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Quantitative material characterization based on the spectral decomposition of X-ray tomographic images

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Summary. — A single-energy CT provides a map of gray levels simply related to X-rays linear attenuation coefficients, which could be very similar for different materials at a given energy. Images acquired at multiple energies allows for a quantitative description of an object. In this work, phantom images were acquired using synchrotron radiation CT at precisely defined energies. A successful attempt was made to differentiate the phantom materials with respect to their decomposition into basis materials.

1. – Introduction

Benefiting from image acquisition at many angles, computed tomography (CT) improved diagnostic power by avoiding tissue superposition often masking signs of malignancy in planar X-ray imaging. An image is reconstructed from the distribution of linear attenuation coefficients μ, which are property of material and X-ray energy. However, a material of different chemical compositions may possess quite similar linear attenuation coefficients. From this point of view, breast imaging becomes a very challenging task since relative attenuation differences in breast tumors and surrounding tissues become negligible [1]. In the energy range of 20–100 keV, used in diagnostic medical imaging, the main contributions to μ are photoelectric effect, mainly dependent on the effective atomic number, Z_{eff}, and Compton scattering, more sensitive to electron density, ρ_e which is closely related to the mass density for most materials.

Since the 1970s, dual-energy computed tomography (DECT) has been developed to separate the two contributions to linear attenuation [2]. In this setup, an object is scanned with X-ray beams of different energy spectra which yield two different μ values. With two sets of measurements available, it is possible to mathematically obtain more quantitative information of the object, such as material composition and mass density [3].

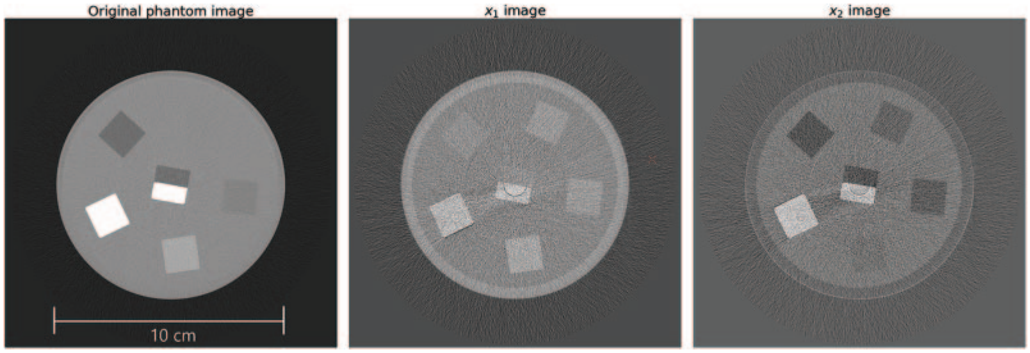

Fig. 1. – The original phantom image compared to the maps of PMMA and Al coefficients.

The quality of this estimation is heavily influenced by the amount of noise arising from the overlap between two spectra. Furthermore, preferential attenuation of low-energy X-rays, known as beam hardening effect, adds uncertainty on the accuracy of results and requires additional computation [4]. An ideal solution to this problem are well-separated monochromatic beams available at synchrotron radiation (SR) facilities. Exposure to monochromatic beams of different energy produce images completely independent from each other and substantially decreases the presence of the mentioned noise.

2. – Materials and methods

Neglecting the minor contribution to beam attenuation coming from coherent scattering, Alvarez and Macovski [2] postulated that μ of a material can be expressed as a linear combination of basis functions describing photoelectric and Compton effects, with respective weights. It is also always possible to change the basis and choose a combination of two materials with their known linear attenuation coefficients, μ_1 and μ_2 to be new basis functions. The change of basis leads to the expression of μ as

$$\mu = x_1 \mu_1 + x_2 \mu_2, \tag{1}$$

where x_1 and x_2 are the coordinates of the material in the reference frame identified by the selected basis. They are concentrations, or amount of both materials "squeezed" inside each geometrical entity in which the target is divided (*i.e.*, each pixel), producing the same attenuation as an original material at any energy. For this work, CT images of breast equivalent phantom were obtained at energies of 25, 28, 32 and 35 keV using a monochromatic beam available at the Elettra synchrotron facility. In an overdetermined system, x_1 and x_2 are estimated using a least-square fit method. The phantom was built for the needs of SYRMA (SYncrotron Radiation MAmmography) Collaboration [5] and consists of five inserts of polyethylene (PE), nylon (PA), PMMA, polyoxymethylene (POM) and polytetrafluoroethylene (PTFE), mimicking tissue found inside of the breast [6]. The choice of the basis materials is based on the imaging application, narrowing the space to a range of materials of interest. For this application empirical choice of PMMA and aluminum (Al) gave satisfactory separation between materials while preserving low measurement uncertainty. Decomposition of image entities into two density maps of weight coefficients for PMMA and Al, denoted by x_1 and x_2, is given in fig. 1.

