1 Introduction

Our research in this program is aimed at developing new methods for what is generically known as the phase retrieval problem. In its classical formulation, phase retrieval amounts to reconstruction of an unknown waveform from the magnitude of its Fourier transform. Currently, the most widely used algorithm for such problems is Hybrid Input-Output (HIO), introduced in 1978 [1]. Notwithstanding many attempts, no better alternative has been established. There is, however, a great interest in developing reconstruction algorithms based on convex optimization techniques, which have been developed extensively in recent decades, both theoretically and practically. Unfortunately, due to the strong non-convexity of the problem, such methods have not met with success. Nevertheless, in our previous research in the framework of the IMG4 MAGNET we showed that incorporating some additional information on the phase can change this situation dramatically. In particular, we developed a convex optimization method for phase retrieval when phase uncertainty is limited by $\pi$ radians. Our method is several orders of magnitude faster than the HIO algorithm in this case, and it demonstrates a much better reconstruction quality when measurements contain noise [5].

In this year we continued our research on the phase retrieval with alternative additional information. This additional information can of course be used together with partial phase information if available. In addition to combining the Fourier magnitude with other sources of information, we developed several methods for reconstruction from defocused images or from interferograms.

Initially, we developed a method for image reconstruction from the Fourier magnitude and a single interferometric pattern. Interferometry is widely used in optics, and is probably the most widely used method for phase estimation. The method and results are described in Section 2. (More details are available in the Y4 annual report.) This method was later
modified (at the suggestion of our research partners, KLA-Tencor) to allow reconstruction from interferograms alone, that is, in the case where reference waves interfere with the sought waveform directly and no Fourier data is available. The method and results are reported in Section 3. In Section 4 we describe a method for image reconstruction from the Fourier magnitude and one or more defocused images. A related setup is considered in Section 5 where input data contains the Fourier magnitude and a blurred (low-resolution) version of the sought image. In Section 6 we report our results for image reconstruction from a series of defocused versions. The latter work was also done at the suggestion of our KLA-Tencor partners.

Finally, we mention here some work that is not reported in detail. In most cases, objects in the phase retrieval problem are assumed to be real-valued. To the best of our knowledge no algorithm exists for reconstruction of a complex-valued object in the original version of this problem. For several reasons the problem of reconstruction of complex-valued objects is much more difficult. We have developed optimization methods for complex-valued objects, however, at this stage the results are of a lower quality than those achieved for real-valued objects. This work is still in progress.

The methods described in this paper are demonstrated on a VLSI circuit image provided by the KLA-Tencor Corporation (see Figure 1)

![Experimental image](image.jpg)

(a) Intensity

(b) Fourier magnitude

Figure 1: Experimental image.

It is important to remark that the methods developed in this work are quite general and can be applied in many areas of optics. They are not limited to the optical metrology which lies in the heart of KLA’s chip verification process.

All methods described in this paper are based on convex optimization techniques. Therefore, we shall say a few words on the algorithms we use, as the results may vary significantly
depending on the optimization routine in use. Since the number of variables is very large (several millions for a typical two-dimensional image and much more in three-dimensional cases), we cannot use Newton or Quasi-Newton methods. Instead, our choice is narrowed to the family of memory-limited algorithms. In practice we used two such algorithms: LBFGS [3] and SESOP [4], which turned out to yield very similar performance. The results reported in this paper were obtained with our implementation of the LBFGS algorithm. As a part of this work we developed an LBFGS version that allows direct use of complex variables. This routine will be of interest to the community of physicist working with inverse problems arising in electromagnetic phenomena.

2 Phase Retrieval Combined with Interferometric Images

In this work we developed a method for image reconstruction based on phase retrieval combined with interferometric images. Here, an unknown wave is combined with one or more known (well controlled) waves and the intensity of the resulting interference pattern is recorded by a CCD. From these patterns one can reconstruct the unknown wave. A schematic view of this process is depicted in Figure 2.
We assume that only two measurements are available: one that includes the reference beam and another without it. Hence, we have in hand the intensity of the sought wave $x(\xi, \eta)$ and the intensity of the sum of $x$ and the reference beam $r$. The intensity of the sum of two complex fields depends on both the amplitude and phase of the unknown field. Thus if

$$x(\xi, \eta) = r(\xi, \eta)e^{j\phi(\xi, \eta)}$$  \hspace{1cm} (1)

