Energy Dependent Information in X-Ray Imaging: Part 1. The Vector Space Description

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ABSTRACT

The energy spectrum of X-rays transmitted through the body contains important information. This information can be extracted by using a vector space description of the attenuation coefficient as a function of energy. The description is consistent with X-ray physics and is extremely accurate. The accuracy versus the number of functions in the basis set is quantified by using a mathematical formulation based on the singular value decomposition. This shows that a two function basis set gives sufficient accuracy for computed tomography and other quantitative medical applications. The vector space formulation can be used to prove that, in general, the line integral of the attenuation coefficient cannot be calculated from a single spectrum transmitted flux measurement. However, complete energy dependent information can be calculated from two flux measurements with different effective source spectra.

1. INTRODUCTION

Energy-selective techniques have a long history in X-ray physics, but it is only in recent times that the use of accurate detectors and computers has allowed this essentially numerical information to be extracted in an imaging system. The introduction of quantitative techniques into X-ray imaging necessitates the development of a firm theoretical foundation for the extraction of the information. That is the purpose of this series of papers.

There are several requirements for this theoretical formulation. First, it should be consistent with the known physics of the interactions of X-rays and matter. Second, it should be applicable within the theory of X-ray imaging techniques which is primarily based on linear systems. A formulation is described in this paper which satisfies both of these criteria and in addition is simple and economical. This formulation uses a vector space description of X-ray attenuation coefficients as a function of energy.

In the first paper this vector space description is introduced and rigorously justified. It is shown to be consistent with known X-ray physics and to represent the attenuation coefficient to an accuracy sufficient for even the most demanding medical applications such as computed tomography. Previous work (Alvarez and Macovski 1976) justified the accuracy on physical grounds. In this paper we introduce a mathematical formulation which computes the accuracy as a function of the number of dimensions of the space. This formulation can then be used to study questions such as the effect of the X-ray energy range and the atomic number range on the representation accuracy. The vector space theory is used to fundamentally analyze the information available from a single broad spectrum measurement as in conventional radiography. We show that, in general, this single measurement can not be used to calculate the line integral of the attenuation coefficient. Next, we show that an energy selective system using two broad spectrum measurements can extract complete energy dependent information under quite general conditions.

2. DESCRIPTIONS OF X-RAY ATTENUATION COEFFICIENTS

Although there are important nonlinearities, the description of X-ray imaging systems is based on linear theory. Linear systems concepts such as point spread function and modulation transfer function have proven invaluable understanding X-ray systems. Any technique for extracting energy dependent information must be linear if it is to utilize this powerful linear systems foundation.

The fundamental physical quantity describing the object, measured by an X-ray imaging system, is the linear attenuation coefficient If this is known, then the data measured by the system can be predicted. Single projection systems (such as used in conventional radiography) measure the line integral of the attenuation coefficient while computed tomography systems measure the attenuation coefficient at points in the object cross section.

While the use of linear techniques may seem obvious, some nonlinear techniques for extracting this information have been introduced. These are the parameterization techniques (Rutherford, *et al.* 1976). These techniques attempt to extract information by using a parametric model of the linear attenuation coefficients of the elements as a function of atomic number, electron density, and X-ray energy. The approach has several problems. First, it is difficult to derive accurate parametric expressions which are valid for the elements and energy range of interest (Hawkes and Jackson 1980). Any errors in these expressions will lead to errors in the calculation of the parameters. Second, and more fundamentally, it is difficult to rigorously generalize these expressions to realistic cases. The models use parameters (such as effective atomic number) which are inherently nonlinearizable in the measured data. Because of this problem, even as simple a situation as a mixture of elements requires an arbitrary definition of average, or effective, parameters which is difficult to justify on physical grounds. As evidence of this difficulty, several papers based on this approach have used different expressions for the effective atomic number (McCullough 1975 and Rutherford, *et al.* 1976).

Vector space techniques expand the attenuation coefficient as a linear combination of known functions of energy multiplied by undetermined coefficients.

$$\mu(E) = \sum_{i=1}^{\infty} a_i f_i(E) \tag{1}$$

Since the coefficients are the only unknown values in the expression, they carry all the information which will be extracted by the imaging system. The systems described in this paper measure these basis set coefficients which are obviously linearly related to the fundamental physical quantity, the linear attenuation coefficient. Furthermore, if the attenuation coefficient varies with position, the vector space expansion will be

$$\mu(x, y, z; E) = \sum_{i=1}^{\infty} a_i(x, y, z) f_i(E) \tag{2}$$

This linear separation of the effects into position-dependent and energy dependent parts fits in naturally with linear systems theory and can be readily applied to X-ray imaging systems.

The choice of basis functions $f_i(E)$ is crucial to this technique. Since the attenuation coefficient is smooth except for a countable number of discontinuities, a suitable set can be found. However, this set could contain a very large number of functions which would make it useless for any practical application. Fortunately, as discussed in the next sections, the minimum number of required functions (the “dimensionality” of the space) is actually quite small.

3. PHYSICAL CONSTRAINTS ON DIMENSIONALITY

The dimensionality of the vector space is an important property of the physical quantity being imaged. It determines the complexity of the procedure for extracting the energy dependent information since the higher the dimensionality, the more complex the procedure. Conversely, the coefficients of the basis functions completely specify the attenuation coefficient. Thus, they represent all that can be deduced about the object from X-ray attenuation measurements.

There are several important physical properties which must be incorporated in any description of the X-ray attenuation coefficient. One of these, the “mixture rule,” states that the cross section for X-ray interactions of an atom is independent of its chemical state. This is, of course, not exactly true. A whole field of X-ray spectroscopy (Agarwal 1979) is concerned with extracting information about the chemical properties from these changes. However, these effects are confined to (at most) a few keV from an absorption edge. Since most biological materials have their absorption edges at energies substantially below those of interest in medical radiography this effect can be ignored. A notable exception is iodine in the thyroid and contrast agents. These are high atomic number materials with K-edges within the medical region. The chemical effects are still quite small but they may affect high precision measurements (and be the basis for sensitive *in-vivo* analysis).

With the mixture rule, the linear attenuation coefficient can be expressed as

$$\mu(E) = \sum_{i=1}^{N} n_i \sigma_i(E) \tag{3}$$

where n_i is the number of atoms per unit volume, and $\sigma_i(E)$ is the total cross section at energy$E$ for element i. This result is important for several reasons. First, it implies that the dimensionality of attenuation coefficient space is less than or equal to the number of distinct elements within the object. For biological objects this is a relatively small number. Second, since the attenuation coefficient of any material is a linear combination of the attenuation coefficients of its constituent elements, it, in turn, is a suitable candidate for a basis function. This result will be used in later discussions.

