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TECHNICAL REPORT NO. 14

Image Analysis

by

Mark G. Moran and Bruce R. Kowalski*

Prepared for Publication

in

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The Harper Encyclopedia of Science defines "image" as "an optical replicant of a luminous or illuminated object formed by a mirror or a lens." (1) In this report, it will be seen how the restrictions implicit in this definition may be relaxed or removed. First, an image need not be a real image or a visual representation. By one method or another an image or a virtual image may be represented purely mathematically. The object which gives rise to the image may do so by interacting with electromagnetic radiation either by absorption or emission. However, it is not necessary to restrict attention entirely to this situation. Various types of scattering experiments also result in the generation of images.

A familiar example of an ordinary two-dimensional image is a photograph. A photograph is a distribution of light intensity and possibly color over a surface. More formally, the information contained in a photograph is encoded by specifying the value of intensity $f(x,y)$ over the points of a surface (x,y) . The set of intensities which constitute the image of $f(x,y)$ is known as the gray scale. Intuitively, the gray scale ranges from the extremes of totally black to totally white. A reasonable assignment of the gray scale may be to specify a monotonically increasing function of the density of perfectly opaque, reflecting dots in a given area. An example is given in Figure 1.

If a photograph is a familiar example of a two-dimensional image, then by similar reasoning, a spectrum can be thought of as a familiar example of a one-dimensional chemical image. A light spectrum is an image which results from encoding the intensity of radiation absorbed or emitted from an object as a function of wavelength. This kind of image is constructed in order to extract specific information from the object under study. Display of an infrared spectrum of a solution of acetone shows a prominent band at about 1730 cm^{-1} . Visual inspection of this image allows interpretation using human experience and ability in recognizing patterns. The location of the band lends insight into the nature

of the species giving rise to it. This signal may also be used to determine the relative amount of species present as well as other details concerning the local environment surrounding it.

Photographs, molecular and atomic spectra and other forms of images, real or virtual, are common to many areas of science and engineering. Chemists are now developing and using instruments capable of generating images of not only one but two and higher dimensionality. Fortunately, there is a great deal known about constructing, transmitting, storing, and improving images, as well as extracting information from them. Powerful mathematical tools primarily developed for application to medical and satellite images have been developed, but by and large are not used in chemistry. Many of the methods which exist to analyze one-dimensional images are also useful when extended to higher dimensional spaces. These methods, when used in conjunction with the observer's intrinsic pattern recognition ability and experience, greatly extend the amount of information that can be extracted from images. The purpose of this report is to introduce the analytical chemist to the great similarity among images produced by a variety of methods and describe a few of the tools that are available for image analysis.

IMAGE CONSTRUCTION

The construction of an image may be tackled by any one of several direct or indirect methods. The image construction process reflects the nature of the information that the experimentalist desires to glean from the image. In carrying out the quantitative analysis of a substance by analyzing the absorption spectrum of a species, one is usually satisfied with knowing the bulk average concentration of the species in the sample. As detection limits are pressed ever lower, and sample matrices become increasingly complex, there are situations where this information is insufficient. In the analysis of a catalytic surface

for instance, it is often desirable to know the concentration of a species as a function of location on the surface. Alternatively, the identity, amount and distribution of pollutants in a body of water or a smokestack plume may be sought. The latter problem could be solved by taking a sufficient number of samples at discrete locations on the object to be analyzed. These values could be used in constructing a spatial "image" of the object. However, a method based on Hadamard modulation spectrometry has been proposed to deal with this class of problems. Figure 2 shows a block diagram of an imaging spectrophotometer based on this principle. (2) The reader will note that except for the two-dimensional mask in the entrance focal plane, this arrangement is the same as the Hadamard multiplex spectrometer described by Decker. (3,4) The singly multiplexed dispersing spectrometer encodes spectral information from all wavelengths at once. This is done by expanding the spectral response in an n -dimensional basis set where the coefficients of expansion are zero or one. The zero coefficient corresponds to the situation where incident radiation falls on the opaque section of the mask, and the unity coefficient corresponds to radiation passing through the mask slots to the detector. The spectrum is reconstructed by solving the resulting set of linear equations generated by the n different mask settings.