represent the wavefront to be detected and reconstructed, and if

$$w(\xi, \eta) = q(\xi, \eta)e^{j\psi(\xi, \eta)}$$  \hspace{1cm} (2)

represents the reference wave whose magnitude $q$ and phase $\psi$ are known. The waves interfere and the intensity of the sum is given by

$$I(\xi, \eta) = r(\xi, \eta)^2 + q(\xi, \eta)^2 + 2r(\xi, \eta)q(\xi, \eta)\cos(\psi(\xi, \eta) - \phi(\xi, \eta))$$  \hspace{1cm} (3)
While the first two terms in this expression depend only on the intensities of the individual waves, the third depends on their relative phase. Hence, from Figure 3 it is clear that there are two possible phase values of the sought image: it is either $\psi + \alpha$ or $\psi - \alpha$. In this work we applied the interferometric imaging to the Fourier transform of the original image, that is, the reference wave was assumed to be incident on, and all measurements are done at the pupil (Fourier) plane. The reconstruction problem is not easy, as this is a combinatorial problem with $2^N$ possible phase values, where $N$ is the number of pixels in our Fourier plane sampling. Thus, a direct approach is infeasible. However, we can perform a relaxation allowing the actual phase to lie anywhere in the interval $[\psi - \alpha, \psi + \alpha]$. This yields exactly the problem of phase retrieval where the phase is known to lie within an interval of uncertainty of up to $\pi$ radians. Therefore, it merges perfectly with the algorithm we developed in our previous work (see Y4 annual report). Hence, to reconstruct the image we perform convex relaxation of the phase requirement. We solve this convex problem first, and only then introduce the
Fourier magnitude requirement. Our experiments demonstrate perfect reconstruction (in the case of perfect data), as shown in Figure 4. It is important to note that this method allows good reconstruction even in the case of a bad (unstable) interferometer, because the phase of the reference beam need not be known with very high accuracy. Instead, one can add the uncertainty of the imperfect phase approximation to the uncertainty interval of the Fourier phase and solve the problem. For example, if the phase of the reference beam is known to lie within the interval $[\psi - \beta, \psi + \beta]$ then the phase interval of the signal would be $[\psi - \beta - \alpha, \psi + \beta + \alpha]$. If the latter interval is larger than $\pi$ radians we can either reduce it to $\pi$ or consider two separate intervals: $[\psi + \alpha - \beta, \psi + \alpha + \beta]$ and $[\psi - \alpha - \beta, \psi - \alpha + \beta]$. Or, if possible, we can add measurements with reference beam phase changed by $\pi/2$ radians.
Figure 4: Phase retrieval with interferometric images allows perfect reconstruction. Subfigures (a) and (b) show the two inputs used in combined phase retrieval and interferometric reconstruction: the Fourier magnitude and the interference pattern obtained by adding a known wave to the Fourier plane. The reconstruction (shown in sub-figure (c)) is perfect.

3 Several Interferometric Images

In the next step we developed a reconstruction method from several interferograms each corresponding to a different phase of the reference wave. The method is based on optimization
techniques for solving the following minimization problem.

$$x^* = \arg \min_x \sum_{i=1}^n \| |x + w_i| - \sqrt{I_i}|^2,$$  

(4)

where $x = x(\xi, \eta)$ is the waveform we want to reconstruct, $w_i = w_i(\xi, \eta)$ denotes the $i$-th reference beam, and $I_i = I_i(\xi, \eta)$ represents the interferogram intensity in the $i$-th measurement. This approach may be compared to the reconstruction described in the previous section. For example, one may ask which method is preferable if we want to minimize the number of measurements, or which is more robust with respect to noise or uncertainties in the measured values. Note that the method described in Section 2 required two measurements in the Fourier plane—with and without the reference beam—while this time the interferograms can be measured at either the object or Fourier plane. In the first case $x$ represents the signal we need to reconstruct, and in the second case it is the Fourier transform of the sought signal. It was demonstrated in Section 2 that two measurements are sufficient for perfect reconstruction if the phase of the reference beam is known precisely. The question is whether two measurements are sufficient if we do not have the Fourier magnitude but two interferograms instead. The general answer is no. This is evident from Figure 5: there are two different signals (shown in solid black and blue) that result in identical measurements (added reference beams are shown in dashed lines).

