Phase imaging based on wavefront propagation

Zhong, Jingshan

2014

Zhong, J. (2014). Phase imaging based on wavefront propagation. Doctoral thesis, Nanyang Technological University, Singapore.

<https://hdl.handle.net/10356/65341>

<https://doi.org/10.32657/10356/65341>

PHASE IMAGING BASED ON WAVEFRONT PROPAGATION

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A thesis submitted to the Nanyang Technological University
in fulfilment of the requirement for the degree Of
Doctorate of Philosophy

2014

Statement of Originality

I hereby certify that the work embodied in this thesis is the result of original research and has not been submitted for a higher degree to any other University or Institution.

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Date

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author

Acknowledgements

First and foremost, I would like to thank my advisor, Dr. Justin Dauwels, for his guidance, advice and wisdom. He encouraged me to think independently but also gave me chances to attend international conferences, visit other labs and learn to work collaboratively with our collaborators. I thank Nanyang Technological University for providing the financial support and training me by teaching assistantship.

I want to express my thanks to my friends at NTU. Especially I would like to thank Yang Feng, Wing Yee Sit, Chen Yan, Yang Xuefeng and Yang Xin in Biomedical Electronics lab at which I stayed for the first two years of my PhD. Importantly I shared precious memories with my labmates in Dauwels' group: Hang Yu, Zhao Wei, Muhammad Tayyab, Jing Jin, Wang Mengmeng, Nikola Mitrovic, Yasir Tahir, Du bo, Dhanya Memon, Sharon Ong, Manuel Vázquez and Srinivasan Kannan. I also had a wonderful time with my other Chinese labmates: Qi Yongbin, Guan Zheming, Jiang Chaoyang, Wei Zhe, Wei Chen and Zhu Qingchang.

I am also indebted to Dr. Laura Waller, assistant professor at the EECS department of UC Berkeley, from whom I learned a lot since my first year of PhD. I appreciate her for the guidance in my research and giving me the chance to visit her lab for half a year in my fourth year of PhD. I also need to thank her post-doc Lei Tian for his

useful discussions in our collaboration and helps in the optics experiments; we also shared a happy time in Berkeley and San Francisco, especially the nice restaurants we visit together. I thank my labmates at Berkeley for their helps and discussions, particularly Aamod Shanker, Daniel Shuldman, Rene Clause, Wang Jingyan and Liu Sijia. I also appreciate the helps and experimental data from the MIT 3D Optical System Group, especially Justin Lee, Huang Yuanhao and Prof. George Barbastathis.

I thank my roommates Zhu Hongyuan, Cui Yingnan, Yuan Quan, Zhang Yuzhe and Yang Qing for their friendship and caring. I would like to thank my undergraduate classmates studying at Singapore: Diao Qiming, Zhao Xun and Zhang Dajiang. I am grateful that we had a chance to study and work together in Singapore after graduating from USTC.

Special thanks must go to my dear parents and cousins for their love and support. Especially I would like to thank my elder sister Zhong Aiyue for her support and encouragement since my junior high school.

Summary

Light is a wave which has both amplitude and phase. Since the vibration of the wave is too fast, phase needs to be recovered from the time-averaged energy—intensity by computational methods. In this thesis, we choose defocus as a way to mix phase into measured intensity images, because it is not only efficient in transferring phase to intensity but also advantageous due to its simplicity and flexibility in the experiment.

In this thesis, we develop computational methods to recover phase from defocused intensity images which contain phase information. We first propose methods based on complex Kalman filtering, which updates the complex field from the noisy intensity images by maintaining pair-wise pixel error correlation. We prove that the pixel-wise correlation is sparse and it reduces computational complexity of the method from cubic to linear of the total number of the pixel numbers.

Secondly, we introduce an exponential spacing measurement scheme to efficiently reduce the number of defocused intensity images. We perform Gaussian process regression over the exponentially spaced intensity images to estimate the axial derivative in the transport of intensity equation (TIE) phase retrieval. It alleviates the nonlinearity error in the derivative estimation by using the prior knowledge of how intensity varies with defocus propagation in the spatial frequency domain.

Finally, we also consider the phase recovery of partially coherent illumination created by any arbitrary source shape in Köhler geometry. By extending the Kalman filtering algorithms to the partially coherent case, we recover not only the phase but also an estimate of the unknown illumination source shape.

In conclusion, we consider the issues of noise, intensity measurement scheme, nonlinearity error in TIE and partially coherent illumination. We validate our techniques experimentally with a brightfield microscope. Since the measurement of defocused intensity images is experimentally simple and flexible, the methods in this thesis should find use in optical, X-ray and other phase imaging systems.

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List of Abbreviations

The following table describes the abbreviations and acronyms used throughout the thesis. The page on which each one is defined or first used is also given.

Abbreviation	Meaning	Page
TEM	transmission electron microscopy	1
CEKF	complex extended Kalman filter	5
ACEKF	augmented complex extended Kalman filter	5
TIE	transport of Intensity equation	6
GP	Gaussian process (GP) regression	6
SGDF TIE	a TIE method by Savitzky-Golay differentiation filter	17
GS	the Gerchberg-Saxton method	18
EKF	extended Kalman filter	25
DFT	discrete Fourier transform	32
RMSE	root mean square error	37
higher order TIE	a TIE method by higher order derivatives estimation	64
GP TIE	a TIE method by Gaussian process regression	66
NA	numerical aperture	87
SMO	source mask optimization	88

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Chapter 1

Introduction

1.1 Quantitative phase imaging

Light behaves as an electromagnetic wave, which has both electric and magnetic field components synchronously oscillating perpendicularly to each other. When light passes through an object, the amplitude and phase of wave field change due to its interaction with the object. Quantitative phase imaging refers to recovering/measuring the optical phase shift in the wave field.

Phase contains important information about the properties of object or sample. In cell imaging application [1], phase shift reveals information of the refractive index variations within structure of cells. In biomedical imaging, phase imaging has useful applications in the refractive index measurement of label-free cells [2], measurement of optical path [3, 4], investigation of cell mass and growth dynamics [5], and reconstruction of 3D structure of cells [6, 7]. Figure 1.1 demonstrates that the phase shift happens when the light passes thorough bovine endothelial cells, and the recovered phase shows the shape and structure of the cells. In transmission electron microscopy (TEM), significant phase changes are introduced by the atomic potentials within the specimen. Phase imaging allows for the measurement of potentials in material and

the measurement of electric and magnetic fields within the specimen [8–10]. Phase imaging also finds wide use in other applications such as X-rays imaging [11, 12], adaptive optics, and edge effect detection in lithography [13].

Figure 1.1: (a) Illustration of phase delay when light passes through an object. (b) Recovered phase of bovine endothelial cells. The phase image shows shape and structure of the cells.

1.2 Quantitative phase imaging from defocused intensity images

Unfortunately, phase cannot be measured directly because the light wave oscillates too fast to be captured by a common commercial camera. It needs to reconstruct phase from the field's time-average intensity which can be easily measured by the camera. The quantitative phase imaging problem can be demonstrated as the need to recover a sample's complex-field, $A(x, y)$, from measurements of intensity, $I(x, y) = |F\{A(x, y)\}|^2$, where $F\{\cdot\}$ is an operator describing the optical system transfer function. At the sample, intensity images contain no information about the phase of $A(x, y)$. However, with a suitable choice of optical system, F , the sample's phase information is translated into intensity variations. Therefore, treating as inverse

problem the complex field $A(x, y)$ is possible to recover from the intensity images, which are measured in the optical system F .

Designing an efficient optical system, F , for obtaining phase-to-intensity contrast is crucial in phase imaging. Various architectures have been proposed, broadly categorized as interferometry [14], Shack-Hartmann sensors [15], grating-based [16] and defocus-based techniques [17, 18]. In fact, any *complex* transfer function will induce some phase contrast (e.g. defocus [18], chromatic aberration [19]). The amount of phase information transferred can be quantified [20], but the ideal choice of F remains a subjective task, since it involves a complicated tradeoff between experimental complexity, cost, accuracy, and the sample itself.

In this thesis, we choose a convenient F - defocus to transfer the phase information into intensity images. The transfer function for defocus has been well-studied [21, 22]. We review the basics of defocus wave propagation in free space starting from the Maxwell's equations in Chapter 2. Importantly, the measurement of defocused intensity images is inexpensive and experimentally simple, even for lensless imagers or non-traditional wavelengths (e.g. X-ray [11], TEM [8]). Figure. 1.2 demonstrates a generalized experimental setup for the measurement of defocus stack. The object/sample is placed at the focal plane. A stack of defocused intensity image can be easily measured by moving the camera or sample to vary the defocus distance, z . The wave propagation by a defocus distance z transfers the phase information to the intensity images. Figure. 1.3 shows a practical example of the imaging system described in Fig 1.2. With an extra z axis motion stage attached, the brightfield microscope can be used to measure the defocused intensity stack.

Figure 1.2: Generalized experimental setup for an imaging system (e.g. a microscope) which captures intensity images at a range of axial defocus distances in order to recover phase. The phase is transferred into the intensity images by defocus.

Figure 1.3: (Left) A brightfield microscope with z axis motion stage attached for capturing through-focus stacks. (Right) A through-focus stack of intensity images obtained by defocusing human cheek cells sample.