The purpose of the $m \times p$ mask in the entrance focal plane is to encode the spectral information in the spatial domain. If this were the only encoding mask in the spectrometer, it would be possible to examine the object with the various mp settings of the mask, store each reading, and subsequently reconstruct a picture of the object. Now, with both the $m \times p$ and the n slotted masks it is possible to gather spatial and spectral information about an object. Using this scheme, a total of mpn different intensity levels have been collected with one detector. Depending on the algorithm used to decode these measurements, n pictures of the object corresponding to n different bandwidths could be displayed,

each having mp spatial resolution elements. Alternatively, mp spectra could be represented, one corresponding to each spatial resolution element.

An image (in the mathematical sense now) can be constructed if the object under scrutiny gives rise to more than one type of response when subjected to a perturbation. An example is the coupled absorption/emission process undergone when a molecule capable of fluorescence is excited by a beam of light at the appropriate wavelength. It is possible to collect simultaneously the excitation and emission spectra of a sample which may consist of a pure species or a mixture. In practice, many more measurements are made than the minimum number dictated by the number of components of the mixture. This provides a solution to the problem of overlapping spectra and also gives a statistical estimate of the validity of the measurements. The excitation and emission spectra can be considered as vectors $|x\rangle$ and $|y\rangle$, where

$$|x\rangle = \{\alpha_1 x_1, \alpha_2 x_2, \dots, \alpha_n x_n\}^T \quad (1)$$

$$|y\rangle = \{\alpha_1' y_1, \alpha_2' y_2, \dots, \alpha_n y_n\}^T \quad (2)$$

x_i , and y_i are scalars proportional to the number of photons absorbed and emitted at wavelength λ_i and λ_j respectively. The mathematical image is constructed by taking the exterior product of these vectors to form the so-called emission/excitation matrix.

$$|x\rangle\langle y| = \begin{bmatrix} \alpha_1 \alpha_1' x_1 y_1 & \alpha_1 \alpha_2' x_1 y_2 & \dots & \alpha_1 \alpha_n' x_1 y_n \\ \vdots & & & \\ \vdots & & & \\ \vdots & & & \alpha_n \alpha_n' x_n y_n \end{bmatrix} \quad (3)$$

Each matrix element specifies a combined intensity of absorbed and emitted radiation at the coordinates λ_i and λ_j . In other words, these values form the gray scale of the image. The isometric projection of the EEM is given in Figure 3.

To date, two mathematical approaches have been used to interpret these types of images; the least squares method (5) and the rank annihilation method (6).

The least squares method defines an error matrix

$$\underline{E} = \underline{M} - \sum_{k=1}^r B_k N^{(k)} \quad (4)$$

where M is the EEM matrix of the mixture and $N^{(k)}$ is the EEM of the pure k^{th} component. The total squared error is thus:

$$e = \sum_i \sum_j E_{ij}^2 = \text{Trace} (E^T E) \quad (5)$$

Ideally, a number β can be formed such that $e^2 = 0$ and $\beta = c_k / c_k^\circ$, the ratio of the concentration of the k^{th} component of the mixture to the concentration of a pure substance containing only component k . In practice, several difficulties arise with this procedure. The major drawback of this type of analysis is that qualitative knowledge of all fluorescing species must be present beforehand. The second technique, that of rank annihilation, is a method of calculating the concentration of a given fluorescing species in the presence of other, possibly unknown fluorophores. The rank annihilation technique involves repetitive diagonalization of the error matrix for different values of β . When the correct value of β equal to c_k / c_k° is chosen, the eigenvalue corresponding to the k^{th} component will vanish. In practice, the best value of β is determined from the minima of the $\mu_k(\beta)$ vs. β plot. The rank annihilation method should also be suitable for other types of two-dimensional data sets such as those produced by GC/IR or GC/MS.

