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Denoising time-resolved microscopy image sequences with singular value thresholding

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ABSTRACT

Time-resolved imaging in microscopy is important for the direct observation of a range of dynamic processes in both the physical and life sciences. However, the image sequences are often corrupted by noise, either as a result of high frame rates or a need to limit the radiation dose received by the sample. Here we exploit both spatial and temporal correlations using low-rank matrix recovery methods to denoise microscopy image sequences. We also make use of an unbiased risk estimator to address the issue of how much thresholding to apply in a robust and automated manner. The performance of the technique is demonstrated using simulated image sequences, as well as experimental scanning transmission electron microscopy data, where surface adatom motion and nanoparticle structural dynamics are recovered at rates of up to 32 frames per second.

1. Introduction

Observing dynamic behaviour using microscopy can play a crucial role in revealing new insights into chemical reactions, structural transformations and biological processes. In these direct observations, length scales can range from millimetres in light microscopy to picometres in aberration-corrected transmission electron microscopy (TEM), whilst observation timescales may reach the femtosecond regime [1]. Important analysis of the image sequences can include particle tracking [2], migration of defects and grain boundaries [3,4], and bond making and breaking [5].

Dynamic imaging brings with it a considerable set of challenges. Acquiring rapid image sequences requires short exposure times for each frame, and the resulting low photon or electron counts lead to a degradation in the signal-to-noise ratio (SNR). Similarly, long observations of radiation-sensitive materials can alter the very processes being observed, causing severe damage to the specimen. Again, this requires the use of low dose imaging and thus a degraded SNR. Developing effective methods to denoise image sequences is therefore essential to expanding the applications of dynamic imaging.

Denoising is a well-studied problem in image processing, and many methods are capable of making significant improvements to the SNR. The related problem of video denoising has also been widely studied, and the most effective schemes for video denoising exploit the temporal correlation between frames. Recently, patch-based methods from image denoising have been extended to image sequences, such as the V-BM4D algorithm [6], which couples motion estimation with noise filtering to achieve state-of-the-art results.

Another promising approach for signal recovery is low-rank matrix approximation [7], which is closely related to the method of principal component analysis (PCA) [8]. Recently, low-rank matrix approximation has been combined with a patch-based approach to denoise dynamic MRI sequences [9]. This exploits the fact that a stack of correlated, vectorized frames from a video will form a matrix with low-rank, the recovery of which can be formulated as a convex optimization problem, known as nuclear norm minimization, and solved efficiently using singular value thresholding [10,11].

In this paper we describe a robust algorithm for denoising time-resolved microscopy image sequences, Poisson–Gaussian Unbiased Risk Estimator for Singular Value Thresholding (PGURE-SVT). The proposed approach, based on low-rank matrix approximation, comprises a number of features designed to address effectively the particular challenges of microscopy image sequences. These include optimal threshold selection, automated estimation of the noise characteristics, and motion estimation of image features. Importantly, the approach preserves, and indeed exploits, the temporal information of the data, and is generally applicable to many types of microscopy, including fluorescence microscopy and TEM. Using simulated image sequences, PGURE-SVT is shown

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to be competitive with the state-of-the-art in video denoising methods. In addition to rigorous evaluation via simulations, an example application to experimental annular dark-field scanning transmission electron microscopy (ADF-STEM) is presented, highlighting the potential of PGURE-SVT to reveal new insights into dynamic processes at the atomic level.

2. Theory

As the volume of data collected in microscopy experiments grows, there is an increasing need to process the datasets in a manner that extracts the key information content. This concept of dimensionality reduction is usually tackled with PCA and related methods, which seek to explain a large dataset in terms of a few principal components by exploiting correlations and structure in the data. Matrices that exhibit correlations between columns (or rows) can be described as low-rank matrices, and it is this attribute that enables the use of PCA. In a microscopy experiment, the underlying data is often low-rank but corrupted by noise, and so the low-rank data must be recovered from these noisy observations. The methods developed here share many principles with PCA, but some distinctive features are particularly advantageous, including robust automation of how much thresholding to apply.

Given a corrupted observation $\mathbf{Y}$ of a low-rank matrix $\mathbf{X}^0$, the goal of low-rank matrix approximation is to recover $\mathbf{X}^0$ as accurately as possible. A natural approach to this problem is to find the optimal solution to:

$$\arg\min_{\mathbf{X}} \|\mathbf{Y}-\mathbf{X}\|_F^2 + \lambda\,\mathrm{rank}(\mathbf{X}) \tag{1}$$

where $\mathbf{X}$ is the decision variable and λ is a regularization parameter [10]. $\|\mathbf{Y}-\mathbf{X}\|_F^2$ represents the square of the Frobenius norm, i.e. the sum of the squared differences of the matrix elements, $\sum_{ij}\left|Y_{ij}-X_{ij}\right|^2$. Stating the problem in this way thus imposes a low-rank constraint on the estimated matrix $\mathbf{X}$, whilst the use of a Frobenius norm ensures $\mathbf{X}$ is also a good fit of the observations, $\mathbf{Y}$. The following section outlines a computationally attractive algorithm for solving Eq. (1), and presents an automated approach for calculating the optimal value of λ under the experimental conditions encountered in microscopy.

