Adaption and application of morphological pseudoconvolutions to scanning tunneling and atomic force microscopy

Andrew D. Weisman

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ADAPTATION AND APPLICATION OF MORPHOLOGICAL
PSEUDOCONVOLUTIONS TO SCANNING TUNNELING AND ATOMIC FORCE
MICROSCOPY

by

Andrew D. Weisman

Rochester Institute of Technology

(1991)

A thesis submitted in partial fulfillment of the requirements for the degree of Master of
Science in the Center for Imaging Science in the College of Graphic Arts and Photography
of the Rochester Institute of Technology

August 1991

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Title of Thesis: Adaptation and Application of Morphological Pseudo-convolutions to Scanning Tunneling and Atomic Force Microscopy

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ABSTRACT

A recently developed class of digital filters known as morphological pseudoconvolutions are adapted and applied to Scanning Tunneling Microscopy (STM) and Atomic Force Microscopy (AFM) images. These filters are shown to outperform, both visually and in the mean square error sense, previously introduced Wiener filtering techniques. The filters are compared on typical STM/AFM images, using both modeled and actual data. The technique is general, and is shown to perform very well on many types of STM and AFM images.
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This thesis is dedicated to my parents, David and Morelyn Weisman.
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Chapter 1

Introduction

1.1 Aims of the study

Both Scanning Tunneling Microscopy (STM) and Atomic Force Microscopy (AFM) are important tools for surface imaging at the sub-micron scale, and it is becoming common to enhance the resulting images by means of digital postfilters, most typically lowpass and Wiener filters.\(^1\)\(^2\) Wiener filtering requires estimates of both the desired image and the noise, and these are difficult to obtain in STM and AFM systems. Moreover, as typically applied, the Wiener filter requires that the image be wide-sense stationary, and while this assumption might be acceptable in certain circumstances, in others it may not. Finally, application of the Wiener methodology presupposes that we wish to employ a linear filter, and in many instances such an assumption is either unwarranted or not relevant.

In this thesis, a recently introduced class of nonlinear spatial-domain filters known as morphological pseudoconvolutions\(^3\)\(^4\)\(^5\), which make very few assumptions regarding image degradation, are applied to STM/AFM data.\(^6\)\(^7\) In pseudoconvolution design, the shape of typical image and noise structure is taken into account. Because the filters are nonlinear, they can be constructed so as to keep the distortion of the underlying image to a minimum. A salient feature of these filters pertaining to microscopy, where minimizing
information loss is critical, is that the filters contain a parameter that allows one to perform desired degrees of filtering, and as the parameter is increased one can actually pass the observed image without alteration.

1.2 Scanning Tunneling Microscopy

Scanning Tunneling Microscopy (STM) is a new branch of microscopy developed in the 1980's that enables one to resolve the surface structure of a conducting substrate down to the atomic level. The idea behind STM is that if an atomically sharp conducting tip (i.e. a metal) is brought within a few angstroms of a conducting substrate, electrons will tunnel between the tip and the substrate. The current depends exponentially on the tip-sample separation. Specifically, for vacuum tunneling the current increases an order of magnitude with roughly an angstrom change in the tip-sample separation. This allows for an extremely sensitive measurement of the height of the sample. In addition, only the atom closest to the end of the tip will contribute to the tunneling current, allowing for atomic resolution laterally. The basic setup for an STM is shown in Figure 1-1.

The tip is moved in both the x and y directions (along the substrate surface) and in the z direction (closer and farther away from the surface) by means of a piezoelectric tube, to which the tip is affixed. Electrodes are placed on the tube (which is in general elongated into the shape of a tube), and when a voltage is applied, the tube contracts or expands (giving the motion in the z direction) and can also be made to bend laterally (for scanning). These movements can be controlled in a very precise manner, thus enabling angstrom
resolution in both the lateral and vertical directions. The STM can be operated in two basic modes: the constant current mode and the constant height mode.

The constant current mode is the most widely used of the two. It gives the topography of the substrate for image dimensions greater than 10Å. It can also be used to image surfaces that are not atomically flat. The tip is lowered towards the surface until a threshold amount of current (on the order of 1nA) is achieved. The tip is then scanned across the surface while a feedback loop monitors the current, attempting to keep the current constant. When the current increases or decreases (i.e. the tip encounters a valley or a mountain), the tip is lowered or raised to compensate. For example, if a valley is encountered while scanning, the current will decrease (because the surface and tip will be farther apart) and the feedback loop will respond by sending a voltage to the tube so that the tip is lowered until the current increases back to the desired level again. This idea is depicted in Figure 1-2. Since the voltage applied to the tube is directly proportional to the current encountered, which is in turn proportional to the relative height of the surface, we may plot an equispaced sampled array of the voltage (z) applied to the tube as a function of position on the substrate (x and y) and thus develop the topography of the surface. This may be displayed in a number of ways, including gray level versus position (thus a gray scale image).

The constant height mode of operation scans the tip over the surface while keeping its height constant from a fixed reference height. The current (which will change when mountains and valleys are encountered) is monitored and can be digitized and plotted as a function of position. This may be seen in Figure 1-3. Because there is no lag time from the feedback circuit present in the constant current mode of operation, images may be taken
at a much faster rate in the constant height mode (one to two orders of magnitude faster). This can be useful in reducing scan-line noise in the image. Because there is an exponential drop-off of the tunneling current with the distance between the tip and the surface, however, the vertical range in the constant height mode is not as large as in the constant current mode. Also, because the tip height does not change, one is at risk of crashing the tip into the surface if a high enough mountain is encountered while scanning. Both modes are capable of giving atomic resolution, however.

1.3 Atomic Force Microscopy

Atomic Force Microscopy (AFM) is another method of atomic level imaging that, unlike STM, does not require the substrate to be a conductor. AFM is similar to STM in that it uses a sharp tip that is lowered very close to the surface which is scanned via a piezoelectric tube, but instead of using the tunneling current to monitor the tip-sample displacement, one uses the force of interaction between the tip and sample to monitor this separation. By monitoring the changing forces on the tip while scanning the surface, imaging may be accomplished. The force on the tip causes a displacement of the cantilever. There are two basic modes of operation for the AFM: the attractive and repulsive modes. Only the repulsive mode will be discussed here, as it is the most widely used of the two and is capable of giving atomic resolution.