Another important physical principle which can be applied is the “sum rule” for the various X-ray interactions. Since X-ray photons may be considered to be discrete, the various types of interactions are independent and mutually exclusive. The total probability of not interacting is the product of the probabilities of not undergoing a particular type of interaction, so, for a particular element, the total cross section is the sum of the cross sections for each type of interaction. There are many possible types of interactions, but for energies in the diagnostic spectrum, three types predominate: Compton scattering, photoelectric absorption, and Rayleigh (coherent) scattering. Expressions can be derived which give these cross sections as a function of atomic number and energy. If these cross sections were separable into multiplicative factors which were functions of atomic number only and energy only, then this would imply that the dimensionality is smaller than the total number of elements. That is, if the cross section for an element i is

$$\sigma_i(E) = \sigma_c(E, Z_i) + \sigma_P(E, Z_i) + \sigma_R(E, Z_i) + \ldots \tag{4}$$

and

$$\sigma_C(E, Z) = K_C(Z) f_C(E) \tag{5}$$

$$\sigma_P(E, Z) = K_P(Z) f_P(E) \tag{6}$$

$$\sigma_R(E, Z) = K_R(Z) f_R(E) \tag{7}$$

then

$$\mu(E) = \left[\sum_{i=1}^{N} n_i K_C(Z_i)\right] f_C(E) + \left[\sum_{i=1}^{N} n_i K_P(Z_i)\right] f_P(E) + \left[\sum_{i=1}^{N} n_i K_R(Z_i)\right] f_R(E) + \ldots \tag{8}$$

Equation. 8 implies that if the expressions are separable, the dimensionality of the vector space is equal to the number of different types of interactions.

In order to study the separability, the cross sections can be plotted on a logarithmic plot. With separable expressions, the curves for different elements will be parallel. Figure 1 shows such a plot for the photoelectric interaction. Although the curves are not parallel, they are close to it. Similar results would be obtained for other types of interactions.

These results indicate that, with measurements of sufficient precision, the effects of individual elements could be resolved. For less accurate measurements, the changes with atomic number would not be resolvable and the dimensionality of the space would be less than the number of elements. The dimensionality must then be considered to be a function of measurement accuracy. Mathematical techniques for quantifying this observation are discussed in the next section.

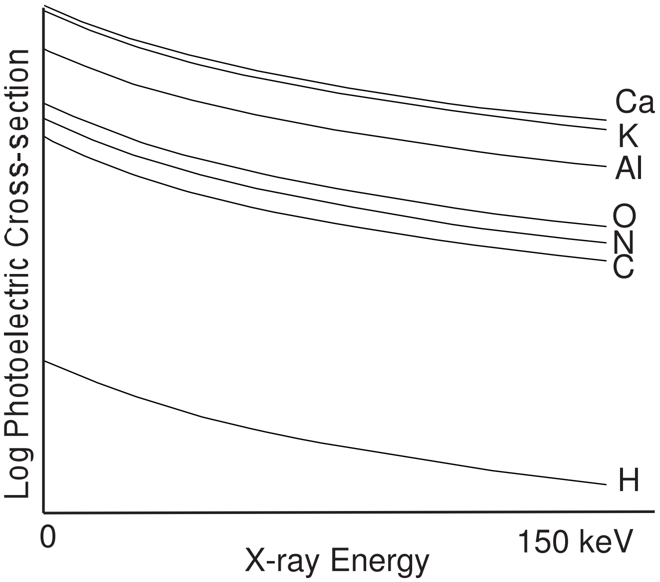

Figure 1. Logarithm of photoelectric cross-section. The curves would be parallel if the cross sections for all elements were represented by a common functional form.

4. THE SINGULAR VALUE DECOMPOSITION

The mathematical tools which will be used to study the dimensionality as a function of measurement accuracy are based on matrix theory. The reason for the applicability of this theory is that the dimensionality of the space is closely related to the rank of a matrix. An important application of the Singular Value Decomposition is to determine the rank of a matrix whose elements are known to contain errors. This same tool will be applied in this section to study the dimensionality of attenuation coefficient space as a function of measurement accuracy.

Consider a matrix whose columns are the values of the attenuation coefficients of various elements at many energies in the medical diagnostic range. If the elements found in biological materials are included, then, by the mixture rule, the columns will span the space of attenuation coefficients of body materials. That is, the attenuation coefficient of any biological material can be expressed as a linear combination of the columns of the matrix.

Analogous to the discussion in the previous section, if the entries in the matrix are considered to be of infinite precision, almost all matrices will have full rank (that is, the rank is equal to the smaller of the number of rows or columns). However, in any physical situation, the matrix entries (the measurements of the attenuation coefficient) will have limited accuracy. In this case, another matrix with less than full rank may be found which is “close” to the original matrix. If the “distance” between the matrices is less than the accuracy of the entries of the original matrix, then the rank of the original matrix is equal to the rank of the approximating matrix to the specified accuracy. This is the concept of numerical rank (Stewart 1973) which will be applied to describe dimensionality of the attenuation coefficient space as a function of measurement accuracy.

In order to define “closeness”, a matrix norm must be introduced. This is a scalar function of the elements of the matrix which is a measure of its size. The norm will be applied to measure the difference between the full rank matrix and its lower rank approximating matrix. There are many candidates for a norm function. Any computationally convenient function can be chosen so long as it satisfies the necessary properties of definiteness, homogeneity, and the triangle inequality. A convenient norm can be defined by reasoning by analogy with a vector norm. The 2-norm for a vector V with components v_i and dimension N is

$$\|V\| = \sqrt{\sum_{i=1}^{N} v_i^2}. \tag{9}$$

The analogous norm for a matrix is called the Frobenius norm. For a matrix B with elements b_{ij} and dimensions M by N the norm is

$$\|B\| = \sqrt{\sum_{i=1}^{M}\sum_{j=1}^{N} b_{ij}^2} \tag{10}$$

A matrix norm defined in this way has all the desirable properties outlined above (Stewart 1973).

The difference between infinite precision and numerical rank can be understood by considering a diagonal matrix, D. The infinite precision rank for this matrix is equal to the number of non-zero entries. The numerical rank can also be determined from these values. In order to do this, the diagonal entries with small absolute value can be replaced by zeros. The limited accuracy rank will be equal to the number of rows or columns minus the number of entries dropped. If the entries are in numerical order and those in columns $r+1$ to N are set equal to zero, the difference between the limited accuracy $\tilde{D}$ and full precision matrices D, is equal to

$$\|D - \tilde{D}\| = \sqrt{\sum_{i=r+1}^{N} d_i^2} \tag{11}$$

If this distance divided by the number of entries is small compared to the error in each of the members, then the numerical rank of the original matrix is equal to the rank of the reduced matrix.