Once the excitation/emission matrix has been collected, a hard copy image of the sample could be constructed from the matrix elements. However, many techniques of analysis involve construction of images by collecting luminescent radiation or particles scattered from an object under study. These techniques

are generally lumped under the term microscopy. A secondary ion mass spectrometer/ion microscope has been built by Morrison et al. (7,8) To extract information from these types of images, they must somehow be sampled in order to convert them to a form amenable to mathematical manipulation. Once this has been accomplished, techniques can be brought to bear which sharpen, enhance, or otherwise modify the image. The aim of these operations is to render the images more suitable for feature extraction. In many cases, hidden features may be brought out more clearly. In other cases, processes which interfere with the collection of a clear image can be corrected for. The remainder of this report will deal with a few of these topics.

SAMPLING THE IMAGE

Proceeding with the working example of a photograph as an image, an image is usually visually seen as a continuous function of grayness over the image plane. A closer examination of the surface reveals this not to be the case. The surface appears to be continuous because the level of quantization exceeds the receiver's ability to discriminate between quantized levels. For mathematical manipulation of the image function, a very high level of spatial quantization is often unnecessary and even undesirable. In general, it is desired to be able to reconstruct or really capture the information inherent in the image function with acceptable fidelity from a minimum number of sampled points. There are no rigid rules to specify a minimum number of sampled points. The total number of bits of information in the sampled image is N^2K . This is for an image quantized as an $N \times N$ spatial array with 2^K brightness levels. The total number of bits must be somehow divided between spatial and gray scale quantization. Usually, a subjective decision is made about the partition. In any case, it is desirable to employ the minimum number of sampled points. The usual procedure is to reduce the number of samples until the degradation becomes intolerable.

The process of conversion of a physical image to an array of points is known as sampling. Consider a two-dimensional image function $f(x,y)$. (The discussion may be generalized to n -dimensions in a very straightforward way.) The function used to select specific values of $f(x,y)$ over the plane is known as the shah function. (9) It is denoted by

$$III(x,y) = \sum_{m=-\infty}^{\infty} \sum_{n=-\infty}^{\infty} \delta(x-m, y-n) \quad (6)$$

The shah function picks out or "sifts" through the function $f(x,y)$ retaining only those values at $f(m,n)$ and destroying all others. Thus it converts an analog signal to a two-dimensional digital signal. Another interesting and useful property of this function is that it is its own Fourier transform. This type of sampling is also known as digital sampling. Care must be taken so that the collection of sampled points is adequate to reconstruct the picture without introduction of serious error. The image function is reconstructed by taking suitably weighted linear combinations of the sample values. In one dimension, this is written as

$$f(t) = \sum_{k=-\infty}^{\infty} f(kT)g(t-kT) \quad (7)$$

where T is the sampling interval, and $y(t-kT)$ is the weighting or interpolation function. It can be shown that if $f(t)$ is a periodic function, the sampling must be conducted in such a fashion that $T \leq \frac{1}{2f_c}$ where f_c is the spatial frequency. This condition insures that the picture function does not overlap with its copies produced in the Fourier domain. Failure to adhere to this condition is the chief cause of the phenomena known as aliasing. In two-dimensional and higher spaces, the consequences of overlap can be more severe. If the picture

function is expanded in terms of orthonormal unit basis vectors \vec{a} and \vec{b} , the sampling criteria can be stated as follows: A function $I(\vec{c})$ whose Fourier transform vanishes over all but a bounded region of frequency space can be everywhere reproduced from its values taken over a lattice space generated by $\vec{ma} + \vec{nb}$ $m, n = 0, \pm 1, \pm 2, \dots$. This is so provided the vectors are sufficiently small to ensure nonoverlapping of the spectrum $I(\vec{w})$ with its images of a periodic lattice generated by $\vec{rp} + \vec{sq}$. This is the so-called reciprocal lattice which is the basis for the function $I(\vec{w})$.

