

THE RECONSTRUCTION PROBLEM IN MICRODOSIMETRY

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Abstract — A generalised formulation of microdosimetry clarifies the linkages between the spatial distribution of energy deposits, their proximity function, and the specific energy. The role of the proximity function suggests that it may replace, for various purposes, the inchoate distribution. The Fourier transform of the proximity function is the product of the Fourier transform of the inchoate distribution with its conjugate. This operation causes the loss of phase information, and the reconstruction problem — the reconstruction of the inchoate distribution from its proximity function — can, therefore, not be resolved by a mere deconvolution. For any finite point pattern one can, however, show that its proximity function permits, in principle, the reconstruction. Numerical examples with 2-dimensional patterns of up to 30 points have consistently led to unique solutions, apart from reflections. While there is a finite algorithm, it is readily seen that the number of steps becomes excessive when the number of points in the pattern increases. The reconstruction problem can, thus, be solved in principle but not necessarily in practice. A more general approach must thus be based on numerical optimisation. The algorithm starts with an assumed initial point pattern and utilises a suitable measure for the difference between its proximity function and that of the original pattern. Minimising this difference can lead to the original or to a similar pattern. With simple algorithms one obtains convergence only for patterns of few points; but improved optimisation methods are likely to provide more general solutions.

INTRODUCTION

The evolution of microdosimetry has been largely determined by the available experimental techniques. The familiar parameters of radiation quality are, therefore, closely linked to measurements. In recent years, however, there has been an increasingly important role for particle track simulations. As emphasised in a preceding contribution to this symposium⁽¹⁾, there is a need for closer links between the practical and the theoretical aspects.

Important quantities in theoretical microdosimetry and in track simulation are closely related to concepts and algorithms of stochastic geometry. The *inchoate distribution* of energy transfers, i.e. the pattern of energy imparted to matter by charged particles, results from a spatial random process, and biophysical arguments in terms of microdosimetry can, therefore, employ a variety of geometric theorems that apply to the random overlap of patterns of energy deposits and the spatial distribution of critical targets in the cell. A theorem of great generality^(2,3) expresses the variance of the overlap in terms of the point-pair distance distributions, and in its application to microdosimetry it provides the fundamental formula^(4,5) for the dose mean lineal energy, \bar{y}_D , which is the most commonly invoked parameter of radiation quality:

$$\bar{y}_D = \frac{1}{\bar{l}} \int_0^{\infty} \frac{s(x) \cdot t(x)}{4\pi x^2} dx \quad (1)$$

\bar{l} is the mean chord length of the reference region, while $s(x)$ is the proximity function of the reference

site (or its substitute, the detector) and $t(x)$ is the proximity function of the inchoate distribution. The latter is the energy weighted distribution of distances between energy deposits and, as such, a basic characteristic of the pattern of energy deposition^(5,6).

The general nature of Equation 1 and various other applications of the proximity function suggest a further exploration of the properties of $t(x)$. The present contribution will deal with one aspect that is of basic mathematical interest, although it appears too complex to permit definite solution. This is the question of whether the proximity function, if known with sufficient precision, contains, in essence, the full information on the spatial distribution of energy imparted. If one had a method to reconstruct from the proximity function the original pattern of energy deposits — or patterns that are in a stochastic sense largely equivalent — the question would be answered positively. The proximity function could then be utilised as a universal tool and would be a compact but complete description of radiation quality.

The subsequent considerations can merely outline the problem, but they may stimulate further investigations and may thus lead to an improved theoretical basis of microdosimetry. As a first step certain essential properties of the proximity function need to be reconsidered. A subsequent section will then explain the reconstruction problem and a tentative approach to its eventual solution.

