transform. Such an approach for multibin systems has been presented by Röbl and Herrmann [7] and successfully applied to real data on a prototype system by Röbl and Proksa [8].

This approach requires accurate knowledge of the forward model, otherwise bias is introduced in the estimates [3], [6]. The forward model is the physical model describing the signal generation in the detector. For a photon counting multibin system, the expected number of counts in bin i , i.e., events with deposited energy E' in the range $[T_{i-1}, T_i]$ is given by

$$\lambda_i(x', \theta) = N_0 \int_0^\infty \Phi(E) D(E) S_i(E) \times e^{-\int_l \mu(\mathbf{r}; E) ds} dE + \varepsilon_i(x', \theta) \quad (2)$$

where

$$S_i(E) = \int_{T_{i-1}}^{T_i} R(E, E') dE' \quad (3)$$

and $\varepsilon_i(x', \theta)$ is the expected number of scatter counts in bin i . N_0 is the expected value of the number of photons, in the unattenuated beam, hitting a detector element x' at a rotation angle θ . The path l connects the X-ray source with the detector element x' , $\Phi(E)$ denotes the energy distribution of the X-ray spectrum, $D(E)$ the detection efficiency. Following the notation of Röbl and Herrmann [7] $R(E, E')$ denotes the probability that an X-ray photon with energy E deposits charge corresponding to an energy E' in the detector and $S_i(E)$ is therefore a bin function, giving the fraction of photons with energy E that are deposited in the i th bin. The parameters of the forward model are thus N_0 , $\Phi(E)$, $D(E)$, $R(E, E')$, $\varepsilon_i(x', \theta)$ and T_i , $i = 1, \dots, N$, where N is the number of energy bins. (N_0 , the unattenuated fluence, is assumed to be measurable with high precision.)

This investigation is concerned with to which accuracy the parameters of the forward model must be known in order to perform material basis decomposition in practice. The approach differs from that taken by Walter *et al.* [6] in at least two aspects. The first is that not only the spectral shape Φ is consid-

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ered, but also other parameters, especially those that are specific to multibin systems like the uncertainty in the set of internal threshold $\{T_i\}$ and the energy response function (the previous investigations were concerned with dual energy methods). The second is the figure of merit applied. When the parameters of the forward model are incorrect the estimates $\hat{a}_1(\mathbf{r})$ and $\hat{a}_2(\mathbf{r})$ will be biased. This bias will add to the variance and result in a mean square error that is larger than the variance of the unbiased estimate ($E[\cdot]$ is the expectation operator and the hat, $\hat{\cdot}$, denotes an estimate)

$$\begin{aligned} \text{MSE}(\hat{a}) &= E[(\hat{a} - a)^2] = E[\hat{a}^2] - 2E[\hat{a}]a + a^2 \\ &= (E[\hat{a}^2] - E[\hat{a}]^2) + (E[\hat{a}] - a)^2 \\ &= \text{var}(\hat{a}) + \text{bias}^2(\hat{a}). \end{aligned} \quad (4)$$

We determine $\text{MSE}(\hat{a})$ for different deviations of the forward parameters from the true values and relate them to the inherent uncertainty, the Cramér-Rao lower bound of the variance, that would remain had the forward model not been misspecified. As a cutoff, we determine the allowable misspecification for each parameter of the forward model would result in a squared bias equal to the variance.

The method is developed and illustrated for a photon counting multibin system with silicon detector diodes [9]–[12] but the methodology applies equally well to other detector materials. A shorter version of this paper has been presented in a conference proceeding [13].

II. BACKGROUND

Since the detection efficiency, response function and spectral shape are continuous functions (or vectorized quantities in practice), assigning a small perturbation or misspecification error to them is nontrivial and can be done in a multitude of ways. Just like Walter *et al.* [6] we derive reasonable misspecification errors of the forward model by ‘first principles’. For example, just like they do, we let a change in X-ray tube acceleration voltage and filter thickness affect the spectral shape. This section is devoted to illustrating how we arrive at misspecifications for the various forward model parameters.

A comment on an underlying model assumption might be in place here: we do not model the parameters of the forward equation as variable over time. They are assumed fixed but unknown. It is how the error in their determination should be modeled and how large the accompanying uncertainty can be before the material basis decomposition breaks down that we want to determine.