IMAGE ANALYSIS METHODS

In this section, a brief review of image analysis methods is given. No attempt is made to be all inclusive due to the depth and breadth of existing techniques. (10) A certain philosophy has been borne in mind during the preparation of this section. The techniques herein are basically distribution-free techniques. That is, no assumptions are generally made about the probability distribution of the gray scale. Considerable ingenuity is often utilized to model, estimate or guess this most useful property. However, on many occasions, images may be sampled, smoothed, enhanced, intensified and utilized without specific knowledge of the probability distribution of gray scale.

Smoothing, Enhancement and Sharpening

Given that an image has somehow been converted to a digital representation, there exists a group of mathematical operations which can possibly enhance the quality of the image. It is important to bear in mind that these operations do not increase the information content of the picture. However, if the image is badly represented, say by blurring or obscured by high frequency noise, then application of image enhancement techniques may be desirable. Operations performed on picture functions may be linear or nonlinear operations. Only linear operations will be discussed here.

The true undistorted image function of an object will be henceforth referred to as $f(x,y)$. Collection of the image function by one technique or another results in a perceived image function denoted by $g(x,y)$. In the absence of distortion (i.e. perfect collection technique) $f(x,y) = g(x,y)$. The mapping of $f(x,y)$ into $g(x,y)$ may be modelled by the following equation: (11)

$$g(x,y) = \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} f(\xi, \eta) h(x-\xi, y-\eta) d\xi d\eta \quad (8)$$

Where g is the distorted image function, f is the true (ideal function) and h is known as the point spread function. If h is known analytically, it is possible to recover f from a knowledge of g . All of this presupposes that h possesses an important property known as linear shift invariance. The degraded image function is recognized as a convolution of an ideal image function with a function describing a degradation process. This model is extremely useful since an important theorem of Fourier analysis can be brought to bear in order to recover f . Taking the Fourier transform of the convolution of two functions f and h is identical to the operations of multiplying the Fourier transforms together.

$$f * h = \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} f(\xi, \eta) h(x-\xi, y-\eta) d\xi d\eta \quad (9)$$

$$F(f)F(h) = F(f*h) \quad (10)$$

where $F(f)$ is the Fourier transform of f . Clearly, then since $g = f*h$

$$F(g) = F(f)F(h) \quad (11)$$

In the transformed space the quotient $F(g)/F(h)$ may be formed and then back transformed to produce f . Such a procedure should result in the recovery of the ideal image function f from the degraded function g . Often, it is useful

to express noise in the degraded picture as an independent, randomly distributed additive function. Viz

$$g = f * h + n \quad (12)$$

then

$$F(g) = F(f)F(h) + F(n) \quad (13)$$

The importance of Equation 8 cannot be underestimated in the process of image enhancement. The proper choice of h can yield a considerably improved, noise free image.

Low frequency noise present in an image can be modelled by the well known diffusion equation.

$$\nabla^2 g = K \frac{\partial g}{\partial t} \quad (14)$$

The motivation for this involves thinking of an ideal picture of a collection of point impulse sources over a field. If $g(x,y, t=0)$ is a representation of an unblurred image, then the real picture function $g(x,y,\tau)$ can be envisioned as the result of a degradation process modelled by a diffusion controlled phenomena from $t = 0$ to $t = \tau$. Expanding $g(x,y, t=0)$ around $t = \tau$ and retaining the first term,

$$g(x,y,t) = g(x,y,0) + \frac{\partial g}{\partial t} \quad (15)$$

$$g(x,y,0) = g(x,y,\tau) - \frac{\partial g}{\partial t} \quad (16)$$

substituting $K^{-1} \nabla^2 g = \frac{\partial g}{\partial t}$

$$g(x,y,t) - K^{-1} \tau \nabla^2 g = g(x,y,0) \quad (17)$$

Thus, the estimation of an unblurred picture from a blurred one may be accomplished by subtracting off the Laplacian of the blurred picture from the blurred picture.