The repulsive mode of imaging with the AFM is performed by bringing the tip into very close range with the sample. The van der Waals force then pulls the cantilever onto the
sample (so that they are in contact), but the very tip of the cantilever feels a repulsive force. The magnitude of this force is measured as the tip moves along the sample. Different schemes for detecting the change in this force while scanning have been documented and implemented, but only one commonly used technique will be presented here.

A simple scheme often referred to as the “beam-bounce" technique is illustrated in Figure 1-4. The substrate is attached to a piezoelectric tube so that it may be moved in both the vertical and lateral directions as in STM (notice that it is actually the substrate that is “scanned” here, while the tip remains stationary). A small metallic rod is bent into a cantilever so that the apparatus consists of a tip connected to an arm, and a minute mirror is placed on the backside of the tip. The arm of the tip is somewhat flexible and is attached to a rigid body so that it may be displaced in the z (vertical) direction freely when forces are encountered. A laser beam coming from an oblique angle is focussed down onto the mirror and from there is reflected onto a position sensitive detector, typically consisting of two photodiodes separated by a 10 micron space. By placing the detector at a relatively large distance from the cantilever, the amount of deflection is magnified and thus small movements may be measured quite easily. The sample is moved until it contacts the tip and the tip bends backwards. As the sample is scanned, bumps and valleys in the surface will cause the tip to move, and thus the laser beam will be displaced on the detector. A feedback loop monitors this displacement, and attempts to keep the beam centered on the detector by adjusting the sample's vertical height by sending voltages to the tube so that it either contracts or expands. This voltage is sampled and recorded as a function of lateral position on the substrate, and thus a surface topography may be developed and displayed as with STM.
As illustrated, the resulting images for both STM and AFM are digital images that may be stored in a computer. Digital image processing techniques may thus be appropriate for filtering out noise incurred during the imaging process. Classical techniques including mean, median, and Wiener filters have been applied\textsuperscript{1,2} with some success, however more effective techniques are desired, as processing images where the input is not always known is precarious.
Figure 1-1: Basic set-up of a Scanning Tunneling Microscope.
Figure 1-2: Set-up for Scanning Tunneling Microscope operated in constant current mode.
Figure 1-3: Set-up for Scanning Tunneling Microscope operated in constant height mode.
Figure 1-4: Basic set-up for Atomic Force Microscope using beam-bounce technique.
Chapter 2

Post-processing techniques previously applied to Scanning Tunneling and Atomic Force Microscopy

2.1 Introduction to linear system analysis

Traditionally, the Modulation Transfer Function (MTF) of an imaging system is studied before image processing is performed to gain knowledge of what the system does to the input to achieve the output one observes. If the MTF is known and the system is found to be linear and shift invariant, one may perform various linear filtering techniques to attempt to correct for the effects of the system. A filter \( \Psi \) is linear if for any images \( f \) and \( g \) and scalars \( a \) and \( b \), \( \Psi(af + bg) = a\Psi(f) + b\Psi(g) \); otherwise it is nonlinear. Linearity represents a restriction on filter design. Linear techniques such as deconvolution and Wiener filtering, however, can be effective for filtering certain types of images.

System linearity means that given an input \( af_1(x, y) + bf_2(x, y) \), where \( a \) and \( b \) are real constants, the output may be written as \( ag_1(x, y) + bg_2(x, y) \). In an optical radiation detector, for example, \( f \) is the intensity of the light incident on the detector, and \( g \) is the
current generated. For an STM operated in constant height mode, \( f \) is the height of the sample defined by a contour of constant Fermi level charge density and referred to an arbitrary zero, and \( g \) is the position of the tip, referred to the same zero. The optical radiation detector can become nonlinear at low light levels and at saturation, where the response may level off, but it may have a linear region between these two extremes. A source of nonlinearity in the STM is its finite response time to changes in the surface topography. This becomes much more pronounced as the scanning speed increases.

System shift invariance means that moving the input laterally before imaging is equivalent to taking the image and then shifting the output. Shift invariance may be expressed mathematically as \( f(x - a, y - b) \rightarrow g(x - a, y - b) \), where \( a \) and \( b \) are real constants. Shift invariance is a more strict definition than it may appear. A system that magnifies an input \( f(x, y) \) into an output \( f(x/k, y/k) \), such as an optical microscope, is not shift invariant because an input of \( f(x - a, y - b) \) is not given by \( f(x/k - a, y/k - b) \), but rather by \( f(x/k - a/k, y/k - b/k) \). The STM does not magnify in this manner, but it is not clear that the STM is shift invariant because a nonlinear response of the scanning piezoelectric may cause the sensitivity to be position dependent.

Although few imaging systems satisfy linear and shift invariance conditions, many are modeled as such in order to utilize linear filtering techniques. To use these techniques, the system MTF must be studied. To gain knowledge of the system MTF, one normally takes an image of a known object, and then compares the output image to this original object. The known object is typically one that contains most frequencies (such as a step or a delta function) so that a system analysis over a large frequency range may be done. Assuming
that the MTF is consistent under different imaging conditions, an algorithm may be developed to correct for its effect to some extent.

In STM/AFM images, however, this process is very difficult to perform, because a "known" input is nearly impossible to consistently create on the atomic scale. One is also faced with the problems of thermal drift over time which inhibits reproducibility of results, different MTFs for different scan speeds, different scan areas, and different substrates producing very different noise effects. All of these factors make the development of a set linear algorithm virtually impossible. What is generally done, therefore, is to use some post-filtering techniques, such as lowpass filtering and median filtering. Wiener filtering, which requires linear system analysis, has also been employed despite these problems.\textsuperscript{1,2}

There is a need for a post-filtering technique that is robust and that does not make many assumptions about the imaging process. Filtering of data of this type, where the goal of the imaging process is to investigate the unknown, must be done in a prudent manner. One does not wish to remove desired information from the image or introduce artifacts. Here, artifacts are structures resulting from the filtering process that may be misinterpreted. As we will see, filtering techniques based in the frequency domain can introduce artifacts of various types.