A. Modeling the Uncertainty in Scatter Counts $\varepsilon_i(x', \theta)$

To perform accurate basis decomposition according to (3), the scatter in each projection must be estimated. As scatter is a spatially slowly varying function, it can be estimated by shielding a fraction of the detector elements from primary rays and thus have them only estimate scatter. Such an approach will inevitably result in some misspecification of the scatter, and we are interested in determining how accurate the estimation must be. In this work we assume the scatter-to-primary ratio of detected counts is $\text{SPR}_0 = 0.15$ in the forward model, and then examine the resulting bias when the actual ratio SPR differs. 15% scatter is a tentative estimate for the modeled silicon

Fig. 1. Effective absorption length x as a function of misalignment angle α and dead layer thickness t .

detector system; 8% internal detector scatter [9] and a similar amount of object scatter. This allows us to draw reasonable conclusions about how much the model assumptions can be allowed to deviate from the truth. (Please note that while the implementation, to mimic reality, assumes a certain number of scatter counts in each energy bin, this number is expressed as a ratio to the signal count for ease of interpretation.)

B. Modeling the Uncertainty of the Detection Efficiency $D(E)$

To increase the detection efficiency of the silicon diodes, they X-rays enter edge on, i.e., in the plane of the wafer they are cut from [9]. This requires a careful alignment. Any misalignment, as captured by the angle α results in a shorter attenuating distance x (cf. Fig. 1) in the silicon. There is also an uncertainty regarding the exact thickness t of the dead layer depicted in the figure. Somewhat simplified, $x(\alpha, t) \approx \min(l - t, d/\sin \alpha)$. One could argue that this underestimates the active length for misalignment errors larger than $\alpha^* = \sin^{-1}(d/(l - t))$, the misalignment angle for which $l - t = d/\sin \alpha$, since transmitted X-rays could interact in adjacent, presumably also misaligned, strips. However, for $d = 0.5$ mm, $l = 32$ mm, and $t \approx 0.5$ mm, $\alpha^* \approx 0.9^\circ$ and this is a rather large angle and any high accuracy alignment procedure can be expected to result in errors smaller than this. For that reason, we model the uncertainty in the detection efficiency as only being dependent on the thickness t of the dead layer

$$D(E; t) = e^{-\mu(E)t} \left(1 - e^{-\mu(E)(l-t)} \right) \quad (5)$$

where $\mu(E)$ is the linear attenuation coefficient of silicon (only the attenuation from incoherent scattering and photoelectric effect is included). $t = 0.5$ mm and Δt , the modeled deviation from the assumed value of t , ranging from -0.2 to $+0.2$ mm, yield the detection efficiency curves in the left panel of Fig. 2.

The error in the assumed linear attenuation coefficient $\mu(E)$ for silicon is estimated to be 1% or less in the literature [14], [15]. This relative uncertainty is of the same order of magnitude as $\Delta t/(l - t)$ and as both parameters are multiplied in the exponent of (5), the uncertainty in the linear attenuation coefficient ought also to be considered. In the right panel of Fig. 2, the detection efficiency for $\Delta t = 0$ mm is shown for a 1% overall increase and 1% overall decrease in $\mu(E)$ compared to tabulated values in XCOM [15].

Fig. 2. Left panel: Detection efficiencies according to (5) for, from top to bottom, $t = 0.3, 0.4, 0.5, 0.6$ and 0.7 mm. Right panel: $D(E)$ for t fixed at 0.5 mm and, from top to bottom, $\mu(E) = 1.01\mu_0(E)$, $\mu_0(E)$ and $0.99\mu_0(E)$ where $\mu_0(E)$ is the tabulated XCOM value.

Fig. 3. Illustration of exaggerated spectral distortion resulting from lower acceleration voltage and increased aluminum filtration.

C. Modeling the Uncertainty of the X-Ray Spectrum $\Phi(E)$

We use tungsten X-ray spectra as modeled by Cranley *et al.* [16]. For the default spectrum $\Phi_0(E)$ $U_0 = 120$ kV acceleration voltage and $d_{0,Al} = 6$ mm aluminum filtration is assumed.

