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Effective Time Averaging of Multiplexed Measurements: A Critical Analysis

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Multiplexing and time averaging of signal are effective noise reduction protocols applied in many analytical measurement systems. The efficacy of these protocols may be reduced by random occurrences of high-magnitude noise that do not conform to the statistical distribution of noise for all other measurements in the data set. This high-magnitude noise, which may have an insignificant probability of occurrence for a single measurement, almost certainly affects data collected in a multichannel, multiplexed modality, such as Fourier transform infrared (FT-IR) spectroscopic imaging employing focal plane array detectors. To recover time-averaging advantages in these cases, we present a general coaddition method that uses two statistical measures, the mean and median of the ensemble of measurements of a signal, to obtain a better estimate of the true signal than that estimated by time averaging alone. This method, termed median filtered time averaging, is shown to be an effective noise removal procedure for FT-IR imaging data. The effects of noise removal on time averaging and multiplexing are examined theoretically and are demonstrated for hyperspectral infrared microspectroscopic imaging data obtained from human skin biopsies by using a rapid data acquisition procedure.

Multiplex detection and time averaging of multiple measurements of a signal are two measurement protocols that are widely applied in the analytical disciplines to improve the inherent sensitivities of a wide range of analytical instrumentation. The multiplex, or Fellgett, advantage results in a significant decrease in data acquisition time, since the improvement for a set of measurements consisting of N resolution elements (as, for example, radiation intensity over a wide spectral range) arises from sampling each element N times, thus raising its signal by a factor of N. Similarly, averaging consecutively acquired measurements of a signal over a period of time, termed signal averaging or time averaging, relies on the measurement of the signal n times to obtain its best estimate. However, the efficacy of both these methods depends on the type and magnitude of noise generated within the instrumentation. Noise in the determination of a signal consists of three statistically independent forms;[1,2] namely, noise that is directly proportional to the signal intensity (for example, fluctuation, modulation, scintillation, or $1/f$ noise) and noise that is either proportional to the square root of the signal intensity (source-limited noise) or independent of signal intensity (detector limited noise). The Fellgett advantage, a maximum of $N^{1/2}$ for signal independent noise, rapidly diminishes as the fraction of noise proportional to the signal is increased.[2,3] Similarly, there is no benefit to be derived from time averaging for noise that increases in a manner directly proportional to the number of measurements. For noise dominated by a contribution varying independently of the measured signal, however, noise reduction may be derived from multiplexing and time averaging the signal, since noise inherent in any measurement is the root mean square of the magnitudes of noise derived from the three independent sources.

One analytical technique that effectively utilizes Fellgett's and time-averaging advantages is Fourier transform infrared (FT-IR) spectroscopy.[4] A linear increase in the sum of the signal with increasing measurement time, compared to a square root dependence of increase in noise in accord with Poisson statistics, leads to an increase in the signal-to-noise ratio (SNR) of measurements that is proportional to the square root of the measurement time. As the measurement time is usually constant for the detection of a signal, the SNR scales with the square root of the number of measurements. This concept has been demonstrated for signals from single element[4] as well as focal plane array[5] (FPA) detectors employed in an FT-IR spectroscopic modality and has become an unquestionably integral component of data acquisition protocols. In this article, we critically examine the concept of time averaging a signal and its application to FT-IR spectroscopy, particularly with respect to its relationship to Fellgett's advantage. We further describe a method that reduces the effects of random, high-magnitude noise and recovers the benefits of both time averaging and Fellgett's advantage.

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FT-IR Imaging and Rapid Data Acquisition. Spatially resolved FT-IR spectroscopy, or FT-IR imaging,[6,7] employing FPA detectors bearing individual pixels that are tens of micrometers in size is a technique that is particularly affected by random noise.[8] The unique array architecture, small detector area, miniaturized electronics, and complicated electrical interfaces required for data acquisition and readout result in larger noise than that commonly encountered in modern, single-element infrared detectors.[9] Further, the small sample area imaged at each pixel usually results in a low radiation throughput per pixel, yielding lower SNRs. This necessitates large data acquisition times for obtaining high SNR data and limits the utility of the technique in settings that require rapid analyses, as, for example, a laboratory imaging large numbers of histological samples. Thus, an active area of research is concerned with an increase in the rates of acquisition to obtain higher SNR data in as short a time period as possible.