AUTOCORRELATION AND PROXIMITY FUNCTION

A preceding contribution to this symposium⁽¹⁾ has referred to the concept of the *directional proximity*

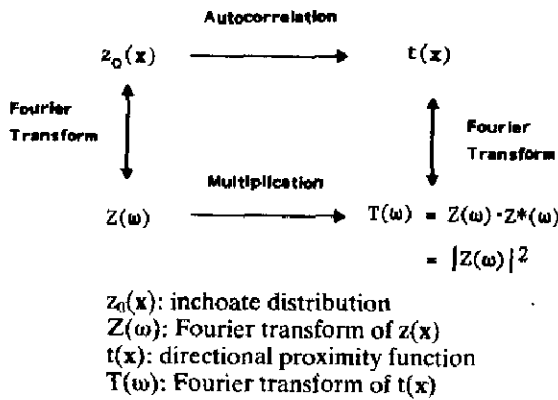


Figure 1. The autocorrelation of the original function $z_0(x)$ corresponds to the multiplication of the Fourier transform, $Z(\omega)$, with its conjugate complex, $Z^*(\omega)$. The latter operation disregards phase information, and is, therefore, not reversible.

function, or the *covariogramme*, which is identical to the familiar autocorrelation function:

$$t(x) = \rho \int z_0(x+s) \cdot z_0(s) ds / \int z_0(s) ds \quad (2)$$

where $z_0(x)$ is the spatial pattern of energy deposits, ϵ_i , at the transfer points, x_i :

$$z_0(x) = \frac{1}{\rho} \sum_{i=1}^n \epsilon_i \delta(x-x_i) \quad (3)$$

where ρ is the density of the material.

The directional proximity function is somewhat too complex to have practical applications in microdosimetry; it can, however, be helpful as a mathematical tool and has, as such, found useful applications^(2,6). Of special interest is the utilisation of the Fourier transform which converts a convolution into a mere multiplication (Figure 1). The interrelations that are indicated in Figure 1 might, at first sight, suggest the possible inversion of the operation that turns the inchoate distribution, $z_0(x)$, into the autocorrelation function. However, the Fourier transform of the autocorrelation function is the product of the Fourier transform of $z_0(x)$ with its (complex) conjugate and this implies the loss of phase information. It is for this reason that the process permits no straightforward inversion.

A solution in terms of the directional proximity function could, nevertheless, be achieved. But this is of theoretical interest only, because of the impracticality of numerical calculations with $t(x)$. A question of far greater pragmatic interest is whether the reconstruction problem might be solved even on the basis of the familiar proximity function, $\tau(x)$, which is a directional average over the autocorrelation function⁽¹⁾.

THE ASSOCIATION OF DISTANCES

This paragraph will first demonstrate — by very simple considerations — the possibility 'in principle' of the reconstruction. But it will be seen that the solution becomes impracticable whenever one deals with even a moderate number of points in a pattern.

For the purpose of the subsequent consideration a simplification of the actual microdosimetric problem will be employed. Instead of the proximity function of a stochastic ensemble of point patterns, we will consider the proximity function of single point patterns, i.e. of single realisations of a stochastic process. In a further simplification all points in the pattern will be assigned equal weight.

A pattern of n points is associated with $m=n(n-1)/2$ distances. If the *association* between the distances were known, the reconstruction would be straightforward.

The notion of the association of distances can be understood by assuming that the points are numbered from 1 to n , and that x_{ik} is the distance between points i and k ; the pattern is then characterised by a symmetrical matrix, X :

$$X = \begin{pmatrix} 0 & x_{12} & x_{13} & \dots & x_{1n} \\ x_{21} & 0 & x_{23} & \dots & x_{2n} \\ x_{31} & x_{32} & 0 & \dots & x_{3n} \\ \dots & \dots & \dots & \dots & \dots \\ x_{n1} & x_{n2} & x_{n3} & \dots & 0 \end{pmatrix} \quad (4)$$

It is sufficient to consider one triangular part of the matrix; from the ordered set of m distances one can then readily reconstruct the point pattern. In the 2-dimensional example this corresponds to the problem of reconstructing a map of the location of cities from their mutual distances.

