Scanning Microscopy

Volume 1994
Number 8 *The Science of Biological Microanalysis*

Article 23

3-14-1994

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Scanning Microscopy Supplement 8, 1994 (pages 289-294) 0892-953X/94$5.00+.25
Scanning Microscopy International, Chicago (AMF O'Hare), IL 60666 USA

SIGNAL AND IMAGE MANIPULATION IN MICROANALYSIS

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(Received for publication September 29, 1993, and in revised form March 14, 1994)

Abstract

Scanning electron microscopes, and transmission instruments equipped for EELS, generate a host of signals and hence of images from each pixel of the specimen. Numerous ingenious ways of coping with this multiplicity of information, which may be very different in character, have been devised, but no detailed study has yet been made of the appropriate mathematical structure, with the aid of which all this information could be manipulated reasonably easily.

One such structure falls within the subject that has come to be known as *Image Algebra*, the principal attraction of which is that we deal directly with entire images and not with individual pixels; the operations involved do of course ultimately take effect at pixel level. Despite its forbidding name, image algebra is intrinsically very simple and has the merit that the notion of "image" is very general. Images can in particular be multi-valued, that is, a set of values can be associated with every pixel. Indeed, a whole image is associated with each pixel, in the case of the very important class of images known as templates. Image algebra has proved to be an extremely fertile subject, generating many new ideas and especially, revealing several unsuspected relationships between different branches of image and signal processing.

The value of this approach will be examined, after a very simple introduction to the basic ideas. The application to image-spectra will be considered as a tangible example. We conclude with some speculations concerning the future of this rich new way of "picturing" images.

Key Words: Multi-valued images, image algebra, imaging-spectrum, spectrum image, morphology.

Introduction

With the arrival and widespread adoption of the various microanalytical modes of microscopy, the meaning of the word "image" became a little less obvious or rather, it ceased to have a single meaning but instead, became attached to several intensity distributions associated with the specimen under study. It could even be associated with a single pixel of the latter, though in this case a different term would be used (energy-loss spectrum) and the image would have only one row of values.

These are not the only extensions of the meaning of the word image that are of interest in electron microanalysis and microscopy. In bright-field image formation in the STEM, it can be useful to record the distribution of intensity in the detector plane for each pixel instead of the total intensity in a certain zone (occupied by the detector) as in the more usual image-forming modes. Here then we have a situation in which a (two-dimensional) image is associated with *every pixel* of the specimen. Again, in routine scanning electron microscopy, we may acquire several signals from each pixel and we are thus confronted with a multi-valued image: several intensity values, provided by different detectors, are associated with each pixel of the latter.

A further degree of freedom arises when we consider the use that is to be made of all this information. If the aim is to establish a map of the elements in the specimen, showing the concentration of the chemical element(s) present at each pixel, the final result will be a multi-valued image, the "intensity-values" of which are now heterogeneous. To each pixel, we shall attach codewords indicating the chemical elements present and the corresponding concentration. The code-words might be the symbols for the elements or their atomic numbers and we shall have to be careful that the arithmetic operations that we may apply to intensities or concentrations do not get applied to these symbolic images. Likewise, at the display stage, the kind of colour coding suitable for representing concentrations (typically coding of saturation or colorimetric purity) will probably be different from that best adapted for representing the various chemical elements (often hue).

The situation is thus complicated and can be confusing to anyone not permanently immersed in the subject. Several helpful tools have been introduced, notably the spectrum-image of Jeanguillaume and Colliex (1989) exploited in depth by Hunt and Williams (1991) and the closely related imaging-spectrum of Lavergne *et al.* (1992). Nevertheless, what is lacking is some general conceptual structure from which these and similar tools, adapted to particular cases, emerge in an obvious way. We can anticipate that the existence of such structure will suggest new tools or at least, shed an original light on those we already know. The purpose of this paper is to show that the mathematical structure known as image algebra is ideal for these purposes. Some preliminary thoughts in this direction were presented at the 10th Pfefferkorn Conference, held in Cambridge, 1991 (Hawkes, 1992).