The SNR of data acquired using FPAs in FT-IR spectroscopic measurements can be increased using many techniques.[10] However, an analysis of the data acquisition process indicates that, for the rapid acquisition of high-fidelity data, a reduction in interferometer stabilization and detector array readout times proves beneficial.[9] In the present paper, a data acquisition method was implemented in which the interferometer is stepped to a specific retardation and allowed to stabilize. Subsequently, the array is triggered to acquire data multiple times with a single frame of data being acquired per trigger. This approach eliminates the need for repeatedly accessing data for coaddition and reduces effective read times. The spectrometer is then stepped to the next sequential retardation and the acquisition protocol is repeated until the entire data set is collected. Multiple images at each retardation are temporarily stored and are averaged after completion of the acquisition process to obtain an interferogram for further processing. The FPA is triggered to initiate data collection at the fastest possible rate to minimize the time required for frame acquisition.

While this strategy was successfully implemented, it was found to lead to a higher noise in the acquired data than that usually observed in data acquired by conventional data acquisition schemes.[9] Since the reduced experimental time does not impact the total time that radiation is detected, the increase in noise is unexpected.[11] An analysis of the acquired data reveals that this increase in noise is due to the random appearance of high-magnitude noise events, or spikes. Since an integrated imaging spectrometer has numerous electrical, optical, and interfacing components that are synchronized, it is virtually impossible either to predict or to eliminate the occurrence of noise spikes without allowing sufficiently large time delays between a synchronization signal and it consequent action. Since random noise spikes cannot be predicted and rigorously tested for thousands of acquisitions for each operational parameter, arbitrarily determined, large time delays are employed for data acquisition. The imposition of these time delays, while effective in virtually eliminating the occurrence of noise spikes, results in rates of data acquisition lower than may otherwise be possible. If an alternative method could be devised to eliminate infrequent noise spikes, then high-fidelity data may be acquired at the fastest possible rate. The following section discusses the effects of noise spikes on the quality of the recorded data and describes a method to take complete advantage of an instrument's inherent capabilities by eliminating this deleterious source of noise.

Random High-Magnitude Noise: Effects and Remedies. An assumption implicit in the time-averaging process is that the noise is distributed in a statistical manner, namely, as given by a Poisson distribution. A single high-noise event, however, negates this assumption and affects adversely the SNR of the acquired data. Clearly, the probability of a high-noise event increases linearly both with the number of resolution elements and with the number of measurements that are coadded in the time-averaging scheme. Further, as more measurements are typically averaged for higher resolution spectra (more multiplex elements), such experiments become especially vulnerable to random high-magnitude noise events. Another technique that is even more susceptible to these effects is one that employs the multichannel detection of time-averaged multiplexed signals, as, for example, FT-IR imaging, since the probability of a high-noise event is further multiplied by the number of channels. As an illustration, a typical experimental protocol that obtains a 1024 element interferogram by coadding four data sets acquired using a 256×256 element array through the averaging of 16 frames for each interferometer retardation increases the probability of a single high-magnitude noise event, p_ϵ, by a factor of 2^{32} in comparison to a single-element detector. Even if the total probability of an extraordinary noise event is 10^{-7} (or, 1 in 10 million measurements), a certainty of hundreds of such spikes exists for a data set acquired using an array as described above. Notably, the probability of a noise spike occurring during the collection of an interferogram under the above circumstances using a single-element detector is only $\sim$0.0001; that is, less than two in every 10 000 experiments conducted may experience an extraordinary increase in noise. Hence, for the detection of multiplexed signals using multichannel detectors, an analysis of the contribution of even an improbable random noise event of high magnitude becomes important.

A. Effect of Noise on Time Averaging. Ordinarily, the noise in a time-averaged measurement increases with the number of measurements, n, as $n^{1/2}$. However, assuming that the noise varies in a manner different from its usual assumed statistical distribution due to n_e nonconforming points, the resultant noise, a_e, becomes

$$a_e = a_0 \sqrt{n - n_e} + \sum_{i=0}^{n_e} e_{\mathrm{i}} \qquad (1)$$

where a_0 is a proportionality constant that is equal to the hypothetical magnitude of noise for a single measurement that corresponds to the observed variation of noise with the number of measurements and e_i is the noise associated with the ith measurement ($0 \leq \mathrm{i} \leq n_e$). Hence, the SNR for a data set

