Multivariate Image Analysis for process monitoring and control

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ABSTRACT

*Information from on-line imaging sensors has great potential for the monitoring and control of quality in spatially distributed systems. The major difficulty lies in the efficient extraction of information from the images, information such as the frequencies of occurrence of specific and often subtle features, and their locations in the product or process space. This paper presents an overview of multivariate image analysis methods based on Principal Component Analysis and Partial Least Squares for decomposing the highly correlated data present in multi-spectral images. The frequencies of occurrence of certain features in the image, regardless of their spatial locations, can be easily monitored in the space of the principal components. The spatial locations of these features can then be obtained by transposing highlighted pixels from the PC score space into the original image space. In this manner it is possible to easily detect and locate even very subtle features from on-line imaging sensors for the purpose of statistical process control or feedback control of spatial processes. The concepts and potential of the approach are illustrated using a sequence of LANDSAT satellite multispectral images, depicting a pass over a certain region of the earth's surface. Potential applications in industrial process monitoring using these methods will be discussed from a variety of areas such as pulp and paper sheet products, lumber and polymer films.

Keywords: Multivariate Image Analysis, Process Monitoring, Principal Component Analysis, Spatial Control, Statistical Process Control

1. INTRODUCTION

Digital imaging sensors have recently become very popular in many off-line laboratory applications, particularly in the biological and medical areas. A large amount of digital image processing literature deals with approaches for image enhancement, restoration, analysis, compression, and synthesis. Most of the methods present are applied off-line and require considerable computer resources (hardware and software) to process the image data

Imaging sensors have been applied to a much more limited extent for monitoring industrial processes. Examples include TV cameras for visually monitoring the state of combustion in engines[7], robot mounted digital cameras for monitoring the sizes and shapes of machine-made parts[8], laser scanners to monitor the surface properties and to detect faults in sheet forming processes[9]. These industrial imaging sensors usually involve only grayscale or binary images. Due to the limited time available to analyze these images, the techniques used for analysis are usually quite simple (e.g. histogram thresholding and area counting).

The purpose of this paper is to investigate an on-line approach to extracting information from time-varying multivariate (3-dimensional) spectral images that will allow for the rapid monitoring, detection, and isolation of process faults and product quality in industrial processes. The approach uses Multivariate Image Analysis (MIA) methods that are based on multi-way Principal Component Analysis (PCA). In section 2 the strength of the approach is illustrated through an application of MIA to a LANDSAT Multispectral Scanner (MSS) satellite image. These methods are then extended to the on-line situation in section 3 where one receives a sequence of images in time and the purpose is to detect and isolate specific features from the images for statistical process control, or feedback control of spatial processes.

2. OVERVIEW OF MULTIVARIATE IMAGE ANALYSIS

Image data when collected in multiple spectral bands produces a multivariate image. It consists of a stack of congruent images, where each image in the stack is measured for a different wavelength, frequency, or energy[10]. Figure 1 illustrates a stack of 4 congruent 512 x 512 pixel images, with each image having a unique wavelength. Alternately, one could view a

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multivariate image as a two-way array of pixel intensity vectors with one vector at each pixel location in the (x, y) image plane (Figure 2).

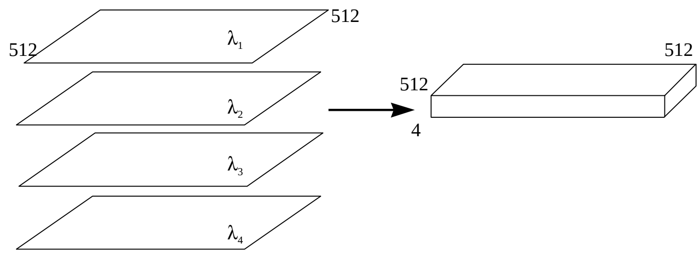


Figure 1 A stack of 4 congruent images (collected in 4 different wavelengths) to form a 512 x 512 x 4 Multivariate Image

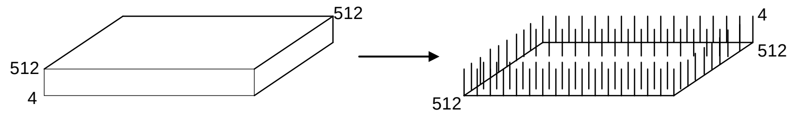


Figure 2 A 512 x 512 x 4 Multivariate Image viewed as a two-way array of 4 x 1 variable