A number of examples in this thesis are introduced via one dimensional signals for clarity of presentation and ease of computation. It should be clear that a signal may be thought of as a one-dimensional image, or equivalently, a cross section of an image may be considered to be a signal.
2.2 Classical filtering techniques

2.2.1 The lowpass filter

In the present section, three classical filtering techniques will be briefly discussed, paying special attention to the Wiener filter. Lowpass filters operate by passing only frequencies lying below a certain cutoff frequency. Filtering is accomplished in one of two ways: (1) the Fourier transform is applied, the transformed image is truncated in frequency, and then the inverse Fourier transform is applied, or (2) the first method is approximated by a convolution in the spatial domain. Digitally, convolution is a moving-window operation that replaces each gray-value in the image by a weighted average of itself and some neighborhood of surrounding gray values. Lowpass filters are linear filters. A basic lowpass filter is the moving mean, which replaces each gray value with the unweighted average of the windowed values.

The underlying assumptions for lowpass filtering are that the noise consists of higher frequencies than the image, and that the higher spatial frequencies in the image do not contain important information. These may or may not be reasonable assumptions. For example, the system may give rise to $1/f$ noise, which is a low frequency noise. This is often the case for STM.\textsuperscript{2,11,12,13} Also, the image may contain different desired edge or texture information that will be lost upon lowpass filtering. An example of texture information in STM is an image containing periodic atomic structure. An edge is made up
of an infinite number of frequencies, and when higher frequencies are truncated, edge sharpness is lost. Thus, if quantitative information is desired from the data, such as width measurements of a polymer strand, the ability to extract this information will be hampered upon lowpass filtering. Also, while lowpass filtering does decrease the amplitude of point noise, it also spreads point noise into neighboring pixels and does not eliminate it. For instance, Figure 2-1 depicts the effect of a three-point mean on point noise. Notice how the spreading effect of the mean causes the output to appear to have structure (an artifact).

2.2.2 The median filter

The median is a nonlinear filter. It replaces the gray value at a pixel by the median of itself and its neighbors in a local window. It completely eliminates point noise in flat regions (Fig. 2-1). Also, whereas the mean blurs edges, the median preserves edges (Fig. 2-2). Because the median filter preserves edge information, one may say that edges are in the invariant class of the median filter. An image f is said to be in the invariant class of a filter \( \Psi \) if \( \Psi(f) = f \). While the median filter does have certain desirable properties, its noise-suppression efficiency is less than the mean's, and the effect of its use is to sometimes give a blotchy output, as well as to flatten higher background variation that may be contained in the uncorrupted image. Specifically, both mean and median filters have detrimental effects on simple highly varying texture information that we may wish to preserve. This may be seen in Figure 2-3. We note that Justusson\(^{14}\) provides a concise account of the statistical effects of median filters, and that a number of approaches have been developed for
designing median-like filters that either enhance edges, possess increased invariant classes, or result in less degradation of the underlying image.15,16,17,18,19

2.2.3 The Wiener filter

The Wiener filter is a relatively optimal filter, which means that it is the most efficient filter of a certain kind with respect to a specific criterion of goodness. Moreover, it depends on joint statistical knowledge concerning the image and noise. The criterion under which the Wiener filter is optimal is the mean square error (MSE). Given that we have n observations $X_1, X_2, ..., X_n$ and wish to use these observations to estimate the value of another variable $Y$, the optimal MS filter is given by the estimation rule $g$ that minimizes (with respect to MSE) the expected value

$$E[ |Y - g(X_1, X_2, ..., X_n)|^2 ].$$

(1)

It is well-known that the optimal filter is given by the conditional expectation $E[ Y | X_1, X_2, ..., X_n ]$. If we restrict the form of $g$ to be a linear combination of the observations,

$$g(X_1, X_2, ..., X_n) = a_1 X_1 + a_2 X_2 + \cdots + a_n X_n,$$

(2)

we obtain a relatively optimal filter known as the optimal linear filter. The weights $a_1, a_2, ..., a_n$ that minimize MSE are found by solving a system of linear equations known as
the Yule-Walker equations.\textsuperscript{20} In noise filtering the observations consist of windowed gray values and Y is the gray value we wish restored.

As it stands, the optimal linear filter is spatially variant, which means that each pixel must be filtered by its own particular set of weights. For the filter to be spatially invariant, which means we can filter by a single weighted sum, we must make an assumption on the class of images under consideration; namely, as a random process, the collection of (noisy) images must be \textit{wide-sense stationary}. This means that second-order statistics must only depend upon the (vector) difference between pixel gray values. The assumption of stationarity in real-world images is quite strong. Under wide-sense stationarity, the optimal linear filter can be expressed by means of the Fourier transform, and in this context it is called the Wiener filter.

Assuming the imaging process is modeled by a linear observation system with uncorrelated, additive, stationary noise, also known as white noise, the Wiener filter is given by

\[
\hat{U}(k_x, k_y) = G(k_x, k_y)[U(k_x, k_y) + N(k_x, k_y)],
\]

where U, N, and \(\hat{U}\) are the Fourier transforms of the uncorrupted image, the noise, and the optimal linear estimate of the uncorrupted image, respectively, and where G, also called the \textit{Wiener filter}, is given by
\begin{equation}
G(k_x, k_y) = \frac{H^*(k_x, k_y)S_u(k_x, k_y)}{|H(k_x, k_y)|^2S_u(k_x, k_y) + S_n(k_x, k_y)},
\end{equation}

where \( S_u \) and \( S_n \) are the power spectra of the uncorrupted image \( u \) and noise \( n \), respectively, and where \( H \) is the frequency response of the system.\(^{21}\) If we assume there is no blurring due to the system, then \( H = 1 \) and the Wiener filter takes the form

\begin{equation}
G(k_x, k_y) = \frac{S_u(k_x, k_y)}{S_u(k_x, k_y) + S_n(k_x, k_y)}.
\end{equation}

This filter is called the **Wiener smoothing filter**. Note that it reduces to 1 when the signal power spectrum is much greater than the noise spectrum and reduces to 0 when the noise dominates the image.