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containing noise spikes, SNR_e, now becomes

$$SNR_e = \frac{nS_0 - |\sum_{i=0}^{n_e} e_i|}{a_0 \sqrt{n - n_e} + \sum_{i=0}^{n_e} e_i} \qquad (2)$$

where S_0 is the true signal. The contribution of noise to the signal is usually neglected for well-behaved noise, since the net effect of the noise on the signal is negligible. Hence, compared to the SNR obtained only with well-behaved noise, the relative SNR can be denoted by

$$\frac{SNR_e}{SNR} = \left[\sqrt{1 - \frac{n_e}{n}} + \left(\frac{\sum_{i=0}^{n_e} e_i}{a_0 \sqrt{n}}\right)\right]^{-1} \qquad (3)$$

The sampling of a signal usually results in the distribution of the measurements about a mean with most of the data points (greater than 99%) being within a few standard deviations. Since any deviation of the measurement from the true value is construed as noise, the distribution of noise is usually characterized by a large number of observations with moderate noise.

B. Effect of Noise on Fellgett's Advantage. The transformation of a multiplexed signal, as for example, interferograms recorded in FT-IR spectrometers, leads to the distribution of noise from any resolution element over every resolution element of the entire spectrum. For shot noise-limited measurements, this effectively negates Fellgett's advantage, while for fluctuation noise limited measurements, it is severely reduced. These factors are well discussed in the literature.[1] Hence, for the remaining discussion, we will assume the noise independent of signal. Under this assumption, the usual conditions of FT-IR spectroscopy are encountered, where Fellgett's advantage is retained and the time averaging of multiplexed signals incorporating random noise is implemented. The noise per resolution element that is not distributed in a statistical manner, b_e, or the excess noise, is given by

$$b_e = \frac{1}{nN} \sum_{j=0}^{n} \sum_{i=0}^{N} e'_{i,j} - a \qquad (4)$$

where e' is the Fourier transform of a noise event, e, a is the resultant noise in the spectrum due to noise a_0 in the interferogram space, and N is the number of resolution elements. The effects of random occurrences of high-magnitude noise, referred to by various authors as "glitches", scintillation, or popcorn noise, are similar to the effects of fluctuation noise on data collected by a multiplex method. The variation of the SNR for the magnitude of fluctuation noise, b, is given by[12,13]

$$SNR = \frac{f(\bar{\nu})\, \Delta\bar{\nu}\xi}{[a^2 + b^2(\bar{\nu}_{max} - \bar{\nu}_{min})\bar{f}^{\,2}]}\sqrt{n} \qquad (5)$$

where $f(\bar{\nu})$ is the spectral energy density distribution as a function of the wavenumber; the spectral range of data collected at a spectral resolution, $\Delta\bar{\nu}$, is given by $(\bar{\nu}_{max} - \bar{\nu}_{min})$ over which the average value of the spectral energy function is $\bar{f}$. The effects of nonconforming noise can be derived by replacing b by b_e in eq 5. For a boxcar spectrum, Fellget's advantage, F_g, derived by multiplexing the signal when compared to a dispersive spectrometer, is then

$$F_g = \left[\frac{1 + g^2}{N^{-1} + Ng^2}\right]^{1/2} \qquad (6)$$

where $g = (b_e\bar{f}\,\Delta\bar{\nu}/a)$ is the ratio of the statistically nonconforming component to the conforming component of noise for each resolution element. The multiplex gain is completely negated when $g^2 = N^{-1}$, and in such cases, it is fruitful to reconsider data acquisition parameters or redesign the experiment. It is clear that if a method could be devised to eliminate the (occasional) occurrences of offending noise observations, a substantial recovery of Fellgett's advantage would be afforded. The benefits of the noise removal procedure can be described by the relative SNR for the data set without such noise sources, SNR_0, compared to the SNR of data set with noise spikes, SNR_e, by

$$\frac{SNR_0}{SNR_e} = 1 + \left[(\bar{\nu}_{max} - \bar{\nu}_{min})\left(\frac{b_e}{a}\bar{f}\right)^2\right] \qquad (7)$$

C. Median Filtered Time Averaging. Acknowledging that a reasonable probability of high-magnitude noise events exists in modern multichannel FT-IR spectroscopic instrumentation, we propose a method to eliminate the effects of this significant noise source. The principle of the filtering scheme is to verify that deviations from the true mean for all observations correspond to less than a predetermined tolerance. Subsequently, the best estimate to the true mean is determined by eliminating possible outliers. For a number of observations conforming to the Poisson distribution, the mean differs little from the median of the set of values. However, in a set of observations that contains a few points varying from the true signal by large deviations, the median signal is the more reliable estimate. Hence, if all measurements in an ensemble are sorted in order of magnitude and the extreme points eliminated until the median and the mean calculated from the remaining observations are nearly equal, the mean then provides a good estimate of the true signal. As the median has been employed to estimate the filtering criterion, we term the process "median filtered time averaging".