Since data in multivariate images consists of several congruent images, each variable vector in such an image contains highly correlated pixel intensity values. Latent variable statistical methods like multi-way Principal Component Analysis (PCA), and multi-way Partial Least Squares or Projection to Latent Structures (PLS) have been successfully used for MIA[11,12,13]. These methods efficiently compress highly correlated data and project it onto a reduced dimensional sub-space through a few linear combinations of the original multivariate data. Multi-way PCA of a three dimensional (n_x x n_y x n_z) digital image array $\underline{\mathbf{X}}$ consists of decomposing it into a series of A (< n_z) principal components consisting of (n_x x n_y) score matrices $\mathbf{T}_a$ and (n_z x 1) loading vectors $\mathbf{p}_a$ plus a residual array $\underline{\mathbf{E}}$, i.e.:

$$\underline{\mathbf{X}} = \sum_{a=1}^{A} \mathbf{T}_a \otimes \mathbf{p}_a + \underline{\mathbf{E}} \tag{1}$$

where ⊗ denotes the Kronecker product. The principal components are ordered in the sense that the first component explains the greatest amount of variance in $\underline{\mathbf{X}}$, the second component explains the next greatest variance, and so forth. The number of components (A) necessary to extract most of the meaningful information can be determined by various procedures[14,15].

This method of multi-way PCA is equivalent to unfolding the 3-way array $\underline{\mathbf{X}}$ into an extended 2-way matrix $\mathbf{X}$, as illustrated in Figure 3, and then performing ordinary PCA on it:

$$\underset{n_x \text{ x } n_y \text{ x } n_z}{\underline{\mathbf{X}}} \xrightarrow{unfold} \underset{(n_x \cdot n_y) \text{ x } n_z}{\mathbf{X}} = \sum_{a=1}^{A} \mathbf{t}_a \mathbf{p}_a^{\mathrm{T}} + \mathbf{E} \tag{2}$$

where $\mathbf{t}_a$ is a ($n_x \cdot n_y$) x 1 score vector, and $\mathbf{p}_a$ is a (n_z x 1) loading vector. The score vectors $\mathbf{t}_a$ (a = 1,…, A) are orthogonal, and the loading vectors $\mathbf{p}_a$ (a = 1, …, A) are orthonormal.

The row dimension of the $\mathbf{X}$ matrix resulting from the unfolding operation is very large (equal to 262,144 for a 512 x 512 image space). Therefore, with essentially all multivariate image data having long and thin unfolded matrices, a kernel algorithm[11] is used. In this algorithm the kernel matrix ($\mathbf{X}^{\mathrm{T}}\mathbf{X}$) is first formed, and then an SVD is performed on this very low dimensional (n_z x n_z) matrix to obtain the loading vectors $\mathbf{p}_a$ (a = 1, …, A). The corresponding score vectors $\mathbf{t}_a$ are then computed via equation 4. The only time consuming step in this kernel algorithm is the (one time) construction of the kernel matrix ($\mathbf{X}^{\mathrm{T}}\mathbf{X}$).

Upon completion of PCA on this long and thin two dimensional matrix $\mathbf{X}$, the ($n_x \cdot n_y$) x 1 score vectors $\mathbf{t}_a$ (a = 1, …, A) can then be reorganized back into (n_x x n_y) score matrices $\mathbf{T}_a$ (a = 1, …, A) giving a representation of the original $\underline{\mathbf{X}}$ array as expressed in equation 1 and illustrated in Figure 3. In this way one can see that the score matrices $\mathbf{T}_a$ (a = 1, …, A) themselves represent images in the original (n_x x n_y) scene space; $\mathbf{T}_1$ being the image with the largest variance, followed by $\mathbf{T}_2$ with the second largest variance, and so forth. A reconstructed multivariate image which eliminates much of the unstructured noise from the original image can be obtained by using only the dominant A principal components:

