Using automatic differentiation as a generalizable approach to ptychographic reconstruction

Saugat Kandel, Stephan O. Hruszkewycz, Chris Jacobsen, Youssef Nashed

Argonne National Laboratory, USA, Northwestern University, USA

Author Email: saugat.kandel@u.northwestern.edu

In recent years, the rapid advance in x-ray synchrotron technology has provided access to x-ray beams at previously inaccessible regimes of high coherence, intensity, and energy ranges. Since x-ray lenses are limited in phase contrast and resolution, nanoscale microscopy in these regimes is largely based on coherent diffraction imaging (CDI) techniques.

Ptychography is a CDI technique that acquires a series of diffraction patterns through latitudinal and longitudinal shifts of the specimen (object), then uses these to reconstruct an image of the not only the object but also the illumination pattern (probe) itself. Simple but powerful, ptychography has become an increasingly popular technique for microscopy in a range of imaging modalities. For complex imaging modalities, however, the reconstruction algorithms are difficult to formulate mathematically. This has limited the uptake of the generalized ptychographic reconstruction method.

In this work, we use the automatic differentiation technique to implement a generalizable gradient descent framework for ptychographic reconstruction. For this approach, we formulate the gradient descent using an amplitude-based variant of the Wirtinger flow phase retrieval algorithm. In our framework, the user needs to only specify the forward propagation model for the specific ptychographic experiment; the gradients are then calculated by backpropagating through this forward model using the Tensorflow deep-learning library. Our use of the popular Tensorflow library provides an additional advantage – access to state-of-the-art machine learning algorithms to accelerate the gradient descent.

We demonstrate the generalizability of our framework through numerical experiments in the near-field and far-field ptychography regimes. Furthermore, we expect that our framework can be straightforwardly extended for applications including, but not limited to, Bragg and multislice ptychography experiments. Our experiments illustrate the promise automatic differentiation holds for solving the general phase reconstruction problem.

![Figure 1](image)

**Figure 1**: (a-d) Far field ptychography (detector-sample distance of 15 m). (a) True object amplitude. (b) True probe amplitude. (c) Reconstructed object amplitude (Normalized RMSE 0.04). (d) Reconstructed probe amplitude (Normalized RMSE 0.02). (e-h) Near field ptychography (detector-sample distance of 4.7 cm). (e) True object amplitude. (f) True probe amplitude. (g) Reconstructed object amplitude (Normalized RMSE 0.04). (h) Reconstructed probe amplitude (Normalized RMSE 0.24).