Measuring more than two interferograms solves this non-uniqueness problem completely. Our experiments demonstrate that perfect reconstruction (from perfect data) is obtained in this scenario, but also with just two images when the reference signal is strong enough; see example in Figure 6.
Figure 5: Two different signals can result in the same measurements. Note that two different signals (solid blue and black lines) can result in identical interferograms (two circles showing the magnitude of the resulting wave). Dashed lines represent two reference waves.
Figure 6: Reconstruction from two or more interferograms yields perfect results. Sub-figures (a) and (b) show the two inputs of interference pattern obtained by adding two known waves to the sought signal. The reconstruction (whose intensity is shown in sub-figure (c)) is perfect.

4 Simultaneous Focus and Phase Retrieval

This time we consider a situation where the Fourier magnitude data is accompanied by one or more defocused images of the sought signal. The illumination is assumed to be coherent, hence the kernel of the defocus aberration in the Fourier plane $(Fx, Fy)$ is equivalent to a
parabolic phase addition [2]. Namely, the signal is multiplied by the complex exponent

\[ \exp \left[ i \lambda f \left( 1 - \frac{f}{z} \right) (F_x^2 + F_y^2) \right]. \tag{5} \]

The case of incoherent illumination\(^1\) is considered in Chapter 5. Let us start with a demonstration of some results and then proceed to the mathematical formulation of the problem and methods of its solution. Figures 7 and 8 depict some of our inputs: defocused and noisy images. The signal to noise ratio (SNR) is 10 dB in Figure 7 and 30 dB in Figure 8. Each of these figures contains two noisy images, one demonstrating a defocus error of one percent and another demonstrating a defocus error of ten percent.

\(^1\)More precisely, we consider a blurred version of the image. The blur can occur due to a defocus error.
Examples of our reconstruction versus that of the HIO algorithm are shown in Figures 9, 10, and 11. These reconstruction results correspond to SNR values of 15, 30, and 45 dB respectively. Note the failure of the HIO algorithm. It seems that its sensitivity to noise is quite high. However, this is not a fair comparison in the sense that our results were obtained with more input data: in addition to the Fourier magnitude we used ten defocused images (focus error range 1-10%). Using ten additional images does improve the reconstruction, but it is also enough to use only one, the results will still be good. We would like to incorporate this additional data into the HIO algorithm as well, however, there seems to be no way to do this. First, projection type algorithms generally do not work well when there are three or more constraints. Second, even if we could formulate the defocused image as a constraint, performing a naive projection on it is meaningless since there is only one solution. Moreover, due to the noise in the data, this solution may be a very poor version of the original image (as actually happens with ill-conditioned kernels).
Figure 9: Reconstruction quality using 10 defocused images (defocus error range 1-10%) is compared to that of the HIO algorithm which cannot use this data. Our results are quite good: the resulting SNR is 13.45 dB higher than the SNR of the inputs. HIO, on the other hand, renders meaningless result. All measurements were contaminated by Poisson noise with SNR=15 dB.
Figure 10: Similar to previous figure, but with Poisson noise of SNR=30 dB.
Our reconstruction method is based on minimization of the following functional:

\[ x^* = \arg \min_x \sum_{i=1}^n \| D_i x - y_i \|^2 + \| F x - r \|^2 + \| x_- \|^2 + \alpha \text{TV}(x), \]  

where \( n \) denotes the number of defocused images (in our experiments \( n \) values vary from one to ten). \( D_i \) and \( y_i \) are the defocus kernel (see Equation (5)) and noisy defocused image magnitude\(^2\) respectively. \( F \) and \( r \) denote the Fourier transform and the measured Fourier magnitude\(^3\). \( x_- \) represents the negative part of \( x \), i.e.

\[ x_- = \min(x, 0). \]  

\(^2\)Actual measurements correspond to the wave intensity, hence, this quantity is the square root of the measurements.

\(^3\)Again, the square root of the measurements.
To alleviate the impact of the noise in the measurements on the reconstructed image we used
the total variation (TV) regularization term [6]:

\[ \text{TV}(x) = \int_\Omega |\nabla x|. \] (8)

In Figure 12 we demonstrate the reconstruction quality of our method (for different TV
weights), with only one defocused image, compared to the quality of the HIO algorithm. Our
results are consistently better by about 25 dB.

