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A FAST CLASSIFICATION METHOD FOR SINGLE-PARTICLE PROJECTIONS WITH A TRANSLATION AND ROTATION INVARIANT*

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Abstract

The aim of the electron microscopy image classification is to categorize the projection images into different classes according to their similarities. Distinguishing images usually requires that these images are aligned first. However, alignment of images is a difficult task for a highly noisy data set. In this paper, we propose a translation and rotation invariant based on the Fourier transform for avoiding alignment. A novel classification method is therefore established. To accelerate the classification speed, secondary-classes are introduced in the classification process. The test results also show that our method is very efficient and effective. Classification results using our invariant are also compared with the results using other existing invariants, showing that our invariant leads to much better results.

Mathematics subject classification: 65D17.
Key words: Classification, Fourier transform, Translation and rotation invariant, Secondary-class.

1. Introduction

Single-particle reconstruction (SPR) is a powerful method in three dimensional electron microscopy [2], which demands that all of the projection images are from the nearly identical macromolecular "particles". The aim of the SPR is to find three dimensional structures of a macromolecule given its two-dimensional noisy projection images at unknown random directions [16].

One of the main problems in electron microscopy is that the object is damaged by the exposure. To avoid the damage, low electron dose is used, and therefore the projection images exhibit very low signal to noise ratios (SNR, below 1/3) and very poor contrast [17]. A way to solve this problem is to put many identical objects onto the stage, which results in many projection images of the same object at unknown orientations [11]. In order to reduce the effect of the high noise and poor contrast, a large number of projection images (from 10^4 to 10^6) are collected and analyzed, which means that the computation load is heavy even for a modern multi-processor computer cluster [18]. Therefore, a primary step of the single-particle analysis is the classification of the measured images according to their similarities. Images in the same class are then averaged to reduce the noise level [3, 8].

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Previous Work

Classification is a procedure that categorizes images into different classes according to their similarities [10]. Existing classification methods are divided into supervised classification and unsupervised classification [2]. Supervised classification is to categorize the images according to the similarity with templates or references, for example, projection matching. Unsupervised classification is to classify the images according to their intrinsic differences. According to the comparison among 2-D projection images, these projection images are classified into different classes. Distinguishing among different image classes requires that the images in these classes are aligned first. As a result, the computational load is heavy because any two projection images need to be aligned before their correlations are computed. Alignment is a difficult task since it is hardly possible to align a highly noisy data set without any deviation [14].

Van Heel et al. [9] propose a multireference alignment method in which the alignment and classification steps are iteratively alternated until convergence. Assuming that a set of class representatives have been selected, the similarities between the aligned images and the representatives are measured. The image is assigned to the class with the maximum similarity. Eventually, the representative of the class is recomputed as the average of the images assigned to the class. This process is repeated till some convergence criterion is met. A possible shortcoming of this classification method is that it depends on the initial selection of the class representatives and it possibly traps in a local minimum. To solve these problems, a multireference alignment algorithm based on a maximum likelihood (ML2D) was devised in [9]. However, ML2D [15] method suffers from the *attraction problem* [17], a phenomena that a class-average with less noise than others attracts more experimental images even if they belong to other classes.

Kerdprasop et al. [5] propose a weighted k-means algorithm for clustering data based on similarity. The clustering process is speeded up by a reservoir-biased sampling technique for data reduction. Recently, Yang et al. [19] describe an iterative stable alignment and clustering approach that can extract homogeneous subsets of images and requires only a small number of parameters and, with minimal human intervention.

Colars et al. [17] propose a novel method of clustering 2D (CL2D) images that is able to address small differences between classes. With this method, all the projection images can be split into specified number classes and at the same time the misclassification error is minimized. The key ideas of the CL2D method are as follows: Firstly, the correlation is replaced by the correntropy, a more effective metric. Secondly, the images are assigned to the class by considering the images are more suitable for the class representative than the other experimental images. This comparison avoids comparing an experimental image to the class averages at different noise levels.

Our classification method is basing on a translation and rotation invariant. We therefore review here a few existing translation and rotation invariants, which have been used in electron microscopy [13, 14]. The detailed descriptions of these invariants are presented in section 2 of this paper. Van Heel et al. introduce in [13] a double auto-correlation function (briefed as DACF) to classify the projection images. At first, the auto-correlation functions (ACF) of the projection images are calculated and converted to the cylindrical coordinates. Then the second ACFs in the angular direction of the ACFs in cylindrical coordinates are computed, resulting in the DACFs. The authors in [13] point out that DACFs overweights the already strong frequency because of the squaring of the Fourier components in calculating the ACF. This disadvantage can be eliminated by using self-correlation function (SCF) instead of auto-