Feature Extraction and Image Classification

The most important manipulations in image processing are those that aid in the extraction of useful information. The goal may be to find objects contained in the image field and classify them into one or more predetermined categories or to automatically categorize entire images. Agricultural crop identification from aerial photographs is an example of the former goal as homogenous regions containing one crop (signal) must first be separated from non-agricultural areas (background) before crop classification can proceed. An example of the latter would be crop classification where the image field contains only a single crop and the object is simply to identify the crop by classification of the entire image.

No matter what the goal, the process begins by extracting features from the prototype images that are then used to develop multidimensional classification rules. This is quite analogous to feature extraction and classification as performed by a number of analytical chemists using the tools of pattern recognition (12) to analyze their data. Although there are no published applications of image classification to analytical chemical data there are numerous applications in other disciplines (13) and as chemical imaging instrumentation becomes more available, application is certain to grow.

Edge Detection

In image analysis, the detection of an edge, an abrupt change in the spatial frequency, can be of crucial importance. Reconstruction of figures present in the image proceeds by detecting all of the unique edges in the image and connecting them in a continuous fashion. The very nature of an edge or as the case may

be, a line, is what makes it possible to detect it by mathematical processes. An ideal edge is shown in Figure 5. The noisy edge in Figure 6 may present a detection problem. However, if edge detection is preceded by local averaging, the local variation in the neighborhood of Z_l will be smoothed sufficiently to proceed.

The most straightforward edge detection technique is to enhance the edge by a high-pass filter. Since the edge is a high frequency phenomena, and blurring is mostly caused by low frequency noise, then this kind of spatial filtering helps in more than one way. However, very high frequencies which constitute a great deal of noise must also be filtered in this process.

Another general class of high frequency detectors is the directional derivative. For an arbitrary function $f(x,y)$ the directional derivative is given by:

$$\begin{aligned} \frac{\partial f}{\partial n} &= \frac{\partial f}{\partial x} \cos\theta + \frac{\partial f}{\partial y} \sin\theta & \Delta_x &= f(i,j) - f(i-1,j) \\ \Delta_y &= f(i,j) - f(i,j-1) & & \\ \Delta_y &= \Delta_x \cos\theta + \Delta_y \sin\theta & & \end{aligned} \quad (18)$$

where θ is measured relative to the vector locating the point i,j and the x axis of the reference frame. If an edge lies between the points j and $j+1$, the operator $|f(i,j) - f(i,j+1)|$ will take on a large value when calculated in this fashion. The major drawback here is that attention must be paid to the direction in which differentiation is carried out. An isotropic (direction independent) operator is clearly desirable in this circumstance. The derivatives of even order, and derivatives of odd order, raised to even powers are endowed with this property. The Roberts gradient (14) is a specific example of such an operator given by,

$$\text{MAX } (|f(i,j) - f(i+1, j+1)|, |f(i+1, j) - f(i, j+1)|) \quad (19)$$

Morrison has used edge detection techniques as well as thresholding techniques in the analysis of polycrystalline iron samples by secondary ion mass spectrometry. (15)

Image Matching

It is often useful to have a method for quantitatively comparing two separate images taken over the same object field. This facilitates the process of taking a relative ratio of images or making a comparison between a "known" and an "unknown" image.

Two image functions may be compared or more specifically, registered by calculating the cross correlation between them,

$$h_1 \otimes h_2 = \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} h_1(x'y') h_2(x'-x, y'-y) dx' dy' \quad (20)$$

and searching for the maximum value of this expression as a function of the offset values x and y . If h_1 and h_2 and $N \times N$ image matrices, the evaluation of the discrete cross correlation is tedious, involving N^4 calculations for each offset value. Fortunately, a generalization of the convolution theorem provides an easier method of evaluation. For the cross correlation of two functions

$$F(h_1)[F(h_2)]^* = F(h_1) \otimes F(h_2) \quad (21)$$

The discrete Fourier transforms of h_1 and h_2 may be evaluated using fast transform procedures (16) which run considerably faster than matrix multiplication routines. Thus, searching for a maxima in large arrays is feasible by this procedure.

