Deep Learning for Bragg Coherent Diffraction Imaging: Detector Gap Inpainting and Phase Retrieval

Thesis

présentée et soutenue publiquement le

Pour l'obtention du titre de

Docteur de l'Université Grenoble Alpes
(mention Physique du rayonnement et de la matière condensée)

par
Matteo Masto

sous la direction de
Dr. Tobias Schülli, Dr. Vincent Favre-Nicolin, Dr. Steven Leake

Composition du Jury

XXXXXXXXXX	PR, XXXXXXXXXX	**Rapporteur**
XXXXXXXXXX	PR, XXXXXXXXXX	**Rapporteur**
XXXXXXXXXX	PR, XXXXXXXXXX	**Examinateur**
XXXXXXXXXX	PR, XXXXXXXXXX	**Examinateur**
Tobias Schülli	ESRF	**Directeur de Thèse**
Vincent Favre-Nicolin	ESRF UGA,	**Directeur de Thèse**
Steven Leake	ESRF	**Directeur de Thèse**

École Doctorale de Physique-Grenoble

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0.1 Introduction

The present document is a draft of my PhD manuscript.

Part I

Bragg Coherent Diffraction Imaging

0.2 Single crystal diffraction

0.3 Phase Problem

Part II

Convolutional Neural Networks

0.4 Introduction on neural networks

0.5 Convolutional

0.6 U-Net and MSD-Net

Part III

Deep learning for Detector Gaps Inpainting

In this chapter the "detectors' gaps problem" in Bragg Coherent Diffraction Imaging and our approach to solve it using Deep Learning are discussed. The main state-of-the-art measures are presented briefly and the topic of image inpainting with Deep Learning is introduced. The focus will then shift to our works that led eventually to the optimal "Patching-based" approach that can also be found in the published paper entitled *"Patching-based deep learning model for the Inpainting of Bragg Coherent Diffraction patterns affected by detectors' gaps"* (https://doi.org/10.1107/S1600576724004163). The chapter is closed with some analyses of the performances of the DL models in a variety of simulated and experimental cases.

0.7 The "Gap Problem"

At time of writing, standard BCDI experiments employ pixelated photon counting detectors to acquire the diffraction patterns. These detectors can guarantee high spatial resolution, noise-free counting and fast read-out times. Two examples of these devices, currently used at the ID01 beamline are the MAXIPIX and EIGER detectors [1, 2]. These detectors are often built by tiling together several sensing chips in order to cover a larger area, and are typically bonded to an Application-Specific Integrated Circuit (ASIC) using bump bonding. This implies the presence, in the overall sensing region, of vertical and/or horizontal stripes that are not sensitive to the impinging radiation. The width of these lines varies depending on the device but normally does not exceed the equivalent of some tens of pixels. Specifically, for the MAXIPIX detector the gap size is 6 pixels wide while the EIGER has two types of larger gaps of 12 pixels and 38 pixels width. The detector gaps problem does not affect BCDI only, but it is shared among other x-ray techniques that deal with single photon-counting pixelated detectors and/or beamstops. We have seen in chapter 0.1 that during a BCDI scan the 2D images acquired by the detector are stacked to form a 3D array. This leads these lines to become planes of missing signal in the dataset. The problems arise when reconstructing the data affected by these gaps. In fact, these regions of non-physical zero intensity deceive the Phase Retrieval algorithms inducing the presence of artifacts in the reconstructions[3].

It follows that the reliability of the reconstructions in this case is compromised as the strain distribution can be deeply affected by the artifacts. A good practice during standard BCDI experiments is to avoid the gaps by moving the detector if possible. However, this tends to be problematic for the case of high-resolution BCDI, i.e. when the diffraction pattern measurement extends to higher q-values, thus covering more than one sensing chip and necessarily crossing a gap region. Under these circumstances it becomes important to reduce the amount of artifacts deriving from the gaps.

0.8 State of the art

Here we will discuss the current strategies employed to treat the detector gaps. As someone could argue, the simplest yet not practical, solution would be to slightly move the detector sideways and acquire a second full scan with the gap hiding a different region of the same Bragg peak, and then merge the two measurements into a single gap-less one. This would in turn increase the acquisition time of more than 2X making it de facto never an option during standard experiments.