1.3 Outline of the thesis

This thesis focuses on developing computational methods to reconstruct both phase and amplitude of complex field from defocused intensity images. The outline of this thesis is as follows:

- Chapter 2 introduces wave propagation starting from the Maxwell's equations, reviews the methods of quantitative phase recovery from defocused intensity images stack, and discusses the basics of the Kalman filters and complex Kalman filters.
- Chapter 3 develops a diagonalized complex extended Kalman filter (CEKF) to infer the phase from a sequence of intensity images taken at different defocus distances. The computational complexity of the proposed algorithm is in the order of $N_z N \log N$, and the data storage requirement scales linearly with N , where N_z is the number of images and N is the number of pixels per image. With the advantage of low complexity, forward and backward sweeps of Kalman filtering can be applied to improve the accuracy of the algorithm. By limiting the number of iterations, one can trade off accuracy vs. complexity.
- Chapter 4 proposes a novel low-complexity recursive filter to efficiently recover quantitative phase from a series of noisy intensity images taken through focus. We first transform the wave propagation equation and nonlinear observation model (intensity measurement) into a complex augmented state space model. From the state space model, we derive a sparse augmented complex extended Kalman filter (ACEKF) to infer the complex optical field (amplitude and phase), and find that it converges under mild conditions. Our proposed method has a

computational complexity of $N_z N \log N$ and storage requirement of $\mathcal{O}(N)$, compared with the original ACEKF method, which has a computational complexity of $\mathcal{O}(N_z N^3)$ and storage requirement of $\mathcal{O}(N^2)$. Thus, it is efficient, robust and recursive, and may be feasible for real-time phase recovery applications with high resolution images.

- Chapter 5 demonstrates a method for solving the Transport of Intensity equation (TIE) from a stack of defocused intensity images taken by a microscope or lensless imager. Our method enables quantitative phase imaging with improved accuracy and reduced data capture, while also being computationally efficient and robust to noise. We use prior knowledge of how intensity varies with propagation in the spatial frequency domain in order to constrain a fitting algorithm [Gaussian process (GP) regression] for estimating the axial intensity derivative. Solving the problem in the frequency domain inspires an efficient measurement scheme which captures images at exponentially spaced focal steps, significantly reducing the number of images required. Low-frequency artifacts that plague traditional TIE methods can be suppressed without an excessive number of captured images. We validate our technique experimentally by recovering the phase of human cheek cells in a brightfield microscope.
- Chapter 6 describes a new method for phase recovery that uses partially coherent illumination created by any arbitrary source shape in Köhler geometry. From a stack of measured defocused intensity images, we recover not only the quantitative phase information but also the illumination source shape, which describes the spatial coherence of the illumination. Our algorithm uses a Kalman filtering approach which is fast, accurate and robust to noise. The method is experimentally simple and flexible, so should find use in optical, electron,

X-ray and other phase imaging systems which employ partially coherent light. The proposed method has potential application where the source information is difficult to measure, such as source mask optimization in lithography and coded illumination microscopy. We provide an experimental demonstration in an optical microscope with various condenser apertures.

- Chapter 7 offers our conclusions and suggests topics for future work.

Chapter 2

Literature review

In this thesis, we use machine learning and signal processing methods to recover phase from defocused intensity images. We review the basics of the related topics in optics, machine learning and signal processing in this chapter. The structure of this chapter is as follows:

- Section 2.1 describes the propagation of coherent light, the importance of phase in the defocused intensity stack and the approximation of wave equation.
- Section 2.2 reviews the methods for quantitative phase recovery from defocused intensity images. The methods are discussed in three main categories: Transport of Intensity Equation (TIE) methods, iterative methods and statistical approaches.
- Finally, Section 2.3 introduces the Kalman filtering, from the most basic linear Kalman filter to the augmented complex extended Kalman filter which is used for the phase recovery in the following chapters.

2.1 Defocus propagation of coherent light

2.1.1 Light as an electromagnetic wave

Light has properties of electromagnetic waves whose electrical and magnetic fields obey the Maxwell's equations [23]. In vacuum and free-charge space, the Maxwell's equations are expressed as:

$$\nabla \times \vec{E} = -\mu_0 \frac{\partial \vec{H}}{\partial t} \quad (2.1)$$

$$\nabla \times \vec{H} = \epsilon_0 \frac{\partial \vec{E}}{\partial t} \quad (2.2)$$

$$\nabla \cdot \epsilon_0 \vec{E} = 0 \quad (2.3)$$

$$\nabla \cdot \mu_0 \vec{H} = 0, \quad (2.4)$$

where $\vec{E}$ is the electric field in 3-D space (x, y, z) , $\vec{B}$ is the magnetic field, μ_0 is the permeability, and ϵ_0 is the permittivity. The equations predict that $\vec{E}$ field and $\vec{H}$ field are possible to be coupled with each other: a time-varying $\vec{E}$ field generates a time-varying $\vec{B}$ fields, and vice versa. Indeed, the Maxwell's equations for *free space* can be manipulated into two vector expressions [23]:

$$\nabla^2 \vec{E} = \epsilon_0 \mu_0 \frac{\partial^2 \vec{E}}{\partial t^2} \quad (2.5)$$

$$\nabla^2 \vec{H} = \epsilon_0 \mu_0 \frac{\partial^2 \vec{H}}{\partial t^2}, \quad (2.6)$$

where the Laplacian ∇^2 operates on each component of $\vec{E}$ and $\vec{H}$. And hence, it results in six scalar wave equations (for $\vec{E}_x, \vec{E}_y, \vec{E}_z, \vec{H}_x, \vec{H}_y$, and $\vec{H}_z$) which take the

same form:

$$\nabla^2 f = \epsilon_0 \mu_0 \frac{\partial^2 f}{\partial t^2}. \quad (2.7)$$

Eqs. (2.5) and (2.6) predict and describe the light as an electromagnetic wave which has time-varying electrical and magnetic fields in the 3D space. Each component in the fields obeys the wave equation in Eq. (2.7). The classical electromagnetic wave theory well explains the wave properties of light such as interference and diffraction, but it fails to interpret the particle properties of light. However, modelling light as an electromagnetic wave is useful in the general situations which only consider the average property of a large number of photons.

2.1.2 Wave propagation

The propagation of wave field can be derived from the wave equation, Eq. (2.7). For a monochromatic and coherent light wave of frequency ν , the $\vec{E}$ field or $\vec{B}$ field (ignoring the polarization effect) may be written explicitly with a scalar function as:

$$f(x, y, z, t) = A(x, y, z) \exp(-j2\pi\nu t). \quad (2.8)$$

The complex function $A(x, y, z)$ of position (x, y, z) has

$$A(x, y, z) = |A(x, y, z)| \exp(-j\phi(x, y, z)), \quad (2.9)$$

where $|A(x, y, z)|$ and $\phi(x, y, z)$ are the amplitude and phase of $A(x, y, z)$.

From the classical electromagnetic wave theory, the field $f(x, y, z, t)$ is a solution of

the scalar wave equation Eq. (2.7). By substituting $f(x, y, z, t)$ back into Eq. (2.7), the *Helmholtz equation* [24], which is free of the time variable, is obtained

$$(\nabla^2 + (\frac{2\pi}{\lambda})^2)A = 0, \quad (2.10)$$

where λ is the wavelength of the light. The complex field $f(x, y, z, t)$ oscillates with frequency of ν at each position in the 3D space (see Eq. (2.8)), and the complex function $A(x, y, z)$ of $f(x, y, z, t)$ obeys the Helmholtz equation.

If it is given that the boundary condition at $z = 0$ equals $A(x, y; 0)$ and the boundary condition at infinity meets Sommerfeld radiation condition [24], the complex function $A(x, y, z)$ in the whole 3D space can be solved from the Helmholtz equation. It gives the Huygens–Fresnel principle for wave diffraction:

$$A(x, y, z) = \frac{z}{j\lambda} \iint A(\xi, \eta; 0) \frac{\exp(j\frac{2\pi}{\lambda}r_{01})}{r_{01}^2} d\xi d\eta, \quad (2.11)$$

where the distance r_{01} is given by

$$r_{01} = \sqrt{z^2 + (x - \xi)^2 + (y - \eta)^2}. \quad (2.12)$$

The distribution $A(x, y, z)$ at any plane z is computed by the integration in Eq. (2.11), which can be understood as defocus propagation from the plane $A(x, y; 0)$ with a distance of z . The measured intensity of a camera placed at z is proportional to $|A(x, y, z)|^2$. At the focal plane $z = 0$, the measured intensity doesn't contain any information of the phase of $A(x, y; 0)$. However, as some amount of defocus is introduced by varying the defocus distance z , the amplitude and phase information is mixed into the measured intensity by defocus wave propagation. Therefore, a stack of

defocused intensity images, measured by varying the defocus distance z , contains the information about the amplitude and phase of $A(x, y; 0)$ (see Fig. 1.2 in Chapter. 1). By treating as an inverse problem, the phase is possible to recover from the defocused intensity images with computational methods.

2.1.3 The Fresnel diffraction and paraxial approximation of wave equation

The Huygens–Fresnel diffraction given in Eq. (2.11) can be approximated with the Fresnel diffraction. By assuming that the defocus distance z is large, the distance r_{01} in Eq. (2.11) is approximated as

$$\begin{aligned} r_{01} &= z \sqrt{1 + \left(\frac{x - \xi}{z}\right)^2 + \left(\frac{y - \eta}{z}\right)^2} \\ &\approx z \left\{ 1 + \frac{1}{2} \left(\frac{x - \xi}{z}\right)^2 + \left(\frac{y - \eta}{z}\right)^2 \right\}. \end{aligned} \quad (2.13)$$

By substituting the approximation of r_{01} back into Eq. (2.11), the Fresnel diffraction is given as

$$A(x, y; z) \approx \frac{e^{i\frac{2\pi z}{\lambda}}}{j\lambda z} \iint A(\xi, \eta; 0) \exp \left\{ j \frac{\pi}{\lambda z} [(x - \xi)^2 + (y - \eta)^2] \right\} d\xi d\eta \quad (2.14)$$

$$= U(x, y; 0) * \left\{ \frac{e^{i\frac{2\pi z}{\lambda}}}{j\lambda z} \exp \left[j \frac{\pi}{\lambda z} (x^2 + y^2) \right] \right\}, \quad (2.15)$$

where $*$ denotes the convolution operation. The convolution in Eq. (2.15) can be written as multiplication in the Fourier domain:

$$\begin{aligned} A(x, y, z) &= \mathfrak{F}^{-1}\{\mathfrak{F}\{A(x, y, 0)\}H(u, v)\} \\ H(u, v) &= e^{i\frac{2\pi z}{\lambda}} \exp[-i\pi\lambda z(u^2 + v^2)], \end{aligned} \quad (2.16)$$

where $\mathfrak{F}(A(x, y, 0))$ is the Fourier transform of $A(x, y, 0)$, $\mathfrak{F}^{-1}$ denotes inverse Fourier transform, and u, v are the spatial frequency variables.