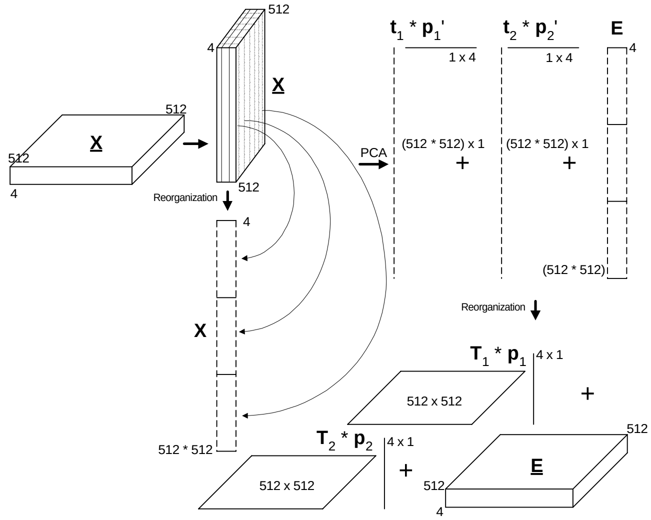


Figure 3 A 512 x 512 x 4 multivariate image reorganized into a (512 · 512) x 4 array followed by PCA decomposition into reduced dimensional sub-space

$$\hat{\underline{\mathbf{X}}} = \sum_{a=1}^{A} \mathbf{T}_a \otimes \mathbf{p}_a \tag{3}$$

where the residual component $\underline{\mathbf{E}}$ has been omitted. However, such Multi-Way PCA (MPCA) methods are not very useful for image enhancement as they are not specifically designed to sharpen edges or enhance other specific features in the image. The power of the MPCA approach lies in its ability to extract and isolate specific image features in a common region of the score space, and then, once the feature is detected, to reveal the locations where it occurs in the scene space. MPCA appears to be more powerful in this image analysis and interrogation aspect as compared to other image analysis methods.

In each dimension ($a = 1, \ldots, A$) MPCA extracts a principal component variable $\mathbf{t}_a$ which is defined as a linear combination of the intensities at each wavelength. The particular linear combination is given by the corresponding loading vector $\mathbf{p}_a$. The vector of values of the principal component at each pixel location in the scene space is defined by the score vector:

$$\mathbf{t}_a = \mathbf{X}\mathbf{p}_a \tag{4}$$

Hence each principal component variable extracts a particular spectral feature (i.e. a linear combination of the intensities over all the wavelengths) from the image. The reorganized score matrix $\mathbf{T}_a$ is a representation of the image in terms of that spectral feature.

A more important analysis of the image comes from the compressed representation of the intensity information at each pixel location in terms of the score values (t_1, t_2, …) of the dominant principal components. These score values summarize the dominant spectral features of the image at each pixel location. If, at different pixel locations in an image, the same feature is present (e.g. surface dirt particles in a sheet forming process), the score value combination (t_1, t_2) would be almost identical for these pixels. Regardless of the spatial locations of the various occurrences of this feature in the image space, MPCA would represent it by the same combination of score values (t_1, t_2). Therefore, by plotting the score values of the dominant principal components (t_1, t_2) for each object (i.e. each pixel location) against each other in a scatter plot, the score combinations for all pixel locations in the scene space having the same spectral characteristics would plot on top of one another or at least in the same neighborhood in this score plot. These score plots will therefore be invaluable in the analysis and monitoring of on-line multispectral images. The above MPCA decomposition of images and subsequent analysis of the results are best presented by way of an example.

2.1. Example: LANDSAT (MSS) Satellite Image

The image used in this example is a LANDSAT (MSS) satellite image of size 512 x 512 consisting of 4 wavelength bands ranging from 500 - 1100 nm. The satellite image depicts a scene of the city of Mobile in Alabama, USA. Figure 4 represents a false color composite image provided by the first score matrix $\mathbf{T}_1$ from the MPCA analysis.