2.1. Nuclear norm minimization

In practice, optimization of the rank function in Eq. (1) is an intractable problem. However, Candés and Recht demonstrated a powerful approach involving minimization of the nuclear norm of the matrix as a convex approximation to the rank function [10]. This approach is based on the singular value decomposition (SVD), defined for an $m \times n$ matrix $\mathbf{Y}$ as:

$$\mathbf{Y} = \mathbf{U}\mathbf{\Sigma}\mathbf{V}^T \tag{2}$$

where $\mathbf{U}$ is an $m \times m$ matrix of left singular vectors, $\mathbf{V}$ is an $n \times n$ matrix of right singular vectors ($\mathbf{V}^T$ represents the transpose of $\mathbf{V}$), and $\mathbf{\Sigma}$ is an $m \times n$ diagonal matrix. The values along the diagonal of $\mathbf{\Sigma}$ are denoted as σ_i, and are known as the singular values of the matrix $\mathbf{Y}$. The SVD is a common method for decomposing datasets in PCA, where the dataset is separated into scores $\mathbf{U\Sigma}$, and loadings $\mathbf{V}$.

Nuclear norm minimization seeks to approximate $\mathbf{X}^0$ by an optimal low-rank solution $\hat{\mathbf{X}}_\lambda$ according to:

$$\hat{\mathbf{X}}_\lambda = \arg\min_{\mathbf{X}} \|\mathbf{Y}-\mathbf{X}\|_F^2 + \lambda\,\|\mathbf{X}\|_* \tag{3}$$

where $\|\mathbf{X}\|_*$ is the nuclear norm of $\mathbf{X}$, which is defined as the sum of the singular values of a matrix, $\sum_i \sigma_i$ [10]. Cai et al. showed that a solution to Eq. (3) can be found in a computationally attractive manner using soft singular value thresholding (SVT) [11], according to:

$$\hat{\mathbf{X}}_\lambda = \mathrm{SVT}_\lambda\left(\mathbf{Y}\right) = \mathbf{U}\mathcal{S}_\lambda\left(\mathbf{\Sigma}\right)\mathbf{V}^T \tag{4}$$

where $\mathcal{S}_\lambda$ is the soft thresholding operator, and for each singular value σ_i:

$$\mathcal{S}_\lambda(\sigma_i) = \max[\sigma_i - \lambda,\, 0] \tag{5}$$

The soft thresholding operator contrasts with the typical hard thresholding approach in PCA, which retains only those components with singular values above a threshold λ [12]. Eq. (5) instead reduces all the singular values towards zero by a fixed amount.

For practical application to image sequences, a refinement to Eq. (4) can be made. Instead of applying a single threshold value to all singular values, a weighted threshold can be applied on the basis that larger singular values correspond to more important image features, and so should be reduced by a smaller amount [13]. Defining the weighted nuclear norm of $\mathbf{X}$ as $\|\mathbf{X}\|_{w,*} = \sum_i w_i\sigma_i$, where $w_i \geq 0$ is a weight assigned to the singular value σ_i, a solution is now sought for:

$$\hat{\mathbf{X}}_\lambda = \arg\min_{\mathbf{X}} \|\mathbf{Y}-\mathbf{X}\|_F^2 + \|\mathbf{X}\|_{w,*} \tag{6}$$

where the parameter λ has been incorporated into the weighted nuclear norm. The approach taken in [13] uses weights w_i in the order $0 < w_1 < \ldots < w_n$ (based on the fact that the singular values of a matrix are always sorted in descending order $\sigma_1 > \sigma_2 > \ldots > \sigma_n$). This ensures the use of soft singular value thresholding remains valid [14]. In the present work we propose to use an exponential weighting scheme to minimize the computational complexity compared to the scheme in [13]. Letting $\sigma_{max} = \max[\mathbf{\Sigma}]$, the exponentially weighted SVT operator incorporating the parameter λ is:

$$\mathcal{W}_\lambda(\sigma_i) = \max\left[\sigma_i - \sigma_{max}\exp\left(-\frac{\sigma_i^2}{2\lambda^2}\right),\, 0\right] \tag{7}$$

and the weighted SVT function is:

$$\mathrm{WSVT}_\lambda\left(\mathbf{Y}\right) = \mathbf{U}\mathcal{W}_\lambda\left(\mathbf{\Sigma}\right)\mathbf{V}^T \tag{8}$$

2.2. Patch-based nuclear norm minimization

In forming a so-called Casorati matrix, whose columns are the vectorized frames from an image sequence, the correlation between frames in the sequence means that such a matrix will be low-rank [15]. In reality, the size of the spatial dimension will often exceed the size of the temporal dimension ($n_x n_y \gg T$, where $n_x n_y$ is the number of pixels in each frame and T is the number of frames), and this may lead to problems with the SVT approach due to limited degrees of freedom [9]. Analyzing the image sequence via a patch-based approach can overcome this problem. The patch-based approach is illustrated in Fig. 1, where a 3×3 pixel patch is extracted from each frame and vectorized to form a column of the Casorati matrix $\mathbf{C}$.

Fig. 2 shows an example of SVT applied to a Casorati matrix formed by vectorized images of a 2D Gaussian peak. The resulting Casorati matrix shown in Fig. 2b is in fact rank 1, as can be seen in the singular value plot in Fig. 2e. These singular value plots can be interpreted in a similar way to a scree plot in PCA, in which most of the variance in the Casorati matrix (and by extension the original image sequence) can be explained by the first component, and the remaining components mainly describe the noise in the

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