This type of image matching has been used by Morrison in the analysis of NBS-662 steel for Niobium and Titanium. (17) As pointed out, this type of

image correlation leads to four dimensional information. There are two concentration dimensions and two spatial dimensions. As existing scattering techniques improve and new ones are developed, these kinds of data analysis methods will be extremely useful in handling the higher dimensional data sets generated.

CONCLUSION

This report has attempted to introduce analytical chemists to the many ways to create and analyze real and virtual images. Images are nothing more than N-dimensional ($N \geq 2$) spectra and therefore, the analysis of images should not present a problem for the analytical chemist for two reasons. First, analytical chemists are quite familiar with one-dimensional spectra. Second, many of the concepts and mathematical operations applied to one-dimensional spectra extend to higher-dimensional data with the appropriate amount of increased computational complexity assumed by the computer. Fortunately, a considerable amount of N-dimensional image analysis mathematics and associated computer software is available. The availability is principally due to the large interest in the field of medicine for analyzing medical images and in remote sensing applications where images come from spacecraft probes and earth satellites. We expect that image analysis will become a standard tool of the analytical chemist in the future as more types of analytical instrumentation are developed or modified to produce higher dimensional images.

CREDIT

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CAPTIONS FOR FIGURES

Figure 1: Example of Gray Scale quantized at $K = 2$. (4 levels)

Figure 2: Hadamard Imaging Spectrometer. The $m \times p$ mask modulates incoming radiation so as to provide spatial resolution. The n slotted mask provides the usual Hadamard modulation.

Figure 3: An isometric projection of a rank one emission/excitation matrix.

Figure 4: The two dimensional shah function. At each point m, n in the x, y plane, the shah function picks out the value $f(m, n)$ when the expression

$$\int_{-\infty}^{\infty} \int_{-\infty}^{\infty} f(x, y) \delta(x-m, y-n) dx dy \text{ is evaluated.}$$

Figure 5: An ideal step edge; cross section orthogonal to the direction of the edge.

Figure 6: A noisy edge superimposed on an ideal edge.

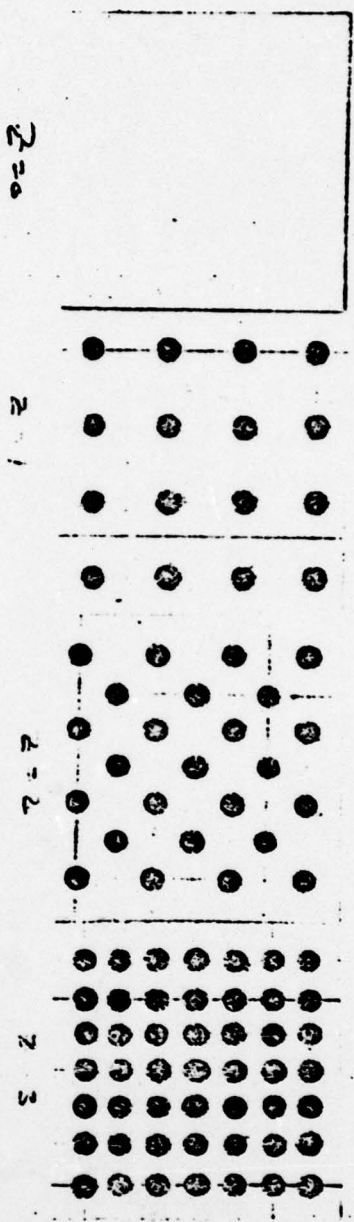
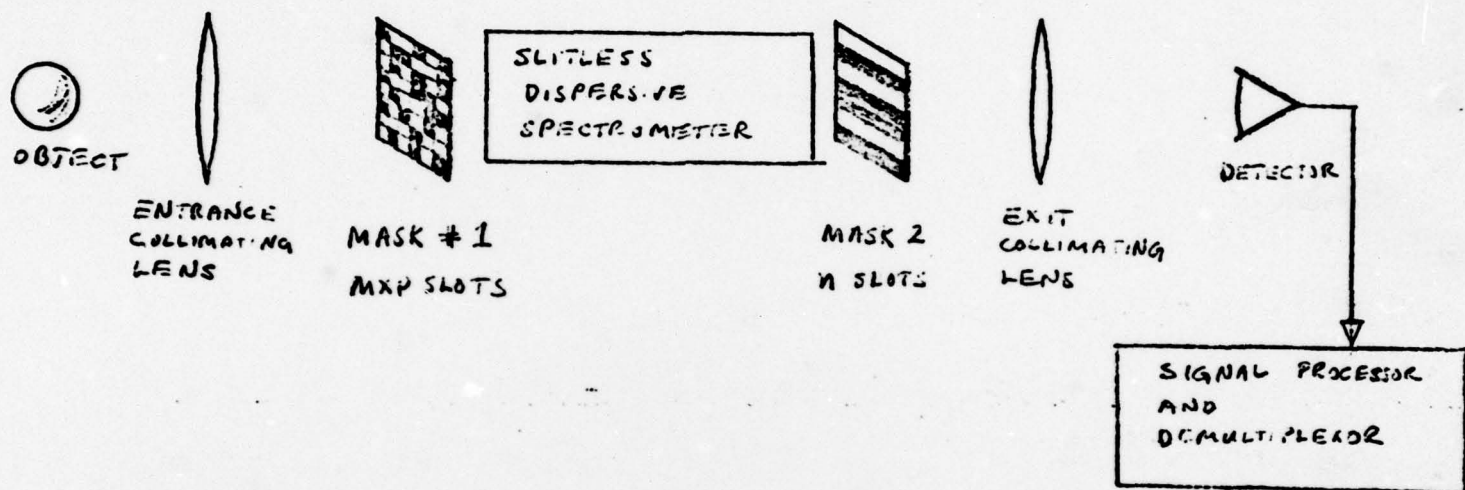