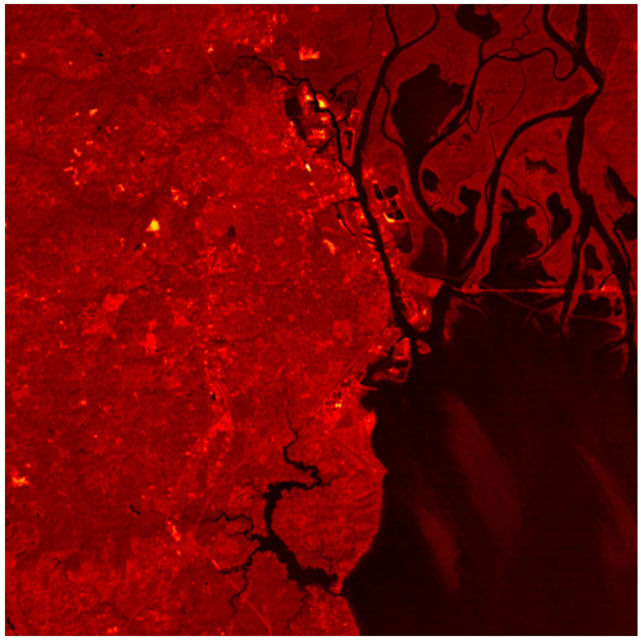


Figure 4 A false color composite of the $\mathbf{T}_1$ score image representing Mobile, Alabama

The cumulative percent sum of squares explained by the first two principal components is 99.7% (95.0% and 4.7%, respectively). Therefore, only A = 2 components will be used in the subsequent analyses. A scatter plot of the first two score vectors ($\mathbf{t}_1$ vs. $\mathbf{t}_2$) is illustrated in Figure 5. In this plot there are 262,144 score combinations plotted, one for each of the 512 x 512 pixel locations in the original image. Since similar features in the original image will yield almost identical (t_1, t_2) score combinations, many points overlap in this scatter plot. Following Geladi et. al.[10] an intensity matrix can be constructed which represents the number of pixels at each point in the score space. The score plot ($\mathbf{t}_1$ vs. $\mathbf{t}_2$) is constructed as a 3D histogram with a grid of 256 x 256 bins. Each bin is filled with a bar giving the count of pixels belonging to that bin. This matrix is then color coded depending upon the number of pixels in each bin (i.e. pixel density) using a color scheme ranging from cold colors (e.g. black) representing bins with a low number of overlapping pixels to hot colors (e.g. white) representing bins having the highest pixel density.

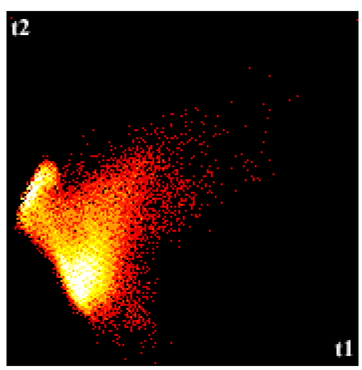
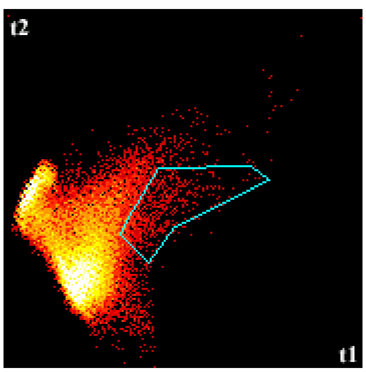


Figure 5 Color coded t1 - t2 score plot of the satellite multivariate image

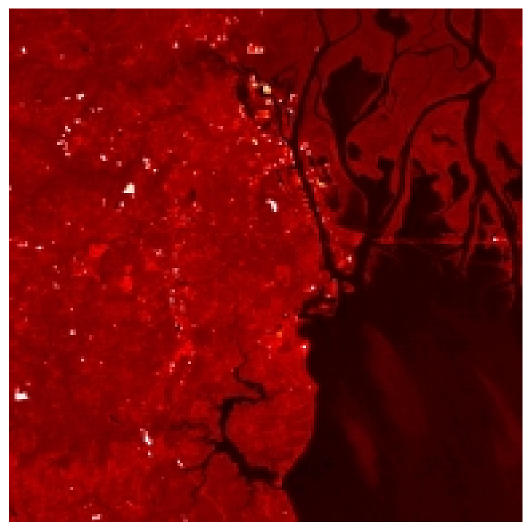
It is relatively easy to detect outlier pixels which are remote from the pixel clusters in the score space. It is also easy to detect high density clusters and the various pixel density gradients that exist both within and between clusters. Figure 5 reveals two major dense classes of pixels which are separated by a prominent area of between-class pixels. As mentioned earlier, pixels having similar spectral features in the multivariate image will have comparable combinations of score values and result in point clusters in the score plot. This fact can be put to use in segmentation of features from the multivariate image through delineating pixel classes in the score plots. In effect, one can delineate a tentative data class corresponding to pixels having similar spectral fingerprints[12].