Representation

The algebraic structure that we shall now describe, in largely qualitative language, has several obvious attractions, notably the ability to express image processing methods coming from very different fields - forensic science, agriculture, textile technology, electron microscopy - in a single language, accessible to all. One merit that is not quite so obvious is surely the principal reason for its success: the main steps of any argument are expressed in terms of whole images, while the inevitable operations at pixel level are relegated to a "second division", to the small print as it were. A necessary consequence is that we must be prepared to find the word "image" used in unfamiliar ways, which are nevertheless no more than natural extensions of its everyday meaning. Thus the diffraction pattern seen in the microscope or obtained with an optical bench or a computer is also an image. These are still single-valued images, one intensity being associated with each pixel. The next degree of complexity is the multi-valued image, in which two or more intensity values are associated with each pixel, the signals from different detectors in a SEM or a STEM for example. We could also include the energy-loss spectrum here, the set of values that represent the spectrum being regarded as the intensity values of the multi-valued image. This corresponds to the idea of a "spectrum-imaging image", employed by Lavergne *et al.* (1992). It may, however, be preferable to think of this as a single-valued image, the values of which are vectors; the elements of the vector are of course the measured values of the spectrum at that pixel. Another example is the complex-valued image, in which phase and amplitude are both of interest, but it is more natural to allow the intensity values to be complex numbers since this situation arises naturally as soon as we form a Fourier transform in the computer.

The final degree of complexity that we need here is not quite so easy to comprehend. Now, the intensity value associated with each pixel of the image is not a single number (real or complex) or even a set of several numbers but is itself an image. Moreover, this image can itself, in principle at least, be single- or multi-valued and its intensity values can be real or complex. Such a situation occurs naturally in the STEM as we have already mentioned and also, in a more subtle fashion, in the image-forming process of the TEM; it also occurs in many image filtering operations, designed to improve the image in some way or to enhance some feature of it. In the case of TEM imaging, this "image-valued image" is the point-spread function. We need not insist on this here but we mention it to show that such images are in practice very common, though we may not often think of them in the these terms.

Another generalization of potential importance, to which very little attention has been paid in electron microscopy and which we shall not discuss further here, concerns *colour*. At the simplest extreme, we could simply treat a coloured image as the superposition of images in the three primary colours, each regarded as "black-and-white" image and consider the problem solved. This is to ignore the fact that colour is most likely to be used to help the microscopist to appreciate a large amount of probably heterogenous information by displaying it in colours, hue and saturation being exploited to convey results of various kinds. It thus becomes important to understand how the observer perceives colour and the role of the colour-matching functions, still a subject of active research (e.g., North and Fairchild, 1993). We cannot go into this here but it will need to be considered whenever digital image information is being fed to the colour inputs of a monitor. The appropriate mapping is easily incorporated into the image algebra that is our subject here.

The mathematical structure that we are seeking must be capable of accepting all these different kinds of image with no special precautions or extensions: its purpose is precisely to express a complex situation in a simple way so we do not want to have to memorize lists of exclusion clauses, dealing with special cases. We then need to add as small a number as possible of operations, preferably of a familiar kind, and we expect to be able to express all our image-handling and image-processing tasks in terms of these few basic operators and the images on which they operate. We can anticipate that a certain amount of housekeeping will also be necessary, notably to remind us of the nature of the images being manipulated: we must not try to add two images if one consists of intensity values and the other of chemical symbols, for example! We might be allowed to form the union of them, however, to insert labels into a half-tone image before the final output stage. Thus operations can be expected to have a meaning only for certain kinds of image, a situation familiar in elementary arithmetic. We may also need to be careful to ensure that the images involved in a calculation are conformable, just as we do when multiplying matrices.

We are now ready to define what we mean by an image and to list the operations that we shall be using. More precisely, we shall explain how these operations work so that if it becomes desirable to add some new operation in the future, it can be fitted in naturally without perturbing those already incorporated. A more formal account of what follows is to be found in the work of Ritter *et al.* (1990) and Ritter (1991).

An image is a set of quantities at a set of points. Formally, we write

$$\mathbf{a} = \{(\mathrm{x}, \mathbf{a}(\mathrm{x})) \mid \mathrm{x} \epsilon \mathrm{X}\}, \ \mathbf{a}(\mathrm{x}) \epsilon \ \mathbf{F} \qquad (1)$$

which states that the image denoted by $\mathbf{a}$ is the set of quantities $\mathbf{a}(\mathbf{x})$ at the points characterized by $\mathbf{x}$, which belong to a set of points $\mathbf{X}$. The quantities $\mathbf{a}(\mathbf{x})$ can be numbers, or sets of numbers or even other images and $\mathbf{F}$ tells us which is the case. The special situation, to which we have drawn attention earlier, in which $\mathbf{a}(\mathbf{x})$ is itself an image, is so important in image processing that such an image is given a particular name, a *template*. Note that in this case, it is necessary to specify not only $\mathbf{X}$, which tell us where the pixels of image $\mathbf{a}$ are situated, but another set, $\mathbf{Y}$ say, which tells us where the pixels of the image $\mathbf{a}(\mathbf{x})$ are situated for each value of $\mathbf{x}$.