Any method that attempts to filter excessive noise from measurements must estimate the allowable noise in a specific and unbiased manner. For FPAs, an estimate of the noise for a measurement of a single data point may be derived from observations at a constant optical retardation. To flat field the array prior to data acquisition, FPA detectors record two observations of signal intensity at constant retardations of maximum and minimum intensity. A number of array frames are captured at each

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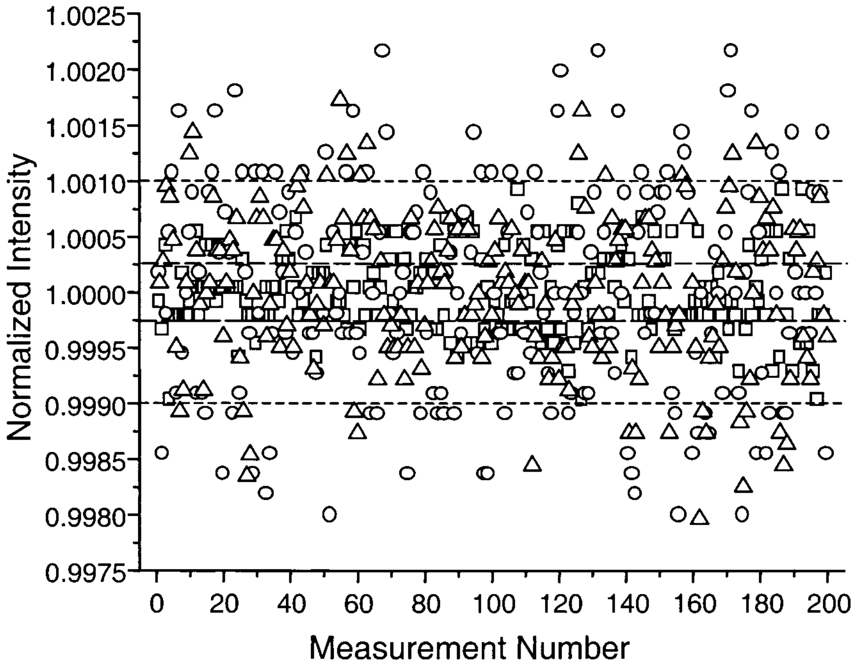

Figure 1. Sequential observations of the same incident intensity from three arbitrarily selected pixels normalized to the ensemble average.

data point, and the average frame is used for calibration. The same frames are stored and analyzed to determine the levels of noise that may be encountered for each observation prior to time averaging the data. These noise levels, typically 8−10 counts for the detector with a 14-bit (16 384 counts) ADC employed in this study, provide a reliable estimate for the tolerances between the median and mean. It must be recognized that the filtering proposed above is not in the spatial domain of acquired data but in the time domain of data acquisition and does not actually involve replacement of any data points by the median of the ensemble. Hence, the concept of median filtered time averaging that we discuss here must not be confused with the spatial median filter applied in image analysis[14] that replaces a noisy pixel value by the median of values of surrounding pixels.

EXPERIMENTAL SECTION

A spectrometer (Bruker IFS 66/s) incorporating a step-scan interferometer optimized for mid-IR operation is interfaced to an IR microscope (Bruker IR Scope II) equipped with an FPA (Santa Barbara Focalplane) detector. The 64 × 64 pixel HgCdTe (MCT) array detector images a sample area of ∼500 μm × 500 μm and is equipped with an optimally sized cold shield[15] and an appropriate band-pass filter. Data were acquired at every fourth crossing of the He−Ne laser to yield an interferogram containing 512 data points, corresponding to a spectral range of 0−3950 cm^{-1}, for every pixel in the array. Operating the assembly in the conventional mode of data collection, we average 20 frames for every spectrometer step for a total data acquisition time of ∼102 s. In the fast mode of data collection, the FPA is triggered 10 times for every interferometer retardation. Only one frame is collected for every FPA trigger and stored to disk, leading to a data acquisition time of ∼28 s. The interferogram data cubes were fast Fourier transformed using triangular apodization to obtain single-beam spectra for every pixel and the ratios of these data to similarly acquired background data sets were calculated to yield absorbance image cubes.