The PyNX software, routinely used for the BCDI phase retrieval at ID01, allows the user to define a mask of the gap regions and ignore those pixels during the execution. In this way the quality of the reconstruction improves, but one can still notice the presence of high-frequency oscillations appearing in both object's modulus and phase. The origin of these artifacts can be found in the diffracted intensity calculated from the reconstructed particle as one can clearly see that the gap-regions is filled with nonphysically high intensity (see Fig. 2)

Another, more invasive, option is to *fill* these gaps with an estimate of the intensity distribution that would be there, before the phase retrieval. These tasks of filling gap in images is usually referred to as "inpainting" and it has been widely studied in the field of photography and imaging [4, 5]. More precisely one could define image inpainting as the task of utilize known information extractable from the image to repair the parts where this information is missing, where for known information the colors, the textures and the semantic features are intended. For traditional inpainting, different techniques have been explored, from the texture synthesis methods pioneered by Efros and Leung [6] to the use of PDEs as Navier-Stokes equations proposed by Bertalmio *et al.* [7] and then again from sparse representations [8] to hybrid methods combining variational and statistical methods [9] More recently Deep Learning models, headed by Convolutional Neural Networks (CNN), have taken the place of more traditional methods as they can attain higher accuracy for more complex inpainting tasks. By undergoing a training process, CNNs can "learn" to recognize and reproduce the semantic features of the training dataset, and thus leverage them during inference as additional information beside the colors and textures of the specific image to restore. As we have seen in **??**, the typical CNN architecture for image generation consists of an encoder, which retains the features of the input image and compresses them into a lower dimensional latent space, and a decoder, which is responsible for the generation of the output image starting from the latent space. The model are then trained according to a loss function that pushes the model's predictions to be close to a given ground truth reference. Since reviewing the vast amount of works about CNN for image inpainting is beyond the scope of this thesis and for more information, we redirect the reader to the reviews published by Elharrouss *et al.* and Xu *et al.* [5, 10].