Pixel class delineation may be carried out in more than one way. An area in the score space may be selected and the corresponding pixels belonging to this area highlighted in the image space. The selected area in the score space is in fact a local model which is chosen to delineate a tentative class of pixel data from the rest. The procedure of selecting an area in the score space is called 'masking' in the MIA literature. Since score plots can themselves be represented as 256 x 256 images, various sizes and shapes of masks can be selected by carrying out simple graphical operations on these score plot images. The pixels contained within the mask can be isolated (into a local model) and projected back to the image space.

This procedure of masking point clusters and outlier pixels in the score space and highlighting the chosen pixels in the image space forms the backbone of the MIA off-line feature extraction strategy. To successfully delineate a class of pixels it becomes imperative to study both the score and image spaces simultaneously. The ability to toggle between the image space and score space is quite fast and easy since both spaces are represented as images in MIA. As a result, it is relatively simple to interrogate the score space by masking several clusters in the score space, and projecting the masked pixels back to the image space. Figure 6(a) re-plots the $\mathbf{t}_1$ - $\mathbf{t}_2$ score plot of Figure 5, but with a polygon mask covering a portion of the lower dense point cluster. The pixel class which has been masked in the score plot of Figure 6(a) is outlined in Figure 6(b) where each pixel with a $\mathbf{t}_1$ - $\mathbf{t}_2$ score combination lying under the mask has been replotted as an overlaid white pixel on the false color image of the first latent variable $\mathbf{T}_1$. From this figure it is evident that the class of pixels masked in the score space belongs to major roadways, paved areas, and building tops in and around the city. Since all the highlighted pixels have similar spectral combinations, they map into the region masked by the polygon in the score space.



(a)



(b)

Figure 6 (a) $\mathbf{t}_1$ - $\mathbf{t}_2$ score plot of the satellite multivariate image with a class- masking of the upper part of the lower dense pixel cluster [masked in maroon]. (b) Overlay of $\mathbf{T}_1$ image with highlighted pixels from class outlined in 6(a)

By repeated use of the masking / highlighting procedure with different polygon masks a *signature* of every feature existing in the image space (regardless of its subtlety or spatial location) can be isolated in the score space. Due to the ability to switch easily between score and image spaces, MIA can also be employed as a reverse mode image analysis tool. Specific pixels belonging to known features of interest in the image space can be highlighted in the score space to determine the region which represents their corresponding score combinations. The area surrounding the highlighted score points can then be masked using a reasonably sized polygon. As a result, subtle features that are subjectively difficult to identify in the image space may easily be identified using the reverse mode application of MIA. The polygon mask used in Figure 6(a) was developed using this methodology. Geladi et al.[10] list several other modes of MIA that employ the use of the image space / score space relationship.

3. REAL-TIME MONITORING WITH MIA

In this section we proceed to the main thrust of this paper - extension of MIA methods to the real-time monitoring of time-varying processes. The purpose in monitoring an industrial process with imaging equipment is to detect and isolate faults or quality defects in the process or product being monitored. For example, in industrial sheet forming processes on-line multivariate imaging could be very useful in detecting and isolating the appearance of various faults in the sheet (e.g. dirt particles, streaks, variations in layer thickness, etc.). The major impediments to the use of on-line imaging at present are the difficulties in handling the large volume of data collected in real-time, and speed limitations in being able to process all these data with current image analysis methods. It is shown in this section that an on-line multi-way PCA approach to MIA can provide a powerful method for monitoring and analyzing many time-varying industrial processes.

The main concepts of this approach are described as follows. A multi-way PCA model is built off-line on a training or calibration image, which contains all typical features that one might be interested in detecting using the on-line monitoring scheme. This training image may be a single image containing all such features of interest, or it may be a composite image put together from sections selected out of many different images. The training image should be of the same dimensions as the subsequent images that are obtained sequentially by the on-line imaging system.