Suppose the matrix of interest B is not diagonal. In this case, the singular value decomposition theorem may be applied to transform this case to the diagonal matrix case just described. According to this theorem, there exist unitary matrices U and V such that

$$B = UDV^H. \tag{12}$$

where D is a diagonal matrix and V^H is the complex conjugate of the transpose of V.

Since U and V are unitary matrices, multiplying by them does not change the value of the norm. Thus the norms of the original and the diagonal matrices are the same. Suppose the columns of the matrices are rearranged so that the diagonal elements of B are in descending order. Let $\tilde{D}$ be the matrix with columns $r+1$ to N equal to zero. The matrix

$$\tilde{B} = U\tilde{D}V^H \tag{13}$$

will have the following important property. No other matrix of rank r will be closer to B than $\tilde{B}$. That is,

$$\|B - \tilde{B}\| = \sqrt{\sum_{i=r+1}^{N} d_i^2} \tag{14}$$

is minimum for all matrices of rank r . Thus, depending on the distribution of the diagonal elements of the transformed matrix B, a matrix of reduced rank may be found which is closer to the original matrix than the error in the terms (with closeness measured in terms of the Frobenius norm). From an experimental point of view, the rank of the original matrix is no larger than that of the reduced matrix.

The mathematical technique for studying dimensionality as a function of the accuracy of the measurements will be complete if a technique can he found for calculating the diagonal elements in the matrix D. The values of the diagonal elements can be calculated by using the singular value decomposition theorem. They are the eigenvalues of the matrix B. Numerical techniques for calculating the singular value decomposition are discussed in the literature (Klema and Laub 1980).

Table 1. Singular Values for Biological Materials

n	Singular Value
1	.948
2	.318
3	.0036
4	.000663
5	.000412
6	.000239
7	.000212
8	.000148
9	.0000361

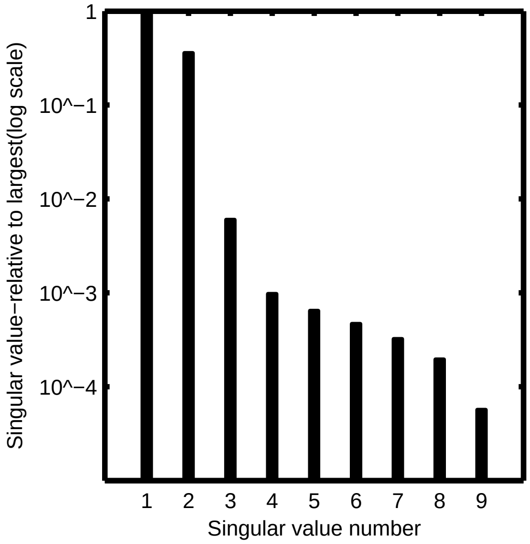

Figure 2. Error vs. number of functions in the basis set for biological materials. The error was computed using the SVD as discussed in the text.

5. APPLICATIONS OF THE SVD TO THE DIMENSIONALITY OF X-RAY ATTENUATION COEFFICIENT SPACE

As described in the two previous sections, any discussion of the dimensionality of a representation of attenuation coefficients must consider the accuracy of the measurement technique. The dimensionality will also depend on other factors such as the set of elements in the object and the X-ray energy region. In this section, quantitative results are presented for the dimensionality of the attenuation coefficients of biological objects in a computed tomography system.

The matrix tools in the previous section, including the singular value decomposition and the concepts of matrix norms, will be applied as follows. First, tabulated values of the attenuation coefficient of various elements are placed in a matrix. The SVD of this matrix is then calculated. By setting entries in the diagonal matrix equal to zero, the closest approximating matrix of a given rank to the original matrix will be calculated as well as the distance between the two matrices. This distance can then be plotted as a function of the rank of the approximating matrix and compared to the expected error in the measurements. The results are based on calculations using tabulated values of the X-ray linear attenuation coefficients from several sources (Veigele 1973 and McMaster *et al.* 1969). The numerical techniques are based on the algorithms developed by Golub and Reinsch (1970) and implemented in the computer software package EISPACK.

Table 1 shows the singular values for a matrix containing the attenuation coefficients of elements with atomic numbers (1,6,7,8,15,16,17,19,20). These span the range of elements commonly found in biological materials. The attenuation coefficients are calculated for a set of energies (30 to 150 keV) that also span the range used in

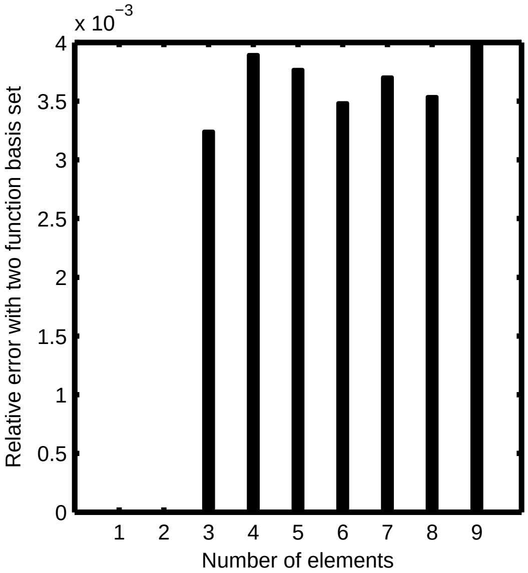

Figure 3. Errors with a two function basis set vs the number of different elements in the material. The elements are those found in significant quantities in biological materials, which were used in Table 1.

medical radiographic applications. These are plotted in Figure 2. Note that the scale is logarithmic so the first two values are much larger than the rest of the values. As discussed in the previous section, this implies that a two function basis set can give an accurate approximation of the values of all the elements in Table 1.

5.1 Dimensionality Versus Atomic Number Range

An important consideration is the effect on the dimensionality of the range of atomic numbers in the set of chemical elements that we are approximating. This was calculated by adding new columns representing the attenuation coefficients of elements with increasing atomic number to the data matrix and then calculating the singular value decomposition of each of these data matrices. The mean relative error with a two function basis set, computed using Equation (14), is shown as a function of the range of atomic numbers in Figure 3. Since there is a small atomic number dependence of the interaction cross- sections, the errors would be expected to increase. As shown, they increase somewhat as the range becomes larger. However, the increase in errors is small so a two function set provides a good approximation. For the complete set of elements and the specified X-ray energy range, the average relative error with a two function basis set is .004. In CT, this corresponds to 4 Hounsfield Units (HU) and this is less than or comparable to the error introduced by X-ray quantum noise.