Note that the approximation in Fresnel diffraction also has the same effect as performing *paraxial approximation* [24] on the Helmholtz equation in Eq. (2.10), which is given as:

$$\frac{\partial A(x, y, z)}{\partial z} = \frac{i\lambda}{4\pi} \nabla_{\perp}^2 A(x, y, z), \quad (2.17)$$

where λ is the wavelength, and $\nabla_{\perp}$ denotes the gradient operator in the lateral (x, y) dimensions only.

2.2 Phase recovery methods from defocused intensity images

2.2.1 Transport of Intensity Equation

The Transport of Intensity Equation (TIE) provides a direct method to solve for phase from a defocused intensity images stack. Transport of Intensity Equation (TIE) [18, 25] reveals the relation between phase and the variation of intensity along the optical

axis z :

$$\left. \frac{\partial I(x, y, z)}{\partial z} \right|_{z=0} = -\frac{\lambda}{2\pi} \nabla_{\perp} \cdot [I(x, y, 0) \nabla_{\perp} \phi(x, y)], \quad (2.18)$$

where $I(x, y, 0)$ is the intensity of the complex field $A(x, y, 0)$ at focus, $\phi(x, y)$ is the phase, λ is the spectrally-weighted mean wavelength of illumination and $\nabla_{\perp}$ denotes the gradient operator in lateral directions (x, y) only.

Figure 2.1 demonstrates a diagram for the TIE-based methods. In the first step, the axial first derivative of intensity $\left. \frac{\partial I(x, y, z)}{\partial z} \right|_{z=0}$ is approximated from the defocused intensity images with numerical methods (because the derivative is difficult to be measured directly). In the second step, the phase is solved with Laplacian inversion (or Poisson solver in some literatures) after both $\left. \frac{\partial I(x, y, z)}{\partial z} \right|_{z=0}$ and $I(x, y, 0)$ in Eq. (2.18) have been already known. We review details of these two steps later in this section.

Figure 2.1: The TIE phase recovery methods can be generally summarized with two steps: estimating the axial first derivative of intensity $\left. \frac{\partial I(x, y, z)}{\partial z} \right|_{z=0}$ from the defocused intensity images and applying Laplacian inversion to solve for phase.

The derivation of TIE is inspired by the paraxial approximation of the wave equation (Eq. (2.17)). It is derived in [18] by subtracting the multiplication result of $A^*(x, y, z)$ and Eq. (2.17) with the multiplication result of $A(x, y, z)$ and the conjugate of Eq. (2.17). The Transport of Intensity Equation can also be understood from the law of conservation of local energy (intensity) [26]: the variation of intensity ($\left. \frac{\partial I(x, y, z)}{\partial z} \right|_{z=0}$) is proportional to the flux of intensity along z ($I(x, y, 0) \nabla_{\perp} \phi(x, y)$ equals the amplitude of Poynting vector).

Besides being simple in the experiment, the TIE method achieves phase accuracy equivalent to that of interferometric methods. It is much less sensitive to coherence in the illumination [27], requires no phase unwrapping, and is computationally efficient [28].

Laplacian inversion

We consider the methods of solving the phase $\phi(x, y)$ from Eq. (2.18) after both $\left. \frac{\partial I(x, y, z)}{\partial z} \right|_{z=0}$ and $I(x, y, 0)$ have been already known. Assume a simple case when $I(x, y, 0)$ is constant [29]. By taking $I(x, y, 0)$ out of the divergence operation, the right hand side of Eq. (2.18) is simplified as Laplacian:

$$\left. \frac{\partial I(x, y, z)}{\partial z} \right|_{z=0} = -\frac{\lambda}{2\pi} I(x, y, 0) \nabla_{\perp}^2 \phi(x, y). \quad (2.19)$$

So the phase can then be recovered by Laplacian inversion (Poisson solver):

$$\Phi(u, v) = F(u, v) / [-4\pi^2(u^2 + v^2)], \quad (2.20)$$

where $\Phi(u, v)$ is the Fourier transform of $\phi(x, y)$, $F(u, v)$ is the Fourier transform of

the estimated first derivative $\left. \frac{\partial I(x, y, z)}{\partial z} \right|_{z=0}$ scaled by the constant term $2\pi/\lambda I(x, y, 0)$, and u, v are the spatial frequency variables.

When $I(x, y, 0)$ is not constant, an auxiliary term $\psi(x, y)$ needs to be introduced and Eq. (2.18) is written with two equations [18]:

$$\nabla_{\perp} \psi(x, y) = I(x, y, 0) \nabla_{\perp} \phi(x, y) \quad (2.21)$$

$$\left. \frac{\partial I(x, y, z)}{\partial z} \right|_{z=0} = -\frac{\lambda}{2\pi} \nabla_{\perp}^2 \psi(x, y). \quad (2.22)$$

The auxiliary term $\psi(x, y)$ is obtained by solving Eq. (2.22) with Laplacian inversion. By dividing both sides of Eq. (2.21) with $I(x, y, 0)$ and taking divergence, we get

$$\nabla_{\perp} \cdot \left[\frac{1}{I(x, y, 0)} \nabla_{\perp} \psi(x, y) \right] = \nabla_{\perp}^2 \phi(x, y). \quad (2.23)$$

Finally, $\phi(x, y)$ is solved with Laplacian inversion again with that the left part of Eq. (2.23) has been already known. Note that the denominator of Laplacian inversion (see Eq. (2.20)) goes towards zero as the spatial frequency goes towards zero, so a small regularization parameter must be added in order to avoid division-by-zero instability. This means that the DC phase term is lost and the TIE methods are sensitive to low frequency noise. And hence, it is important to improve the accuracy in the estimation of $\left. \frac{\partial I(x, y, z)}{\partial z} \right|_{z=0}$, especially for the low frequency components.

Estimation of the first derivative of intensity $\left. \frac{\partial I(x, y, z)}{\partial z} \right|_{z=0}$

Limitations of the TIE method mainly stem from noise and nonlinearity in the intensity derivative estimate, both of which we address here. Nonlinearity error comes from the estimation of the intensity derivative, $\left. \frac{\partial I(x, y, z)}{\partial z} \right|_{z=0}$, from through focus im-

ages. We cannot measure this linear (first) derivative directly and so it is usually estimated by finite difference methods. The first method [18] only estimates the first derivative from two intensity image plane defocused by a small distance Δz over the focus:

$$\left. \frac{\partial I(x, y, z)}{\partial z} \right|_{z=0} \approx \frac{I(x, y, \Delta z) - I(x, y, -\Delta z)}{2\Delta z}. \quad (2.24)$$

However, intensity is not linear through focus, due to diffraction, and so any nonlinearity in the through focus intensity corrupts the derivative estimate [30, 31]. Nonlinearity error can be removed by using multiple defocus intensity images through-focus in higher order TIE method [32]. It performs polynomial fitting on each pixel's intensity vs. z plot in order to extract the first order derivative. This provides some inherent noise stability and mitigates the nonlinearity error. However, there is a danger of over-fitting (fitting to noise) and the optimal order to use will be phase dependent, making it a difficult parameter to optimize. The Savitzky-Golay differentiation filter (SGDF) TIE [33] was proposed to solve this trade-off between the order of fitting and noise in higher order TIE. It recovers phase images with different orders of polynomial fitting, then combines these phase images into a final reconstructed phase with band-pass filters. Limitations are that the fitting becomes unstable when the order is large [34] and the derivation assumes equally spaced focus steps, which we show to be non-ideal in Chapter 5.

2.2.2 Iterative methods

The iterative methods for phase recovery refer to the algorithms which repeatedly and iteratively update the desired complex field with the constraint of measured

defocused intensity images. The Gerchberg-Saxton (GS) method [35] is probably the first and earliest iterative method. It only needs two measured intensity images: the intensity at focal plane and the modulus at Fourier plane. The GS method updates the unknown complex field by propagating forward and backward between spatial and Fourier domain. As shown in Fig. 2.2, the following steps need to be proceeded:

- (i) Initialize the estimated complex field at plane 1.
- (ii) Propagate the estimated complex field from plane 1 to plane 2, and replace the intensity of the estimated complex field with Intensity 2.
- (iii) Propagate the estimation back to plane 1, and replace its intensity with Intensity 1.
- (iv) Repeat until the error is small enough.

Figure 2.2: A scheme of the GS algorithm. Intensity 1 and Intensity 2 are the measured intensity images at Plane 1 and Plane 2, respectively.

There are three main elements in the description of the GS method in Fig. 2.2: the way of the estimation being updated from the measured intensity, the measurement position of intensity planes, and the number of intensity images. Any change of these three elements brings new variation of iterative methods. Potential improvements in the

estimation update were introduced in Error-reduction algorithm, the Gradient-search algorithm, Input-Output-algorithm, and Yang-Gu in [17, 36, 37]. Instead of using Fourier transform, methods using Fresnel transform as the complex transfer function in the intensity measurement were developed in [38–41]. The iterative methods of multiple defocused intensity images were proposed in [42–45]. The methods using multiple intensity images have similar procedure as the GS method; the estimated complex field is first propagated within the measured intensity planes and updated by replacing the intensity of the estimated field with the measured intensity [43, 45].

The GS method can be explained as a subset of projection over convex sets (POCS) method, which is developed to calculate the intersection of sets in an alternative projection manner. In phase recovery, each intensity image formulates a set (or constraint) of the potential solutions for the unknown complex field; then the GS method (or POCS) is used to find an intersection of those sets by alternative projection. Since the set of intensity constraint is nonconvex, the GS method only converges a stationary point and does not guarantee a global minimum [46]. The GS method can also be understood as a kind of gradient descent methods or error-reduction method [17, 47], which minimizes the least error between estimation and measurement. But the convergence speed for the GS method could be slow, partly due to the property of gradient descent methods [47]. In the case of strong noise, the constraints set of intensity measurement may not have intersections. However, soft or fuzzy projections [48] could be applied to guarantee a common intersection.