The Wiener filter requires an estimate of the power spectrum of both the noise and the image. While this may be a reasonable requirement for general large scale imaging systems that take certain classes of images, it is not for either the STM or the AFM. In addition to the Wiener filter's requirement of system linearity and shift invariance, it also requires stationarity of the image. This means that the image must have some basic frequency or texture that does not change across the image. In typical STM/AFM atomic scale images, images of uniform crystalline surfaces can be described as stationary, while images of absorbed molecules on these same surfaces are not stationary. Edges separate the molecule and the surface, and stationarity does not hold. The Wiener filter will have the tendency to blur edges, and thus inhibit our ability to make quantitative measurements. Blurring the edges of an image also has the effect of making the image aesthetically undesirable to view,
as our eyes respond more strongly to edge information than to many other types of information.\textsuperscript{22}

The Wiener filter is optimized with respect to MSE, which is strictly a \textit{linear} metric deriving from inner product spaces. It is well known that our eyes respond in a non-linear manner\textsuperscript{22}, and given that it is the eyes of the scientist that are probing and analyzing the image, it is not necessarily appropriate to use a linear metric to optimize an image for human viewing.

While the Wiener filter does have drawbacks relative to filtering STM/AFM data, it is used somewhat successfully under the conditions that the image is slowly varying and homogeneous, there are no edges in the image, and the noise is not too great, is consistent, and is known to a good extent. These situations, however, do not always exist, and it is then that a nonlinear filter can perform better.
Figure 2-1: Effect of three point mean and median filters on point noise, where \( f(x) \) is the input. Note how the mean filter spreads the noise while the median filter eliminates this noise.
Figure 2-2: Effect of three point mean and median filters on a digitized step, where \( f(x) \) is the input. Note how the mean blurs the step while the median preserves the step.
Figure 2-3: Effect of three point mean and median filters on simple variation, where $f(x)$ is the input. Both have detrimental effects here.
Chapter 3

Morphological pseudoconvolutions

3.1 Motivation behind pseudoconvolutions

Both mean and median filters have the side effect of degrading high-frequency texture information in the underlying image. It would therefore be highly desirable to recover this useful information after mean or median filtering has been performed. If we could utilize the desirable white noise suppression properties of the mean filter but also preserve edge and texture information, for example, we would have an excellent white noise filter. If it were possible as well to use the point noise suppression and edge preservation properties of the median filter, but also preserve texture information, we would then have a useful pair of filters to work with.

In the microscopy field, given that we do not always know what we are looking for, we would like to see less information lost due to filtering. A good filter should not introduce artifacts, and should have a controllable parameter which would allow all of the original input to be restored after a certain point, thus allowing the image to be filtered as little as
desired. The information should be restored in a manner such that the noise is last to come back, and that all of the desired information is in the invariant class of the filter. Increasing a filter's invariant class is the underlying idea behind a new set of filters known as pseudoconvolutions\textsuperscript{3,4,5} that arise in mathematical morphology.

3.2 Introduction to mathematical morphology

Mathematical morphology is a branch of image processing utilizing primitive shapes, known as \textit{structuring elements}, that are "fit" into an image. The degree to which a structuring either fits or does not fit determines the degree to which the image is or is not filtered. Here, only two basic morphological operations are presented, referring the reader to the literature (see Giardina and Dougherty\textsuperscript{23}, Serra\textsuperscript{24}, or Haralick, Sternberg, and Zhuang\textsuperscript{25}). Morphological pseudoconvolutions will then be introduced.

A filter is said to be morphological if it is both translation invariant and increasing. A filter $\Psi$ is translation invariant if $\Psi(f_x + y) = \Psi(f)_x + y$, where $f_x$ is the translation of $f$ by $x$ and $f_x + y$ is the offsetting of $f_x$ by $y$. A filter $\Psi$ is increasing if, given that $A \ll B$, $\Psi(A) \ll \Psi(B)$, where $A \ll B$ means that all points in the set $A$ are below all points in the set $B$, or the domain of $A$ is a subset of the domain of $B$, and for all $j$ in the domain of $A$, $A(j) \leq B(j)$. Notice that both the moving mean and median are morphological filters by definition.
The two most fundamental morphological operations are erosion and dilation. Erosion of $f$ by the structuring element $e$ is defined by

$$\left(f \ominus e\right)[j] = \max\{k: \text{ej} + k << f\},$$

(6)

where $\text{ej}$, the spatial translation of $e$ by $j$, is defined by $\text{ej}(i) = e(i-j)$. The erosion of $f$ by $e$ at $j$ is found by translating $e$ to $j$ and determining the maximum amount $e$ can be "pushed up" and still remain beneath $f$. An example of erosion is given in Figure 3-1. Owing to the shape of the structuring element, erosion reduces maximum noise (noise spikes) while preserving the underlying image. Dilation of $f$ by $e$ is defined similarly by

$$\left(f \oplus e\right)[j] = \min\{k: \text{ej} + k >> f\},$$

(7)

where $\text{ej}$ is the reflection of $e$ through the origin defined by $\text{ej}(j) = -e(-j)$. Geometrically, dilation marks the origin position at which the "flipped" structuring element would hit the signal if it were raised above the signal and then lowered. This is illustrated in Figure 3-1, where the input is dilated by the structuring element $e$. Here, dilation reduces minimum noise (dropouts in the signal) but preserves the underlying signal. It is interesting to recognize that the movement of an STM tip over a sample may be thought of as a dilation of the sample by a structuring element of the same shape as the tip. The tip, like a structuring element, will fit into some places on the sample but not into others.

The structuring element used in Figure 3-1 is employed in the pseudoconvolutions introduced in Refs. 3, 4, 5. Here, the structuring element is defined in one dimension by
\[ e[-1] = e[1] = -\lambda, \text{ and } e[0] = 0, \]
where \( \lambda \) is a filter parameter chosen by the user and the argument of \( e \) is the pixel index. As one can see from the previous example, the greater \( \lambda \), the less work the erosion/dilation does, or the more the input signal is preserved. As \( \lambda \) approaches infinity, no filtering is done, and as \( \lambda \) approaches zero, the data is flattened. One would therefore like to adjust \( \lambda \) so that the structuring element just "fits" into the signal, and not into the noise.

Since the *shape* of the structuring element plays as much of a role as its size, one would like the shape to be of a type that will not fit into the noise, but will fit into the type of image one wishes to preserve. The structuring element shown in Figure 3-1 is not ideal for the type of images found in STM, as it tends to fit slightly into the noise found in these images, and because its shape is not characteristic of the type of structures found in STM. The underlying principle of pseudoconvolutions, however, will prove very useful.