From the off-line analysis of this image masks are developed in the score space, which correspond to each feature in the image space that one desires to monitor. Upon applying the fixed PCA model to the new images as they become available, values of the scores are computed for the dominant principal components $\mathbf{t}_a$ (Equation 4) using the loading vectors $\mathbf{p}_a$. The pixel densities in the score space can then be updated for the new image. By monitoring the changing score point cluster intensities under the mask in the score plot one can then track the appearance and disappearance of the corresponding feature in the current image. Upper tolerance limits can be set on the pixel densities in each mask area. Violation of these limits in future monitoring could be handled as in any Statistical Process Control (SPC) monitoring scheme. Upon discovering violation of the SPC tolerance limits for any feature being monitored, one can investigate further by switching to the image space to reveal those pixel locations where the fault feature was present. The locations of this feature might help indicate possible assignable causes, which can be corrected. This on-line monitoring approach is now illustrated by way of an example.

3.1. On-line monitoring of a surface feature from LANDSAT (MSS) images

A modified version of the LANDSAT (MSS) multispectral satellite image example (depicting Mobile, Alabama) introduced in the earlier example is used here to illustrate the main ideas of feature monitoring using MIA. The original $512 \times 512 \times 4$ multivariate image is segmented into nine sections of $256 \times 256 \times 4$ multivariate images as the LANDSAT satellite moves in a north to south trajectory over Mobile.

It is important to select a training image that contains representative samples of all the features of interest to build a good PCA training model. In the satellite image example the feature of interest chosen to be monitored from various landscape features in and around Mobile is the presence of sand pits. This feature is not as obviously detectable through simple visual observation of the image space. As the satellite moves over the region, those pixels belonging to sand pits would be monitored using the MIA scheme. A good representative training multivariate image must contain ample pixels belonging to the above feature of interest. The center $256 \times 256 \times 4$ pixel sub-section of the full scene (Figure 4) in the original multivariate image adequately meets this requirement.

The PCA training model is calibrated by masking various point clusters with a customized local area score mask. The size and shape of the masks is determined by using the previously discussed iterative procedure of feature extraction from multivariate images. The score space mask that adequately represents the sand pits in the image space is illustrated in Figure 7. This figure also highlights four other masks that adequately capture various landscape features around the Mobile, AL region. Using the customized local area mask for sand pits in Figure 7, along with the reduced loading matrix $\mathbf{P}_{tr}$, the calibration of the PCA training model is complete.

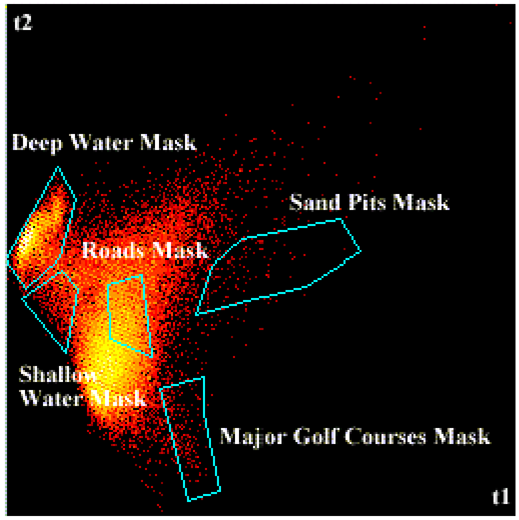


Figure 7 Detailed t1 - t2 score plot of training image with highlighted masks that adequately represent the four features of interest

To emulate a moving satellite gathering scans of the earth surface only the left half of the scene is used (i.e. columns 1-256). This half of the full scene is further divided into 9 overlapping equal sized scans of 256×256 pixels in all four spectral bands. Since the LANDSAT satellite moves in a north to south trajectory while gathering images of the earth surface, the first $256 \times 256 \times 4$ scan is located in the top left hand corner of the image. Each successive scan is gathered as the satellite moves south in a certain time, which is represented here as 32 rows. As a result, the second $256 \times 256 \times 4$ scan spans rows 33 to 288 whereas the ninth scan spans rows 257 to 512 in the left half of the full scene.

The 9 input multivariate images are decomposed into their score spaces with the help of the PCA training model. Each $256 \times 256 \times 4$ pixel multivariate image is rearranged into a $65{,}536 \times 4$ two-way array $\mathbf{X}_{test}$ and multiplied with the training loading vectors $\mathbf{p}_1$ and $\mathbf{p}_2$ to produce the corresponding score vectors $\mathbf{t}_1$ and $\mathbf{t}_2$. These score vectors are rearranged into 256×256 pixel intensity arrays and viewed as score images, as well as plotted against each other as color coded scatter plots. As a result of the decomposition, 9 $\mathbf{t}_1$-$\mathbf{t}_2$ score plot images can be plotted. Since the satellite scans over the Mobile region in a north-south trajectory it is expected that scan #1 captures regions that are mainly north of the city, whereas scan #9 captures areas that are south of the city.

