Artificial Intelligence and Augmented Intelligence for Automated Investigations for Scientific Discovery

Exploring Coherent Diffractive Imaging using AI
Project Report
Project Dates: 01/07/2021-17/09/2021
University of Southampton

Project Student: Gavin Man
Supervised by: Professor William Brocklesby, University of Southampton

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1. Project Details

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3. Lay Summary

Diffraction requires certain lenses in order to see the pattern that is imprinted. However, this is problematic in the case of X-rays, as the lenses would need to be of an extremely high grade which is not widely available or economically viable. This is seen in the example of X-rays in hospitals where the image produced are of shadows where the X-ray diffraction patterns are produced by having the film exposed to radiation and particles are ionised and electrons trapped cause an X-ray image to be imprinted.[1] This process makes it difficult to produce very precise images as can be seen in the additional blurriness seen in hospital X-rays and therefore computational methods are explored to circumvent this.

4. Aims and Objectives

The aim is to explore suitable solutions to solving issues with limited information such as phase for generating accurate images for diffraction data such as in X-rays. Both analytical and computational methods for obtaining graphical diffraction patterns are explored.

The pattern of scattered light from an object is given by its Fourier transform. When light is detected with a normal Charge Coupled Device (CCD) no detailed phase information is present, only $|E|^2$ the absolute value. Information is obtained when a positive potential is applied to a portion of pixels that have photos of high enough energy to strike the surface which caputres the electrons information into a two-dimensional array.[2]

For all applications, the image process requires solving inverse problems which include which object produced a particular pattern. This is very feasible when the complete phase information is already known but very difficult when the complete phases are not already known.[3]

Given insufficient information to be able to generate suitable diffraction images from present methods, neural networks have been able to replace or complement solutions to problems that also involve a range of imaging tasks.[4]

5. Methodology

Fourier Transforms

Different types of Fourier transforms were explored including the continuous version with infinite bounds to determine an object, $f(x)$, to its Fourier transform $F(u)$ where x is an M-dimensional spatial coordinate and u is an M-dimensional spatial frequency coordinate.

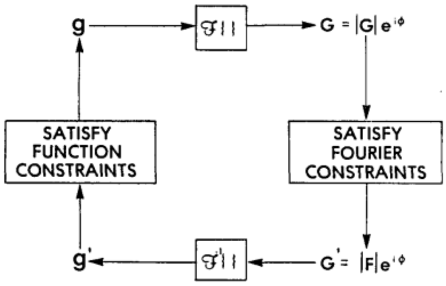
$$\mathrm{F(u)} = \int_{-\infty}^{\infty} \mathrm{f(x)}\, \mathrm{e}^{-\mathrm{i}2\pi \mathrm{u}\cdot \mathrm{x}}\, \mathrm{dx}$$

However, for most cases where $M = 2$ and for 2D cases where square arrays are assumed, the discrete Fourier Transform is used instead along with its inverse.[5] Both of these were experimented with sample data sets using Python.

$$Discrete\ Fourier\ Transform$$
$$\hat{x}_n = \sum_{k=0}^{N-1} x_t e^{-2\pi ikn/N}$$

Phase Retrieval

Recovering the phase would be complex-valued; therefore a suitable strategy would be to use the Gerchberg-Saxton algorithm.[6] The Gerchbberg-Saxton algorithm is an iterative phase retrieval algorithm for when the complete wave function whose intensity in the two different planes, diffraction and imaging planes, of an imaging system is known.[7]



(Fig. 1. Block diagram of Gerchberg-Saxton algorithm.[5])

Another phase retrieval technique explored was Ptychography. This relatively young method is used to reconstruct intensity and phase images of samples from groups of diffraction patterns.[8] Ptychography utilises a stack of low-resolution images derived from overlapped apertures to reconstruct a super-resolved image.[10]

One of the issues from diffraction patterns is the phase information lost. Ptychography utilises data sets of many inference patterns during displacement then an algorithm is used to invert the data into suitable images.[8] Seeing the evolution of various types of imaging and the emerging field is very insightful as to how new techniques are initially criticised and explored before being trusted and used as a standard technique.

Ptychography scans a spot over the sample. Fourier Ptychography (FP) scans the angle of the light beam illuminating the sample. Maths related to calculating the objects are both related. Unlike holography, ptychography is a non-interferometric imaging technique and therefore more easily implemented.