5.2 Dimensionality versus Energy Range

As the range of energies increases, the dimensionality would also be expected to increase. If the range does not encompass K-edges or regions (such as that greater than $2m_ec^2$) where pair-production becomes important, the increase should not be large. These intuitive considerations are supported by the data in Figure 4. This plots the mean relative error as a function of energy range. The upper energy was fixed at 500 keV while the lower energy was varied. Thus at the lower energies in the plot the range is larger. The data set contained the biological element set used in Figure 2.

5.3 Dimensionality with K-edge in Energy Range

If the energy range contains a discontinuity in the attenuation coefficient of one of the elements, the results are substantially different. Figure 5 shows the singular values for a set of elements including iodine for an energy range from 30 to 150 keV. Note that this range includes the K-edge of iodine at 33.2 keV. The dimensionality of the space is now equal to three for even moderate accuracies.

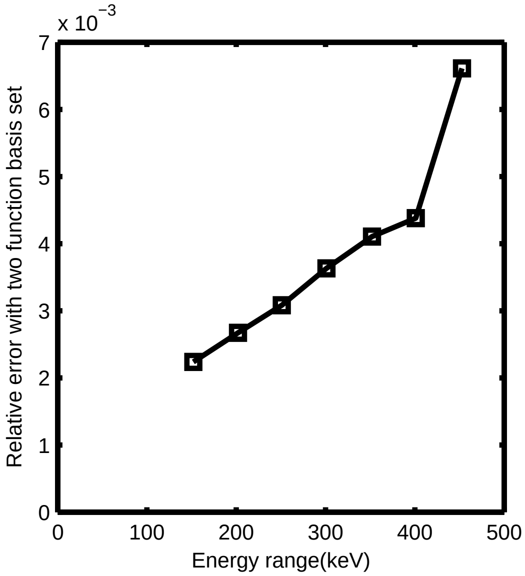

Figure 4. Error with a two function basis set *vs.* x-ray energy range. The range is the maximum minus the minimum x-ray energy.

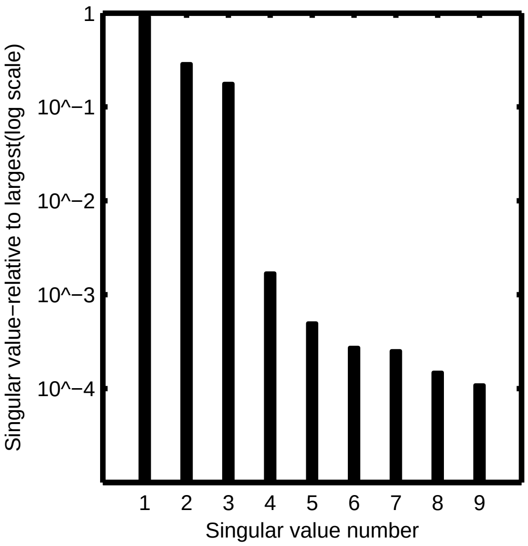

Figure 5. Singular values with K-edge in energy range. Note that now three functions are required.

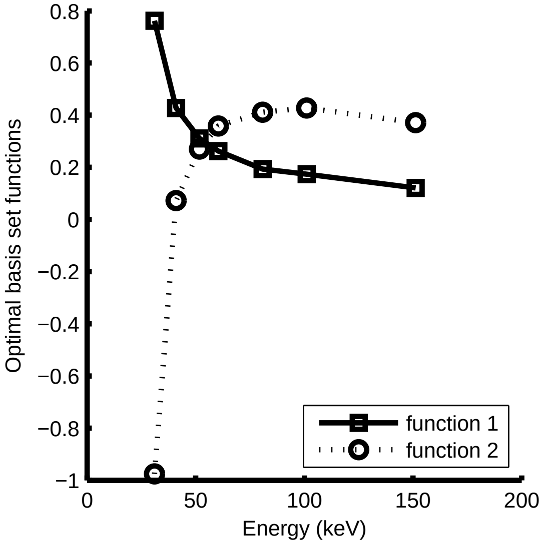

Figure 6. Optimal basis set functions. These functions result in the minimum error in approximating the attenuation coefficients with two functions.

5.4 Discussion

The results presented in this section indicate that the dimensionality of x-ray attenuation space is equal to two even for the accuracies achieved in computed tomography. Although the use of a broader energy range or the inclusion of high atomic number materials increases the errors with a two function basis set, these are still substantially less than the errors due to quantum noise. Thus, for almost all uses in medical radiography

$$\mu(E) = a_1 f_1(E) + a_2 f_2(E) \tag{15}$$

where $f_1(E)$ and $f_2(E)$ are attenuation coefficients of elements with atomic numbers similar to those found in the body.

Two details of the calculations should be considered. The most important is the effect of errors in the data. Although the data used are considered to be the most accurate available, they still contain errors. While these errors probably would not affect the conclusions, they may change the numerical values of the smaller singular values. Another consideration is the effect of energy sampling. Theoretically, the attenuation coefficients should be considered to be continuous functions of energy while our results are based on samples. The effect of these samples was studied by increasing the number while keeping the energy range fixed. For a large enough number of samples, the results converged to a single set of singular values. A sufficient number of energy samples was used so that the results should be close to those with a very large number of samples.

6. THE OPTIMAL BASIS SET FUNCTIONS

As discussed previously the SVD gives the optimal approximating matrix of a given rank to the original matrix. By studying equation (12), it is clear that the optimal basis functions are the first r columns of the matrix U. Figure 6 is a plot of the first two columns of this matrix. Since$U$ is unitary, the columns are orthogonal. These two columns can be considered to be samples of the optimal basis set functions at the energies used in the attenuation coefficient matrix.

7. VECTOR SPACE DESCRIPTIONS OF MIXTURES AND LINE INTEGRALS

A linear vector space representation allows simple geometrical representations to be used to describe the attenuation of mixtures and line integrals. This model consists of a set of rules for manipulating the coefficients directly without regard for the energy functions. These rules are derived in this section.