An objective feature-monitoring scheme is obtained by monitoring the pixel densities of the corresponding point clusters under the masks in the score space of Figure 7. The pixel densities under the sand pits mask in the nine score space images covering the north to south movement of the satellite are monitored by enumerating the exact number of pixels belonging to the feature of interest for each satellite scan. The total number of pixels belonging to this feature are recorded and plotted as control charts for all nine scan images. Highlighting the masked pixels and overlaying them in the score image can obtain exact spatial locations of the sand pits in the image space. The resulting control charts for the feature pixel counts and the highlighted spatial locations of these pixels in the image space are illustrated in Figures 8. The score image used to highlight the spatial locations of pixels belonging to the sand pits is a false color image of the first score vector $\mathbf{T}_1$. The bar chart in Figure 8 shows the exact number of pixels belonging to the feature of interest for all nine scan images. This can serve as an on-line monitoring chart for the variation of sand pits throughout the sequence of the 9 multivariate images.

The information extracted from these multivariate images and plotted in Figures 8 can be used for Statistical Process Control (SPC), or automatic feedback control. In a SPC scheme the height of the bars corresponding to the frequency of occurrence of each type of fault would be monitored in successive images. Whenever any one of these bars exceeds a predetermined threshold or tolerance an alarm would be given and the process operator or engineer would look for an assignable cause. This would be greatly aided by highlighting the spatial location of the faults in the image space as shown in Figures 9. The results could also be used in an automatic feedback control scheme if spatial actuators were present which could be used to affect the particular feature being monitored. For example, if the feature corresponded to the thickness of a particular layer in a multi-layer sheet coating operation and spatial actuators were available to adjust the flow of coating material for that layer in the region of interest, then feedback control algorithms could be used to maintain the layer thickness uniform across the sheet. The above SPC and spatial feedback control strategies would rely upon the successful extraction of various features, evaluating their intensity of occurrence, and identifying their spatial locations in the image.