### 3.3 Morphological pseudoconvolution development

Pseudoconvolutions are defined in the following manner: Given a filter \( \Psi \) (here we will take \( \Psi \) to be the mean or median), the corresponding pseudofilter \( \Psi' \) is given by:

\[
\Psi'(f) = \min\{ f \ominus e, \max[f \ominus e, \Psi(f)] \}, \tag{8}
\]

where \( f \) is the image and \( e \) is the previously defined structuring element. In words, the pseudofilter is computed by taking the maximum of the image filtered by \( \Psi \) and the eroded
image, and then the minimum of this result and the dilated image. In effect we employ the original filter, and then bring back more information of higher variation, the amount of which corresponds to the choice of $\lambda$. In particular, all local variation smaller than lambda is preserved. Figure 3-2 gives an example of this process on a signal.

As mentioned previously, the main import of morphological pseudoconvolutions is their ability to preserve certain classes of structure that would otherwise be lost under the original filter. In particular, one property that morphological pseudoconvolutions possess is that the invariant class of structure of the original filter $\Psi$ will be a subclass of the invariant class of the corresponding pseudofilter, or $\text{Inv}(\Psi) \subset \text{Inv}(\Psi')$. For example, since steps are invariant under median filtering, steps are also invariant under pseudomedians, but fast varying texture may also be invariant under pseudomedians.

Another desirable property of pseudoconvolutions is that if the original filter is morphological, then the corresponding pseudofilter will also be morphological. This is a highly desirable property indeed, as the basic properties intrinsic to morphological filters, namely translation invariance and increasing, are important (and often assumed) when filtering is performed.

Notice also that if $\lambda = 0$, then the original filtering operation (mean or median) is the result. Conversely, as $\lambda$ tends toward infinity, no matter what filter has been chosen, the result will be the original unfiltered image. A proper $\lambda$ must therefore be chosen to bring back an acceptable amount of image while not bringing back too much noise.
Pseudoconvolutions are especially effective on noise that is not necessarily uniform across the image, but occurs in bursts. This is because they act somewhat adaptively across the image; that is, they treat some parts of the image that may contain more or less noise differently than other parts. This is very useful in STM/AFM imaging because the type of noise processes that occur tend to be highly non-uniform. If the structuring element fits in one region of the image, no filtering will be done. If, however, in a noisier region of the image the same structuring element does not fit, filtering will be performed. This is seen in Figure 3-1.

Pseudoconvolutions are general in the sense that any filter may be used in conjunction with them, (for example we could have a pseudoWiener filter) but here only pseudomeans and pseudomedians are studied. The decision to use either the pseudomean or pseudomedian is made based on the image and noise content, following the same guidelines as whether to use the mean or median. If, for example, the image is slowly varying and has white noise, the pseudomean should be used; if, however, there are desired edges and/or undesired sparse point noise in the image, the pseudomedian is preferable (see Refs. 3, 4 for a statistical analysis regarding this choice).
Figure 3-1: Example of erosion and dilation on a signal by the structuring element e, where f(x) is the input. The erosion eliminates maximum noise and the dilation eliminates minimum noise.
Figure 3-2: Example of a three point pseudomean on a signal by the structuring element e.
Chapter 4
Application of morphological pseudoconvolutions to STM/AFM images

4.1 Adaptation of morphological pseudoconvolutions to STM/AFM type data

Upon first using pseudoconvolutions, improvement over previously used methods was found in many images. However, because of the sharpness of the structuring element, some line noise in STM images resulting from the 1/f noise was brought back along with useful information, the reason being that the sharp peak of the structuring element increasingly fits into the lines as \( X \) grows. White noise was also noticeable as \( X \) increased, for the same reason.

The structuring element introduced in Refs. 3, 4, 5 was used to bring out highly varying texture information and preserve edges in the presence of point noise. STM and AFM images do not generally have edges or texture as sharp as that discussed in Ref. 3. Because most structures have a rounded shape (atoms, absorbed molecules, etc.),...
structuring element is chosen to be a paraboloid of revolution sampled in a 5x5 mask (see Figure 4-1). This allows the structuring element to fit very well into the desired information, while not passing the noise.

With its new shape, the structuring element probes more fully the data, and thus point noise and white noise are not allowed through. The desired image, however, is restored (with relatively small λ) and there is strong improvement over the mean and median. Also, with the new filter mask (using 25 points as opposed to 5 in Ref. 3), line noise is not allowed through, because the structuring element now does not fit into thin lines.

Although rigor will not be provided here, the same properties as in Ref. 3 hold true for pseudoconvolutions with the new structuring element. As λ approaches infinity, for example, the filter becomes very sharp and thus all of the original data passes. This process, however, is not as abrupt as with the previous structuring element.

4.2 Development of criteria for evaluating pseudoconvolutions

The usual method for evaluating the effectiveness of a filter in a certain environment is to first create noise and ideal image models appropriate to that environment. The noise model is added to the image model and this noisy image is filtered by the filter in question. The filtered image is then compared to the ideal image.
4.2.1  Mean Square Error - metric for comparison

The standard basis of comparison is global MSE. The global MSE is found by taking the squared difference between each pixel in the ideal image and the corresponding pixel in the filtered image, summing all of these squared differences, and dividing the sum by the total number of pixels. As mentioned before, this is not necessarily the best metric for the eye. We will use it, however, for lack of a better one, and also to follow standard practices. One must keep in mind, however, that edges, which have a strong influence on our eyes\textsuperscript{22} and on quantitative analysis, will not have a strong influence on the overall MSE because they do not make up much of the total image area, and thus the blurring of them will not make much of an overall numerical difference. In order to illustrate this point, the MSE of a filtered edge is included in the analysis.

4.2.2  Development of noise model

Often, the noise of an imaging system is estimated by collecting several images, averaging them, and subtracting this average from one of the images. Such an approach presents statistical pitfalls. In particular, there are problems in applying this method to STM and AFM images. Thermal and piezoelectric drifts cause offsets in subsequent images and make a pixel by pixel comparison difficult. For example, if the image consists of a number of bumps, and the bumps do not align between images, then the misalignment of the bumps will appear as noise.
Another possible method, useful if the image information is at a lower frequency than the
noise, is to subtract the moving average of the image from the image itself. One advantage
of pseudoconvolutions over linear filters, however, is their ability to preserve step
information. If this averaging method is used, step information in the original image would
appear as noise in the frequency domain. This is because steps would be averaged out, as
they consist of high frequency information. Because of these problems, the source of
noise in STM images will be considered, and then this noise will be simulated.