2.2.3 Statistical approach

A few statistical approaches in estimation theory have been proposed as well; an approximation to the maximum likelihood estimator is derived in [49, 50]. However, it is iterative, easily gets stuck in a local maximum and faces trade-off between noise and accuracy. In [51] an extended Kalman filter is proposed to recover phase from a stack of noisy defocused intensity images. The Kalman filter provides a theoretically near-optimal solution to compute an estimate from the noisy measurement. In the state-space model, it uses the wave propagation as state transition and approximates the Poisson noise in the intensity measurement as Gaussian. However, in order to achieve the noise reduction, it requires to maintain and update the covariance matrix which records the pair-wise pixel noise correlation. This demands a high computational complexity and storage requirement in the algorithm implementation, and hence it is impractical for the real-time applications when the size of image is large.

2.3 An introduction to the Kalman filter

2.3.1 Linear Kalman filter

The *Kalman filtering* is a method to estimate the statistics of states from the noisy measurements. Since its first publication in 1960 [52], the Kalman filter has found its use in control systems, navigation, out-space vehicles, and so on. In linear Kalman filter, the state $\mathbf{x}_k \in \mathbb{R}^n$ is governed by a linear stochastic difference equation,

$$\mathbf{x}_k = \mathbf{A}\mathbf{x}_{k-1} + \mathbf{u}_k, \quad (2.25)$$

with its measurement $\mathbf{y}_k \in \mathbb{R}^m$

$$\mathbf{y}_k = \mathbf{C}\mathbf{x}_k + \mathbf{v}_k. \quad (2.26)$$

The matrix $\mathbf{A}$ in Eq. (2.25) is the state transition matrix which relates the state $\mathbf{x}_k$ at time k with the previous state $\mathbf{x}_{k-1}$ at time $k-1$. The matrix $\mathbf{C}$ is the observation matrix which maps the current state $\mathbf{x}_k$ into its measurement $\mathbf{y}_k$. The variables $\mathbf{u}_k$ and $\mathbf{v}_k$ represent the Gaussian noise in the process and measurement, which has

$$\mathbf{u}_k \sim \mathcal{N}(0, \mathbf{W}_k) \quad (2.27)$$

$$\mathbf{v}_k \sim \mathcal{N}(0, \mathbf{R}_k). \quad (2.28)$$

With the state-space model (Eqs. (2.25) and (2.26)), the Kalman filter is able to maintain the first two moments of the state distribution:

$$E[\mathbf{x}_k] = \bar{\mathbf{x}}_k \quad (2.29)$$

$$E[(\mathbf{x}_k - \bar{\mathbf{x}}_k)(\mathbf{x}_k - \bar{\mathbf{x}}_k)^T] = \mathbf{M}_k, \quad (2.30)$$

where $\bar{\mathbf{x}}_k$ is the mean and $\mathbf{M}_k$ is the covariance matrix which records the pair-wise error correlation of the state estimation. The Kalman filter estimates the mean and covariance matrix in the state distribution by a form of feedback control, in which the prediction step predicts the estimation and the update step corrects the estimation with the measurement.

In the prediction step, the Kalman filter obtains the *a priori* estimation of the state $\mathbf{x}_k$ from the estimation of the previous state $\mathbf{x}_{k-1}$. The mean $\hat{\mathbf{x}}_k$ and covariance $\hat{\mathbf{M}}_k$

of the *a priori* estimate can be derived from Eq. (2.25) of the state-space model:

$$\hat{\mathbf{x}}_k = \mathbf{A}\bar{\mathbf{x}}_{k-1} \quad (2.31)$$

$$\hat{\mathbf{M}}_k = \mathbf{A}\mathbf{M}_{k-1}\mathbf{A}^T + \mathbf{W}_k. \quad (2.32)$$

In the update step, the *a posteriori* estimate is derived by correcting the *a priori* estimate with the measurement $\mathbf{y}_k$. The *a posteriori* estimation $\bar{\mathbf{x}}_k$ is computed as a linear combination of the *a priori* estimation $\hat{\mathbf{x}}_k$ with a weighted difference between the measurement $\mathbf{y}_k$ and a measurement prediction $\mathbf{C}\hat{\mathbf{x}}_k$:

$$\bar{\mathbf{x}}_k = \hat{\mathbf{x}}_k + \mathbf{G}_k(\mathbf{y}_k - \mathbf{C}\hat{\mathbf{x}}_k). \quad (2.33)$$

The weight $\mathbf{G}_k$ (or the Kalman gain) can be derived by minimizing the square error $E[(\mathbf{x}_k - \bar{\mathbf{x}}_k)^T(\mathbf{x}_k - \bar{\mathbf{x}}_k)]$, which is equal to the trace of the covariance matrix $\mathbf{M}_k$. It follows

$$\mathbf{G}_k = \hat{\mathbf{M}}_k\mathbf{C}^T(\mathbf{C}\hat{\mathbf{M}}_k\mathbf{C}^T + \mathbf{R})^{-1}, \quad (2.34)$$

$$\bar{\mathbf{x}}_k = \hat{\mathbf{x}}_k + \mathbf{G}_k(\mathbf{y}_k - \mathbf{C}\hat{\mathbf{x}}_k), \quad (2.35)$$

$$\mathbf{M}_k = \hat{\mathbf{M}}_k - \mathbf{G}_k\mathbf{C}\hat{\mathbf{M}}_k. \quad (2.36)$$

The Kalman filter provides the least mean square error estimation when the state-space model is linear. Note that an alternative derivation of the Kalman filter from the perspective of Bayesian inference will be explained in details in Section 2.3.2. The prediction step predicts the *a priori* estimation and the update step obtains the *a posteriori* estimate by correcting the *a priori* estimation. By this prediction-correction process, the Kalman filter maintains the first two moments of the state distribution.

Since the Kalman filter updates the state distribution immediately with the new measurement, it has a nice property of being able to process the data in a recursive manner.

2.3.2 The Kalman filter by Bayesian inference

The prediction and update steps in the Kalman filter can be explained as an instantiation of Bayesian inference [53]. The variables are assumed to be Gaussian distributed, which only requires first two moments of the state distribution. The aim becomes to obtain the distribution of the state $\mathbf{x}_k$ conditioned on all k measurements

$$p(\mathbf{x}_k | \mathbf{y}_1, \mathbf{y}_2, \dots, \mathbf{y}_k). \quad (2.37)$$

Suppose the distribution of the state $\mathbf{x}_{k-1}$ from the previous $k - 1$ measurements is given as:

$$p(\mathbf{x}_{k-1} | \mathbf{y}_1, \mathbf{y}_2, \dots, \mathbf{y}_{k-1}) = \mathcal{N}(\bar{\mathbf{x}}_{k-1}, \mathbf{M}_{k-1}). \quad (2.38)$$

we can derive from Eq. (2.25) of the state-space model that the *a priori* distribution of the state

$$p(\mathbf{x}_k | \mathbf{y}_1, \mathbf{y}_2, \dots, \mathbf{y}_{k-1}) = \mathcal{N}(\hat{\mathbf{x}}_k, \hat{\mathbf{M}}_k), \quad (2.39)$$

where the mean $\hat{\mathbf{x}}_k$ and the covariance matrix $\hat{\mathbf{M}}_k$ can be written as:

$$\hat{\mathbf{x}}_k = \mathbf{A}\bar{\mathbf{x}}_{k-1} \quad (2.40)$$

$$\hat{\mathbf{M}}_k = \mathbf{A}\mathbf{M}_{k-1}\mathbf{A}^T + \mathbf{W}_k. \quad (2.41)$$

From the measurement equation in Eq. (2.26), the joint probability distribution of the state $\mathbf{x}_k$ and the measurement $\mathbf{y}_k$ can be expressed as:

$$p\left(\begin{bmatrix} \mathbf{x}_k \\ \mathbf{y}_k \end{bmatrix} \middle| \mathbf{y}_1, \mathbf{y}_2, \dots, \mathbf{y}_{k-1}\right) = \mathcal{N}\left(\begin{bmatrix} \hat{\mathbf{x}}_{k-1} \\ \mathbf{C}\hat{\mathbf{x}}_k \end{bmatrix}, \begin{bmatrix} \hat{\mathbf{M}}_k & \hat{\mathbf{M}}_k\mathbf{C}^T \\ \mathbf{C}\hat{\mathbf{M}}_k & \mathbf{C}\hat{\mathbf{M}}_k\mathbf{C}^T + \mathbf{R} \end{bmatrix}\right) \quad (2.42)$$

So the conditional distribution of $\mathbf{x}_k$ given the new measurement $\mathbf{y}_k$ and the previous $k - 1$ measurements is

$$p(\mathbf{x}_k | \mathbf{y}_1, \mathbf{y}_2, \dots, \mathbf{y}_k) = \mathcal{N}(\bar{\mathbf{x}}_k, \mathbf{M}_k), \quad (2.43)$$

with the mean and covariance updated with

$$\mathbf{G}_k = \hat{\mathbf{M}}_k\mathbf{C}^T(\mathbf{C}\hat{\mathbf{M}}_k\mathbf{C}^T + \mathbf{R})^{-1}, \quad (2.44)$$

$$\bar{\mathbf{x}}_k = \hat{\mathbf{x}}_k + \mathbf{G}_k(\mathbf{y}_k - \mathbf{C}\hat{\mathbf{x}}_k), \quad (2.45)$$

$$\mathbf{M}_k = \hat{\mathbf{M}}_k - \mathbf{G}_k\mathbf{C}\hat{\mathbf{M}}_k. \quad (2.46)$$

And hence, after the distribution $p(\mathbf{x}_0)$ is initialized, the *a posteriori* distribution of states can be updated recursively from new measurements by following Eqs. (2.39) and (2.43).