The operations that enable us to manipulate such images are few in number and very familiar: addition, multiplication and maximum; whenever possible, we extend this list to include subtraction, division and minimum. Together with a certain amount of convenient notation, this is all we need to manipulate images, however complicated, and to represent all the methods of image processing. The newer ideas involving neural networks prove to have been anticipated, in the sense that all the corresponding mathematics was already included in image algebra, just waiting to be recognized.

Let us now consider the imaging-spectrum and spectrum-image in closer detail. In the imaging-spectrum, a set of N energy-filtered images is recorded, which we denote $\mathbf{a}_i$, $i = 1,2,...N$. Each of these is a single-valued intensity image and corresponds to a particular energy loss. Such a set of images can be obtained with a TEM equipped with a filter: the entire area of the specimen to be imaged is illuminated simultaneously with a beam travelling parallel to the axis.

The spectrum-image is obtained by scanning a small probe over the specimen, typically in a STEM equipped for parallel EELS (PEELS). The entire energy-loss spectrum is recorded for each probe-position and hence for each pixel of the specimen. When the probe has scanned the whole specimen-area, we thus have a multi-valued image $\mathbf{b}$, each pixel-value of which represents an energy-loss spectrum.

The imaging-spectrum and the spectrum-image of course contain the same information. The relation between them is trivial: $\mathbf{b} = (\mathbf{a}_1, \mathbf{a}_2, ..., \mathbf{a}_N)$. The various types of information coded in $\mathbf{b}$ are immediately accessible as projections in various directions. These and other variants are known collectively as "flavours" (Hunt and Williams, 1991) and all can be included in $\mathbf{b}$ with only minor modification. Hunt and Williams identify six such flavours, most of which are already present in $\mathbf{b}$, notably E (spectral data from a single point), which is $\mathbf{b}(\mathbf{x})$ for the point $\mathbf{x}$; xE (spectral data from a line scan), which is $\mathbf{b}(\mathbf{x})$ for y= constant, say, with $\mathbf{x}$= (x, y); xyE (spectral data from each point in a 2D image), which is $\mathbf{b}$ itself. xyzE (spectral data from each point in a 3D image) can be accommodated simply by regarding $\mathbf{x}$ as (x, y, z) instead of (x, y). The line scans available now require two coordinates to be held fixed, if the line is parallel to one of the coordinates; in addition, a new possibility arises, namely, spectral data from each point in a 2D section through the image cube (or parallelepiped!).

Hunt and Williams also include two time-resolved flavours, tE (time-resolved spectral data from a point) and xtE (time-resolved spectra data from line scans). In this case, it may be preferable to regard $\mathbf{b}$ as a multi-valued image, the individual values at each pixel being not scalar but vector quantities. We then write

$$\mathbf{b} = (\mathrm{b}_1, \mathrm{b}_2, \mathrm{b}_3 ... \mathrm{b}_T) \qquad (2)$$

in which each b_j, $j = 1,...,T$, is an entire spectrum, for the j-th member of the time series. The flavour tE is then just $\mathbf{b}(\mathbf{x})$, as before, for a particular value of $\mathbf{x}$ and xtE is again $\mathbf{b}(\mathbf{x})$ for y= constant, for example, or more generally for ax+by = constant for an oblique line-scan.

So far, we have done little more than define a notation. How do we use it? For this, we need to see what can be done with the three basic operations (+, x and $\vee$) and their complements (-, /, and $\wedge$) beyond the most obvious uses. Let us consider the combination of addition and multiplication, the latter between an image and a template and the former over the resulting products. A special symbol is used for this combination, which reduces in the simplest case of a space-invariant template to a convolution. We write

$$\mathbf{a} \oplus \mathbf{t} = \{(\mathbf{y}, \mathbf{b}(\mathbf{y}); \mathbf{b}(\mathbf{y}) = \Sigma \mathbf{a}(\mathbf{x}).\mathbf{t}_{\mathbf{y}}(\mathbf{x})\} \quad (3)$$

in which the summation is over $\mathbf{x}$. This enables us, with suitable definition of the template $\mathbf{t}$, to describe in a homogenous way all the convolutional filters that are employed in image enhancement.