The noise in STM images arises from a number of sources. These sources include noise
generated by the feedback circuit, inadequate damping of vibrations, variation in the tunnel
junction characteristics, and piezoelectric and thermal drift over time. The magnitude of
each of these noise sources depends on the conditions under which the sample is imaged.
For example, mobile molecules entering the tunneling gap will in general cause spikes in
the tunneling current and thus some response in the tip to sample spacing, while in vacuum
this noise source will for the most part be absent. The size of the scan and the rate at which
the scan is taken will determine the spatial frequency of the noise. As an extreme example,
thermal drifts can be eliminated by scanning the sample sufficiently fast.

Many physical processes possess a 1/f noise spectrum, which has been observed in the
STM current spectrum by a number of researchers.2,11,12,13 However, since the image is
collected in time as the probe is scanned along the x axis, there will be no correlation
between adjacent points on different scan lines, and the noise spectrum along the y axis will
be white noise.1 The noise spectrum is therefore obtained by generating white noise in the
spatial domain, taking the Fourier transform, multiplying each point of the Fourier
transform by $1/k_x$, where $k_x$ is the wave number in the scan direction, and then calculating the inverse Fourier transform.

4.2.3 Development of image model

Because STM and AFM image features are not always observable with other techniques, it is not always clear what an ideal image should look like. The graphite surface has been extensively studied in air and sources of noise have been discussed by several research groups. An ideal image consist of a triangular lattice. However, asymmetric tips often cause a distortion of these atoms. Even though the image is distorted, the symmetry of the graphite lattice constrains the structure to have 3-fold symmetry, and since the microscope can resolve only the lowest Fourier components, an image is well approximated by a summation of three cosine waves oriented at 120 degree angles. This sum is therefore taken to represent the ideal image. It is displayed in Figure 4-2, along with a cross section of the data.

4.3 Comparison of pseudoconvolutions with Wiener filtering

Pseudoconvolutions are compared with the Wiener filter method discussed by Park and Quate both qualitatively and relative to MSE. In their method, the spectrum is chosen as $1/f$ in the $k_x$ (scan) direction, and independent of frequency (white) in the $k_y$ direction. It should be noted that they employ a form of the Wiener filter that demands uncorrelated
noise, whereas 1/f noise is a strongly correlated noise. The power spectrum estimate of the (uncorrupted) image is taken to be that of the input (noisy) image, and a weighting parameter adjusts the amplitude of the noise so that from eqn. (5) the filter reads:

$$G(k_x, k_y) = \frac{1}{1 + [(\alpha/k_x)/S_u(k_x, k_y)]}$$  \hspace{1cm} (9)

where \(\alpha\) is the parameter in question, and we have divided through by \(S_u\) to show the direct influence of the noise spectrum and the signal spectrum on the filter. In practice, \(\alpha\) is adjusted until an acceptable amount of filtering has been accomplished.

Several important points should be made clear here. First, for reasons previously discussed, a graphite lattice is chosen for the image model. As can be seen in Figure 4-2, this model is not only slowly varying, but is also essentially wide-sense stationary. The model is therefore an excellent environment for Wiener filtering. Second, the 1/f\(_x\) noise has been chosen and implemented, and a Wiener filter that contains as its noise estimate the very same noise present in the image has then been chosen. In a real imaging environment, the noise will not be given in this manner and will most likely change, thereby making a perfect noise estimate unobtainable. In sharp contrast to the present Wiener filter, pseudoconvolutions will remain symmetric, and thus will filter equally in both the x and y directions. Lastly, the numerical basis for comparison is MSE, which is not only a linear metric, but is precisely the goodness measure the Wiener filter minimizes.
The presence of \(1/f\) noise causes horizontal lines to appear in the input image. This is referred to as \textit{scan-line} noise. Three noise conditions are simulated, in which only the amplitude of the scan-line noise is adjusted. For noise A, the amplitude of the scan lines is half of the amplitude of the image, for B the amplitude of the scan lines is approximately that of the image, and the amplitude of noise C is 1.5 times that of the image.

4.4 Results and analysis for graphite model

Because the simulated graphite image has no edges and the simulated noise contains no point noise, the appropriate filter is the pseudomean. Also, \(\alpha\) and \(\lambda\) have been adjusted to minimize MSE in the Wiener filter and the pseudomean, respectively. One should keep in mind that the motivation behind using pseudoconvolutions is not simply to minimize MSE as in the Wiener case, but to bring back useful information without a great deal of noise gain. We expect a plot of MSE versus \(\lambda\) to stay relatively constant over a range where the structuring element fits into the image and not the noise. For larger \(\lambda\), the structuring element fits into the noise and MSE will increase more rapidly with \(\lambda\). If MSE stays constant or goes up slowly while we acquire more information, this is fine. If MSE actually goes down with increasing \(\lambda\) for a region, this is all the better.

A cross section through the maxima of Figure 4-2 given by 
\[
\cos(4\pi y/3a) + 2\cos(2\pi y/3a),
\]
where \(a\) is the nearest neighbor carbon atom spacing, shows two valleys, one shallow and one deep. The difference in the depth of the valleys is due to the higher frequency component; however, the shallower of the two is more difficult to recover after adding
noise. A gauge of a filter's effectiveness is the restoration of the small valley upon filtering. This is exactly the type of information that may be important in order to gain greater knowledge of a real sample.

Figures 4-3(a) and 4-3(b) show the plots for noise types A, B, and C, for the Wiener filter and pseudomean, respectively. A 5x5 mean was used for the pseudomean. MSE is normalized by dividing by the MSE of the unfiltered noisy image. This is then multiplied by 100 to show the percentage of the unfiltered MSE.