The proximity function gives the m distances but not their association. However, there is only a finite number of possible associations and from this one concludes that, in principle, one can reconstruct the original pattern from the proximity function by forming all possible associations and by attempting the reconstruction in each case. There is, of course, no certainty that the reconstruction has only one solution. But if the solution is not unique, one is, at least, certain to obtain the original pattern as one of the solutions.

The somewhat striking conclusion is, that the reconstruction problem has a solution. It would however be a fallacy to infer from this fact the necessary existence of a practicable solution. To understand the problem one may consider the number of possible associations of the distances.

There are $m!$ possibilities to order the distances into the triangular scheme. The number of 'essentially different' associations is smaller, because the numbering of the n points is arbitrary and without effect on the spatial patterns. The

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number of 'essentially different' associations is therefore:

$$M = \frac{m!}{n!} = \frac{(n(n-1)/2)!}{n!} \quad (5)$$

Table 1 gives the values *m* for point numbers up to *n*=12. It is evident that the simple method of exhausting all associations is impracticable for *n*>6. *One concludes, therefore, that the reconstruction problem can be solved in principle, but not necessarily in practice.*

THE PROBLEM OF MULTIPLE SOLUTIONS

The reconstruction problem would be of comparatively little interest if there were a large number of solutions to the same proximity function. This aspect of the problem will, therefore, be briefly considered in general terms and will then be examined by some numerical computations.

Although it may be difficult to obtain general statements, one may intuitively expect, that the solution is — apart from translations, rotations, and reflections — unique or that there is at most a small number of solutions. This expectation is based on the simple observation that the problem is largely overdetermined for a sufficiently large point pattern. Consider the *k*-dimensional case. There are then *k*·*n* coordinates of the points, but translation and rotation of the pattern reduce the number of degrees of freedom to *k*(*n*-2)+1. The proximity function, on the other hand, contains the *m*=*n*(*n*-1)/2 distances as parameters, and Table 2 shows that, even for moderate point numbers, the problem is substantially overdetermined. The conclusion is that an arbitrarily chosen increasing step function will not be a proximity function, and that a proximity function may have multiple solutions only in exceptional cases where there are

certain symmetries in the point patterns (see, for example, Reference 7). It will be of particular interest to identify constraints that a monotonous function must meet to be a proximity function, but the problem transcends the scope of this contribution.

Since general conclusions are difficult, we have examined the uniqueness of the solutions of the reconstruction problem by numerical examples. As shown in the preceding section, the exploration of all distance associations is impracticable. If, however, the distances are precisely known, the problem is greatly simplified. Entire classes of associations are then readily seen to be impossible, and a finite algorithm becomes possible.

For simplicity we have examined merely the 2-dimensional case. Beginning with the largest distance, *x*_{max}, one can search for five more distances that are able to form with *x*_{max} the four sides of a quadrangle and its two diagonals. Once this initial quadrangle is determined one proceeds to find triplets of distances that connect a further point to a triplet of points that have already been constructed. This finite algorithm is feasible with patterns of up to about 30 points, and then requires computing times which can be many hours on a PC.

Figure 2 shows examples of patterns that have been reconstructed by this straightforward method. They are arbitrarily selected from several dozen cases that have been computed, and the essential point in the present context is that the inferred patterns were in all cases identical to the initial patterns or their mirror images. This suggests that the reconstruction problem has, in essence, unique solutions. The explicit computations have been utilised merely to explore the problem of the uniqueness of reconstructed patterns. It is not a suitable general procedure because it requires precise knowledge of the distances and because it leads to excessive computing times for point numbers in excess of about 30. It is also considerably more time consuming in the 3-dimensional than in the 2-dimensional case.

Table 1. Number of points in a pattern, the corresponding number of point-pair distances and the total number of distance associations.