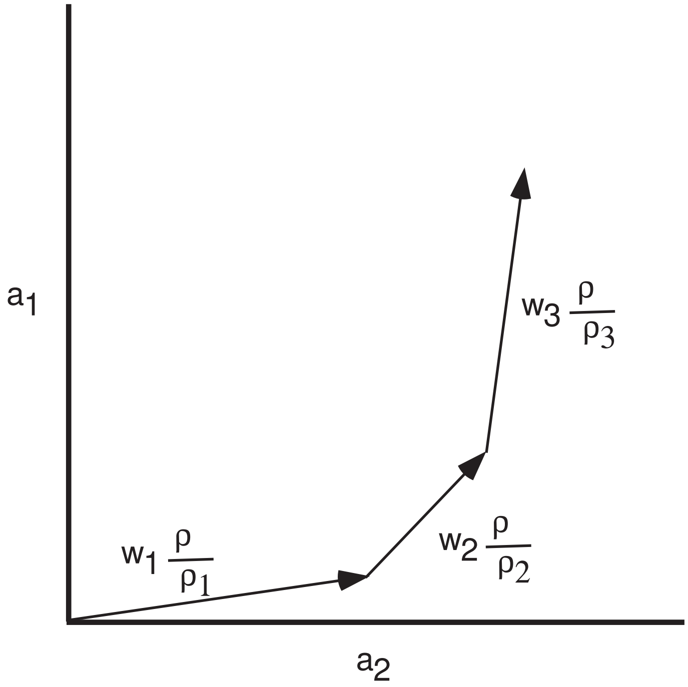

Figure 7. Vector interpretation of the basis set coefficients of a mixture.

The fundamental law is the mixture rule. By this rule, the total, linear attenuation coefficient μ is related to the attenuation coefficients of the constituents by

$$\frac{\mu}{\rho} = \sum_{i=1}^{N} W_i \frac{\mu_i}{\rho_i} \tag{16}$$

where $\rho$is the overall density, W_i is the fraction by weight of element i in the mixture and ρ_i is its density.

Thus, if the basis set coefficients for the elements in the mixture are (a_{1i}, a_{2i}) then the basis set coefficients for the mixture are:

$$a_1 = \sum_{i=1}^{N} W_i \frac{\rho}{\rho_i} a_{1i} \tag{17}$$

$$a_2 = \sum_{i=2}^{N} W_i \frac{\rho}{\rho_i} a_{2i} \tag{18}$$

This can be considered to be a weighted vector sum and given a graphical interpretation as shown in Figure 7.

The line integrals of a mixture have a similar interpretation. The line integral of an inhomogeneous object is

$$L(E) = \int \mu(x, y, z; E) ds \tag{19}$$

Introducing the vector space description of the attenuation coefficient, the line integral is

$$L(E) = f_1(E) \int a_1(x, y, z) ds + f_2(E) \int a_2(x, y, z) ds \tag{20}$$

Denoting the line integrals of the basis set coefficients as A_1 and A_2 the line integral is then

$$L(E) = A_1 f_1(E) + A_2 f_2(E) \tag{21}$$

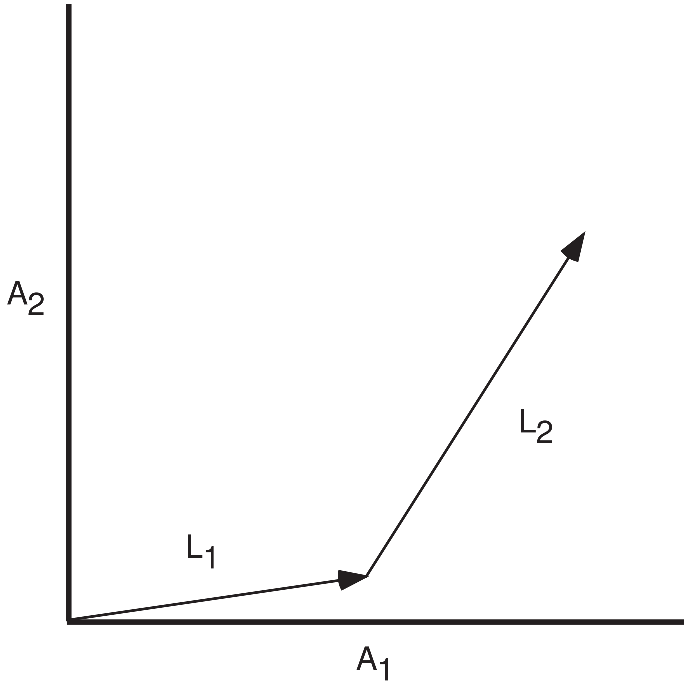

Figure 8. Vector interpretation of line integrals of basis set coefficients for a mixture.

If the object is composed of a single material with coefficients (a_1, a_2) and has a thickness l the line integrals will be

$$A_1 = a_1 l \tag{22}$$

and

$$A_2 = a_2 l. \tag{23}$$

If it is composed of several materials in different regions with coefficients (a_{1i}, a_{2i}) and thicknesses l_i , the line integrals are

$$A_1 = \sum_{i=1}^{N} a_{1i} l_i \tag{24}$$

and

$$A_2 = \sum_{i=1}^{N} a_{2i} l_i. \tag{25}$$

An object modeled to be a mixture of several materials with the ratio of the amounts of the materials varying gives similar results. In any case, due to the linear nature of the vector space model and the sum rule, the total line integrals can also be modeled to be weighted vector sums of the line integrals of the materials in the object. This is illustrated in Figure 8.

8. THE CALIBRATION MATERIAL BASIS SET

Note that the results of the previous sections are independent of any parameterization of the cross sections for the various interactions. All that is necessary is that the attenuation coefficient of a given element be expressible as a linear combination of the attenuation coefficient of other elements. Since the attenuation coefficients of real materials are a linear combination of the attenuation coefficients of their elements (by the mixture rule)

Table 2. Accuracy of Calibration Material Basis Set

Z	a_1	a_2	rms fractional error (%)
1	2.2298	-0.27396	0.29026
2	1.1211	-0.13334	0.17917
3	0.96715	-0.10971	0.09164
4	0.98483	-0.10255	0.0652
5	1.0087	-0.08729	0.03254
6	1.0557	-0.05785	0.02771
7	1	0	0
8	0.92372	0.08147	0.02035
9	0.76582	0.18902	0.06501
10	0.6782	0.33074	0.09362
11	0.47834	0.49541	0.12483
12	0.28195	0.72698	0.18738
13	0	1	2e-005
14	-0.31465	1.3321	0.29977
15	-0.68005	1.6622	0.38051
16	-1.0716	2.1168	0.14641
17	-1.6213	2.6063	0.30005
18	-1.9095	2.8529	0.22294
19	-2.7208	3.7283	0.287
20	-3.3678	4.5083	0.40408

and since the attenuation coefficients of the elements are a linear combination of two elements, the attenuation coefficient function of any two distinct materials can be used as a basis set (Alvarez 1976). This approach is preferable to a parameterization approach for two reasons. First, it is more accurate for a given dimensionality. Second, it allows calibration of the solution of equations for the energy selective information to be in terms of lengths instead of complex measurements based on attenuation coefficients.