![Figure 12: Phase retrieval with focusing: in addition to the Fourier magnitude one defocused
image is available (1% focusing error). Higher values of the total variation weight produces
better results in case of noisy images, however, for very clean images the weight must be
reduced.](image)

Even better results can be obtained if we add more defocused images as is evident from
Figure 13 where ten defocused images were available (focusing error of 1-10%). It is also
important to note that the reconstruction quality is not very sensitive to the weight of the
regularization term. This is a good property meaning that the reconstruction is robust and there is no need for parameter tweaking.

![Figure 13: Phase retrieval with focusing: in addition to the Fourier magnitude ten defocused images are available (1-10% focusing error). Higher values of the total variation weight produces better results in case of noisy images, however, for very clean images the weight must be reduced.](image)

5 Simultaneous Deblurring and Phase Retrieval

In this section we consider the situation where the Fourier magnitude is available together with a low-resolution and noisy image. This situation resembles what we had in Section 4 and can be viewed as an approximation to a case of incoherent illumination. Besides poor focus, these low-resolution images can be available from some inferior optical device, i.e., a cheap microscope or telescope. In either case a Gaussian kernel is a good approximation of the actual blurring kernel. In the results demonstrated below we use a Gaussian kernel of size $7 \times 7$ and standard deviation equal to 1.5. As before, to approximate real conditions,
all the measurements (both the low-resolution images and Fourier magnitude data) were contaminated by additive Poisson noise. To visualize the input data and reconstruction result we demonstrate in Figures 14, 15, and 16 the blurred (and noisy) input image for 15, 30, and 45 dB SNR respectively. The Fourier domain inputs are not shown, however the amount of noise is the same as that of the blurred images. As is evident from the experiments, our reconstruction consistently provides results that are 20 dB better than those of the HIO algorithm. In Figure 17 we demonstrate the reconstruction results for a broad range of SNR: from 10 to 50 dB.

Figure 14: Measurement SNR is 15 dB. Our method reconstruction yields 24 dB, while HIO produces only 2.1 dB.
Figure 15: Measurement SNR is 30 dB. Our method reconstruction yields 37.80 dB, while HIO produces only 12.54 dB.
Figure 16: Measurement SNR is 45 dB. Our method reconstruction yields 49.20 dB, while HIO produces only 25.58 dB.
The results demonstrate that our reconstruction is consistently better than that of the HIO algorithm, due to the fact that we are able to incorporate additional information.

The optimization problem was formulated as follows:

$$x^* = \arg \min_x \|Hx - y\|^2 + \|\|Fx\| - r\|^2 + \|x_-\|^2 + \alpha \text{TV}(x),$$

(9)

where the objective function is comprised of a set of penalty terms: one for each data source and a regularizing term $\alpha \text{TV}(x)$. The terms are as follows. The first source of information is the blurred images, hence, we introduce the term $\|Hx - y\|^2$ where $H$ is the blurring kernel and $y$ is the blurred (and noisy) measurement\(^4\). Then we add the Fourier domain data: $\|\|Fx\| - r\|^2$. Here $F$ represents the Fourier transform and $r$ is the measured Fourier magnitude\(^5\). The final piece of information is the non-negativity of the object, hence we add the term $\|x_-\|^2$, where $x_-$ represents the negative part of $x$ (see Equation (7)).

\(^4\)Strictly speaking $y$ is the square root of the measured data because all sensors record the wave intensity rather than amplitude.

\(^5\)Again, what is actually measured is $r^2$. 

Figure 17: Reconstruction quality versus measurements SNR.
6 Reconstruction From Multiple De-focused Images

In this work we consider image reconstruction from its defocused and noisy variants. That is, unlike what was done in Chapter 4, we drop the Fourier domain data altogether. Although this setup is not related directly to our main target: image reconstruction from the Fourier magnitude, it is potentially beneficial for the KLA-Tencor’s inspection procedure. Besides this, we would like to find out what measurements are more valuable: given a certain limit on the amount of input data, should we trade off the Fourier magnitude for another defocused image?