RESULTS AND DISCUSSION

It is instructive to examine the characteristics of individual intensity measurements as a function of the ensemble average. Figure 1 shows successive intensity measurements normalized to the ensemble average for three different pixels on the FPA. The incident radiation remains the same during the course of measurement; the observed mean intensity for all three pixels is the same, yet the dispersion in measured intensity values is different. Clearly, if all points are taken into account (for example, for the observations denoted by the circles), and the SNR is determined by the inverse of the deviation from the mean, a SNR of ∼500 would be observed. If a similar exercise is carried out for observations denoted by squares, a SNR of ∼1000 would be observed. However, it may be noted that a large majority of points from all three observations lie between the inner patterned lines, indicating a SNR of 2000 if the guidelines above are followed. Clearly, the effect of outlying points on the observed SNR is not straightforward, since the number of observations and their distribution density convolutes the estimate of the mean. This exercise, however, emphasizes the point that the presence of a few outliers in an ensemble of observations decreases the confidence in the measurement and results in enhanced levels of noise. The selective elimination of a few outlying observations would result in a narrower distribution of the magnitude of measurements and may lead to a higher confidence in the determination of their mean.

Large-magnitude, outlying observations of the intensity are observed as spikes in a plot of multiple measurements of the signal. For example, in recording an interferogram for which the intensity at each optical retardation is sequentially measured 10

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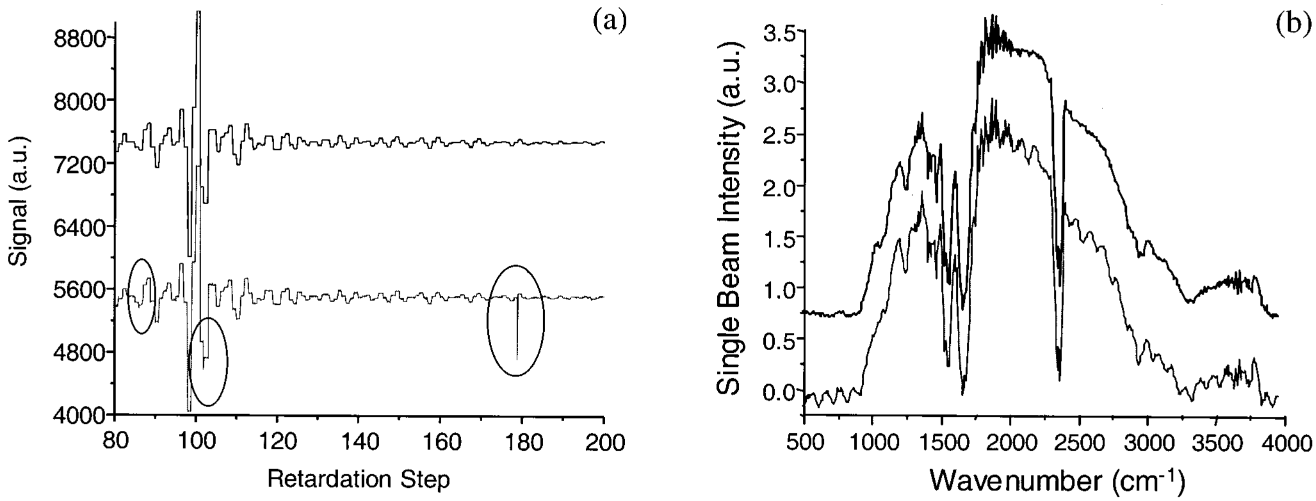

Figure 2. (a) Portions of interferogram measured at the same pixel in an FPA before (lower trace) and after (upper trace) median filtering the data. Visually detectable noise spikes are circled in the lower trace. (b) The corresponding single-beam spectra, obtained by Fourier transform of interferograms obtained by averaging all points at each retardation, clearly demonstrate the reduction in noise for filtered data (upper trace) compared to the single beam obtained from the acquired data (lower trace). Spectra have been offset for clarity.

times, the lower trace in Figure 2a reveals the outliers in the form of spikes, as indicated by the ellipses. Ideally, no such outliers should be observed, and corrective action can be taken to eliminate them by median filtering the data and replacing the outliers by the mean of the remaining values, as shown in the upper trace in Figure 2a. For each data set from which the traces are extracted, 10 observations at each retardation are averaged with the resulting interferogram being Fourier transformed to obtain a single-beam spectrum. The single-beam spectra corresponding to the interferograms in Figure 2a are shown Figure 2b. Removal of the noise spikes results in a significantly higher SNR spectrum (upper trace).

