Sparse Phase Retrieval

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Coherent X-ray Diffraction Imaging (CXDI) is a technique for the 2-dimensional (2D) and 3D reconstruction of nanoscale structures. The detector receives the photons scattered by the object, and ideally, the diffraction pattern gives the power spectrum of the electron density. Since we are only provided the power spectrum and the phase is lost, we need to retrieve the phase in order to reconstruct the structure from the diffraction image.

Let $f_{xy} \geq 0$ be the electron density of a molecule projected onto a 2D plane. We consider the discretized coordinate, $x, y = 1, \cdots, M$ and ideal diffraction pattern is $|F(u,v)|^2$ where, $F(u,v)$ is the Fourier transform of $f(x,y)$ as follows,

$$F_{uv} = \frac{1}{M} \sum_{x,y} f_{xy} \exp\Big(\frac{2\pi i(ux+vy)}{M}\Big). \tag{1}$$

A widely used phase retrieval method is the hybrid input-output (HIO) method [1], [2]. The HIO method set a support region and assume $f_{xy} = 0$ outside the support and estimate the phase with an iteratively process. It effectively solves the problem for high signal-to-noise ratio measurements.

Recently, a new type of coherent beam, x-ray free electron lasers (XFELs), became available. This new technology can potentially provide a novel mean to determine the three-dimensional (3D) structure of biomolecules from the diffraction data of single molecules instead of conventional crystallography [3], [4]. One of the crucial processes of single molecule imaging is the phase retrieval from a very weak diffraction due to the "single" molecule. Figure 1a shows a simulated electron density of a biomolecule. If the power spectrum is obtained as in Fig. 1b, the HIO method will successfully reconstruct the 2D density. However, the simulated result of the diffraction pattern would not be any better than Fig. 2a. The diffraction image is so noisy that the HIO method does not even converge.

Here, we propose a new approach, the sparse phase retrieval (SPR) method [5], for retrieving phases of diffraction data which will be obtained by XFELs. Instead of assuming the support region, we use the Bayesian statistics as in [6], employing a sparse prior. Let N_{uv} be the number of the photons detected at (u,v) of the detector. It is natural to assume each N_{uv} follows a Poisson distribution independently,

$$p(\boldsymbol{N}|\boldsymbol{F}) = p(\boldsymbol{N}|\boldsymbol{f}) = \prod_{uv} \frac{|F_{uv}|^{2N_{uv}} \exp(-|F_{uv}|^2)}{N_{uv}!}, \tag{2}$$

where, $\boldsymbol{N} = \{N_{uv}\}$, $\boldsymbol{F} = \{F_{uv}\}$, $\boldsymbol{f} = \{f_{xy}\}$, and the fact $\boldsymbol{F}$ is a deterministic function of $\boldsymbol{f}$ was used. Assuming a sparse prior of $\boldsymbol{f}$ as $\pi(\boldsymbol{f}) \propto \prod_{xy} \exp(-\rho_{xy} f_{xy})$, where $\rho_{xy} \in \Re_+$, we compute the maximum a posteriori (MAP) estimator, and the SPR method computes the MAP estimate for the density reconstruction. The estimate $\hat{\boldsymbol{f}}$ is the maximizer of the following function,

$$\ell(\boldsymbol{f}|\boldsymbol{N}) = \sum_{uv} \big(N_{uv} \ln |F_{uv}|^2 - |F_{uv}|^2\big) - \sum_{xy} \rho_{xy} f_{xy}.$$

The sparse prior automatically sets many entries of $\boldsymbol{f}$ equal to 0 without specifying the support region and the sparsity is adjusted by modifying ρ_{xy}. Figure 2b shows the density reconstructed by the SPR method. Compared to the HIO method, the SPR method gives better results under the noise. This is a new promising direction for phase retrieval in practice.

References

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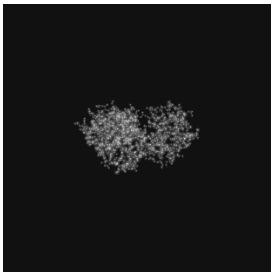
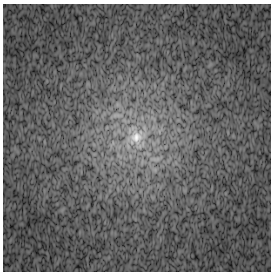
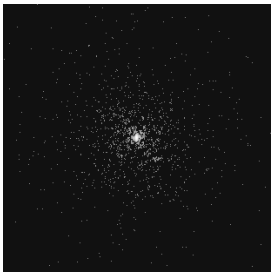


(a) Electron density of lysozyme.

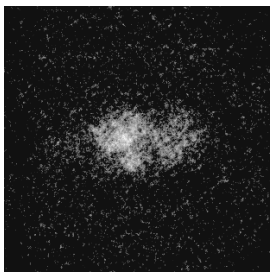


(b) Ideal diffraction pattern.

Fig. 1. (a) 2D electron density of a protein, lysozyme. (b) An ideal 2D diffraction image of lysozyme without noise.



(a) Simulated diffraction pattern.



(b) Reconstructed density.

Fig. 2. (a) A simulated diffraction image of lysozyme under a realistic situation. (b) A reconstructed density images with SPR method.