Number of points, <i>n</i>	Number of distances, <i>m</i> = <i>n</i> (<i>n</i> -1)/2	Number of associations, <i>M</i> = <i>m</i> !/n!
3	3	1
4	6	30
5	10	30,240
6	15	1.8×10 ⁹
7	21	1.0×10 ¹⁶
8	28	7.6×10 ²⁴
9	36	1.0×10 ³⁶
10	45	3.3×10 ⁴⁹
11	55	3.2×10 ⁶⁵
12	66	1.1×10 ⁸⁴

Table 2. Number of points in a pattern, the corresponding number of degrees of freedom of coordinates in different dimensions, and the number of point-pair distances.

Number of points, <i>n</i>	Number of degrees of freedom of coordinates			Number of distances, <i>m</i>
	<i>R</i> ¹	<i>R</i> ²	<i>R</i> ³	
5	4	7	10	10
10	9	17	25	45
20	19	37	55	190
50	49	97	145	1225
100	99	197	295	4950

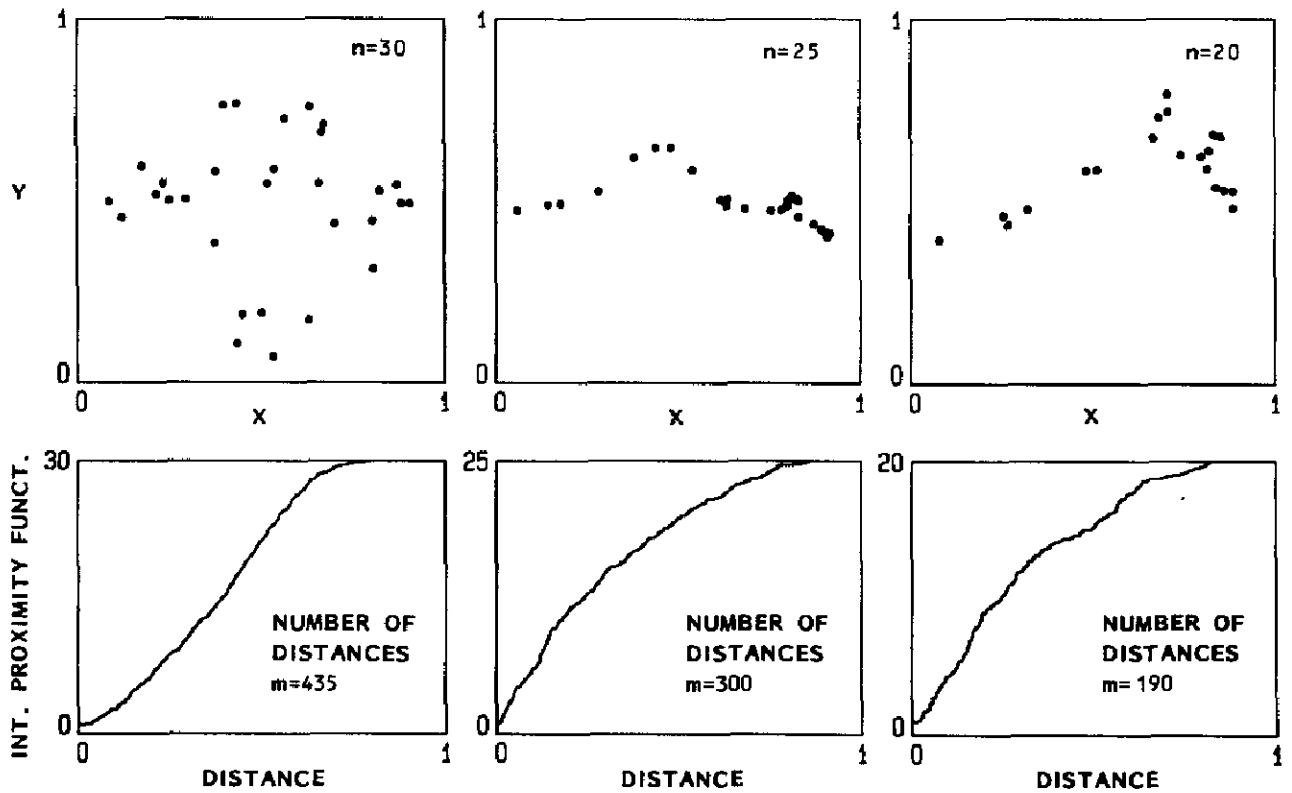


Figure 2. Examples of 2-dimensional point patterns and their proximity functions. These point patterns — and a considerable number of further examples — have been reconstructed directly from their proximity functions; all solutions were, apart from reflections, identical to the original patterns.

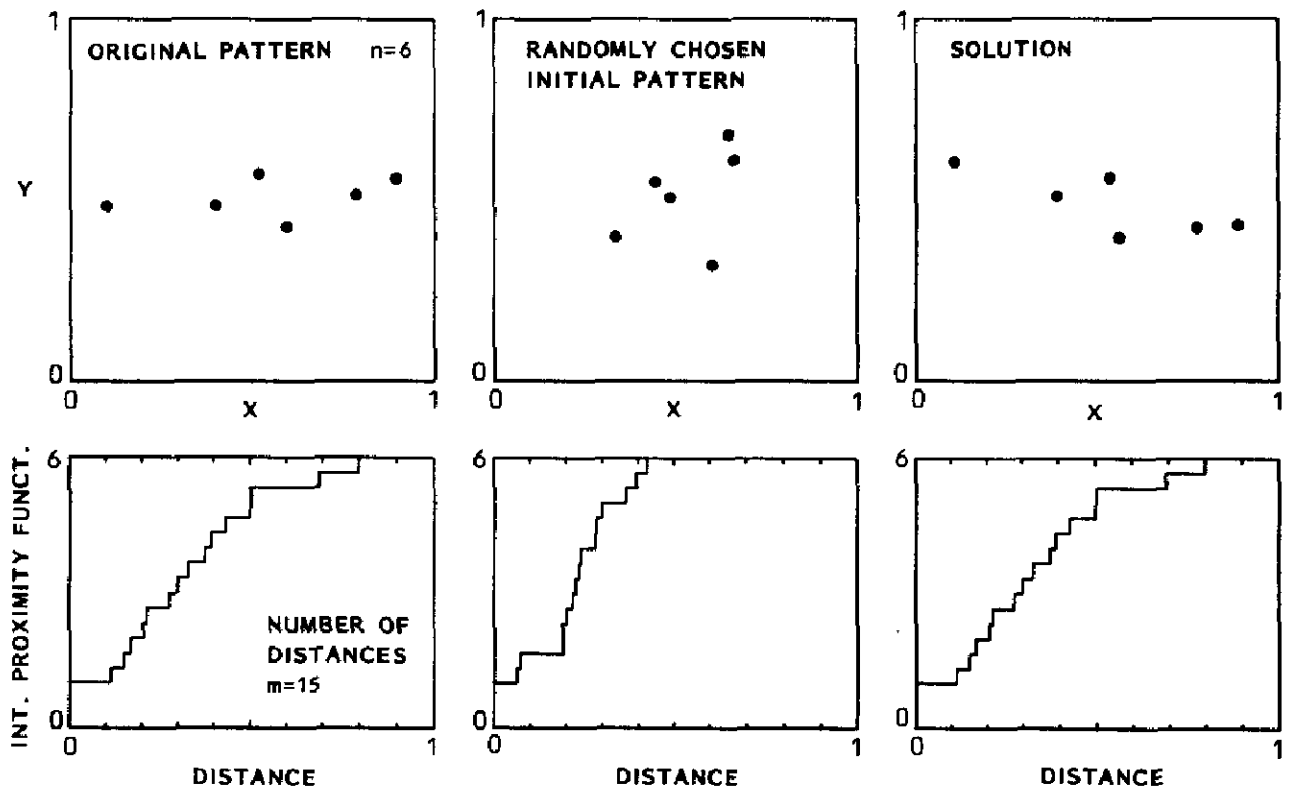


Figure 3. Original pattern, randomly chosen initial pattern, and the solution of the optimisation procedure. The lower panels give the corresponding integral proximity functions. The solution is congruent to the original pattern.