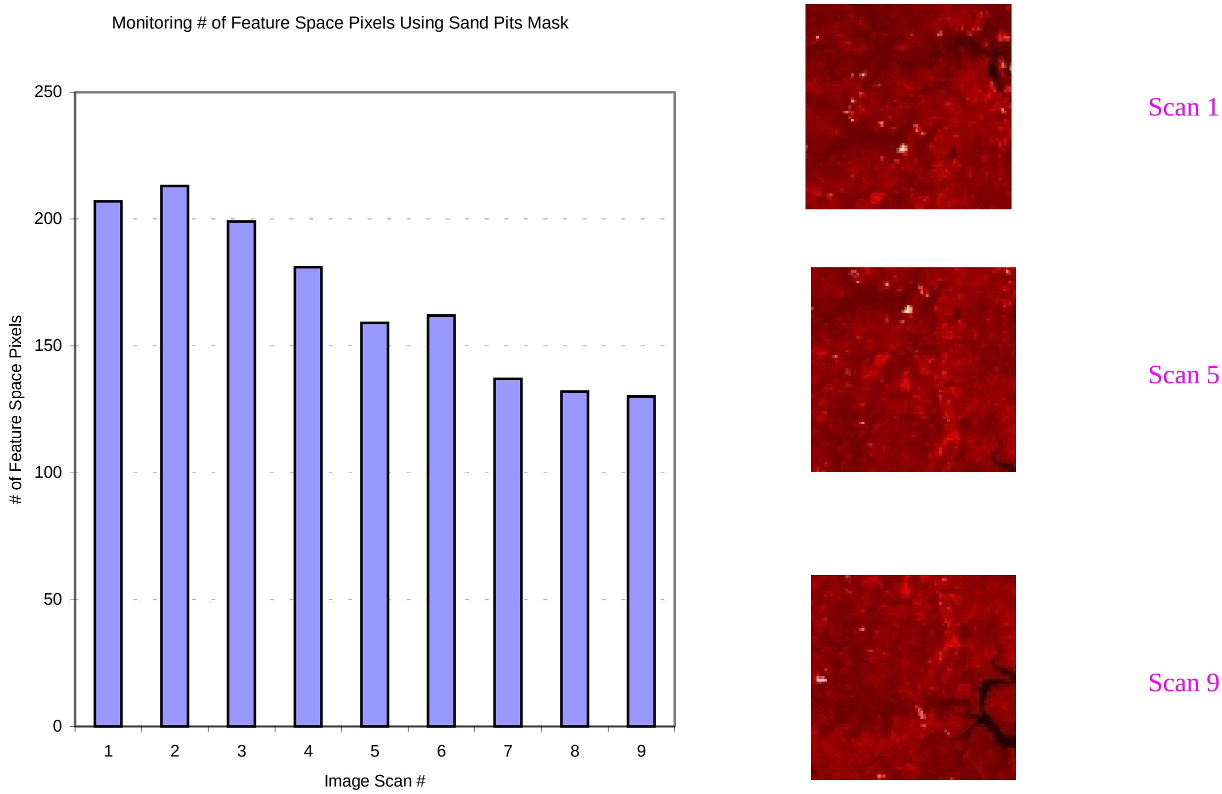


Figure 8 Bar chart of total number of pixels belonging to sand pits areas through scans 1-9 with highlighted spatial locations of these feature pixels in the image space for scans 1,5, and 9

4. INDUSTRIAL APPLICATIONS OF MIA FOR PROCESS MONITORING AND CONTROL

Although MIA based on PCA and PLS are very poor at performing traditional image analysis tasks such as image enhancement, reconstruction, etc., in general it is more powerful at extracting the often subtle information from time varying images that typically occur in process monitoring and control environments. This stems from the fact that in time varying process images it is often not the detailed shape, location or orientation of the features in the image that is important , but rather the amount of the feature occurring anywhere in the image. In multi-way PCA features with similar spectral features, no matter where they occur in the image, are extracted and located in the same region of the score space. This allows one to work almost entirely in the score space for most process monitoring and control problems.

This aspect of MIA via PCA and PLS is being exploited in numerous industrial applications in the McMaster Advanced Control Consortium (MACC – a consortium involving the advanced control research group in the chemical engineering department at McMaster University and approximately 20 international companies). On-going projects include texture/roughness analysis and monitoring of sheet and film products as presented in another paper in this conference (Bharati and MacGregor, 2000). Projects involving the monitoring of different gels and faults in polymer films, and the classification of wood products use a similar analysis to that presented for monitoring features of the earth's surface in the LANDSAT example. The extraction of quality information from images of pulp and paper sheets, from images of food products, and from time varying images of flames in industrial boilers and incinerators utilize different variants of MIA and multivariate image regression (MIR).

4. CONCLUSIONS

In this paper we have investigated the extension of Multivariate Image Analysis techniques based on multi-way PCA methods to real-time monitoring situations. Using a LANDSAT (MSS) satellite image sequence as an example these methods were shown to efficiently utilize large amounts of digital image data that might typically arise from on-line multispectral imaging sensors. Information gathered from the data can be used for analyses such as detecting and isolating faults or quality features in the process or product, and to do so in a time frame that is reasonable for some industrial situations.

The key points in the approach are as follows. All modeling and model calibration (mask determination, etc.) is performed off-line on a representative training image. On-line monitoring is then achieved quite rapidly by using the fixed loading vectors of the primary principal components from the model to update the score vectors. All monitoring is then performed in the score space by enumerating the pixel densities in masked regions of the score scatter plots. The number of defects or product features present in the image space is proportional to these densities. If the pixel density exceeds a pre-set upper control limit, one can toggle back to the image space to view the locations and structure of the defects. Depending upon the type, severity, and location of the faults one may stop the process to rectify any assignable cause, mark the image number and fault locations for rectification in the next stage of the process, or apply spatial feedback control strategies to compensate for the occurrence of certain features.

In spite of the ready availability of multivariate imaging systems in off-line settings, there has been very little application of such systems to industrial processes for on-line monitoring. One of the many reasons for this has been the lack of suitable image analysis techniques capable of handling the large volumes of data and extracting the relevant information in a sufficiently short period of time. The on-line MIA approach proposed in this paper addresses some of these problems, and we hope that it will expand the use of multivariate imaging sensors for monitoring industrial processes.

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