When the actual acceleration voltage is U and the aluminum thickness d_{Al} , the X-ray spectrum $\Phi(E; U, d_{Al})$ will be different from $\Phi_0(E)$ and this is how we model uncertainties in the spectral shape.

In Fig. 3, $\Phi(E; U, d_{Al})$ and $\Phi_0(E)$ are depicted for $U = 110$ kV and $d_{Al} = 4$ mm (greatly exaggerated deviations from model for illustrative purposes).

D. Modeling the Uncertainty of the Reference Thresholds $\{T_i\}$

As an interacting photon deposits energy (in units of keV) in the diode material, charge carriers are generated which are subsequently fed through an analog circuit to generate a voltage pulse (in units of mV). The relationship between energy and pulse height is linear

$$u_j(E) = g_j E + m_j \quad (6)$$

where index j indicates that the response is channel dependent, i.e., differs between channels.

When the set of thresholds $\{T_i\}$, $i = 1, \dots, N$ are implemented, N global (i.e., channel independent) reference voltages U_i are applied to the N discriminators [17]. Due to the channel variation of the gain g_j (in units mV/keV) and the offset m_j (in units mV), these reference voltages will correspond to different

deposited energies in each channel (which can be thought of as a detector element)

$$T_{ij} = (U_i - m_j)/g_j. \quad (7)$$

In an energy weighted image, such channel inhomogeneities would result in ring artifacts if not properly compensated for [18] and [19]. When material basis decomposition is applied to the sinogram data, the inhomogeneities require that different forward equation parameters are used for each channel j , according to (7). A problem of misspecification might occur however since m_j and g_j are only known up to certain precision (and their values are known to drift with temperature, albeit in a predictable fashion) [10].

In the ideal case, the gain g_j (in units mV/keV) and offset m_j (in units mV) for each channel can be determined from a synchrotron source, as done in previous work [11], [12], [10]. In the limit case of infinite exposure the statistical error of the estimates will approach zero. Under one set of typical synchrotron radiation exposure conditions [10], the relative errors Δg and Δm (i.e., the estimated uncertainty in the estimates of $\hat{g}_j$ and $\hat{m}_j$ due to finite statistics) was $\Delta g = 0.019$ mV/keV and $\Delta m = 0.55$ mV. This should be compared to the average gain and offset values of $\bar{g} = 1.64$ mV/keV and $\bar{m} = 6.87$ mV [10]. The uncertainties Δg and Δm translate to an uncertainty ΔT_i of the bin thresholds. For a threshold at $T_i = 30$ keV this uncertainty is approximated by (not taking correlation between g and m -estimates into consideration which would lower the estimate)

$$|\Delta T_i| = T_i \sqrt{\left(\frac{\Delta m}{U_i - \bar{m}}\right)^2 + \left(\frac{\Delta g}{\bar{g}}\right)^2} = T_i \sqrt{\left(\frac{\Delta m}{T_i \bar{g}}\right)^2 + \left(\frac{\Delta g}{\bar{g}}\right)^2} \quad (8)$$

which evaluates to 0.48 keV. We model the threshold uncertainty effect by evaluating the bias for uncertainties in the thresholds ranging from $\Delta T = -1$ keV to 1 keV. All thresholds are assumed to move in parallel by ΔT , which is a likely consequence of a global change in temperature [10].

E. Modeling the Uncertainty of the Response Function $R(E, E')$

The derivation of the response function for a silicon strip detector system has been presented in the literature [9]. Given that an interaction of a photon of energy E has occurred, the fraction that undergoes photoelectric interaction to the fraction of Compton interactions is given by the ratio of the corresponding photon cross sections. From the above section we now expect that there is an uncertainty in tabulated value of these cross sections.

For Compton interactions the distribution of deflection angles is given by the Klein-Nishina differential cross section, and this approach assumes free outer shell electrons. This is a second potential source of error. Given the X-ray photon deflection angle and an initial electron at rest, the deposited energy is obtained via the Compton scatter formula.