Similar calculations are needed in the study of spectra. Thus by forming difference spectra or second-difference spectra, small edges can be detected just as small contrast changes in images are accentuated by differentiation or by forming the digital Laplacian. The effect of studying the whole image $\mathbf{b}$ in this way may be expressed as follows:

$$\mathbf{c} = \mathbf{b} \blacklozenge \mathbf{t} = \{(\mathbf{x}, \mathbf{c}(\mathbf{x}); \mathbf{c}(\mathbf{x}) = \mathbf{b}(\mathbf{x}) \oplus \mathbf{t}\} \quad (4)$$

and any of the numerous ways of recognizing peaks can be applied to the processed spectra that are stored as $\mathbf{c}(\mathbf{x})$. This offers immense flexibility for not only can the template be space-variant but it can also be parametrized so that, for example, different linear operations are performed on different ranges of the spectrum and these need not be the same for all pixels.

Another technique that is proving invaluable in EELS elemental mapping is based on multivariate statistical analysis (introduced a decade earlier by Frank and van Heel in connection with data-handling for three-dimensional reconstruction), as Trebbia, Bonnet and colleagues have shown (Bonnet *et al.*, 1992; Trebbia and Bonnet, 1990; Trebbia *et al.*, 1990). The essential step here is the reorganization of a set of images into a single larger composite image. This is scaled and multiplied by its transpose and information is extracted from a study of the eigenfunctions and eigenvalues of the resulting matrix. We discussed this analysis at some length in Hawkes (1993) and the only point worth insisting on here is the possibility of regarding the image set as a template of particularly simple structure, since it has only a single column of pixels, each of which is an image with a single row of pixels, those of one of the original images redistributed in line. When that paper was composed, the importance of the template-to-matrix mapping was not clear and its utility in this context was merely speculated on. Recent developments have made it clear how useful it is likely to prove, and we return to it briefly below.

The manipulation of signals, from scanning instruments in particular, frequently involves the family of operations that are known collectively as mathematical morphology, a name that was more appropriate when the subject came into being than today, when it is recognized as just one of the branches of image processing, admittedly a very large one. These are essentially nonlinear operations between an image and a second, usually much smaller image, known as a structuring element. Just as all the linear filtering operations employed in image enhancement can be represented as a convolution product of the image and a second small image so these nonlinear morphological operations can be thought of as a different kind of "product" between a similar pair of images. It is fair to say that image algebra has completely transformed our perception of these morphological procedures, for not only has it revealed the close relation between the structuring elements of morphology and the templates of image algebra but it has also shown that the basic operations of morphology - dilation and erosion - are exactly equivalent to recognized image algebra calculations. Moreover, the latter can be represented as matrix-vector product, a particularly useful finding. The fact that the latter is a linear operation may seem to conflict with our earlier observation that morphology is intrinsically nonlinear; in fact, however, the steps that convert the structuring-element, for example, into a matrix are non-linear, though very simple and easy to implement and the product itself is defined more generally.

For a more formal but still extremely readable account of these ideas, the work of Davidson is strongly recommended, notably Davidson (1992, 1993).

Conclusion

The image algebra is thus a very powerful unifying force, bringing together the whole of image enhancement and image restoration, convolutional and morphological filtering as well as the numerous linear and non-linear fields of image restoration (Wiener-like filtering, phase determination, three-dimensional reconstruction,...). A preliminary attempt has been made to express image analysis and image description in the language of image algebra, but much still remains to be done there.

This vast edifice is built on the modest foundations presented in the beginning of this proselytizing introduction to the subject, namely, the definition of the image and the three operations of addition, multiplication and maximum.

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Discussion with Reviewers

R.D. Leapman: One practical difficulty that arises in the analysis of spectrum-images concerns the formulation of the right algorithm to apply to the data. For example, in EELS spectrum-images, we may need to take account of plural scattering effects, to compensate for energy and specimen drift, to correct for beam current fluctuations and detector gain variations and to take account of overlapping edges, etc. Image algebra clearly provides us with a unified formal structure for all the necessary mathematical operations. However, it also seems that some sort of expert system or artificial intelligence may be needed to optimize the analysis strategy for handling the vast quantity of data that is typically acquired. To what extent can image algebra help us with this?
Author: I agree entirely that the algebra should be forced to supply as much guidance as possible as well as providing a framework. Probably the most useful reply today is to say that work on neural networks and on fuzzy set theory in this field has already begun and that these are likely to be vital elements when constructing some kind of expert system.