The presence of noise spikes can be deduced from a plot of the deviation from the mean for each retardation. The mean for 10 observations per step after median filtering the data is subtracted from each observation. The residual intensity, as shown in Figure 3, is largely distributed in a statistical manner. The inset displays the small number of observations that show significantly larger (either positive or negative) deviations from the distribution of the majority of the values. These outliers are precisely those to be eliminated by the use of median filtering. Although the origin of these noise events, which are of unusually high magnitude in our data, is not examined in detail in this paper, they probably arise from either bad or failing pixels, electrical noise in contacts, or electrical buffer over-runs due to a high rate of sampling. Clearly, by judicious application of median filtering, time delays between synchronization events need not be overestimated by eliminating the effects of random electrical anomalies, resulting in improved duty cycles. Additionally, some pixels that were previously classified as unusable due to numerous noise spikes may be recovered, leading to improved image integrity. The irreproducible nature of the noise makes detection and elimination difficult, and perhaps wasteful of time, if the data acquisition procedure in question is only used for certain cases.

We have a considerable interest in applying FT-IR imaging to discriminate between histologically similar indicators of various skin diseases. Figure 4a shows an infrared bright-field image of a thin section of a human skin biopsy. The corresponding absor-

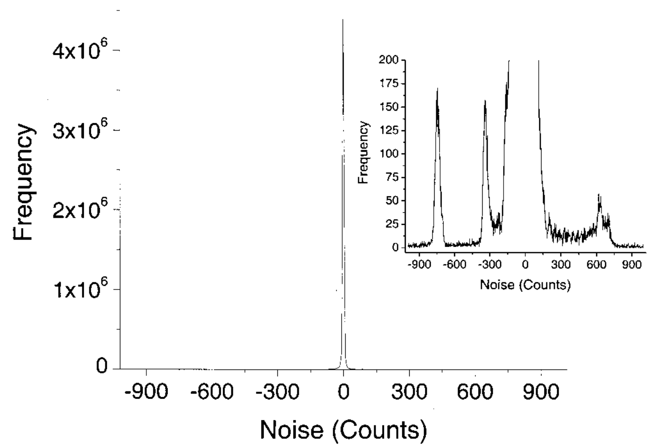

Figure 3. Noise in a measurement calculated by subtracting the mean of an ensemble of observations at similar intensities. The resultant distribution shows the bulk of values conforming to a statistical distribution with some measurements displaying large positive and negative deviations (inset).

bance image of the amide III vibrational mode peak at 1245 cm^{-1} obtained by conventional acquisition of data is shown in Figure 4b. In this conventional mode, large time delays are allowed for interferometer stabilization, data acquisition by averaging 20 frames at each interferometer retardation, and data readout leading to a data cube acquisition time of ~102 s. In contrast, when data are acquired at the frame rate of the FPA, while allowing time for the interferometer to stabilize for a smaller time with no additional readout time being required, a large fraction of the dead time during data acquisition is eliminated, thus, creating a more efficient process. The image obtained from the rapidly acquired data set is shown in Figure 4c. The noise in the acquired data is considerably greater than expected based on the integration time.[9] When that same data set and its corresponding background data set are median filtered, in the context described here, an image of considerably superior quality, as shown in Figure 4d, is obtained. The agreement between the image and the one acquired using conventional methods is excellent. The

