The Use of Regularized Least Squares Minimization for the Deconvolution of SEM Images

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Major advances are currently taking place in image processing algorithm development. When combined with today’s high speed computers utilizing multicore processing and very large memories the door is opened to the practical application of regularization techniques to the restoration of SEM images with improved spatial resolution. It is well recognized that an observed SEM image can be thought of as the convolution of a point spread function (psf) arising from measurement broadening and the true structure imaged. However, even with the abovementioned advances, a variety of additional limitations arise that are preventing the practical implementation of deconvolution to SEM image restoration. These factors include noise as well as a lack of detailed knowledge of the psf since no experimental technique is currently available to directly measure it with level of spatial resolution required. Furthermore, the problem is complicated by other factors such as specimen drift, contamination, the three dimensionality of specimen, signal excitation volume considerations, non-linearity in the scanning system and also non-linear behavior in the detection chain [1].

Fortunately, the problem is not as intractable as it might seem, if attention is carefully paid to all of the above details. First consider the mathematical description of deconvolution. For the purpose of subsequent analytical calculations, even though the true image and the observed image are m by n matrices it is standard practice to express them as column vectors and the convolution process can then be represented as:

\[ I_c = AI_t + k \] (1)

where \( I_c \), \( I_t \) and \( k \) are \( m \times n \) by 1 vectors for the blurred image, true image and noise respectively. In the absence of noise the determination of \( I_t \) could be viewed as a minimization of \( \| I_c - AI_t \|_2^2 \) where \( A = \text{circ}(b) \) is the block circulant \( m \times n \) by \( m \times n \) matrix of the psf, here designated as ‘b’. If \( A \) is known, the minimization becomes a least squares problem of some size for images that are typically at least 500 by 500 pixels. Unfortunately, if even a small amount of noise is present the problem can become quickly ill-posed and a useful solution can not be found.

The ill-posedness of the simple least squares problem can be eliminated by incorporating regularizers in the least squares objective. Typical choices for such regularizers include the l2 norm and the total variation (TV) term [2]. These terms allow a solution to be obtained by trading off the least squares minimization requirement with the regularizer. For instance, when the TV regularizer is used, the resulting minimization equation has the form:
\[ \min_{l} \left( \frac{\lambda}{2} \| I_c - \text{circ}(b) I_l \|_2^2 + \sum_i \| \text{circ}(w_i) I_l - z_i \|_1^2 + \| z_i \|_1 \right) \]  

This function is not differentiable, as is needed for the minimization, but can be made so through the use of an auxiliary vector \( z_i \) with \( i = 1, \ldots, l \) to form the equation:

\[ \min_{l} \left( \frac{\lambda}{2} \| I_c - \text{circ}(b) I_l \|_2^2 + \sum_i \frac{\beta}{2} \| \text{circ}(w_i) I_l - z_i \|_2^2 + \| z_i \|_1 \right) \]  

As the solution to equation (3) approaches that of equation (2) and equation (3) can be solved by iterative block coordinate descent. The problem in (3) can be efficiently solved using the Fourier transform of the images for even the relatively large images [2], and we have developed an interactive MATLAB code implementing this algorithm. Representative results are given in figure 1 for both \( l_1 \) and \( l_2 \) (Tikhonov) regularizations. Improved resolution is definitely present and work is progress to quantify the amount as well as to assess the most effective penalty factors and their associated parameters.

References:
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Figure 1. Titanium spheres imaged with an LaB6 source SEM: a) 18 nm/pixel reference image with the probe size smaller than the pixel size, b) restored image using \( l_1 \) regularization of image c) obtained with a 67 nm probe size. All images have the same number of pixels. The arrow in b) clearly demonstrates improved resolution relative to the same region in c).