Since charge generation is a stochastic process, the generated charge and thus the measurable energy deposition, follows a distribution around the value predicted by the photoelectric effect

and the Compton scatter formula. The deviation from Poisson statistics (the actual distribution is narrower) is captured by the Fano factor and its accurate determination is elusive [20]. Thus different tabulated values exist for silicon, in the vicinity of $F = 0.11$. This introduces an additional source of possible forward model specification error.

All generated charge carriers are not collected in the correct detector element as some dissipate to neighboring detector elements. The extent of this charge sharing is highly stochastic and depends on interaction location and initial charge cloud size and shape. For events depositing charge at the border of a neighboring pixel the fraction of the charge collected in the correct pixel have an expected value of 50% and this results in a highly leftward-skewed distribution of detected energies around the deposited energy. This distribution can be estimated [9] by making assumptions regarding electric field strength, charge drift velocity and diffusion speed but such modeling is prone to errors (for instance the diffusion coefficient depends on temperature which cannot be assumed to be known exactly). To complicate matters more, pile-up at high photon flux will also distort the collected energy spectrum [21], by a degree varying with the flux. The channel dependent electronic noise, which can only be ascertained with a certain precision, of course also presents an obstacle to the exact determination of the response function.

Recall that the purpose of this investigation is to determine which degree of model misspecification is acceptable before the material basis decomposition method breaks down. For this purpose, it is actually not important to model the correct response function in detail—it is the deviation from the assumed that matters and this deviation must be quantifiable.

Let $\gamma_0(E, E'')$ be the true, but unknown, distribution of initially released energy E'' from the primary interaction of a photon with energy E . Now let $h_0(E', E'')$ be a distribution that captures charge sharing, pile-up, the Fano-spreading and the electronic noise and, for an initial deposition of E'' in a detector element, yields the probability of collecting E' . The real response function is now

$$R_0(E, E') = \int_{-\infty}^{\infty} \gamma_0(E, E'') h_0(E', E'') dE''. \quad (9)$$

It holds that $\int \gamma_0(E, E'') dE'' = \int h_0(E', E'') dE' = \int R_0(E, E') dE' = 1$.

When we want to estimate the response function by $R(E, E')$, a first step is to determine $\gamma(E, E'')$ by taking the probabilities of photoelectric effect and Compton scatter into consideration and, for Compton events, the Compton scatter formula [9]. A next step would be to estimate the degradation due to pile-up, charge sharing, the statistics of electron-hole formation and electronic noise as captured by $h(E', E'')$, our estimate of h_0 , and form $R(E, E') = \int_{-\infty}^{\infty} \gamma(E, E'') h(E', E'') dE''$. It should hold that $\int R(E, E') dE' = 1$.

The distribution of deflection angles θ are given by (10) [9]

$$\frac{d\sigma}{d\theta} \propto \left(1 + \cos^2 \theta + \frac{k^2(1 - \cos \theta)^2}{1 + k(1 - \cos \theta)} \right) \times (1 + k(1 - \cos \theta))^{-2} \sin \theta \quad (10)$$

Fig. 4. Response functions. R is the faulty approximation of R_0 obtained by assuming a internal energy resolution from charge sharing, pile-up and electronic noise (h being a Gaussian with 4 keV standard deviation instead of h_0 , a Gaussian with 3 keV standard deviation).

where k is the ratio of the photon energy E and the electron mass energy at rest. Combined with the deposited energy E'' of (11) for a given deflection angle θ

$$E'' = E \left(1 - \frac{1}{1 + k(1 - \cos \theta)} \right) \quad (11)$$

$\gamma_0(E, E'')$ is obtained.

For simplicity, we let $h_0(E, E')$ be a Gaussian distribution with standard deviation 3 keV which is incorrectly modeled by a Gaussian h with standard deviation 4 keV. (The Gaussian shape is motivated by previous simulation work showing that charge sharing and pile-up do not lead to a severe left-skewed distribution at reasonable flux [21] and the standard deviation is based on a measured value of 2.2 keV for the pure electronic noise [10] with some margin for the statistical spread around the peak, the pile-up and the charge sharing.) In the below illustration, it is assumed that γ_0 is correctly estimated by γ .