From the mathematical point of view, the problem is similar to what we had seen in Section 4 apart from the fact that the Fourier domain data is absent. We solve the following optimization problem

\[
x^* = \arg \min_x \sum_{i=1}^{n} \|D_i x - y_i\|^2 + \|x_+\|^2 + \alpha \text{TV}(x),
\]

Where the parameters \(D_i, y_i\) represent the defocus kernels and defocused noisy images respectively, in the way defined in Equation (6). Since the setup is very similar to what we had in Section 4, in this work we mainly check whether the reconstruction is possible and how important the Fourier domain information is: whether it provides any benefits over another defocused image in terms of reconstruction quality. Input examples can be found in Figures 7 and 8. The reconstruction examples for ten defocused images available as inputs are shown for SNR values of 15 dB, 30 dB, and 45 dB in Figures 18, 19, and 20 respectively.
Figure 18: Reconstruction from just defocused images compared with the reconstruction from defocus and Fourier magnitude. Reconstruction quality is very close, although addition of the Fourier data provides slightly better results. In this setup we use 10 defocused images (focus error range 1-10%) for reconstruction from the defocus only. When reconstructing from defocus and Fourier magnitude, we used only 9 defocused images (focus error range 1-9%) so that the number of measurements in both setups will be the same. All measurements were contaminated with Poisson noise with SNR=15 dB.
(a) Original

(b) Measurements: defocused (1%) version with noise (30 dB SNR)

(c) Reconstruction from the defocus and Fourier data: 42.09 dB SNR

(d) Reconstruction from the defocus data only: 42.25 dB SNR

Figure 19: Same as previous figure, but with Poisson noise of SNR=30 dB.
The results suggest that there is no particular benefit in measuring the Fourier magnitude instead of recording an additional defocused image. This may be true when the number of measurements is large (10 in this case). However, it is not necessary so when the number of measurements is small. Let us look at the case of two measurements only: once these are two defocused images and another time they are a defocused image and Fourier magnitude. Figures 21, 21, and 23 depict the reconstruction results for SNR of 15 dB, 30 dB, and 45 dB respectively.
Figure 21: Reconstruction from just defocused images compared with the reconstruction from defocus and Fourier magnitude. Reconstruction from defocused images provides better results. In this setup we use 2 defocused images (focus error range 1-2%) for reconstruction from the defocus only. When reconstructing from defocus and Fourier magnitude, we used only 1 defocused image (focus error 1%) so that the number of measurements in both setups will be the same. All measurements were contaminated with Poisson noise with SNR=15 dB.
Figure 22: Same as previous figure, with Poisson noise of SNR=30 dB.
Now we see that the Fourier data provides better results for higher SNR values. The difference is not big, but there is something more than the reconstruction quality. The optimization problem in our formulation includes one adjustable parameter: the weight of the regularization term $\alpha$. In the comparison above we used the best results available, i.e., the best value $\alpha$ that we could find. In practice, finding the best parameter value may be time-consuming and thus undesirable. Hence, for better evaluation of a particular data importance we must compare the sensitivity of reconstruction with or without that particular data. In Figures 24 and 25 we test whether the Fourier data gives better robustness to the reconstruction in case of two and ten measurements respectively.
Figure 24: Adding Fourier domain data make the reconstruction less dependent on the regularization parameter, hence, more robust.
Figure 25: When the number of measurements is large, it does not make much difference whether one takes the Fourier magnitude or another defocused image.
It turns out that if the number of total measurements is small it is better to take one defocused image and Fourier magnitude. In case of many measurements it does not really matter whether one uses the Fourier data or another defocused image.

7 Conclusions

This research focuses on the numerical solution of inverse problems arising in optics: phase retrieval, reconstruction from interferometric data, de-blurring, image reconstruction from its defocused versions, and combinations thereof. Special emphasis was put on tests with incomplete and corrupted data. The main idea is to formulate the problem in an appropriate way that will be suitable for modern numerical optimization techniques. Note that straightforward application of optimization algorithms is not sufficient in most cases. The problem must be formulated/modeled (this stage may include relaxations/approximations) in a certain way to allow successful solution. For example, there were many attempts in the past to solve the original phase-retrieval problem by convex optimization methods. All such attempts have failed due to the high non-convexity of the problem, even additional data, e.g., a phase uncertainty interval, does not help if used in a naive way. In this work we extend our previous results by incorporating new types of additional data—which is possible precisely due to the flexibility of these optimization methods—obtaining methods that are quite effective and robust with respect to noise. Our research spans a broad range of data and prior information, including defocused images, blurred and noisy images, interferograms and partial information on the phase. These results are of significant practical value, even though they are so far demonstrated only on synthetic examples. They do, however, require (nearly) coherent signals, which is why we could not apply them directly to data provided to us by KLA-Tencor. Working with incoherent signals should be possible, as our results with blurred data suggest, but this has not yet been accomplished in practice.
References