2.3.3 Extended Kalman filter

In Section 2.3.1 and 2.3.2, the state-space model is governed by the linear stochastic difference equations (Eqs. (2.25) and (2.26)). When the state-space model is governed by nonlinear stochastic difference equations, the estimate of state uses an extended Kalman filter (EKF) method [54] which is realized by linearizing the covariance of the state. Assume that the state $\mathbf{x}_k$ is governed by the nonlinear stochastic difference equation,

$$\mathbf{x}_k = \mathbf{f}(\mathbf{x}_{k-1}) + \mathbf{u}_k, \quad (2.47)$$

with its measurement

$$\mathbf{y}_k = \mathbf{h}(\mathbf{x}_k) + \mathbf{v}_k. \quad (2.48)$$

where the variables $\mathbf{u}_k$ and $\mathbf{v}_k$ again represent the Gaussian noise in the process and the measurement. The nonlinear transition function $\mathbf{f}(\mathbf{x}_{k-1})$ relates the previous state $\mathbf{x}_{k-1}$ to the current state $\mathbf{x}_k$. The nonlinear measurement function $\mathbf{h}(\mathbf{x}_k)$ maps the state to the measurement.

The Kalman filtering maintain the estimation of the mean and covariance of the state. In the linear Kalman filter, the covariance propagation can be realized by using the state transition matrix or the observation matrix (see Eq. (2.32)). However, the nonlinear function makes it complicated to propagate the covariance matrix of state. This is solved by performing a Taylor-series expansion on the nonlinear function

$\mathbf{f}(\mathbf{x}_{k-1})$ at the estimation $\bar{\mathbf{x}}_{k-1}$:

$$\mathbf{x}_k = \mathbf{f}(\bar{\mathbf{x}}_{k-1}) + \mathbf{A}(\mathbf{x}_{k-1} - \bar{\mathbf{x}}_{k-1}) + \mathbf{u}_k, \quad (2.49)$$

where $\mathbf{A}$ is the Jacobian matrix of partial derivatives of the function $\mathbf{f}$

$$\mathbf{A} = \left. \frac{\partial \mathbf{f}}{\partial \mathbf{x}_{k-1}} \right|_{\mathbf{x}_{k-1} = \bar{\mathbf{x}}_{k-1}}. \quad (2.50)$$

Suppose the *a posteriori* estimate of the state $\mathbf{x}_{k-1}$ from the previous measurement has a mean of $\bar{\mathbf{x}}_{k-1}$ and covariance of $\mathbf{M}_k$. The mean and covariance of *a prior* estimate in the prediction step can be computed as:

$$\hat{\mathbf{x}}_k = f(\bar{\mathbf{x}}_{k-1}) \quad (2.51)$$

$$\begin{aligned} \hat{\mathbf{M}}_k &= E[(\mathbf{x}_k - \hat{\mathbf{x}}_k)(\mathbf{x}_k - \hat{\mathbf{x}}_k)^T] = E[(\mathbf{x}_k - f(\bar{\mathbf{x}}_{k-1}))(\mathbf{x}_k - f(\bar{\mathbf{x}}_{k-1}))^T] \\ &\approx \mathbf{A}\mathbf{M}_{k-1}\mathbf{A}^T + \mathbf{W}_k. \end{aligned} \quad (2.52)$$

The linearization can also be performed for the nonlinear equation $h(\mathbf{x}_k)$ in the measurement process. The posterior distribution is then estimated with the similar approach in the linear Kalman filter. In the Bayesian inference perspective, the linearization step is understood as an approximation of the non-Gaussian distribution with Gaussian one [53].

2.3.4 Complex Kalman filter

In the previous sections, we reviewed the Kalman filter whose states are real numbers. In this section, we introduce variations of the Kalman filter when the states are

complex numbers. When the linear state space model in Eqs. (2.25) and (2.26) has the state $\mathbf{x}_k \in \mathbb{C}^n$ and the measurement $\mathbf{y}_k \in \mathbb{C}^m$, the corresponding filter is named linear complex Kalman filter. When the transition function $f(\mathbf{x}_{k-1})$ and the measurement function $h(\mathbf{x}_k)$ are nonlinear, Complex Extended Kalman Filter (CEKF) [55] can be derived with the linearization step (see Section 2.3.3).

However, the covariance matrix $E[(\mathbf{x}_k - \bar{\mathbf{x}}_k)(\mathbf{x}_k - \bar{\mathbf{x}}_k)^H]$ is not sufficient for a complete-description because of the fact that the state $\mathbf{x}_k$ is complex. In [56], a complex state $\mathbf{x}^a$ is proposed by combining the state $\mathbf{x}_k$ with its conjugate $\mathbf{x}_k^*$

$$\mathbf{x}^a = \begin{bmatrix} \mathbf{x}_k \\ \mathbf{x}_k^* \end{bmatrix}. \quad (2.53)$$

The covariance of the state $\mathbf{x}^a$ can be written as:

$$\begin{aligned} & E[(\mathbf{x}_k^a - \bar{\mathbf{x}}_k^a)(\mathbf{x}_k^a - \bar{\mathbf{x}}_k^a)^H] \\ &= \begin{bmatrix} E[(\mathbf{x}_k - \bar{\mathbf{x}}_k)(\mathbf{x}_k - \bar{\mathbf{x}}_k)^H] & E[(\mathbf{x}_k - \bar{\mathbf{x}}_k)(\mathbf{x}_k - \bar{\mathbf{x}}_k)^T] \\ E[(\mathbf{x}_k - \bar{\mathbf{x}}_k)(\mathbf{x}_k - \bar{\mathbf{x}}_k)^T]^* & E[(\mathbf{x}_k - \bar{\mathbf{x}}_k)(\mathbf{x}_k - \bar{\mathbf{x}}_k)^H]^* \end{bmatrix}, \end{aligned} \quad (2.54)$$

where the pseudo-covariance $E[(\mathbf{x}_k - \bar{\mathbf{x}}_k)(\mathbf{x}_k - \bar{\mathbf{x}}_k)^T]$ together with the covariance matrix $E[(\mathbf{x}_k - \bar{\mathbf{x}}_k)(\mathbf{x}_k - \bar{\mathbf{x}}_k)^H]$ provide a full description for the second order statistical property of the complex variable $\mathbf{x}_k$.

The state space model for the augmented complex linear Kalman filter is expressed as [56]:

$$\mathbf{x}_k^a = \mathbf{A}^a \mathbf{x}_{k-1}^a + \mathbf{u}_k^a; \quad (2.55)$$

$$\mathbf{y}_k^a = \mathbf{C}^a \mathbf{x}_k^a + \mathbf{v}_k^a, \quad (2.56)$$

where $\mathbf{x}_k^a = \begin{pmatrix} \mathbf{x}_k \\ \mathbf{x}_k^* \end{pmatrix}$, $\mathbf{y}_k^a = \begin{pmatrix} \mathbf{y}_k \\ \mathbf{y}_k^* \end{pmatrix}$, $\mathbf{u}_k^a = \begin{pmatrix} \mathbf{u}_k \\ \mathbf{u}_k^* \end{pmatrix}$, $\mathbf{v}_k^a = \begin{pmatrix} \mathbf{v}_k \\ \mathbf{v}_k^* \end{pmatrix}$, $\mathbf{A}_k^a = \begin{pmatrix} \mathbf{A}_k & 0 \\ 0 & \mathbf{A}_k^* \end{pmatrix}$ and $\mathbf{C}_k^a = \begin{pmatrix} \mathbf{C}_k & 0 \\ 0 & \mathbf{C}_k^* \end{pmatrix}$. The covariance matrix of the process and observation noise, $\mathbf{u}_k^a$ and $\mathbf{v}_k^a$, become

$$\mathbf{W}_k^a = \begin{bmatrix} \mathbf{W}_k & \mathbf{P}_k \\ \mathbf{P}_k^* & \mathbf{W}_k^* \end{bmatrix}, \mathbf{R}_k^a = \begin{bmatrix} \mathbf{R}_k & \mathbf{Q}_k \\ \mathbf{Q}_k^* & \mathbf{R}_k^* \end{bmatrix}, \quad (2.57)$$

where $\mathbf{P}_k$ and $\mathbf{Q}_k$ are the pseudocovariance of $\mathbf{u}_k$ and $\mathbf{v}_k$.

For the case when the transition function $f(\mathbf{x}_{k-1})$ and the measurement function $h(\mathbf{x}_k)$ are nonlinear, a state space model for the Augmented Complex Extended Kalman Filter (ACEKF) can be derived with the linearization. However, the Taylor expansion for the nonlinear functions are expressed as:

$$\mathbf{x}_k = \mathbf{f}(\bar{\mathbf{x}}_{k-1}) + \left. \frac{\partial \mathbf{f}}{\partial \mathbf{x}_{k-1}} \right|_{\mathbf{x}_{k-1}=\bar{\mathbf{x}}_{k-1}} (\mathbf{x}_{k-1} - \bar{\mathbf{x}}_{k-1}) + \left. \frac{\partial \mathbf{f}}{\partial \mathbf{x}_{k-1}^*} \right|_{\mathbf{x}_{k-1}^*=\bar{\mathbf{x}}_{k-1}^*} (\mathbf{x}_{k-1}^* - \bar{\mathbf{x}}_{k-1}^*) + \mathbf{u}_k, \quad (2.58)$$

$$\mathbf{y}_k = \mathbf{h}(\hat{\mathbf{x}}_k) + \left. \frac{\partial \mathbf{h}}{\partial \mathbf{x}_k} \right|_{\mathbf{x}_k=\hat{\mathbf{x}}_k} (\mathbf{x}_k - \hat{\mathbf{x}}_k) + \left. \frac{\partial \mathbf{h}}{\partial \mathbf{x}_k^*} \right|_{\mathbf{x}_k^*=\hat{\mathbf{x}}_k^*} (\mathbf{x}_k^* - \hat{\mathbf{x}}_k^*) + \mathbf{v}_k. \quad (2.59)$$