The use of a real material basis set is more accurate than the parametrization approach because it removes errors due to inaccuracies in the expressions for the energy dependence of the interactions (Lehmann 1982). The relative accuracy of these approaches is illustrated in Table 2. This shows the root mean square (rms) fractional error in fitting the mass attenuation coefficients (Veigele 1973) of elements with atomic numbers from 1 to 30. The real material basis set used the attenuation coefficients of nitrogen and phosphorus (atomic numbers 7 and 15) as the basis functions. The basis set coefficients were determined by least squares fitting to the data. This was compared to the effective atomic number and electron density parameterizations of McCullough (1975) and Rutherford (1976). Note that for all elements tested the real material basis set had smaller errors.

The use of a real material attenuation coefficient basis set has important practical advantages in the calibration procedure used to solve for the energy-selective information. Suppose the attenuation coefficient functions of the calibration materials themselves are used as the basis set (Alvarez 1976). Then the basis set coefficients in the calibration phantom are simply zero or one.

$$\mu_1(E) = 1 * f_1(E) + 0 * f_2(E) \tag{26}$$

$$\mu_2(E) = 0 * f_1(E) + 1 * f_2(E). \tag{27}$$

The line integrals of the basis set coefficients are then just the thicknesses of the calibration materials along the path of the X-ray beam. That is

$$A_1 = \sum_{i=1}^{N} a_{i1} l_i \tag{28}$$

with a similar result for A2 . Since the accuracy of the information extraction technique (Alvarez and Macovski 1976) rests on the measurement of these line integrals, this transformation of the line integrals to length measurements substantially improves the quantitative usefulness of the technique.

9. CALCULATION OF LINE INTEGRAL $\int \mu(X, Y, Z : E) DS$ FROM A SINGLE MEASUREMENT

X-ray imaging systems do not measure the attenuation coefficient directly. Rather, they measure the flux transmitted through the object. Neglecting scatter and assuming an infinitesimally narrow beam, the flux is given by

$$I = \int S(E) e^{-L(E)} dE \tag{29}$$

where $S(E)$ is the energy spectral density of the source, and $L(E) = \int \mu(x, y, z : E) ds$ is the line integral of the linear attenuation coefficient. In many quantitative applications, such as computed tomography and digital radiography, it is desired to calculate the line integral at a single energy from the flux. in this section, we show that, even if the spectrum is known, this is not possible except in special circumstances. The best that can be done in a practical clinical situation is an approximation which will be accurate only under a limited set of conditions.

Using the vector space description of the attenuation coefficient, the line integral at a single energy E is

$$L(E_0) = A_1 f_1(E_0) + A_2 f_2(E_0) \tag{30}$$

For a given energy, the basis functions $f_1(E_0)$ and $f_2(E_0)$ are constant and the problem of the calculation of a line integral may be generalized mathematically as follows: Is there any way to calculate a linear combination of the line integrals of the basis set coefficients from a single flux measurement? The following theorem answers this question.

> If the spectrum is not monoenergetic and if the object consists of more than one material, then an invertible function $g(I)$ does not exist such that
>
> $$g(I) = k_1 A_1 + k_2 A_2 \tag{31}$$
>
> where $k_1$and $k_2$are constants.

By the discussion above, this theorem includes the calculation of the line integral as a special case.

First, consider the special case of an object known to consist of a single material. In this case the flux can be used to calculate the line integrals. These are given by equation (22) and the object vectors are constrained to lie along a straight line passing through the origin of the vector space. The flux is a function only of the material thickness l

$$I(A_1, A_2) = I(l) = \int S(E) exp(-a_1 l \left[f_1(E) + \frac{a_2}{a_1} f_2(E) \right]) dE \tag{32}$$

Note that (a_1, a_2) are constants for the single material case.

The derivative

$$\frac{dI}{dl} = -\int \left[a_1 f_1(E) + a_2 f_2(E) \right] S(E) exp(-a_1 l \left[f_1(E) + \frac{a_2}{a_1} f_2(E) \right]) dE \tag{33}$$

is always less than zero since S(E) and the attenuation coefficient

$$\mu(E) = \left[a_1 f_1(E) + a_2 f_2(E) \right] \tag{34}$$

are always greater than zero. Thus the flux is a monotonically decreasing function of the material thickness and the flux can be used to calculate the thickness l (and therefore the line integral).

The proof of the impossibility for the general material case is in two steps. First, we show that if the invertible function g exists the contour curves of $I(A_1, A_2)$ must be straight lines. Next we show that these contour curves are not straight lines thus proving the result by contradiction. For the first part of the proof, consider the composite function $h(A_1, A_2) = g[I(A_1, A_2)]$. If g exists then

$$h(A_1, A_2) = k_1 A_1 + k_2 A_2 \tag{35}$$

where $k_1$and $k_2$are constants. The function g is invertible so, if $h(A_1, A_2)$ is equal to a constant c then $I(A_1, A_2)$ is equal to the unique constant $g(c)$ on this line which then must be a contour curve of $I(A_1, A_2)$. Thus if $g(I)$ exists the contour curves of I are straight lines.