Referring to the curve for noise A, the minimum MSE is almost identical for both filters. Note the drop of about 3% MSE in the pseudomean from the mean at $\lambda = 30$. The drop in MSE from the original noisy image is approximately 67% for both. The fact that the pseudomean performs as well as the Wiener filter in this environment relative to MSE is remarkable. Figures 4-4(a), 4-4(b) and 4-4(c) show the unfiltered image with noise A, the optimally Wiener filtered image, and the optimal pseudomean filtered image, respectively. Even though the drop in MSE is the same in both cases, the Wiener filter has introduced an asymmetry into the previously six-fold rotationally symmetric graphite image. The graphite image arises from the sum of six equal amplitude Fourier coefficients located on the vertices of a hexagon. However, Wiener filtering decreases the amplitude of the Fourier coefficients with a larger $k_x$ relative to those with a smaller $k_x$. The same general phenomenon can arise from multiple tips, and gives rise to the triangular array of ellipses in Figure 4-4(b). The effect of Wiener filtering can also be seen in the cross section. For a cross section perpendicular to the scanning direction, the amplitude is given as $\cos(4\pi y/3a) + 2\cos(2\pi y/3a)$. The first term, which is of higher spatial frequency, is decreased in the
filtering and this eliminates the shallow valley. In Figure 4-4(c), however, the image filtered by the pseudomean more closely resembles the original image. The 6 fold rotational symmetry is maintained and the cross section shows that the small valley is preserved. The restoration of the valley results because the optimal parabola fits into and thus restores it after the mean has blurred it out. This image is preferable to the Wiener filtered image because we have not lost (possibly vital) structure.

Referring to the plots for noise B, the pseudomean does about 4% better than the Wiener filter. This is because the signal to noise ratio is unity, and thus the assumption that the (uncorrupted) image power spectrum is approximated by the input spectrum in the Wiener filter function is not a good one. Figures 4-5(a), 4-5(b), and 4-5(c) show the unfiltered image, the optimally Wiener filtered image, and the optimal pseudomeaned image, respectively. Even though the difference in MSE between the two filtered images is not great, the pseudomeaned image has been much better restored. One can still make out the small valley in many places across the image in the pseudomeanded image, but the Wiener filtered image remains obscured by noise.

Referring to the plots for noise C, the pseudomean does several percent better than the Wiener filter. Referring to Figures 4-6(a), 4-6(b), and 4-6(c), we see that the Wiener-filtered image is severely degraded by noise, while the pseudomean does quite well in preserving the overall structure. For both, the small valley is far too degraded to be recovered, but the pseudomeaned image could be analyzed globally to determine atomic spacing, while this would be more difficult in the Wiener filtered image.
4.5 Analysis on edges

The Wiener filter and the pseudomedian are compared on a modeled bar, shown in Figure 4-7 oriented at an angle 30° to the horizontal. This may represent a polymer strand or a molecule on a background. To quantify the effect of filtering, MSE is taken only in the neighborhood of the bar so that the edges will have a greater influence on the results than before. Because the Wiener filter operates asymmetrically, a comparison for a series of bars at 15° increments through 90° is performed.

Noise B was used because the structure of the image is simple, so a good filter should be able to recover it in a reasonable amount of noise. Figure 4-8 plots MSE versus angle of rotation of the bar from the horizontal for both the Wiener filter and pseudomedian derived from a 5x5 median. Also, the optimal λ was approximately 20% of the step height for all points.

From the first point on the plot (θ=0) it is clear that the Wiener filter performs quite poorly on horizontal edges, improving MSE by only 7%. Poor performance results because the edges of the bar are similar to the scan-line noise that the filter would optimally remove. The original noisy image, along with both the optimal Wiener and pseudomedian filtered images are shown in Figures 4-9(a) 4-9(b) and 4-9(c), respectively. Referring to Figure 4-9(b), it is clear that the Wiener filter performs poorly on information in the horizontal (scanning) direction. The pseudomedian, however, does quite well. A cross section is given to show the restoration of the bar. The small amount of high frequency noise
noticeable in the cross section does not show up to our eyes when the image is viewed. A quantitative analysis regarding the size and shape of the structure may be done on the image filtered by the pseudomedian, but not on the image filtered by the Wiener filter.

As the angle from the horizontal increases, the Wiener filter's performance improves, while the pseudomedian's performance remains fairly constant, and the two curves start to converge at 45°. This is as expected: The pseudomedian is symmetric, so we expect performance that is independent of angle; the Wiener filter is heavily biased towards filtering information oriented in the horizontal direction, so it will preserve off-horizontal information more effectively. The Wiener filter performs better than the pseudomedian (in the MSE sense) for θ>75°, because the bar is nearly vertical: the information now lies perpendicular to the noise, so the Wiener filter is effective. The pseudomedian’s results stay relatively constant, giving consistently impressive results at all angles. Note that the slight change in apparent trend for both filters in the region 45° - 75° results from the noise distribution in the particular realization we are using. Figures 4-10(a) 4-10(b) and 4-10(c) show the noisy image, along with the optimal Wiener and pseudomedian filtered images, respectively, when the bar is perfectly vertical. Even though the Wiener filter gives better MSE for θ near 90°, the performance of the pseudomedian is close to that of the Wiener filter, thereby demonstrating the pseudomedian's versatility.
4.6 Empirical results and analysis

In Figure 4-11(a), an unfiltered 128x128 STM image of calf thymus DNA is shown. DNA has been imaged by a number of research groups, with some groups arguing that they have identified molecular structure.\textsuperscript{28,29,30} This sample was prepared by placing a drop of a 7mM DNA water solution on a cleaved graphite substrate and allowing the drop to evaporate. The remaining residue was imaged in air. In A form, or at low humidity, DNA is known to have a helical geometry with a pitch of 24-28Å and a width of 22Å.\textsuperscript{31} When these helices are constrained to lie flat on a surface, they will appear as zigzagging strands. In the image, one can identify three zigzagging strands running vertically starting at the bottom of the image. The left strand is much wider than the other two. Possible causes are friction between the tip and the DNA, or motion of the DNA induced by the tip. Both these occurrences would cause the imaging system to reveal more motion between the tip and the DNA than exists in reality.

The presence of 1/f noise, which appears as horizontal lines, makes it difficult to locate the edges of the DNA strand, because the edges lie in the same direction as the line noise. Specifically, the bright horizontal noise lines fool the eye into thinking that these lines are edges of the DNA. A determination of the pitch, which is gauged by the strand edges, may be incorrectly deduced because the edge of the strand could be misjudged.