0.9 Model design

0.10 Patching approach

0.11 Results in detector space

0.12 Results in real space

0.13 Fine-tuning

0.14 Performances assessment

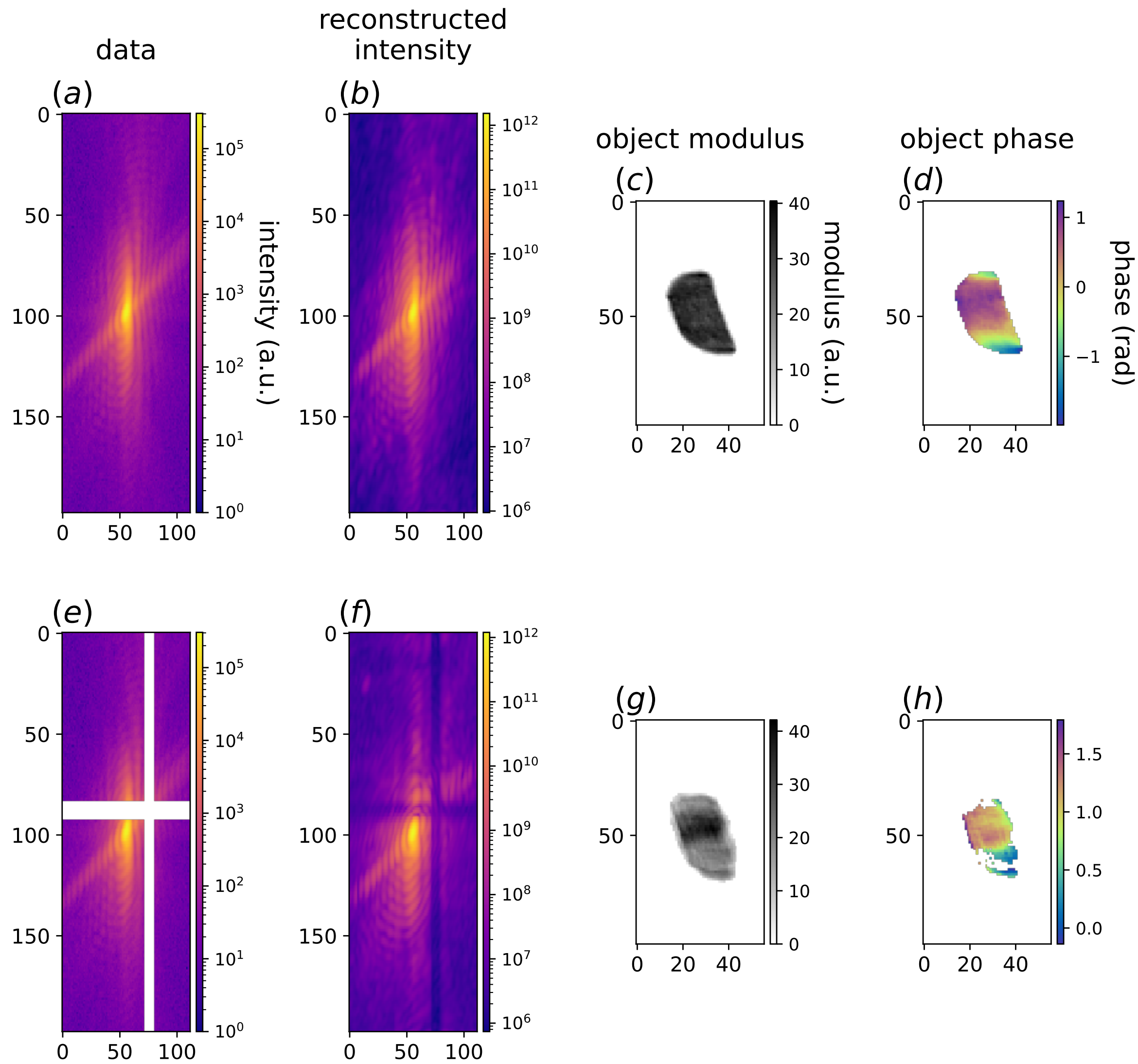

Figure 1: Effect of detector gaps in BCDI reconstructions (a) The central xz slice of an experimental diffraction pattern. **(b)** The same slice of the diffracted intensity calculated from the retrieved object. **(c - d)** xz slice of the modulus and phase respectively of the particle obtained from the phasing of the gap-less dataset. **(e)** Same slice as in **(a)** with an artificially added 9 pixel-wide, cross-shaped gaps to mimic the detector's ones. **(f)** The same slice of the diffracted intensity calculated from the retrieved object when not masking the gap regions. **(h - g)** xz slice of the modulus and phase respectively of the particle obtained from the phasing of the gap-affected dataset. The distortions caused by the gaps are evident.

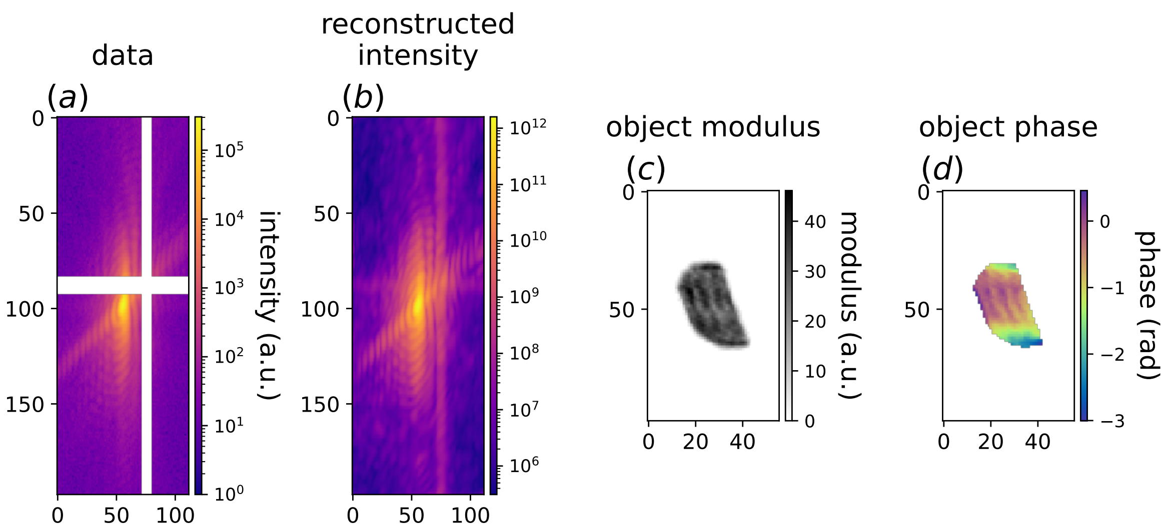

Figure 2: Masking the gap region during phasing (a) The central xz slice of an experimental diffraction pattern. **(b)** The same slice of the diffracted intensity calculated from the retrieved object. Comparing this figure with 1**(b)** one can see that when excluding the gap region from the phasing with a mask, the calculated intensity shows bright non-physical streaks instead of the gaps. **(c - d)** xz slice of the modulus and phase respectively of the particle obtained from the phasing of the gap-less dataset. Despite the much higher quality of the reconstruction, one can notice some oscillatory artifacts appearing in both the modulus and the phase of the retrieved object.

Part IV

Deep learning for Phase Retrieval

We enter now the core topic of the thesis. Most of the efforts during this PhD have been dedicated to the Phase Problem.

0.15 State of the art

0.16 Highly strained crystals

0.17 Reciprocal space phasing

0.18 Phase symmetries breaking

0.19 Model design

0.20 Results on 2D case

0.21 Results on 3D case

0.22 Refinement with iterative algorithms

0.23 Experimental results

Part V

Conclusions

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Annexes

Appendix A

Appendix