Two response functions $R_0(E, E')$ and $R(E, E')$ are depicted in Fig. 4. (That the response function drops for small detected energies around 0 keV is an artefact of the assumed Gaussian form of h_0 and h . This does not matter for the model as the lowest threshold T_1 is set to 5 keV for rejection of electronic noise.)

III. METHOD

Recall that the goal is to find how large misspecifications of the forward model that can be tolerated before the bias component of the mean square error of (4) is larger than the variance part. This appears straight forward: the CRLB of the variance of the A_1 -estimate is given by [7]

$$\sigma_{A_1}^2 \geq \mathcal{F}_{11}^{-1} \quad (12)$$

where

$$\mathcal{F}_{jk} = \sum_{i=1}^N \frac{1}{\lambda_i} \frac{\partial \lambda_i}{\partial A_j} \frac{\partial \lambda_i}{\partial A_k} \quad (13)$$

and the bias is obtained by solution of the maximum likelihood problem given the observed bin counts $\{m_i\}$

$$\begin{aligned} A_1^*, A_2^* &= \arg \max_{A_1, A_2} P(\{m_i\}; A_1, A_2) \\ &= \arg \min_{A_1, A_2} \prod_{i=1}^N (\lambda_i - m_i \log \lambda_i) \end{aligned} \quad (14)$$

where $\lambda_i = \lambda_i(A_1, A_2)$ according to (3) [7]. For the bias calculation the expected value of counts in each bin was used, i.e., we apply the approximation $\mathbb{E}\hat{A}(\{m_i\}) \approx \hat{A}(\{\lambda_i\})$.

The results will unfortunately depend on dose and on the size of the region of interest (ROI) that is examined; for larger dose or when averaged over a larger area, the random variance component of (4) will decrease whereas the contribution from the bias will not (at least in the case of a homogenous cylindrical object where the central volume is considered). Thus we have to select typical X-ray fluence for which the comparison is carried out, and also determine how the size of the region of interest affects the result. First however, we show how variance and bias in the projection domain is translated to the reconstructed image domain.

A. Relationship Between $\text{var}(A)$ and $\text{var}(a)$

Hanson [23] has shown how the single-pixel variance in a reconstructed image depends on the variance of a projection measurement

$$\sigma_{\hat{a}_1}^2 = \frac{\sigma_{\hat{A}_1}^2(\lambda)}{N_\theta a^2} k^2. \quad (15)$$

$a = 1$ mm is the size of the detector elements (and distance between samples) and N_θ the number of projection angles. k is a unitless factor depending on filter kernel for the filtered back-projection and determined to $k = 0.62$ for MATLAB's `iradon` with cropped Ram-Lak ramp filter [24]. (The Appendix of [24] contains a general method for determining k of (15).)

B. Relationship Between $\text{bias}(A)$ and $\text{bias}(a)$

One would easily be lead to believe that the bias in the middle of the reconstructed image of a homogenous cylinder with diameter L is given by $\text{bias}(a) = \text{bias}(A)/L$ since by definition

$$A(x', \theta) = \int_l a(\mathbf{r}) d s = aL \quad (16)$$

for a central ray l . When estimates are biased, as in the case of a misspecified forward equation, one cannot however be sure that $\hat{A}(x', \theta) = \hat{a} \int_l d s$ for all possible path lengths $\{\int_l d s\}$ in the sinogram/projection domain. If the relative bias does depend on the path length it is not at all clear how a bias in the projection domain (A -space) translate to the image domain (a -space). The basic problem is similar to a characteristic of the Fourier transform: a change at *one* point in the Fourier domain of a function alters the spatial representation of the function at *all* points. The same holds for the filtered back projection due to the filtering step and thus, if relative biases differ across projections for instance due to path length, this will propagate unpredictably to the image domain bias.

Fig. 5. Effect of errors in the assumed amount of scatter.

A sufficient condition for $\text{bias}(a) = \text{bias}(A)/L$ to hold in the central region of reconstructed image of a homogenous cylinder with diameter L is

$$\hat{A} = c a \int_l d s \quad (17)$$

with constant c for different path lengths $\int_l d s$. If (17) holds, we have $\text{bias}(A) = \hat{A} - A = (c - 1)a \int_l d s$ since $A = a \int_l d s$ by definition. In the reconstructed domain, we have $\text{bias}(a) = \hat{a} - a$ where $\hat{a}$ is obtained via the inverse radon transform of $\hat{A}$ of (17). Due to the linearity of the transform, $\hat{a} = c a$ and $\text{bias}(a) = (c - 1)a$. Thus, it follows that $\text{bias}(A) = L \text{bias}(a)$.