The noise amplitude in Figure 4-11(a) is on the order of the signal amplitude. An attempt to use a Wiener filter to correct this image is shown in Figure 4-11(b). Notice how some edges in the original image lie essentially parallel to the scan direction, where the Wiener
filter does poorly, as was demonstrated in the case of the horizontal bar in the previous section. To eliminate the scan-line noise and see any apparent change in the original image, one must choose \( \alpha \) in eqn. (9) to be much larger than that of the parameter found to be optimal for the graphite image model under similar noise conditions. The resulting image contains only periodic strands of negative slope (going down the image from left to right), whereas the original image contained strands of both positive and negative slope giving the zigzagging pattern characteristic of DNA. The resulting structures can be easily misinterpreted, because they are spatially periodic.

Referring to eqn. (9), we can discern the reason for this effect. If \( \alpha \) is too large, thereby giving a strong positive bias to the noise estimate, image components corresponding to moderately sized noise components will be overly suppressed along with the noise. Consequently, parts of thin strands possessing small positive slope are eliminated along with the scan lines (that have zero slope), while parts of strands containing the larger negative slope remain. The problem here is that when using frequency based filters, including the Wiener filter, if the noise and image contain similar frequency components, one has the choice of either leaving the noise contributed components, or eliminating both the image and noise content at these frequencies.

Non-linear filters, however, can recover image information of similar frequency to that of the noise. Application of the pseudomean to Figure 4-11(a), shown in Figure 4-11(c), allows a clear identification of the position of the strands, most clearly seen at the bottom-center of the image running vertically. A 7x7 mean was applied and subsequently operated on by a \( \lambda=35 \) structuring element. Such a large convolution window was used to ensure
that the scan-line noise was eliminated. The useful information is then recovered with the parabolic structuring element, since the shape allows the element to fit into the DNA, but not the lines. The scan-line noise is no longer a dominating feature of the image. Comparison of Figures 4-11(a) and 4-11(c) shows that no artificial structures are introduced.

The STM can also potentially identify molecular features in absorbed polymers.32,33 In Figure 4-12(a), an unfiltered 256x256 image of 3.1x10^{-5} g/mL of polyhexylthiophene dissolved in toluene is shown, prepared the same way as the DNA sample. This image shows three strands, one at the left of the image, and two near the center of the image, one apparently crossing the other. In the upper right corner there is some structure appearing as protrusions along the strand, but this structure is obscured by noise. These protrusions may be due to the hexyl side groups of the polymer. To verify this, one would like to accurately describe their spacing.

Determining the edges of the protrusions is difficult, because the presence of scan-line noise causes these edges to appear at different locations in each scan line. The pseudomedian was chosen (with a 5x5 median, found to be empirically optimal) in order to get rid of the point noise (noticeable in the background) and to preserve the edges. The structuring element in the pseudomedian eliminates this noise by not fitting between these scan lines. The edges of the protrusions in the filtered image, shown in Figure 4-12(b), are uniform from one scan line to the next, and one can better quantitatively determine their spacings and relate them to the expected spacing in the polymer.
Figure 4-1: Parabolic 5x5 structuring element mask for use with pseudoconvolutions, and one-dimensional cross section for $\lambda = 1$. 
Figure 4-2: Simulated graphite for image model shown with cross section. Notice large and small valleys in cross section.
Figure 4-3: Plots of normalized mean square error versus filtering parameter for noises A, B, and C for (a) images filtered by Wiener filter and (b) images filtered by pseudomean.
Figure 4-4: Graphite image model (a) corrupted by noise A (b) filtered by Wiener filter and (c) filtered by pseudomean, shown with cross sections.

Notice how the Wiener filter introduces an asymmetry to the image.
Figure 4-5: Graphite image model (a) corrupted by noise B (b) filtered by Wiener filter and (c) filtered by pseudomean, shown with cross sections.
Figure 4-6: Graphite image model (a) corrupted by noise C (b) filtered by Wiener filter and (c) filtered by pseudomean, shown with cross sections.
Figure 4-7: Modeled bar for analysis of edges shown with cross section.
Figure 4-8: Plot of normalized mean square error versus angle of rotation of modeled bar for Wiener filter and pseudomedian.
Figure 4-9: Modeled bar shown horizontally (a) corrupted with noise B (b) filtered by Wiener filter and (c) filtered by pseudomedian, shown with cross sections.
Figure 4-10: Modeled bar shown vertically (a) corrupted with noise B (b) filtered by Wiener filter and (c) filtered by pseudomedian, shown with cross sections.
Figure 4-11: Image of DNA shown (a) as raw data (b) filtered by Wiener filter and (c) filtered by pseudomean. Notice how the Wiener filter cuts out information with positive slope, while the pseudomean preserves the overall structure.
Figure 4-12: Image of Polyhexylthiophene shown (a) as raw data and (b) filtered by pseudomedian.
Conclusions/Recommendations

Morphological pseudoconvolutions have been applied to STM images and, with respect to certain kinds of important information, have been shown to perform favorably when compared to a common Wiener filter employed in STM imaging. While the latter works well on information in the vertical direction, it performs less well on information oriented in the horizontal direction, this difference owing to the manner in which the Wiener filter is designed relative to the directional noise model. Just as key is the way in which morphological pseudoconvolutions preserve small structure that is often blurred by linear filters, as well as their tendency to avoid the introduction of artifacts. Regarding the two pseudoconvolution classes discussed, pseudomeans are especially effective on slowly varying information, such as atomic structure, whereas pseudomedians are particularly effective at restoring edges and eliminating point noise, while at the same time not degrading the underlying image texture.

The paraboloid structuring element used in this study was not optimized in a mathematical framework, but was rather developed from an empirical approach, taking into consideration a specific image model. The study of the optimization of non-linear filters has just begun, and to further this, a metric for optimization has not even been agreed upon. It would be highly useful to use the simple graphite model presented in this study as a test case for the study of non-linear optimization. In addition, as it is well known that global MSE (while it is widely used for comparison purposes) is not necessarily the best metric for the eye, the development of a new, realistic metric that takes into consideration how the eye responds to stimuli would be most useful.
References