However, ptychography is found to face problems in reconstructing images.[11] This arises from the scanning which produces mechanical vibrations.[11] Additionally, ptychography as a computational imaging technology may face accuracy issues from the deviations in aperture position. This is because the resolution and quality of the reconstructed image are directly affected by the accuracy of the aperture position, and deviations result in either poor reconstruction quality or failure in reconstructing the image.[10]

Another problem that Ptychography faces is limited in the attainable resolution in the reconstruction process, arising from limitations in illumination source, the depth of field problem, and limitations in photon flux.[11] For instance, the depth of field problem is more acute in X-ray imaging.[4] The depth of field problem arises from the limitations in assuming that a 2D projection is sufficient in representing a 3D object viewed from a specific angle, because the Frensel propagation effects renders this assumption invalid when the object’s thickness exceeds a thickness equal to the optic’s depth of focus (DOF).[4]

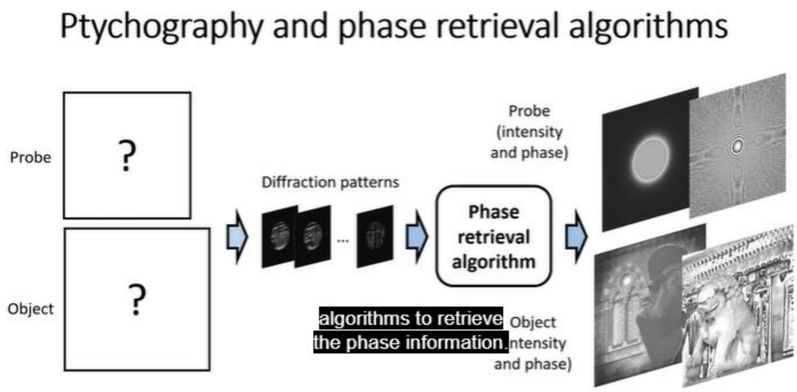
$$DOF = \frac{2}{0.61^2}\frac{{\delta_t}^2}{\lambda} \cong 5.48\frac{{\delta_t}^2}{\lambda}$$

(Optic’s Depth of Focus
where δ_t is the achieved transverse spatial resolution
and λ is the wavelength of the beam.[4])

Present reconstruction approaches are based on nonlinear optimization, which requires calculating the far-field intensities that one would expect to measure, based on one's present guess of the object.[4] This is so that the simple projection model can be replaced with a wave propagation model that depicts the way in which illumination propagates through the guessed object.[4] This then enables the reconstruction of objects that extend beyond the depth of focus or objects that violate the first Born approximation.[4] However, due to the short wavelength and high penetrating power of X-rays, the depth of field problem is difficult to overcome especially when X-ray nanoimaging is scaled up to larger objects such as entire tissues.[12]

Onerous computational requirements also result in difficulties in practically implementing ptychography, such as requiring the collection of data sizes approximately 10-20 times larger than the desired image size of the sample in the point-by-point scan.[4] Time taken to acquire such large data sizes is also lengthy because of the innate scanning procedure.[4] While procedures to reduce data-acquisition duration exist and are commonly used in full-field X-ray microscopy and electron microscopy (e.g. imaging larger sample volumes, capturing dynamic phenomena under operando conditions), applying such procedures to ptychography is still challenging and an area for further development.[4] It is important to improve time resolution to allow for higher-dimensional analysis, for instance in doing ptychography as a function of incident X-ray energy for spectroscopic imaging.[4]

An alternative way to improve the speed of imaging is to utilise compressive-sensing techniques to make up for relatively sparse data acquisition.[4] However, due to a necessary overlap constraint in solving the phase retrieval problem, compressive sensing is challenging when attempting to use it in ptychography.[4] Furthermore, the process of continuous scanning (critical to the scanning of some specimens) is limited by acceleration limits on optics, hence making it difficult to design a scheme to uniformly acquire data across the whole image while reducing the total length of the trajectory.[4]



(Fig. 2. Abstract of Ptychography[9])

In summary, ptychography is currently limited by the large data size required to process a high-resolution image as well as the lengthy time required to obtain and process such large data sizes on top of the limited types of data. This leads us to explore other methods, notably using Neural Networks for reconstruction.