Equation (17) unfortunately does not hold for all path lengths $\int_l d s$ and different misspecifications. However, in the Appendix (Fig. 12) we show, via simulation, that $\hat{A} \approx c a \int_l d s$ for $\int_l d s \in [0.85, 1]L$ for a range of misspecified forward parameters. Since the inverse Fourier transform of the ramp filter (used to convolve the detector response with before back projection) is quite narrow and well centralized, detector readings far away from the center have very little effect on the values in the middle of a reconstructed image. In the present investigation we therefore consider it sufficient to examine the effect of path lengths corresponding to small off center shifts as captured by $\int_l d s \in [0.85, 1]L$. Under these circumstances (17) holds approximately and thus $\text{bias}(a) \approx \text{bias}(A)/L$.

C. Decrease of Variance as a Function of ROI Area

The correlation structure in the reconstructed image makes the variance in an ROI consisting of M pixels decaying faster than M^{-1} . In the limit of a continuous image, with perfect bandlimited interpolation of the projection data before backprojection, the variance depends on M as $M^{-3/2}$ [25]. In previous work [24], we have shown (with a discrete image and typical interpolation) that the variance decreases as $M^{-1.33}$.

For an ROI consisting of M pixels, the standard deviation will thus have decrease by a factor of $M^{-0.66}$. For a 10×10 pixel (1 cm $\times$ 1 cm) large ROI this evaluates to $100^{-0.66} = 0.0479$. Since quantitative CT will most likely be carried out over ROIs much larger than a single pixel, we chose to compare the bias with the variance over a 100 pixel large ROI.

Fig. 6. Effect of errors in the assumed dead layer thickness.

Fig. 7. Effect of errors in the assumed linear attenuation coefficients.

Fig. 8. Effect of errors in the assumed X-ray spectrum stemming from different filtration than assumed.

Fig. 9. Effect of errors in the assumed X-ray spectrum stemming from a different acceleration voltage than assumed.

Fig. 10. Effect of uncertainty in thresholds.

Fig. 11. Effect erroneous response function.

D. Assumed Forward Model Parameters

The homogenous cylindrical object with $L = 20$ cm diameter consisting of 50% soft tissue and 50% adipose tissue (ICRU 44 [22]). The bases $f_1(E)$ and $f_2(E)$ of (1) are taken as the linear attenuation coefficients for the same materials. The unattenuated X-ray fluence, N_0 , must be selected as the total number of X-rays per reconstructed pixel area for an entire

gantry revolution. (Note that the lower bound of the variance in the reconstructed image is independent of the number of angles and depends only on N_0 since $\lambda = \lambda(N_0/N_\theta)$ in (12) and $\sigma_{\hat{A}_1}^2(\lambda(N_0/N_\theta))/N_\theta = \sigma_{\hat{A}_1}^2(\lambda(N_0))$.) Assuming a typical current of 360 mA the X-ray tube model of Cranely *et al.* [16] with a 120 kVp tungsten anode spectrum, 6 mm Al filtration, 7° anode angle and 1000 mm source-to-isocenter distance gives $8.1 \cdot 10^8$ photons $\text{mm}^{-2} \text{s}^{-1}$ on the detector. With 3 revolutions

Fig. 12. Constancy of c of (17) evaluated for different path lengths. Columns from left to right depict the scatter (as captured by assuming an SPR of 14% and 16% instead of 15%), effects on changes in the detection efficiency (as captured by assuming a dead layer thickness of 0.4 mm and 0.6 mm instead of 0.5 mm), a change in input spectrum from varying the aluminum filtration and, last column, a change in threshold values. $\Delta c = \max(c) - \min(c)$.

per second as a typical rotation speed $N_0 = 2.7 \cdot 10^8$ are directed towards a central pixel area of $1 \text{ mm} \times 1 \text{ mm}$ (which is the area henceforth assumed).