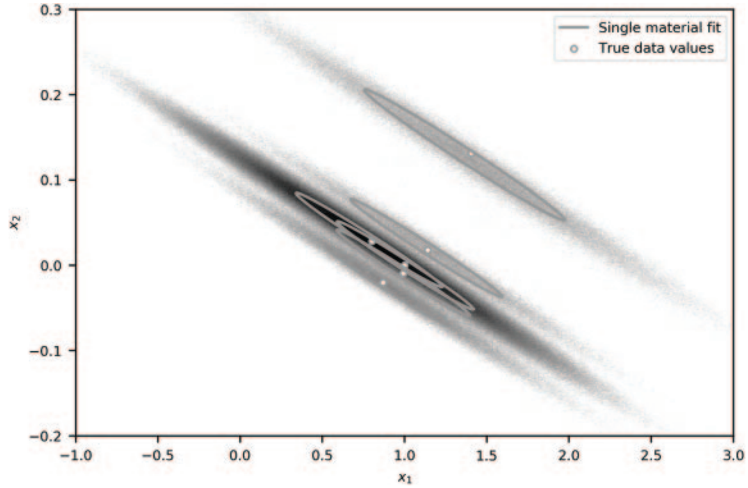

Fig. 2. – The two-dimensional histogram in logarithmic scale showing clusters of similar gray levels indicating different phantom materials. Ellipses are a product of two-dimensional Gaussian fit for each material separately. Dots show the "true" positions calculated from the dataset [8].

Table I. – *List of output parameters in the two-dimensional Gaussian fitting method for the phantom materials.*

Material	Major axis spread	Minor axis spread	Tilt
Water	0.146	0.00739	−0.122
PE	0.383	0.00653	−0.122
PA	0.406	0.00686	−0.123
PMMA	0.418	0.00685	−0.123
POM	0.465	0.00748	−0.123
PTFE	0.614	0.00992	−0.124

3. – Results

For material characterization, the two-dimensional arrays x_1 and x_2 were flattened into vectors and plotted against each other in form of a two-dimensional histogram. In fig. 2 the x-axis represents weights x_1 of PMMA and the y-axis weights x_2 of Al in the linear combination of these materials, and the brightness of a two-dimensional bin (*i.e.*, a coordinate in the two-dimensional histogram) the number of pixels with that specific combination of the two weights. For the visualization of each bin's frequency, a logarithmic scale is used.

The unique generating mechanism of spots representing specific materials is apparent [7]. The direction of major spreading is about two orders of magnitudes larger than the spread in the direction orthogonal to it and all spots have a similar tilt. These parameters were estimated upon fitting a sum of $N = 6$ two-dimensional elliptic Gaussian functions to the full histogram dataset (see table I).

The positions, that are in fact the concentrations x_1 and x_2, are identified with the centroid values of Gaussians. Ellipses in fig. 2 show the contribution of single material

Table II. – *Numerical values of material positions estimated through the Gaussian fitting method and positions calculated using known μ values (dots in fig. 2).*

Material	x_1	x_2	$x_{1,t}$	$x_{2,t}$
Water	0.784	0.029	0.802	0.028
PE	0.893	−0.023	0.869	−0.020
PA	0.991	−0.009	0.992	−0.009
PMMA	1.004	−0.0002	1	0
POM	1.133	0.020	1.141	0.018
PTFE	1.364	0.129	1.406	0.131

separated from the others. The accuracy of the estimated peak positions is cross-checked when these values are directly compared with the ones calculated using "known" linear attenuation coefficients published in [8]. These are precisely defined positions marked as points in fig. 2. The values of both, experimental and calculated positions, $x_{1,t}$ and $x_{2,t}$, are given in table II.

4. – Conclusion

In this work, the first step toward a quantitative description of breast content is described. The proposed theoretical model was successfully applied to experimental data and used to remove the degeneracy between materials with similar μ. Although significant overlapping existing due to the large presence of PMMA, used for the construction of the phantom, and water filling, coordinates were discriminated with good accuracy. From this decomposition, material density and effective atomic number of materials can be extracted, allowing a non-destructive chemical characterization of the sample. Such a path was explored in [7]. Furthermore, the proposed method for quantitative description could be used with polychromatic sources once a photon-counting detector is set to multiple energy thresholds. Such a transition could suffer from increased noise introduced into a decomposition procedure. For this reason, future work will address other sources of information for material separation, such as spatial correlations in x_1 and x_2 maps which vanish once a two-dimensional histogram is created.

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REFERENCES

[1] Piai A. *et al.*, *Phys. Med. Biol.*, **64** (2019) 155011.
[2] Alvarez R. E. and Macovski A., *Phys. Med. Biol.*, **21** (1976) 733.
[3] Contillo A. and Taibi A., *EPL*, **117** (2017) 48003.
[4] Coleman A. J. and Sinclair M., *Phys. Med. Biol.*, **30** (1985) 1251.
[5] Longo R. *et al.*, *J. Synchrotron Rad.*, **26** (2019) 1343.
[6] Contillo A. *et al.*, *Radiol. Oncol.*, **52** (2018) 329.
[7] Vrbaski S., Master Thesis, Kaunas University of Technology, 2020.
[8] Azevedo S. G. *et al.*, *IEEE Trans. Nucl. Sci.*, **63** (2016) 341.