R.D. Leapman: Is there any simple-to-use image algebra software that is available for the small computer.
Author: There is IA C and IA Fortran but I do not know whether there are pocket versions of these yet.

M. Bond: A number of us are familiar with the term "voxel". How is this term related to multi-valued images? Would the spectrum-image described for EELS be an example of a voxel? Please comment on the usefulness of the term and its relevance in the field of image algebra.
Author: The term pixel has come to be associated with a small area of a two-dimensional single-valued image, while voxel is used when small volumes are in question, notably in three-dimensional reconstruction.The term voxel has been used exclusively with three spatial dimensions in mind but there is no reason why two spatial dimensions and a third dimension representing energy, say, or time should not be envisaged — or one spatial dimension and one energy and one time. In such contexts, I think that it is very convenient to have a separate word. In algebra, however, it is not quite so obvious that a new term is helpful. Personally, I prefer to think of pixel-values that may be scalars or vectors or arrays associated with a coordinate that may have any number of components: 2 for a simple pixel, 3 for a voxel, or even more, energy associated with a volume element
as a function of time needs five!

M. Bond: Please clarify and expand on the idea of measuring the intensity distribution in the plane of the detector [of the STEM] for each pixel. Does this imply that intensity variations are within the image plane as opposed to perpendicular to the image plane? Does this imply that such an approach would be most useful in a "coarsely pixelated" image?
Author: In a STEM, we may imagine that the probe illuminates a pixel and the electrons are then distributed over the detector plane. Each detector collects all the electrons that fall on it and the signal is sent to the monitor. In effect, the detector adds all the local currents that fall on its own pixels. If, however, such a

simple detector is replaced by one that records the distribution of electrons in the detector plane from a single specimen pixel, we have a much more fine-grained idea of the specimen. The intensity variations are indeed in the detector plane, for each specimen pixel illuminated by the probe. The coarseness or fineness of the sampling is not in question though it is of course of practical importance.

M. Bond: Please give an example of image morphology in AEM.
Author: Morphology has mostly been used in SEM, for measuring geometrical properties. But it is just as promising in EELS, for "cleaning" noisy spectra, for example.

N. Bonnet: I have appreciated the overview of the different kinds of images as a very general mathematical structure and the possible gathering of the numerous image processing methods within the general class of image algebra. Knowing that different groups of methods can be understood within a common formalism is not only reassuring but also probably contains potential for the invention of more powerful image processing algorithms. But besides this elegant generalization, I have the impression that image algebra has not yet produced really new approaches for image processing and has not helped to solve problems that could not be solved by "classical" image processing algorithms. Is it possible to guess to which kinds of problems image algebra could bring a significant contribution in the future?
Author: It was probably inevitable that, during the first few years of its existence, image algebra should have been dominated by the applied mathematicians who invented it, with the result correctly described by the reviewer. The situation is now changing, and papers are beginning to appear in the image-processing literature in which "real" problems are studied by a mixture of traditional and image-algebraic methods. Image algebra has already shed light on the murky waters of grey-level morphology, though much remains to be done there. I think that there is much to be hoped for in the newer and more obscure aspects of image processing, morphology as I have already mentioned, but also the use of neural networks, for classifying very large data sets with object-oriented learning rules, for example. However, the mathematics is now all ready; what we need is for the practicing members of the image-processing community to try it out.

N. Bonnet: Traditionally, there are two main groups of methods for extracting chemical information (characteristic energy-loss peaks) from data sets in the form of image series: either a local modelling of the different spectra, following methods developed in spectroscopy, or a global analysis of the whole data set, by multivariate statistical analysis, for instance. Each of these groups of methods has its own drawbacks: the need to choose a model and statistical problems for the former; the need to choose a metric distance and sensitivity to outliers and artefacts for the latter. For these reasons, new methods are beginning to be investigated, which try to place the analysis on a quasi-local (or regional) scale.

Do you think that image algebra could cope with this kind of problem in the near future? Could you also give some more indications concerning the nature of the templates that could be used for processing spectrum-images?
Author: Image algebra is general enough to represent clearly and compactly the kind of procedures described but I am not sufficiently aware of the details of these new methods to be able to speculate on the contribution that the algebra might make. On past experience, however, one can be optimistic. So far as the nature of the templates to be used for processing spectrum–images is concerned, several replies are possible: for smoothing, the templates would represent the corresponding structuring elements of mathematical morphology, but structuring elements of other families, notably "grey-level" (not flat) elements, would be needed for recognizing and perhaps labelling peaks.