FIG 1 Illustration of gray scale quantized @ $K=2$

Note: [This figure will need four squares of equal area
 covered with opaque dots at roughly the density levels
 given above.

FIG 2



FIG

HADAMARD IMAGING SPECTROMETER

Figure 3

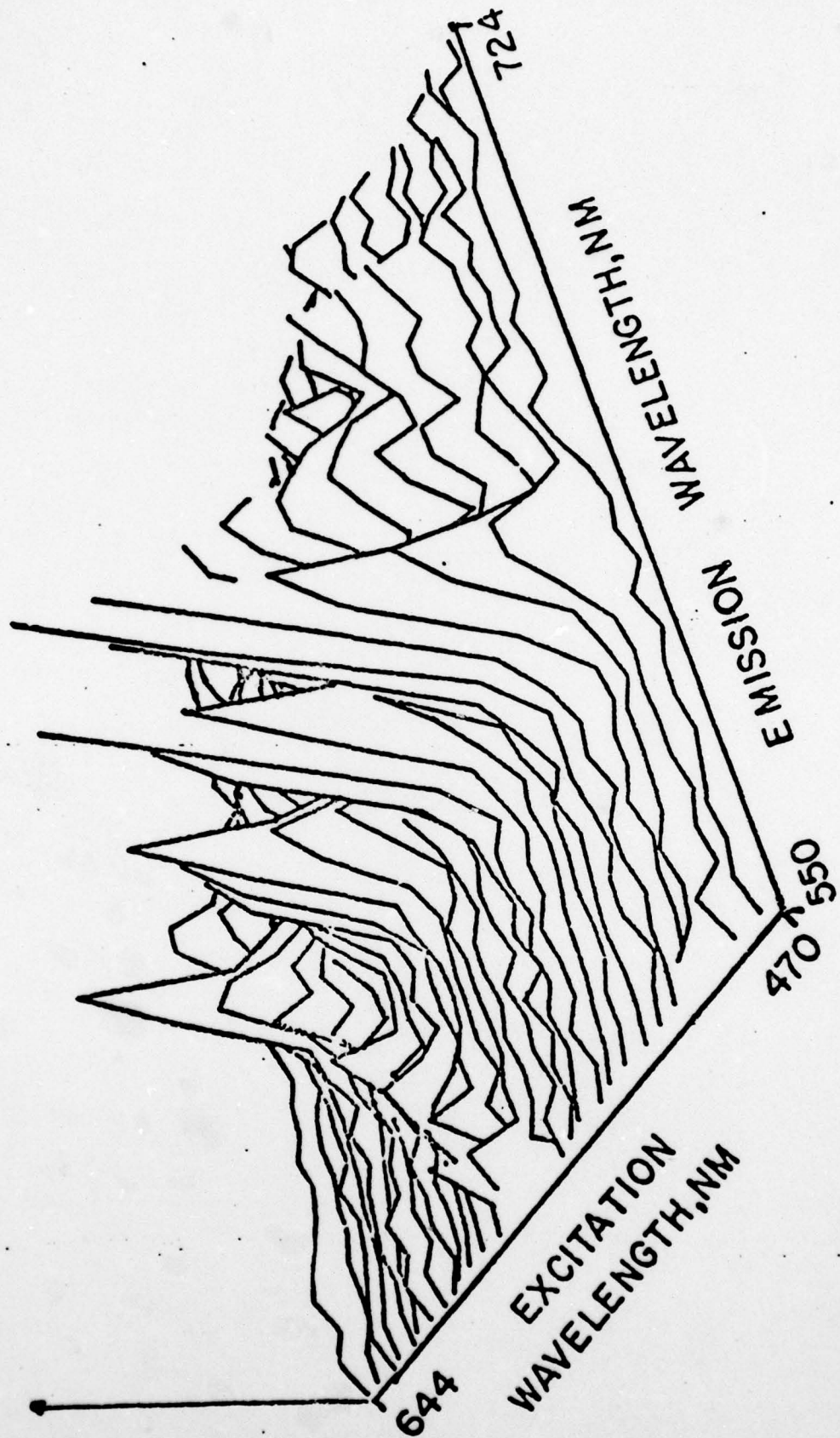
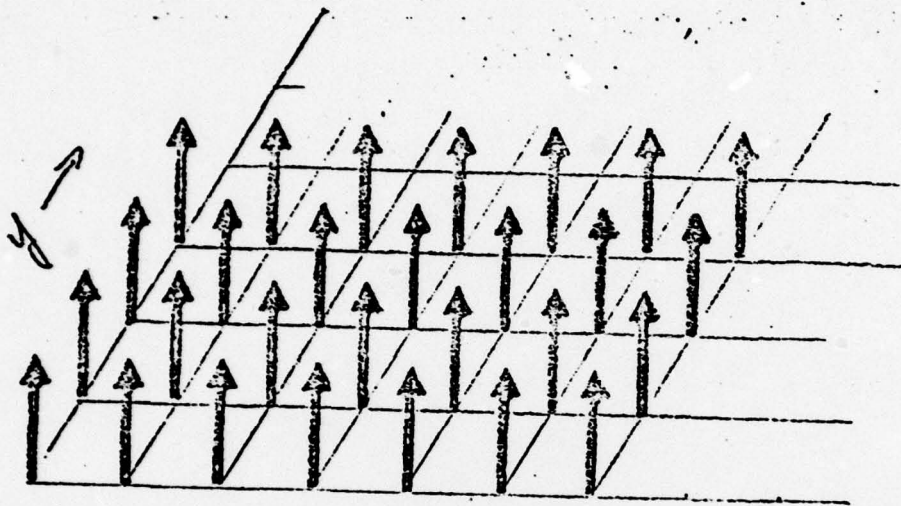


FIG 4

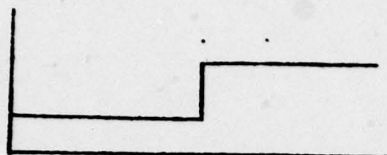
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$$\Pi(x, y) = \sum_{n=-\infty}^{\infty} \sum_{m=-\infty}^{\infty} \delta(x-n, y-m)$$

FIG 5

INTENSITY
(GRAY SCALE)



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FIG 6

INTENSITY

