Researchers use 'complexity' as a guiding tool to make phase retrieval easier for coherent X-ray imaging

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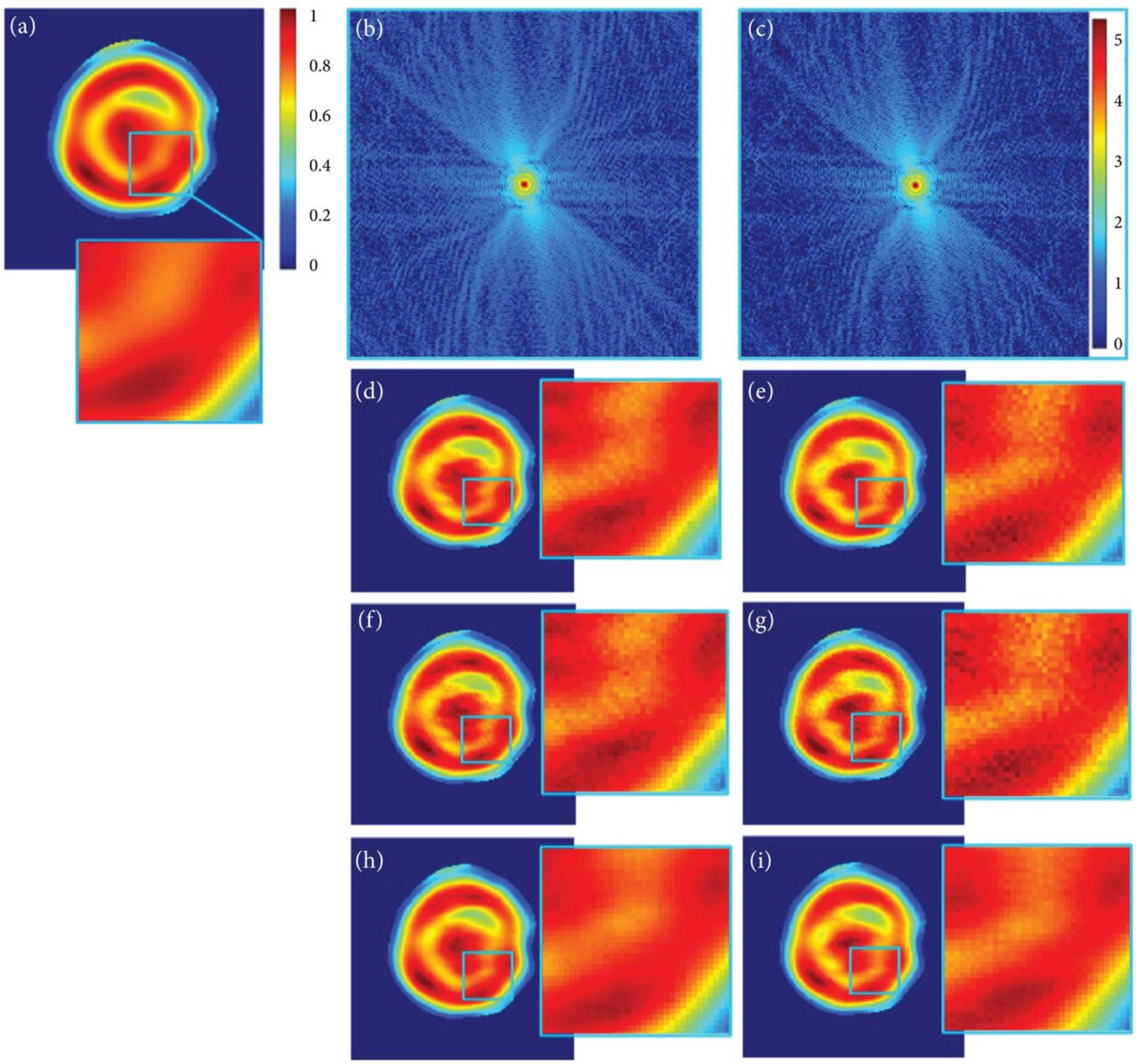

Reconstruction from noisy diffraction data using RAAR-ER and CG-RAAR algorithms. (a) Ground-truth amplitude for red blood cell (RBC) object (phase not shown). Simulated noisy oversampled Fourier intensity data of RBC in (a) corresponding to average light levels of (b) 1000 photons/pixel and (c) 500 photons/pixel. The data are shown as $|G|^{0.1}$ for the display purpose. Solutions recovered after (d, e) 1000 iterations of RAAR alone and (f, g) after concluding the solution in (d) and (e) by 100 ER steps and (h, i) 1000 CG-RAAR iterations from the noisy data shown in (b) and (c), respectively. For both the noisy data cases, the CG-RAAR solution can be clearly seen to be free from artifacts. All the solutions are displayed in colorbar range [0,1]. Credit: *Intelligent Computing* (2022). DOI: 10.34133/2022/9819716

Since their discovery by Roentgen in 1895, X-rays have become an effective tool for doctors to take images of their patients' bones, organs and vessels, and make better diagnoses. Scientists have continued this quest to acquire high-resolution images of interesting objects. Only this time, with much-advanced imaging hardware at hand, they are looking at micro- and nano-sized objects across the structural biology, material science, chemistry, and medical science fields while trying to determine their structures.