The measurement matrix $\mathbf{A}^a$ of the augmented linearized state-space model

$$\mathbf{A}^a = \begin{bmatrix} \left. \frac{\partial \mathbf{f}}{\partial \mathbf{x}_{k-1}} \right|_{\mathbf{x}_{k-1}=\bar{\mathbf{x}}_{k-1}} & \left. \frac{\partial \mathbf{f}}{\partial \mathbf{x}_{k-1}^*} \right|_{\mathbf{x}_{k-1}^*=\bar{\mathbf{x}}_{k-1}^*} \\ \left. \frac{\partial \mathbf{f}}{\partial \mathbf{x}_{k-1}^*} \right|_{\mathbf{x}_{k-1}^*=\bar{\mathbf{x}}_{k-1}^*}^* & \left. \frac{\partial \mathbf{f}}{\partial \mathbf{x}_{k-1}} \right|_{\mathbf{x}_{k-1}=\bar{\mathbf{x}}_{k-1}}^* \end{bmatrix}. \quad (2.60)$$

The observation matrix $\mathbf{C}^a$ of the augmented linearized state-space model can be derived in a similar way. For the case of the measurement $\mathbf{y}_k \in \mathbb{R}^m$, the measurement

matrix $\mathbf{C}^a$ can be written as:

$$\mathbf{C}^a = \begin{bmatrix} \left. \frac{\partial \mathbf{h}}{\partial \mathbf{x}_k} \right|_{\mathbf{x}_k = \hat{\mathbf{x}}_k} & \left. \frac{\partial \mathbf{h}}{\partial \mathbf{x}_k^*} \right|_{\mathbf{x}_k^* = \hat{\mathbf{x}}_k^*} \end{bmatrix}. \quad (2.61)$$

Although that the state-space models for the discussed complex Kalman filtering have complex state and complex covariance matrices, they follow the similar rules as the prediction and update steps introduced in Section 2.3.1.

Chapter 3

Diagonalized complex extended Kalman filter for phase imaging

3.1 Introduction

In [51] the augmented complex extended Kalman filter (ACEKF) method was used to solve for phase with significant noise corruption. However, the memory requirements are of order N^2 and the computational complexity is of order N^3 . The ACEKF method is infeasible for practical mega-pixels image (e.g. 1000×1000 pixels), and the long computation time is impractical for real-time applications. In this chapter we introduce a novel approach-diagonalized complex extended Kalman filter (CEKF) to the problem of amplitude and phase estimation. Just as the method of ACEKF in [51], it is based on the Kalman filter. However, we make certain convenient approximations to significantly reduce the computational complexity, without jeopardizing the quality of the reconstruction. Moreover, the diagonalized CEKF is iterative and can trade off computational complexity vs. reconstruction accuracy.

This chapter is organized as follows. In Section 3.2, we give a brief description of the problem. We present our state-space model in Section 3.3. We derive the

proposed diagonalized CEKF algorithm in Section 3.4. We show experimental results in Section 3.5, and offer concluding remarks in Section 3.6

3.2 Problem description

We aim to estimate the 2D complex-field $A(x, y, z_0)$ at the focal plane z_0 , from a sequence of noisy intensity images $I(x, y, z)$ captured at various distance $z_0, z_1, z_2, \dots, z_{N_z}$. We assume a linear medium with homogeneous refractive index and coherent (laser) illumination, such that the complex-field at z_0 fully determines the complex-field at all other planes. The complex optical field at z is $A(x, y, z) = |A(x, y, z)|e^{i\phi(x, y, z)}$, where $|A(x, y, z)|$ is the amplitude, and $\phi(x, y, z)$ is the phase. Propagation is modeled by the homogeneous paraxial wave equation:

$$\frac{\partial A(x, y, z)}{\partial z} = \frac{i\lambda}{4\pi} \nabla_{\perp}^2 A(x, y, z), \quad (3.1)$$

where λ is the wavelength of the illumination, and $\nabla_{\perp}$ is the gradient operator in the lateral (x, y) dimensions. The noisy measurements $I(x, y, z)$ usually adhere to a (continuous) Poisson distribution:

$$p[I(x, y, z)|A(x, y, z)] = e^{-\gamma|A(x, y, z)|^2} \frac{(\gamma|A(x, y, z)|^2)^{I(x, y, z)}}{I(x, y, z)!}, \quad (3.2)$$

where γ is the photon count detected by the camera and $!$ means factorial. The measurement at each pixel $I(x, y, z)$ is assumed statistically independent of any other pixel (conditioned on the optical field $A(x, y, z)$).

3.3 State space model of the optical field

We discretize the optical field $A(x, y, z)$ as a raster-scanned complex column vector $\mathbf{a}_n$, and we similarly discretize the intensity measurement $I(x, y, z)$ as column vector $\mathbf{I}_n$:

$$\mathbf{a}_n \equiv \begin{bmatrix} A(x_1, y_1, z_n) \\ \vdots \\ A(x_{N_x}, y_1, z_n) \\ A(x_1, y_2, z_n) \\ \vdots \\ A(x_{N_x}, y_{N_y}, z_n) \end{bmatrix}, \quad \mathbf{I}_n \equiv \begin{bmatrix} I(x_1, y_1, z_n) \\ \vdots \\ I(x_{N_x}, y_1, z_n) \\ I(x_1, y_2, z_n) \\ \vdots \\ I(x_{N_x}, y_{N_y}, z_n) \end{bmatrix}, \quad (3.3)$$

where $N_x \times N_y$ is the total number of pixels in one intensity image.

We denote by $B(u, v, z)$ the 2-D Fourier transform of $A(x, y, z)$. The column vector $\mathbf{b}_n$ is again raster-scanned from $B(u, v, z)$, and hence can be expressed as

$$\mathbf{b}_n = \mathbf{K} \mathbf{a}_n, \quad (3.4)$$

where $\mathbf{K}$ is the discrete Fourier transform (DFT) matrix. Since $\mathbf{K}$ is unitary, we can write

$$\mathbf{K} \mathbf{K}^H = \mathbf{K}^H \mathbf{K} = \mathbf{U} \quad (3.5)$$

where $\mathbf{U}$ is the identity matrix or unit matrix and $\mathbf{K}^H$ denotes the hermitian of $\mathbf{K}$.

Let us assume the distance between two consecutive planes is a constant Δz . Then,

we can define the propagation matrix from z_{n-1} to z_n as from the Fresnel diffraction theory [24]:

$$\mathbf{H} = \text{diag}\left(\exp\left[-i\lambda\pi\left(\frac{u_1^2}{L_x^2} + \frac{v_1^2}{L_y^2}\right)\Delta z\right], \dots, \exp\left[-i\lambda\pi\left(\frac{u_M^2}{L_x^2} + \frac{v_N^2}{L_y^2}\right)\Delta z\right]\right), \quad (3.6)$$

where L_x and L_y are the width and height of the image, respectively. It can be observed that the matrix $\mathbf{H}_n$ is diagonal and unitary.

In order to fit within the Kalman filter framework, we approximate the Poisson observation model as in Eq. (3.2) with a Gaussian distribution of the same mean and covariance. In particular, we consider the approximate observation model:

$$\mathbf{I}_n = \gamma |\mathbf{a}_n|^2 + \mathbf{v}, \quad (3.7)$$

where $\mathbf{v}$ is a vector of Gaussian noise with zero mean and covariance $\mathbf{R} = \gamma \text{diag}(\mathbf{a}_n^*)\text{diag}(\mathbf{a}_n)$.

Here $\mathbf{a}_n^*$ denotes the complex conjugate of $\mathbf{a}_n$, and $\text{diag}(\mathbf{a}_n^*)$ is a diagonal matrix with its corresponding diagonal entries equal to the elements in the vector $\mathbf{a}_n^*$. In particular, the observation model is further linearized as

$$\mathbf{I}_n = \gamma |\hat{\mathbf{a}}_n|^2 + 2\gamma \text{diag}(\hat{\mathbf{a}}_n^*)(\mathbf{a}_n - \hat{\mathbf{a}}_n) + \mathbf{v}, \quad (3.8)$$

where $\hat{\mathbf{a}}_n$ is the state predicted from the previous $n - 1$ observations.

In summary, a simplified state-space model for the problem at hand is:

$$\text{state : } \mathbf{b}_n = \mathbf{H}_n \mathbf{b}_{n-1} \quad (3.9)$$

$$\text{observation : } \mathbf{I}_n = \mathbf{J} \mathbf{b}_n - \gamma |\hat{\mathbf{a}}_n|^2 + \mathbf{v}, \text{ with } \mathbf{v} \sim (\mathbf{0}, \mathbf{R}), \quad (3.10)$$

where

$$\mathbf{R} = \gamma \text{diag}(\hat{\mathbf{a}}_n^*) \text{diag}(\hat{\mathbf{a}}_n) \text{ and } \mathbf{J}_n = 2\gamma \text{diag}(\hat{\mathbf{a}}_n^*) \mathbf{K}^H. \quad (3.11)$$

Notice that both the observation matrix, $\mathbf{J}$, and the noise covariance, $\mathbf{R}$, depend on the predicted state vector $\hat{\mathbf{a}}_n$.

3.4 State estimation by diagonalized complex extended Kalman filter

In this section, a modified Kalman filter for the state-space model given by equations (3.9)-(3.10) is derived. Since the observation equation is non-linear, the resulting algorithm is suboptimal. However, the estimates of b_n that it produces are accurate enough for our purposes, and its simplicity makes it amenable for real-time implementation. From the equations of the extended Kalman filter [52, 54], we have the three following steps:

(1) **Initialization:** $\mathbf{b}_0$ and error covariance matrix.

(2) **Prediction:** $\hat{\mathbf{b}}_n = \mathbf{H}\mathbf{b}_{n-1}; \hat{\mathbf{M}}_n = \mathbf{H}\mathbf{M}_{n-1}\mathbf{H}^H$.