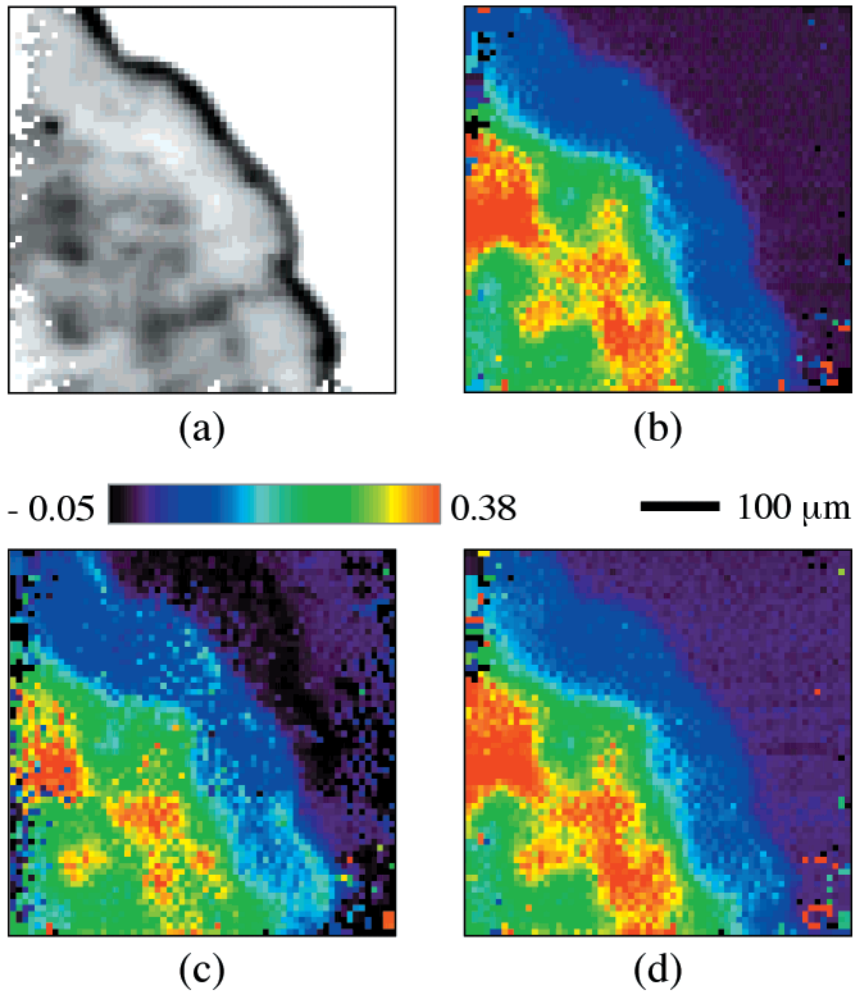

Figure 4. (a) Infrared bright-field image of skin section. (b) Absorbance distribution of the amide III stretching mode at 1245 cm^{-1} for a data set acquired in 102 s is displayed as indicated by the color bar. (c) Absorbance distribution for the same region as obtained from a rapidly acquired data set. (d) Absorbance distribution after the data in (c) was median filtered.

distribution of a baseline-corrected absorbance over the field of view is shown in Figure 5 for the conventional, rapidly acquired, and corresponding median filtered data sets. Comparing the absorbance distribution of conventionally acquired data with that from the rapidly acquired data set, it is apparent that the noise in the rapidly acquired data set precludes the correct determination of the distribution of absorbance. The absorbance distribution is, however, accurately reproduced after the data is median filtered.

If all measurements remain within selected tolerance limits, as determined by the noise during flat fielding, the benefits of median filtered time averaging are the same as that achieved by conventional time averaging alone. Clearly, the benefits of median filtering are most apparent when the noise in some observations results in large deviations from the mean. However, by neglecting a number of data points, n_e, from the total number of observations, n, a lower than expected SNR will result, as the eliminated points no longer contribute to the time-averaging process. The improvement in SNR will now only scale as $\sim(n - n_e)^{1/2}$. The number of observations (out of 10) remaining per resolution element as a function of the tolerance limit employed after median filtering the rapidly acquired data set are shown in Figure 6a. As expected, a large fraction of observations is eliminated as the tolerance is decreased. It is difficult to predict the number of observations

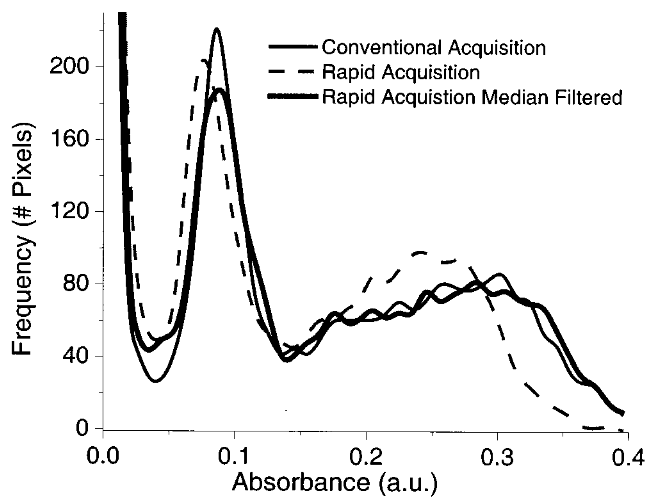

Figure 5. Baseline-corrected absorbance distribution at 1245 cm^{-1} for the data set obtained by a conventional acquisition route, rapidly acquired protocol, and median filtering of the rapidly acquired data.