For the default parameter values, the Cramér-Rao lower bound of the variance of the A_1 -estimate is given by (12) and (13) in conjunction with (3). Combined with (15) this yields $\sigma(\hat{a}_1) = 0.68$ (unitless) (which should be related to $\mathbb{E}(\hat{a}_1) = 0.5$ (also unitless)). For an ROI with $M = 100$, $\sigma(\hat{a}_1)$ is 0.033. This is the value the bias should be compared to.

IV. RESULTS AND DISCUSSION

A. Effect of Uncertainty in Scatter Counts $\varepsilon_i(x', \theta)$

In Fig. 5, the bias resulting from misspecification of the scatter counts is illustrated. When large regions are considered the misspecifications can be rather large (0.2 instead of 0.15 is a 33% error) before the bias has a significant effect on the MSE.

B. Effect of Uncertainty of the Detection Efficiency $D(E)$

In Figs. 6 and 7, the result of misspecification of the detection efficiency by erroneous dead layer assumption and faulty linear attenuation coefficients. Clearly, the quantum noise will dominate the error for realistic ROIs and errors of the forward model.

C. Effect of Uncertainty of the X-Ray Spectrum $\Phi(E)$

That basis decomposition is very sensitive to assumptions regarding X-ray tube acceleration voltage is known [6]. Our result, illustrated in Figs. 8 and 9, confirms this. While the thickness of any aluminum filter can certainly be determined with

a very high accuracy, the actual X-ray tube voltages can easily differ by a few kV from stipulated values. This in itself is not a problem, since the actual X-ray spectra for each tube setting can be accurately measured. Instead it is the reproducibility of the voltage that is critical, and typically modern X-ray tubes reproduce the peak voltage with an uncertainty of only 0.01%. Thus Fig. 9 indicates that the bias introduced this way will be dominated by the statistical error in the quantitative determination of the basis function coefficients a_1 and a_2 .

D. Effect of Uncertainty of the Reference Thresholds $\{T_i\}$

Fig. 10 indicates that misspecified thresholds are very detrimental to quantitative CT. For parallel shifts in the thresholds of 0.1 keV or more (as compared to assumed values in the forward model), the bias introduced will dominate the MSE. This indicates that thresholds uncertainties of much more than 0.15 keV cannot be tolerated for quantitative CT *if* threshold uncertainties all line up in the same direction (otherwise the effect will be less serious) and *if* it is deemed essential to perform the decomposition at the quantum limit (where statistical noise makes up the lion's share of the mean square error). At the very least, the level is indicative of what good calibration methods should strive for.

E. Effect of Uncertainty of the Response Function $R(E, E')$

In obtaining $R(E, E')$ of Fig. 4, $h(E', E'')$ was assumed to be Gaussian with a standard deviation of 4 keV instead of 3 keV. The resulting bias for different choices of the Gaussian standard deviation is shown in Fig. 11. Clearly, for reasonable deviations of h from h_0 , the statistical limitation (variance) outweighs the bias.

V. CONCLUSION

We have presented a method to determine allowable misspecification in based photon counting multibin system under the assumption that one wants to perform close to quantum limited quantitative CT. With quantum limited we mean that the statistical noise should dominate over the bias introduced by the misspecifications. We have also quantified the allowable misspecifications for a particular silicon strip detector system. The results show that the bin edges are the most critical parameters of the forward model and that they need to be determined with an accuracy of 0.15 keV given the assumptions of this particular investigation (silicon detector and thresholds that all shift in parallel). Devising calibration methods, preferably not relying on synchrotron radiation, whereby the thresholds of individual channels can be determined accurately is therefore very important to be able to reap the expected benefits of spectral CT.

APPENDIX

In this section we show that c of (17) is close to constant for some different forward model misspecifications. For values of the path length $\int_l ds$ ranging from $0.85L$ to L , $\hat{A}_1$ is estimated by (14) [by insertion of the erroneous forward parameter in (3)]. c is then determined by $c = \hat{A}_1 / \int_l a_1 ds$ and plotted against path length expressed as a ratio to the diameter L in Fig. 12. Relative changes of c seem to be confined to around or less than 1% over the interval, for which reason we can model it as approximately constant.

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