Coherent X-ray imaging (CXI), a technique largely enabled by X-ray free electron lasers (XFELs), applies to such structural analysis. But to reconstruct an image from incomplete, noisy Fourier intensity data obtained by a typical CXI experiment, which involves retrieving the undetectable phase information, is nontrivial. It is addressed by phase retrieval algorithms—advisably, in an iterative fashion.

Iterations, in other words, running the algorithms hundreds of times, are expected to provide more stable and reliable solutions when a problem is not amenable to be solved directly. But sometimes the quality of solutions does not improve even after a large number of iterations, resulting in the so-called stagnation problems.

To break this impasse, researchers from Indian Institute of Technology Delhi have been working since 2018 and proposed a novel approach involving a complexity parameter for guiding the phase retrieval algorithms. On Oct. 10, they published their latest research on this topic in *Intelligent Computing*.

"In recent works, we have proposed a novel approach that we call 'complexity-guided phase retrieval' (CGPR) that is meant to address the typical stagnation problems with phase retrieval algorithms," the researchers said. "This methodology uses a complexity parameter which is computed directly from the Fourier intensity data and provides a measure of fluctuations in the desired phase retrieval solution."

In their previous research, the researchers developed the CGPR methodology mainly with simulated noisy data in combination with the Fienup's hybrid input-output (HIO) algorithm, a well-known algorithm for phase retrieval.

"In this paper, our effort is to understand the nature of phase retrieval solution from a new perspective of the complexity parameter," the researchers said. For the first time, the researchers have put their complexity-guidance idea to test for experimental data available from the Coherent X-ray Imaging Data Bank (CXIDB) database, used along with the relaxed averaged alternating reflection (RAAR) phase retrieval algorithm, another well-known algorithm popular in the CXI community.

CXIDB is a great initiative that provides access to raw coherent X-ray diffraction data that can presently be recorded at just a couple of synchrotron facilities globally. Ready availability of this data allows researchers anywhere in the world to design and test newer phase retrieval algorithms.

The research team started by observing the complexity behavior of the iterative solutions obtained using the popular RAAR-ER methodology, which is a combination of a larger number of RAAR iterations followed by a smaller number of error reduction (ER) iterations. The quality of the recovered solutions and their resolution was assessed by evaluating the phase retrieval transfer function (PRTF).

They observed both the single run of the RAAR-ER algorithm and the averaged solutions, since the latter—hundreds of trial solutions first obtained based on random initial guesses, then averaged with phase adjustment—are considered to be more reliable than the former.

And both kinds of solutions, as they found out, consisted of undesirable grainy artifacts that had smaller feature size compared to the PRTF-estimated resolution and thus considered to be "spurious." This inconsistency was what drove the researchers to add the complexity-guidance component to the RAAR algorithm and present the so-called complexity-guided RAAR (CG-RAAR) algorithm.

CG-RAAR was first tested with simulated noisy data (with two noise levels) that did not have missing pixels, and then applied to the real cyanobacterium diffraction data (noisy, with missing pixels) from the CXIDB database for further validation.

"It is worth highlighting that the single run of CG-RAAR produces solutions with much reduced artifacts, and as a result, the number of trial solutions required for the averaging process with this methodology is less than the half number that are needed for the traditional RAAR-ER method," the researchers observed. Meanwhile, the CG-RAAR solution had the smallest features consistent with the PRTF-estimated resolution.

According to the researchers, the main idea behind complexity-guidance is to match the complexity of RAAR solution with the desired ground-truth complexity. "CG-RAAR essentially provides a regularized solution that does not contain spurious grainy features. The regularization is controlled in this methodology by means of the complexity parameter, thus making the solution consistent with the data," they added.

In conclusion, the complexity-guidance concept, when combined with traditional phase retrieval algorithms like HIO and RAAR, can offer a better noise-robust estimate of the object. "We believe that complexity-guidance as an idea may potentially be integrated into existing software tools and can improve the performance of existing phasing algorithms in coherent X-ray imaging," the researchers concluded.

More information: Mansi Butola et al, Robust Phase Retrieval with Complexity-Guidance for Coherent X-Ray Imaging, *Intelligent Computing* (2022). DOI: 10.34133/2022/9819716

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