



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

Thesis

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par
Matteo Masto

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

Composition du Jury

XXXXXXXXXX	PR, XXXXXXXXXXXX	Rapporteur
XXXXXXXXXX	PR, XXXXXXXXXXXX	Rapporteur
XXXXXXXXXX	PR, XXXXXXXXXXXX	Examineur
XXXXXXXXXX	PR, XXXXXXXXXXXX	Examineur
Tobias Schüllli	ESRF	Directeur de Thèse
Vincent Favre-Nicolin	ESRF UGA,	Directeur de Thèse
Steven Leake	ESRF	Directeur de Thèse

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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 more than double the acquisition time making it, de facto, never an option during standard experiments.

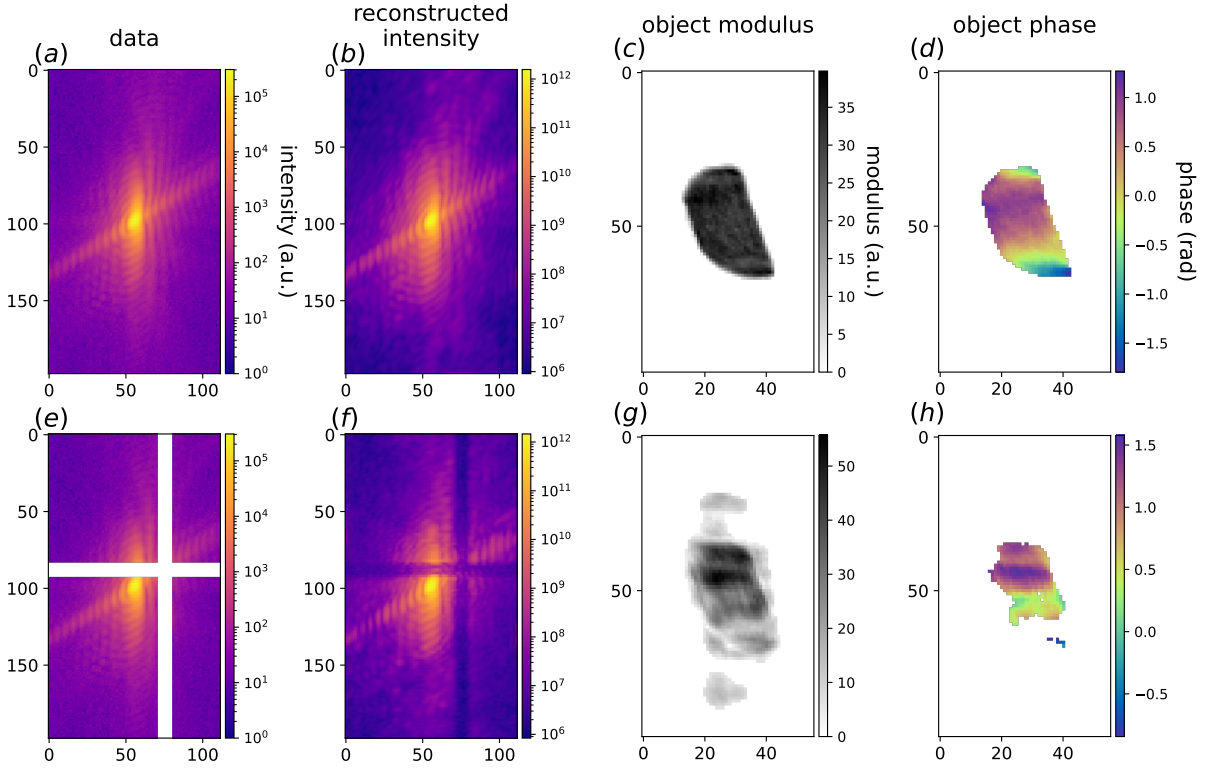


Figure 1: Effect of detector gaps in BCDI reconstructions (a) The central xz slice of an experimental diffraction pattern. (b) The same slice of the diffracted intensity calculated from the retrieved object. (c - d) xz slice of the modulus and phase respectively of the particle obtained from the phasing 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.

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”. The following paragraph mentions the most relevant inpainting methods to give a context for our work.

0.8.1 Background on Image Inpainting Research

Computational image inpainting has been widely studied in the field of photography and imaging for many years [4, 5]. The inpainting problem can be defined as the task of utilizing known information extractable from the image, to repair the parts where this information is

