Phase Retrieval and Support Estimation in X-Ray Diffraction

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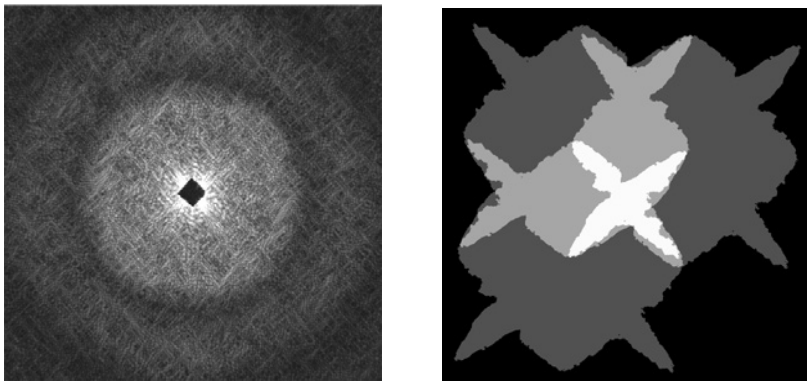
Phase retrieval algorithms originally developed for astronomy [1] and wavefront sensing [2,3] can also be used to reconstruct an image from an X-ray diffraction pattern of a nonperiodic object. Iterative transform algorithms, including the "hybrid input-output algorithm," transform back and forth between object space and Fourier space, enforcing the constraints and measured data in each domain. Gradient search algorithms typically optimize over an objective function that quantifies the difference between the collected Fourier data and the computed Fourier transform of a model estimate of the object. An analytic expression for the gradient enables efficient computations within an algorithm such as conjugate gradient search.

Important to the convergence of phase retrieval algorithms is determining a constraint for the support of the object, i.e., the set of points outside of which the object is known to be zero (or some constant). We have developed algorithms for placing upper bounds ("locator sets") on the support of the object from the support of its autocorrelation function [4-6], which can be computed by Fourier transforming the measured x-ray intensity data. Figure 1 shows an example on data provided by Henry Chapman at LLNL and Malcolm Howells at LBNL, from a collection of microscopic gold balls. The existence of the beam stop, preventing the measurement of the lower spatial frequencies, presents an additional challenge.



(a) (b)

Figure 1: (a) X-ray diffraction data, (b) upper bound on object support, shown in white: the intersection of three translated versions of the support of the autocorrelation function computed from (a).

References

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