that will remain after filtering is applied, as it depends on the experimental variables. However, a large decrease in the number of observations to be coadded diminishes the benefits of averaging

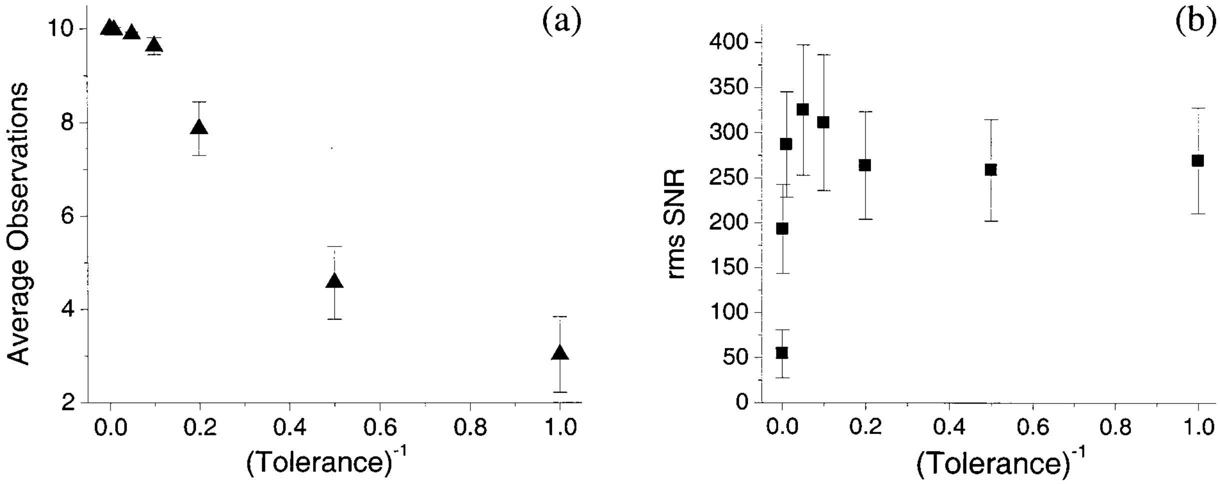

Figure 6. (a) Number of data points remaining ($n - n_e$) after outliers were eliminated by median filtering as a function of the tolerance employed in the filtering process. (b) Observed SNR for median filtering with different levels of tolerance.

and will result in a higher level of noise. Such an effect is observed for this data set when the SNR of spectra are plotted as a function of tolerance as shown in Figure 6b. A maximum is observed at a tolerance level of ~10−20 units where greater than 95% of the points were included in the averaging (Figure 6a). Even though the dispersion in their values was larger than others, the benefits of averaging a larger number of observations provided better quality data. In general, such behavior will be observed for median filtering any data set. An optimal compromise between a small tolerance and the inclusion of the maximum number of observations possible will achieve the best results. The results do not vary sharply with the tolerance level selected, and hence, a set tolerance level can be determined for a system that may only need periodic updating.

CONCLUSIONS

Median filtered time averaging uses two statistical measures of acquired data, namely, the median and the mean, to present a more accurate estimate of the true signal. The proposed averaging process is a form of a self-recalibration feedback that provides another safeguard or corrective mechanism in an analytical system for achieving optimal performance. Consequently, the occurrence of larger than expected noise-related errors is negligible in, for example, an integrated FT-IR imaging system. Median filtered time averaging of data, as suggested in this paper, is especially useful when noise-contributing events may be easily recognized but may not be readily corrected by either a change in sample-handling procedures or simple hardware alterations. Median filtering of data is also useful in removing noise spikes from the acquired data, a difficult task using unsupervised numerical transform techniques.[16] The method results in improvements in the quality of data, which is achieved with very little cost in terms of computational time. At a minimum, the results obtained after median filtering will be as good as those obtained by conventional time averaging. Our assessment is that median filtered time averaging will find general applicability in many types of analytical measurements.

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