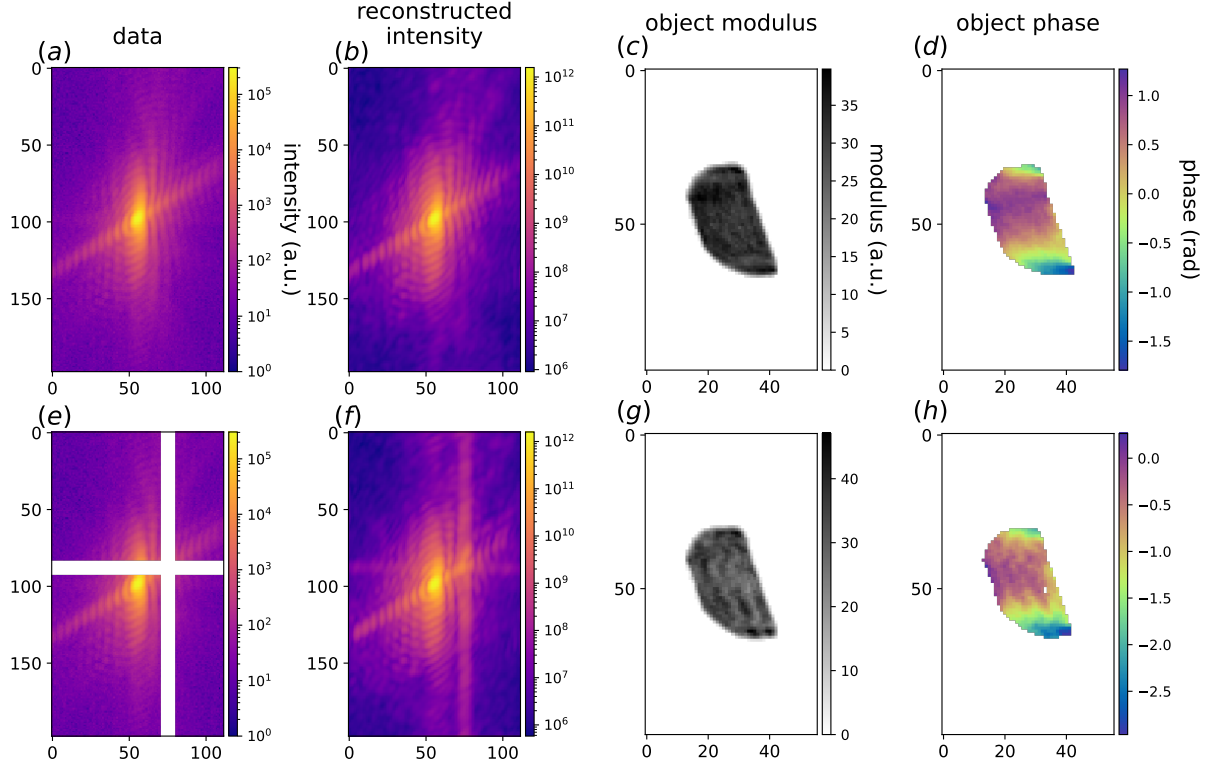


Figure 2: Masking the gap region during phasing (a) The central xz slice of an experimental diffraction pattern. (b) The same slice of the diffracted intensity calculated from the retrieved object. Comparing this figure with 1(b) one can see that when excluding the gap region from the phasing with a 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 affected data with a mask of the gap regions. 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.

missing, where for known information the colors, the textures and the semantic features are intended. In the history of image inpainting a clear cut can be observed when deep learning methods have started to be employed. 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 instead, 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. In some cases, the loss function can be replaced by another CNN that is trained to discriminate true images from the ones predicted by the model. These complementary networks are known as

Generative Adversarial Networks (GAN), firstly proposed by Goodfellow *et al.* [10], and have also been used for image inpainting (e.g. [11]). 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, 12]. as well as this blog article [13]. For what concerns the application of DL based inpainting for scientific imaging, early works date back to 2018 as in the case of Sogancioglu *et al.* for x-ray human chest 2D radiographic images [14] and to 2020 for 2D microscopic images [15]. A couple of years later Tanny Chavez and coauthors published a paper comparing the performances of different CNN models for the inpainting of 2D x-ray diffraction images [16]. The work is precisely addressing the gap problem for x-ray detectors used for powder diffraction measurements and is awarding UNet and Mixed Scale Dense (MSD) models for the best performances on experimental data. The DL models outperform interpolations obtained with biharmonic functions across 7 and 17 pixel-wide gaps. This work has been of inspiration for the design of our DL model for BCDI gaps inpainting. In the same year, another work on DL based inpainting for x-ray detector gaps was published by Alfredo Bellisario and coauthors [17]. The authors tested a UNet-like model on the inpainting of 2D simulated, noiseless coherent diffraction patterns against gaps of different sizes (2 to 20 pixels) along the central row. The gaps were placed such that the center of the peak was covered, a choice that, as we will see later, yields better results than predictions on peripheral areas. To our knowledge, at the time of writing, no other works about deep learning based inpainting for X-ray detector gaps are present in the literature.

0.9 Model design: 2D case

On the heels of the last mentioned works we have started to tackle the detector gaps problem for BCDI using CNNs. For simplicity, we started off with 2D case, using simulated diffraction patterns and inpainting randomly placed vertical gaps of different width. First, we created a training set of simulated data, composed of pairs of gap-affected images and corresponding gap-free ground truths, then built a UNet-like model and trained it in a supervised fashion.

0.9.1 Dataset creation

The creation of training datasets of simulated 2D BCDI patterns for both the gap-inpainting and phase retrieval tasks has followed the procedure described in this paragraph.

In first place, once chosen the size of the array, a randomly shaped polygon is created in the center using `scipy.spatial.ConvexHull` function. This guarantees the object to have a compact support with homogeneous electron density as assumed for BCDI. Subsequently, a random phase field of the same size with variable phase range and correlation length is generated thus the complete complex object is formed. In order to make the object more realistic a Gaussian filter and Gaussian random noise are applied to the object's modulus, so to smoothen the edges and simulate real cases respectively. At this point the object is resized to the shape required to match the chosen oversampling ratio and the 2D Discrete Fourier Transform is computed. As last stage, Poisson noise is added to the diffraction patterns with different magnitudes to simulate various X-ray flux conditions.

Datasets contain a number of diffraction patterns in the order of thousands and for each of

them the random variables are different as well as the oversampling ratios.

0.10 Patching approach

0.11 Results in detector space

0.12 Results in real space

0.13 Fine-tuning

0.14 Performances assessment

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