TWO DIMENSIONAL ARMA MODELS AND PARAMETER ADJUSTMENT TO ESTIMATE THE CTF OF THE ELECTRON MICROSCOPE

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A powerful parametric spectral estimation technique, 2D-ARMA (Auto Regressive Moving Average) modeling, has been applied to contrast transfer function (CTF) detection in electron microscopy. Parametric techniques such as AR (auto regressive) and ARMA models allow a more exact determination of the CTF than traditional methods based only on the Fourier Transform (FT). Previous works[1] revealed that AR models can be used to improve the CTF estimation and the detection of its zeroes. ARMA models reduce the model order and the computing time, and more interestingly, increase the achieved accuracy. ARMA models are generated from electron microscopy (EM) images, and then a stepwise search algorithm is used to determine all the parameters of a theoretical CTF model in the ARMA model previously calculated. Furthermore, this adjustment is truly 2D in order to properly treat astigmatic images. The user only needs to know a few *a priori* parameters of the experimental conditions for his micrographs, which turns this technique into an automatic and very powerful tool.

The ARMA model for an image[2] is defined by means of a difference equation expressing the relationship between a pixel and its surroundings, through the AR and MA coefficients, denoted by $\theta_{AR}(\mathbf{r})$ and $\theta_{MA}(\mathbf{r})$ respectively. The power spectrum of the image is then calculated from the ARMA model as:

$$S_I^{ARMA}(\boldsymbol{\omega}) = \left| \upsilon \frac{1+\sum_{\mathbf{r}\in R}\theta_{MA}(\mathbf{r})e^{-2\pi i(\boldsymbol{\omega}\cdot\mathbf{r})}}{1-\sum_{\mathbf{r}\in R}\theta_{AR}(\mathbf{r})e^{-2\pi i(\boldsymbol{\omega}\cdot\mathbf{r})}} \right|^2$$

In order to extract the values of the CTF physical parameters, a CTF model is adjusted to the power spectrum obtained with ARMA. The process performs a 2D surface adjustment, and no radial average is done in any way, in order to detect and adequately treat astigmatic images. Due to the large number of local minima that exist in the search space, an algorithm that gradually approaches the solution, fitting the CTF with parameters having physical meaning, has been developed.

RESULTS

We have tested our programs with simulated and real data coming from experiments of negative staining microscopy, carbon coated holey grids and holey grids cryomicroscopy. First of all, a quantitative test comparison between the ARMA models and the periodogram averaging (a FT based method) was done using simulated data. Periodogram averagings and ARMA models were calculated over 1470 images with simulated CTFs varying the defocus and the image size. The results obtained from the comparison of the ARMA models with the periodogram averaging using a suitable fitness figure were concluding: ARMA estimation was better in all the 1470 cases. These experiments also revealed that there existed a group of consensus ARMA models performing optimally for nearly all cases.

The method was applied to real micrographs obtained with different techniques and microscopes: negative staining, cryomicroscopy, and carbon coated cryomicroscopy. Figure 1 shows that the ARMA models allow a clearer determination of the CTF rings in a case where the classical methods encounter difficulties to detect the CTF.

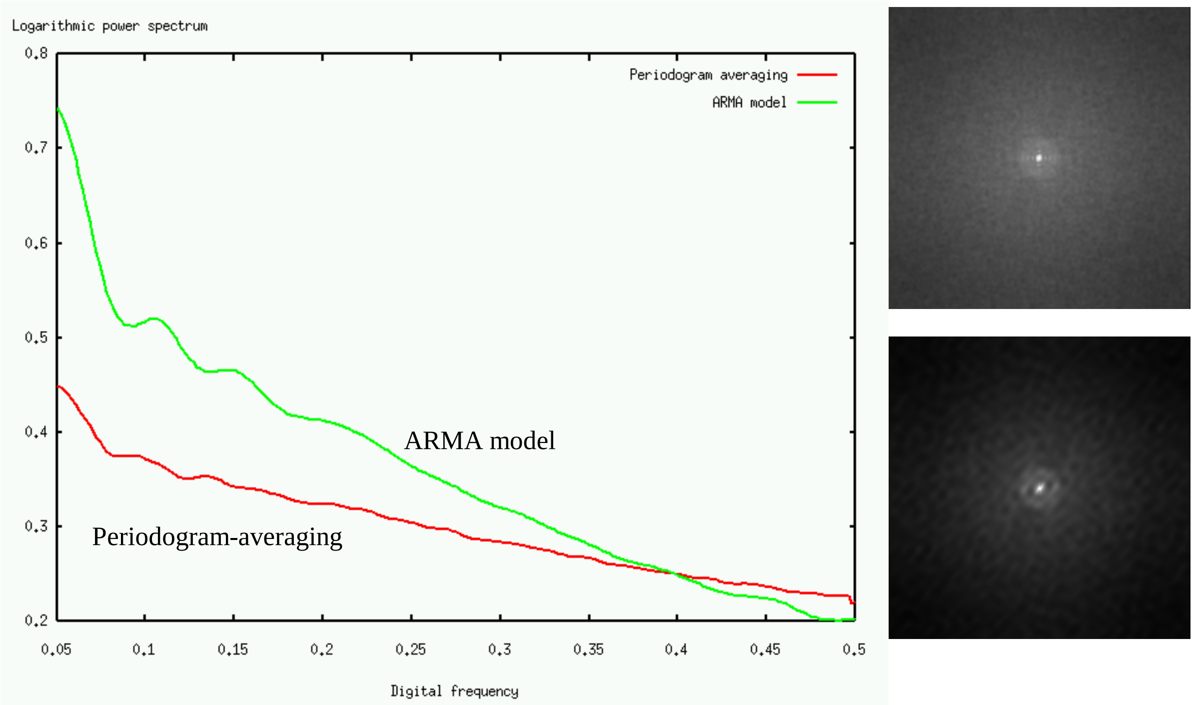

Figure 1. Results of CTF estimation for holey grids cryomicroscopy micrographs. Upper right: periodogram averaging. Lower right: ARMA estimation. Left: Radial averages of the CTF estimations. When the common practice of radial averaging is used, ARMA allows to see the first three zeroes of the CTF, while with the periodogram averaging only two are seen, and are definitely less noticeable.

REFERENCES

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