(3) **Update:**

$$\mathbf{G}_n = \hat{\mathbf{M}}_n \mathbf{J}^H (\mathbf{J} \hat{\mathbf{M}}_n \mathbf{J}^H + \mathbf{R})^{-1} \quad (3.12)$$

$$\mathbf{b}_n = \hat{\mathbf{b}}_n + \mathbf{G}_n (\mathbf{I}_n - \mathbf{J} \hat{\mathbf{b}}_n) \quad (3.13)$$

$$\mathbf{M}_n = \hat{\mathbf{M}}_n - \mathbf{G}_n \mathbf{J} \hat{\mathbf{M}}_n. \quad (3.14)$$

The matrix $\mathbf{G}_n$ is known as the Kalman gain, whereas $\mathbf{M}_n$ is the covariance matrix, providing a measure of the uncertainty in the estimate $\mathbf{b}_n$. The computational complexity of Eqs. (3.12)-(3.14) is in the order of N^3 . It can be reduced significantly by constraining the state covariance matrix to be diagonal. We will show that in order for this condition to hold at all times, it suffices to initialize the algorithm with a diagonal covariance matrix (that is, $\mathbf{M}_0 = \alpha_0 \mathbf{U}$). With this choice of initialization, Theorem 3.1 provides a simple update rule for the covariance matrix $\mathbf{M}_n$, whereas Theorem 3.2 provides a simplified expression for $\mathbf{b}_n$. In order to prove those theorems, we have first derived two simple lemmas (Lemma 3.1 and 3.2). For the sake of brevity, all the proofs are shown at Appendix A.

Lemma 3.1 *If $\mathbf{M}_{n-1}$ is diagonal, then $\hat{\mathbf{M}}_n = \mathbf{H}\mathbf{M}_{n-1}\mathbf{H}^H = \mathbf{M}_{n-1}$.* ■

Lemma 3.2 $\mathbf{R} = (4\gamma)^{-1} \mathbf{J}\mathbf{J}^H$. ■

Theorem 3.1 *If $\mathbf{M}_0 = \alpha_0 \mathbf{U}$, then $\mathbf{M}_n = \alpha_n \mathbf{U}$ with $\alpha_n = \frac{\alpha_{n-1}}{4\gamma\alpha_{n-1}+1}$.* ■

Theorem 3.2 *The update formula for state is*

$$\mathbf{b}_n = (1 - 4\alpha_n\gamma)\hat{\mathbf{b}}_n + 4\alpha_n\gamma\mathbf{J}^{-1}\mathbf{I}_n.$$

■

The resulting algorithm, referred to as diagonalized CEKF, is summarized in Table 3.1. Note that the inverse of $\mathbf{J}$ in Eq. (3.17) can be computed efficiently by Fast Fourier Transform (FFT). Thus, if N_z images are available and the number of each image is N , then the overall computational complexity of the proposed algorithm is $\mathcal{O}(N_z N \log(N))$.

Table 3.1: Diagonalized CEKF for inferring an complex field.

(1) Initialization: $\mathbf{b}_0$ and error covariance matrix $\mathbf{M}_0 = \alpha_0 \mathbf{U}$.	
(2) Prediction: $\hat{\mathbf{b}}_n = \mathbf{H}\mathbf{b}_{n-1}$; $\hat{\mathbf{M}}_n = \mathbf{M}_{n-1}$.	
(3) Update:	
$\hat{\mathbf{a}}_n = \mathbf{K}^H \hat{\mathbf{b}}_n$	(3.15)
$\mathbf{M}_n = \alpha_n \mathbf{U}, \text{ with } \alpha_n = \frac{\alpha_{n-1}}{4\gamma\alpha_{n-1} + 1}$	(3.16)
$\mathbf{b}_n = (1 - 4\alpha_n\gamma)\hat{\mathbf{b}}_n + 4\alpha_n\gamma\mathbf{J}^{-1}\mathbf{I}_n,$	(3.17)

Here we analyze the convergence of the algorithm. In Theorem 3.1 the covariance matrix is updated using: $\alpha_n = \frac{\alpha_{n-1}}{4\gamma\alpha_{n-1} + 1}$. Because $\alpha_0 > 0$ and $\gamma > 0$, it is easy to observe $\alpha_n > 0$ and $\alpha_n < \alpha_{n-1}$. Therefore, α_n in the covariance matrix $\mathbf{M}_n$ becomes nearer to zero after each update. The covariance matrix $\mathbf{M}_n$ acts as a measure for the uncertainty of the estimate of the state [57], so the uncertainty keeps reducing when a new observation is available.

3.5 Experimental results

In order to assess the performance of the proposed method, two sets of images have been considered. **Data set 1** consists of 100 images of size 100×100 pixels artificially generated to simulate a complex field propagating from focus in $0.5 \mu m$ steps over a distance of $50 \mu m$ with illumination wavelength of $532 nm$. Pixels are corrupted by Poisson noise so that, on average, each pixel detects $\gamma = 0.998$ photons. **Data set 2** comprises 50 images of size 150×150 pixels acquired by a microscope. A test phase object is made by etching the PMMA substrate with electron beam. The depth of the etched trenches is $190 nm$, measured by an atomic force microscope. The wavelength

was again 532 nm, and the defocused intensity images were captured by moving the camera axially with a step size of $2\ \mu\text{m}$ over a distance of $100\ \mu\text{m}$. Fig. 3.1 shows the images of synthetic data (Data Set 1) and experimental data (Data Set 2).

Figure 3.1: (a) Data Set 1: synthetic images with strong noise. (b) Data Set 2: experimental data acquired by a microscope (150×150 pixels).

3.5.1 Data Set 1 (synthetic data)

Since the ACEKF method in [51] has a computational complexity of $\mathcal{O}(N_z N^3)$ and bulk storage requirements of $\mathcal{O}(N^2)$, each image has been divided into 4 blocks of size 50×50 each. Nevertheless, this approach still takes 1.4×10^4 seconds. The complexity of our method is $\mathcal{O}(N_z N \log N)$, and hence it is not necessary to divide the image. Indeed, the proposed method takes only 0.30 seconds to process the 100 (all) images.

Fig. 3.2 shows the intensity and phase images recovered by both ACEKF and the proposed method, along with the true intensity and phase images. The average (across all pixels) root mean square error (RMSE) of our method as compared to that of ACEKF is given in Table 3.2, with all phase results in units of radians. Both

methods clearly lead to artifacts in both the intensity and phase recovered images: traces of the phase image can be seen in the intensity image and vice versa. As we will show in Section 3.5.3, those traces can be removed through an iterative algorithm.

Figure 3.2: Recovered intensity and phase[radian] images of Data Set 1 by ACEKF and the proposed diagonalized CEKF.

It can also be observed in Fig. 3.2 that the images recovered by ACEKF exhibit a block effect that shows artifacts in the form of straight lines crossing the images. This is due to the latter being processed in segments rather than as a whole. The proposed method can handle the entire images efficiently and hence, no segmentation artifacts occur.

In both the proposed diagonalized CEKF method and the ACEKF method, the estimation error decreases as images are processed, as illustrated in Fig. 3.3, which compares the RMSE incurred for increasingly more images being added. Ultimately, both methods seem to converge to similar estimation errors for both the intensity and

phase. However, our low-complexity method converges faster than ACEKF.

Figure 3.3: Intensity error and phase error for Data Set 1, as a function of the number of images (total = 100).

Table 3.2: Comparison between the diagonalized CEKF and ACEKF.

	Complexity	Time[s]	Storage	Intensity/Phase Error	Block Effect
ACEKF [51]	$\mathcal{O}(N_z N^3)$	1.4×10^4	$\mathcal{O}(N^2)$	0.0091/0.01388	Yes
Diagonalized CEKF	$\mathcal{O}(N_z N \log N)$	0.30	$\mathcal{O}(N)$	0.0079/0.01664	No

Table 3.2 summarizes the results of the diagonalized CEKF and ACEKF for Data Set 1.

3.5.2 Data Set 2 (experimental data)

Fig. 3.4 shows the intensity and phase images estimated by the proposed method when using Data Set 2, which was collected from the experimental data. Running the algorithm takes 0.32 seconds whereas ACEKF takes 8.0×10^3 seconds, with blocks of size 40×40 . The recovered intensity and phase images do not exhibit a block effect, but have some phase errors inside the lettering of MIT. As we will show in next section, the results can be further improved by means of an iterative algorithm.

Figure 3.4: Estimated intensity and phase[radian] of Data Set 2 by diagonalized CEKF and ACEK.

3.5.3 Iterative algorithm

Instead of carrying out *one* forward sweep of Kalman recursions, we now alternate forward and backward sweeps multiple times. This will allow us to trade off computational complexity for accuracy. When the forward recursion ends at the last image, a backward recursion is started, initialized by the current estimate of the (last) image. Likewise, when the backward recursion ends at the first image, a forward recursion is started with the current estimate of the first image as initialization.

Table 3.3: RMS for iterative method

Number of Iterations	1	5	20	60
RMS for Intensity Image	0.0078	0.0072	0.0071	0.0071
RMS for Phase Image	0.0165	0.0158	0.0152	0.0147

The recovered intensity and phase images for Data Set 1 and different numbers of iterations are displayed in Fig. 3.5. Each iteration consists of a forward and backward sweep of the Kalman recursions. It shows how the artifacts gradually vanish as the number of iterations increases. This is also assessed numerically in Table 3.3, which shows the RMSE of the intensity and phase images recovered for different numbers of

Figure 3.5: Estimated intensity and phase [radian] for Data Set 1 at iterations 0, 5, 20 and 60, with computational time of 0.30s, 3.18s, 12.11s, and 37.04s respectively.

Figure 3.6: Estimated intensity and phase [radian] for Data Set 2 at iterations 0, 5, 20 and 60, with computational time 0.32s, 3.39s, 12.90s, and 39.50s respectively.

iterations. The difference in the RMSE is small but the image quality improvements can be appreciated by comparing the reconstructed images in Figs. 3.5 and 3.6.

Fig. 3.6 shows the recovered phase and intensity images for the Data Set 2 with different numbers of iterations. It can be seen that the pixels of the MIT logo in the

recovered phase images look brighter after a few iterations. Although the computational complexity increases linearly with the number of iterations, the computational time of the algorithm is in the order of tens of seconds, which is still rather low.