The proof that the contour curves of $I(A_1, A_2)$ are not straight lines rests on the fact that the basis functions $f_1(E)$ and$f_2(E)$ are linearly independent. The equation of the contour curves is

$$c = \int S(E) exp\left[-A_1 f_1(E) - A_2 f_2(E)\right] dE \tag{36}$$

Differentiating this expression implicitly gives the value of the slope of the contour curve through any point (A_1, A_2).

$$\frac{dA_2}{dA_1} = -\frac{\int f_2(E) S(E) exp\left[-A_1 f_1(E) - A_2 f_2(E)\right] dE}{\int f_1(E) S(E) exp\left[-A_1 f_1(E) - A_2 f_2(E)\right] dE}. \tag{37}$$

If the contour is a straight line, then this slope must be a constant and equal to, say, α along the line $A_2 = \alpha A_1 + \beta$. That is,

$$\frac{dA_2}{dA_1} = \alpha = -\frac{\int f_2(E) S(E) exp\left[-A_1 f_1(E) - (\alpha A_1 + \beta) f(E)\right] dE}{\int f_1(E) S(E) exp\left[-A_1 f_1(E) - (\alpha A_1 + \beta) f(E)\right] dE} \tag{38}$$

for all A_1. Multiplying by the integral in the denominator and gathering terms on one side of the equation shows that if the contours are straight lines, then

$$\int \left[\alpha f_1(E) + f_2(E)\right] S(E) exp\left[-A_1 f_1(E) - (\alpha A_1 + \beta) f(E)\right] dE = 0. \tag{39}$$

Since this must be true for all A_1, if the spectrum $S(E)$ (which is non-negative) is not a delta function, then there exists a constant a, such that

$$\alpha f_1(E) + f_2(E) = 0 \tag{40}$$

for all energies E. That is, if the contour curves are straight lines, then the basis functions are linearly dependent. This is not true, so the contour curves of $I(A_1, A_2)$ are not straight lines and the proof is completed.

It is instructive to consider the monoenergetic spectrum case where $S(E)$is a delta function, say $\delta(E - E_0)$. In that case, the contour curves of $I(A_1, A_2)$ are straight lines with slope

$$\frac{dA_2}{dA_1} = -\frac{f_2(E_0)}{f_1(E_0)}. \tag{41}$$

This does not imply that the basis functions are linearly dependent since equation (41) has to be satisfied only at one energy.

Although the theorem just presented shows that, in general, a linearizing function does not exist, there may be cases where a good approximate linearizing function can be defined (Alvarez 1976). In computed tomography, errors in estimating the line integral result in beam hardening artifacts and techniques have evolved to minimize these errors (Stonestrom *et al.* 1980). One possibility is to have a spectrum which is near to monoenergetic. This can be achieved by prefiltering the incident beam. Another possibility is to use a water bath so that the effective object attenuation approaches a single material case. The most complex approaches use information from all the projections along with *a-priori* models of body tissue composition to calculate corrected line integrals. Although these techniques reduce the artifact problem, they will only work under specialized circumstances and will fail if the object does not fit their assumptions.

10. INVERTIBILITY OF THE DUAL ENERGY EQUATIONS

The previous section demonstrated that the line integral can not be calculated from a single flux measurement. In this section we show that under quite general conditions complete energy dependent X-ray attenuation information, i.e., the attenuation at any energy in the diagnostic region, can be calculated from two flux measurements with different source spectra. This is done by deriving a procedure to calculate the line integrals of the basis set coefficients A_1 and A_2. In a single projection system these can be used with Equation (21) to calculate the line integral at any energy. In a CT system the line integrals can be reconstructed to give cross sectional images of the value of the basis set coefficients, Then using the fundamental vector space decomposition the attenuation coefficient can be calculated at any energy. In either case, the results represent all the information which can be inferred from X-ray attenuation measurements.

Using the expression for the attenuation coefficient line integral $L(E)$, (21) in the equation for the transmitted flux (29), shows that the flux is a function of two independent variables, A_1 and A_2 (the source spectrum is assumed to be constant). Since there are two variables this single measurement cannot in general be inverted to yield the line integrals. However, suppose another measurement is made with a different effective source spectrum. This could be effected either by using an energy resolving detector or by varying the spectrum by switching the X-ray tube voltage. This gives two functional relationships

$$I_1(A_1, A_2) = \int S_1(E) exp[-A_1 f_1(E) - A_2 f_2(E)] dE \tag{42}$$

$$I_2(A_1, A_2) = \int S_2(E) exp[-A_1 f_1(E) - A_2 f_2(E)] dE \tag{43}$$

and therefore defines a transformation between the measured quantities (I_1, I_2) and the desired quantities (A_1, A_2). An important question is under what conditions this transformation is invertible.

Before discussing the situation in general, two simple but important cases will be discussed. The first case is the use of two monoenergetic spectra with energies E_1 and E_2. In this case the flux measurement can be linearized by taking the logarithm of the flux measurements (42). The result is that the logarithms of the measurements and the line integrals are related by the linear equations

$$log\left[\frac{I_1}{I_{10}}\right] = -A_1 f_1(E_1) - A_2 f_2(E_1) \tag{44}$$

$$log\left[\frac{I_2}{I_{20}}\right] = -A_1 f_1(E_2) - A_2 f_2(E_2) \tag{45}$$

where I_{10} and I_{20} are the measurements with zero object thickness. These equations can be solved uniquely for the line integrals if the determinant of the coefficients is not equal to zero:

$$\begin{vmatrix} f_1(E_1) & f_2(E_1) \\ f_1(E_2) & f_2(E_2) \end{vmatrix} \neq 0 \tag{46}$$

That is if

$$\frac{f_1(E_1)}{f_2(E_1)} \neq \frac{f_1(E_2)}{f_2(E_2)} \tag{47}$$

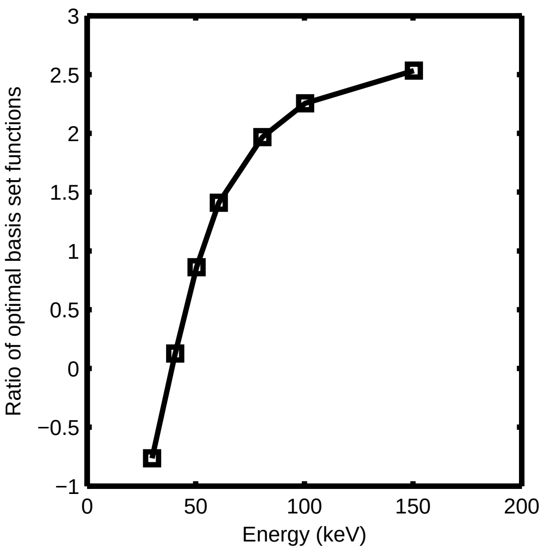

Figure 9. Ratio of optimal basis set functions. Since the ratio is not constant, the condition in Equation 47 is satisfied.

Figure 9 shows a plot of the ratio of the basis set functions versus energy in the medical diagnostic region. Note that the ratio is monotonically decreasing. Thus, the condition in equation (47) will be true if the two energies are different.