USE OF OPTIMISATION PROCEDURES

Since there is no practicable finite algorithm for large patterns, one may base — as in similar mathematical problems — the search for solutions on optimisation algorithms. Such algorithms can, even for functions of many variables, identify maxima or minima. To solve the reconstruction problem, one needs to 'guess' an initial point pattern, determine its proximity function, and choose a suitable measure to quantify its deviation from the proximity function of the unknown original pattern. Varying the assumed pattern one can then, by use of the optimisation algorithm, identify the minimum of the measure of the deviation and, thereby, search for the original pattern.

We have formulated an optimisation algorithm in terms of the sum of the squares of the differences between the ordered distances. The conjugate gradient algorithm then requires for each iteration step the reordering of distances between point pairs before the computation of the 'economic function' that measures the deviations between the proximity functions.

The large number of potential associations of distances suggests that the optimisation procedure may frequently converge toward secondary minima, instead of the absolute solution; it is also not unlikely that the facility of convergence depends greatly on the complexity of the underlying pattern, with easiest convergence for a uniform random distribution of points. The question of convergence is central to optimisation problems, but we have not, at this stage, employed the various techniques to overcome the difficulty.

The unrefined application of the conjugate gradient algorithm converges adequately only for small point numbers. Figure 3 gives the example of a pattern of six points and the corresponding integral proximity function which was readily identified. Figure 4 gives an example of incomplete convergence, where the derived pattern is substantially different from the original configuration, although the proximity functions are nearly the same, at least on a linear scale of distances.

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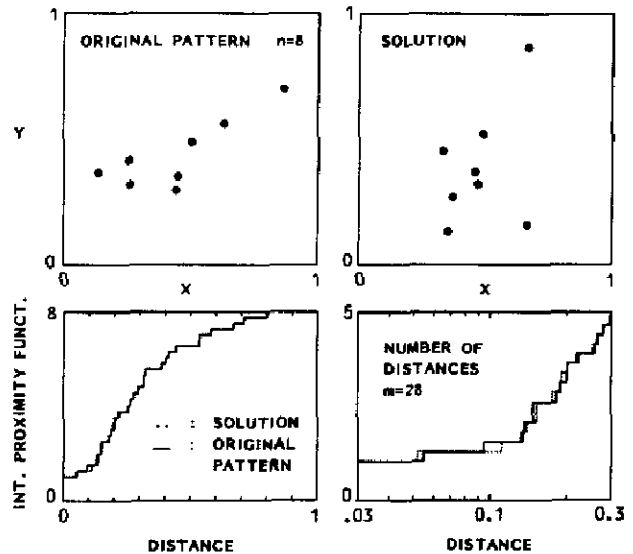


Figure 4. Original pattern and the solution of the optimisation procedure in a case of incomplete convergence. The corresponding proximity functions (lower panels) are largely equal, but the patterns differ considerably.

The incomplete convergence highlights the difficulty of the reconstruction problem, but one must note that the remaining differences of the proximity functions appear more substantial on a logarithmic scale of the distances, which indicates that a more suitable 'economic function' may lead to improved convergence. One notes, furthermore, that two patterns may appear very different over all, but may nevertheless exhibit largely equivalent stochastic properties, as they are relevant for the problems of microdosimetry.

The reconstruction problem is far from a solution but it points towards a multitude of questions that are essential to a better understanding of microdosimetry and any numerical description of radiation quality.

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