6. Conclusions & Future Work

Neural Network Reconstructions for Phase retrievals

Ptychography requires computational reconstruction to recover the complex field of the super-resolved object.[10] Various algorithms have been proposed to tackle the nonlinear inverse FP problem.[10] The Gerchberg-Saxton-type algorithm[13] is used in Fourier ptychography (FP), but it reinforces constraints in the image domain and the Fourier domain.[10] The Wirtinger flow framework that resembles gradient descent-based optimization[14,15], as well as PhaseLift (a convex relaxation-based phase retrieval algorithm)[16] has been applied or explored within the context of ptychography.

In the context of ptychography, neural network reconstruction would take the role of complementing or replacing solutions to ptychography's imaging tasks, such as super-resolution, inpainting, deconvolution, or denoising.[4] Deep neural networks are advantageous for they have the potential to surpass classical optimization techniques for imaging tasks, by imposing constraints on the reconstructed image by having the image remain on a learned manifold.[4]

Advantages of methods involving Network Networks

As a data-driven method, neural networks can be incorporated into the imaging and reconstruction process in ptychography, specifically within ptychography-related algorithms.[10] Neural networks would have the potential to address accuracy issues in ptychography that arise from deviations in aperture position by correcting these deviations at the level of algorithms.[10] For example, the simulated annealing (SA) algorithm has been able to function as a self-calibration method to correct deviations in the position of the aperture. To minimise the cost function, the SA algorithm can be incorporated to locate the optimal aperture position, with the refined position utilised to update the object's corresponding region in the Fourier domain with the classical GS-type iteration.[10]

Trainable FP neural networks have also been proposed that can correct the irregularities in each aperture position deviation alongside object reconstruction, by constructing an FP neural network in accordance with an FP forward model that contains the aperture positional deviation.[17] The FP neural network then sets the imaginary and real parts of the object, along with each aperture's positional deviation as the weights of the convolutional layer.[10] This results in a predicted image FP being the output of the FP neural network, with the results from experiments and simulations showing that the neural network could accurately locate aperture positions to improve the FP image reconstruction quality.[10]

Neural networks also have the potential to address certain aspects such as the depth of field problem, which contribute to the problem of limited attainable resolution due to time and data collection constraints in ptychography. Researchers have proposed and designed a convolutional neural network (CNN) known as ESTNet to quickly and accurately estimate depth, via training the ESTNet with a light-field data set and coupling it with an encoding-decoding structure, with this CNN presenting promise in balancing computational time with accurate depth estimation.[18]

Neural networks offer potential in optimising and accelerating the ptychographic reconstruction process. For instance, an end-to-end CNN could potentially allow the CNN to learn the mapping from a stack of low-resolution images to a high-resolution image.[10] Research that utilised a simple three-layer CNN for ptychography reconstruction demonstrates that the CNN could attain a faster speed than the iterative algorithms[19] Another adapted variation of the CNN, known as a generative adversarial network (cGAN), has also been shown to yield a 50x speedup in ptychography reconstruction for dynamic cell videos in contrast with the model-based frequent pattern mining (FPM) algorithm[20] Neural networks are also able to suggest a viable route to compressive sensing to reduce the time taken for data collection, by constraining either the likelihood and prior terms, or both.[21]

Future Outlook

The applications of neural networks in ptychography and X-Ray imaging are still relatively new, likely a result of the phase-retrieval problem and its nonconvexity that demand special attention when applying machine learning models.[4] Additionally, it is still challenging to apply machine learning neural network methods to large-scale 3D imaging problems, due to the training process growing proportionately with the size of the degrees of freedom in the phase-retrieval problem.[4] However, the potential of applying neural networks in ptychography is promising. For instance, certain studies have demonstrated that machine learning-based regularisation could lift the overlap constraint in ptychography.[4] Neural networks could also be applied to solve other difficult puzzles in spectroscopy, and other fields. For instance, fast convolutional neural networks (CNN) can be used in high-resolution microscopy, to obtain a higher precision in estimating illumination angles, with the CNN producing solid results which can exceed traditional approaches with a nearly three-fold reduction in estimation errors.[22] Considering the progress made in computational hardware in the last few years, with quantum computing on the horizon, neural networks have been observed to be computationally feasible, and could produce more precise estimations and time reductions to produce more accurate reconstructions at higher quality in the field of imaging.[22]

7. Outputs, Data & Software Links

Presentation Poster Presented August

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