Another useful special case is when the object is known to consist of a single material. As discussed in the previous section, a single flux measurement suffices if the exact composition is known. The thickness can be calculated as previously discussed and equation (22) can then be used to calculate the line integrals. For the general case, the following theorem is useful (Fulks 1969 page 284):

> Let F be a continuously differentiable mapping defined on an open region D in E2, with range R in E2 , and lets its Jacobian be never zero in D. Suppose further that C is a simple closed curve that, together with its interior (recall the Jordan curve theorem), lies in D, and that F is one-to-one on C. Then the image T of C is a simple closed curve that, together with its interior, lies in R. Furthermore, F is one-to-one on the closed region consisting of C and its interior, so that the inverse transformation can be defined on the closed region consisting of T and its interior.

which I paraphrase as

> If the Jacobian of a continuously differentiable two dimensional mapping is nonzero throughout an open region D and if the mapping is one to one on a simple closed curve C which lies in D, then the mapping is one to one on C and its interior.

By using this theorem the following result can be established:

> If two spectra with different maximum energies and such that suitably defined average energies of the spectra transmitted through an object are not equal over a region of the (A_1, A_2)plane containing the points for the object, then the two flux measurements (given by equation (42)) can be used to uniquely calculate the values of the line integrals.

In order to establish this result using the previously quoted theorem the Jacobian must be shown to be nonzero throughout a region in the (A_1, A_2) plane and the transformation must be shown to be invertible on a closed simple curve in this region. The region shown in Figure 10 will be used. It consists of the first quadrant of the plane. This is a region of theoretical and practical importance because a basis set consisting of the attenuation

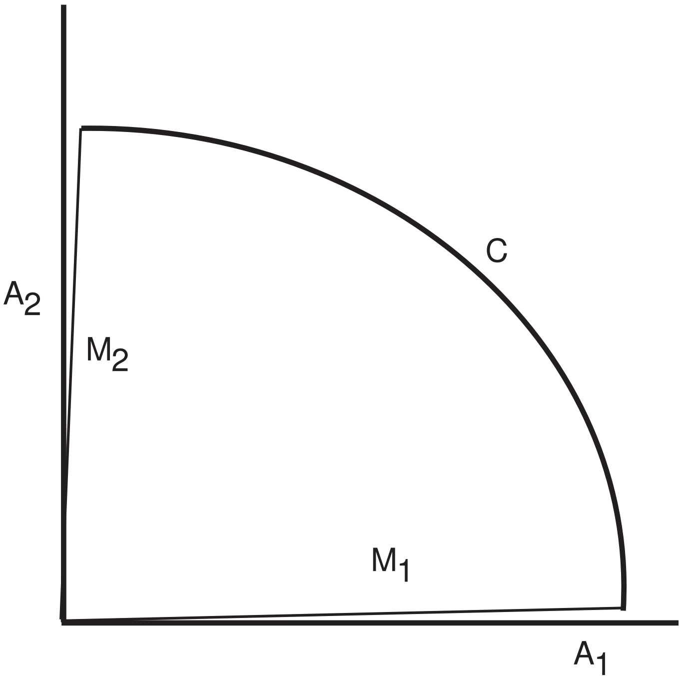

Figure 10. Closed contour used in proof of invertibility. The contour consists of the two axes, drawn slightly offset to show the contour, and a large portion of a circle to close it.

coefficients of the calibration materials is usually used, Since only positive equivalent thicknesses of the calibration materials can be used, this region must contain all the measured values. The closed curve will consist of the axes and a portion of a circle (with a large radius so that all points in the object are included) centered on the origin joining the axes. This curve is also shown in Figure 10.

Instead of using the flux measurement directly, suppose the logarithm of the flux is used. The results will be equivalent so long as the flux is greater than zero. With the log, the components of the Jacobian of the transformation are

$$J_{ij} = -\frac{\int f_j(E) S_i(E) exp[-A_1 f_1(E) - A_2 f_2(E)] dE}{\int S_i(E) exp[-A_1 f_1(E) - A_2 f_2(E)] dE} \quad i,j = 1,2 \tag{48}$$

Note that by defining two normalized spectra

$$\overline{S_i}(E) = \frac{S_i(E) exp[-A_1 f_1(E) - A_2 f_2(E)]}{\int S_i(E) exp[-A_1 f_1(E) - A_2 f_2(E)] dE} \quad i = 1,2 \tag{49}$$

the Jacobian can be written as

$$J = \begin{bmatrix} -< f_1 >_1 & -< f_2 >_1 \\ -< f_1 >_2 & -< f_2 >_2 \end{bmatrix} \tag{50}$$

where $<>_i$ denotes the average using the normalized spectrum $\overline{S_i}(E)$. Thus the condition for the Jacobian not being zero is equivalent to

$$\frac{< f_1 >_1}{< f_2 >_1} \neq \frac{< f_1 >_2}{< f_2 >_2}. \tag{51}$$

This condition must be tested for individual spectra.

In order to complete the proof of invertibility, the transformation must be shown to be invertible on a closed curve in the domain. The simply cases discussed at the beginning of this section may be used for this proof. The parts of the curve along the axes are special cases of the single material case. By the previous results, these cases are invertible. The circle of large radius is an approximation of the single energy case. For large radius there will be high attenuation. With beam hardening, the transmitted spectrum with large attenuation approaches a monoenergetic spectrum at the maximum energy in the spectrum. If the maximum is different for each spectrum, we can approach the known invertible monoenergetic case arbitrarily closely by making the radius larger and larger.

If the Jacobian can be shown to be non-zero throughout a region of line integral values including those of the object, then these results guarantee that the flux measurements can be inverted to give the line integral values. Consider x-ray tube voltage switching as an example. In the tube spectrum, the maximum energy is the tube voltage times the electron charge. So, if the two voltages are different, these results imply that the equations will be invertible to compute the line integrals from the transmitted fluxes with the two voltages. The line integrals are all the information that can be produced by a single projection system. If a CT system is used then the line integrals can be reconstructed to give the values of the basis set coefficients in the object's cross-section. Techniques for extracting medically useful information from these line integrals or coefficients will be discussed in the second paper in this series (Alvarez and Lehmann 1982).

11. CONCLUSIONS

The X-ray linear attenuation coefficient as a function of energy can be accurately described by a vector space model. The accuracy of this description depends on the number of functions in the basis set. By using the singular value decomposition theorem of matrix algebra, the dependence of the errors on the dimensionality of the space can be quantified. For an energy range which does not include discontinuities in the attenuation coefficient, a two function basis set provides excellent accuracy.

The vector space decomposition has many important uses. It provides a theoretical framework for understanding the effect of energy dependent attenuation on conventional X-ray systems. These results have important implications for quantitative X-ray systems such as computed tomography and digital fluoroscopy. The vector space formulation can also be used to design and analyze systems which extract energy dependent information. This includes both energy-selective computed tomography and digital radiography systems.

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