3.6 Conclusions

We have proposed the diagonalized CEKF method to recover the phase and amplitude of a complex optical field from noisy defocused intensity images. It requires vastly less storage than existing methods (linear vs. quadratic), and it is substantially less complex (close to linear vs. cubic), while attaining high reconstruction accuracy. Moreover, it allows to trade off between complexity and accuracy. Although the data used in this chapter is measured by moving the camera with a constant step-size, the proposed method can be applied to data of non-constant step-size as well.

Chapter 4

Sparse augmented complex extended Kalman filter for phase reconstruction

4.1 Introduction

The Kalman filter is a well-known recursive algorithm for estimating dynamically changing quantities from a set of noisy measurements. In [51, 58], Kalman filtering was used to solve for phase from the defocused intensity stack which is in the presence of significant noise corruption. In the linear Kalman filter, with Gaussian noise statistics, the Kalman filter is the optimal estimation method. However, intensity is a nonlinear measure of complex field, and noise in images generally follows Poisson statistics, so the solution will not be provably optimal. In order to account for nonlinear measurements, a linearization step needs to be added to approximate the nonlinear measurements and the Poisson noise.

In Chapter 3, a diagonalized complex extended Kalman filter (diagonalized CEKF) was proposed to recover phase from a stack of defocused intensity images. Although

the diagonalized CEKF is computationally efficient and robust, the diagonalized CEKF requires a iteration step to further improve the estimation accuracy. It needs to cycle through the set of intensity images repeatedly, yielding a more accurate phase reconstruction after each cycle, and the computational complexity increases with each cycle. This limitation is caused by the fact that the state in the state space model of diagonalized CEKF is complex. An augmented complex state is required to provide a full description of the second order statistics of complex state [56]. In [51], an augmented complex extended Kalman filter (ACEKF) is used in order to deal with complex numbers in the state. The resulting ACEKF outperforms many previous algorithms in noise robustness, but at the cost of very high computational complexity of $\mathcal{O}(N_z N^3)$ and storage requirement of $\mathcal{O}(N^2)$. The memory storage requirements are particularly limiting - for example, an image with pixel counts on the order of megapixels requires terabytes of data to be stored and processed - thus, the algorithm is infeasible for large images and impractical for real-time applications.

In this chapter, we propose the sparse ACEKF which still use the same augmented state space model as ACEKF. With assumption that phase is small, we derive theorems to simplify the update equations of ACEKF. It eventually results in a low-complexity noise-robust phase reconstruction algorithm. The proposed method has a computational complexity of $N_z N \log N$, while ACEKF requires $N_z N^3$. However, our method still achieves better phase reconstruction than both ACEKF and the diagonalized CEKF.

This chapter is organized as follows. In the Section 4.2, we turn the propagation and observation models from scalar wave optics into an augmented state space model in signal processing. In Section 4.3, we derive the proposed sparse ACEKF algorithm. In Section 4.4, we analyze the convergence and stability of the new ACEKF. In

Section 4.5, we compare results of different methods using synthetic and experimental data. We offer concluding remarks in Section 4.6.

4.2 Problem description and state space model of the optical field

Our problem is still to estimate the 2D complex-field $A(x, y, z_0)$ at the focus z_0 , from a sequence of noisy defocused intensity images $I(x, y, z)$ captured at various distance $z_0, z_1, z_2, \dots, z_{N_z}$. The defocused complex optical field z is denoted with $A(x, y, z) = |A(x, y, z)|e^{i\phi(x, y, z)}$, where $|A(x, y, z)|$ is the amplitude, and $\phi(x, y, z)$ is the phase.

We follow the same notations as in the Chapter. 3. We discretize the optical field $A(x, y, z)$ as a raster-scanned complex column vector $\mathbf{a}_n$, the intensity $I(x, y, z)$ as $\mathbf{I}_n$, and the Fourier transform of $A(x, y, z)$ as $\mathbf{b}_n$. The discrete Fourier transform (DFT) matrix is denoted with $\mathbf{K}$, and the conjugate of $\mathbf{K}$ with $\mathbf{K}^H$.

From the Fresnel diffraction theory [24], the relation between two complex fields defocused with distance Δz can be expressed in Fourier domain as:

$$\mathbf{b}_n = \mathbf{H}\mathbf{b}_{n-1}, \quad (4.1)$$

where $\mathbf{H}$ is the wave propagation matrix which is diagonal and unitary (also see Eq. (3.6)).

Since the Kalman filter need to maintain the first two moments of state's statistical property, we approximate the Poisson noise in the intensity measurement with a Gaussian distribution of the same mean and covariance. In particular, we consider

the approximate observation model:

$$\mathbf{I}_n = \gamma |\mathbf{a}_n|^2 + \mathbf{v}, \quad (4.2)$$

where $\mathbf{v}$ is a vector of Gaussian noise with zero mean and covariance $\mathbf{R} = \gamma \text{diag}(\mathbf{a}_n^*)\text{diag}(\mathbf{a}_n)$.

The vector $\mathbf{a}_n^*$ represents the complex conjugate of $\mathbf{a}_n$, and $\text{diag}(\mathbf{a}_n^*)$ is a diagonal matrix with its diagonal entries equal to the elements in $\mathbf{a}_n^*$.

In order to obtain a augmented state space model, the nonlinear observation model with complex state in Eq. (4.2) is linearized according to [56]:

$$\mathbf{I}_n = \gamma |\hat{\mathbf{a}}_n|^2 + \gamma \text{diag}(\hat{\mathbf{a}}_n^*)(\mathbf{a}_n - \hat{\mathbf{a}}_n) + \gamma \text{diag}(\hat{\mathbf{a}}_n)(\mathbf{a}_n^* - \hat{\mathbf{a}}_n^*) + \mathbf{v}, \quad (4.3)$$

where $\hat{\mathbf{a}}_n$ is the state predicted from the previous $n - 1$ observations, and Eq. (4.3) is the first order Taylor series expansion of Eq. (4.2) with respect to $\hat{\mathbf{a}}_n$.

Summarizing, the augmented state space model is given as:

$$\text{state: } \begin{bmatrix} \mathbf{b}_n \\ \mathbf{b}_n^* \end{bmatrix} = \begin{bmatrix} \mathbf{H} & 0 \\ 0 & \mathbf{H}^* \end{bmatrix} \begin{bmatrix} \mathbf{b}_{n-1} \\ \mathbf{b}_{n-1}^* \end{bmatrix} \quad (4.4)$$

$$\text{observation: } \mathbf{I}_n = \begin{bmatrix} \mathbf{J}_n & \mathbf{J}_n^* \end{bmatrix} \begin{bmatrix} \mathbf{b}_n \\ \mathbf{b}_n^* \end{bmatrix} - \gamma |\hat{\mathbf{a}}_n|^2 + \mathbf{v}, \text{ with } \mathbf{v} \sim (\mathbf{0}, \mathbf{R}), \quad (4.5)$$

where

$$\mathbf{R} = \gamma \text{diag}(\hat{\mathbf{a}}_n^*)\text{diag}(\hat{\mathbf{a}}_n) \text{ and } \mathbf{J}_n = \gamma \text{diag}(\hat{\mathbf{a}}_n^*)\mathbf{K}^H. \quad (4.6)$$

We adopt the augmented state space model because the ACEKF with the state aug-

mented outperforms CEKF [58] in both estimation error and convergence [56]. If the state is not augmented, such as in CEKF algorithm, the covariance $\mathbf{E}[\mathbf{b}_n \mathbf{b}_n^H]$ is not sufficient for a complete description of the complex state. Since the state in ACEKF is augmented from $\mathbf{b}_n$ to $[\mathbf{b}_n \ \mathbf{b}_n^*]^T$, it introduces both the covariance $\mathbf{E}[\mathbf{b}_n \mathbf{b}_n^H]$ and the pseudo-covariance $\mathbf{E}[\mathbf{b}_n \mathbf{b}_n^T]$. The covariance $\mathbf{E}[\mathbf{b}_n \mathbf{b}_n^H]$ and pseudo-covariance $\mathbf{E}[\mathbf{b}_n \mathbf{b}_n^T]$ together provide a more comprehensive statistical description of the complex state.

4.3 State estimation by sparse augmented complex extended Kalman filter

The state covariance matrix of the augmented state has the form:

$$\mathbf{S}_n = \begin{bmatrix} \mathbf{S}_n^Q & \mathbf{S}_n^P \\ (\mathbf{S}_n^P)^* & (\mathbf{S}_n^Q)^* \end{bmatrix} \quad (4.7)$$

From the update equations of ACEKF [51, 52], we have the following steps:

1. Initialize: b_0 , $\mathbf{S}_0^Q$, and $\mathbf{S}_0^P$.
2. Predict:

$$\hat{\mathbf{S}}_n^Q = \mathbf{H} \mathbf{S}_{n-1}^Q \mathbf{H}^H, \quad (4.8)$$

$$\hat{\mathbf{S}}_n^P = \mathbf{H} \mathbf{S}_{n-1}^P \mathbf{H}. \quad (4.9)$$

3. Update:

$$\mathbf{S}_n^Q = \hat{\mathbf{S}}_n^Q - (\hat{\mathbf{S}}_n^Q \mathbf{J}_n^H + \hat{\mathbf{S}}_n^P \mathbf{J}_n^T)(\mathbf{J}_n \hat{\mathbf{S}}_n^Q \mathbf{J}_n^H + \mathbf{J}_n \hat{\mathbf{S}}_n^P \mathbf{J}_n^T + \mathbf{J}_n^* (\hat{\mathbf{S}}_n^Q)^* \mathbf{J}_n^T + \mathbf{J}_n^* (\hat{\mathbf{S}}_n^P)^* \mathbf{J}_n^H + \mathbf{R})^{-1} (\mathbf{J}_n \hat{\mathbf{S}}_n^Q + \mathbf{J}_n^* (\hat{\mathbf{S}}_n^P)^*), \quad (4.10)$$

$$\mathbf{S}_n^P = \hat{\mathbf{S}}_n^P - (\hat{\mathbf{S}}_n^Q \mathbf{J}_n^H + \hat{\mathbf{S}}_n^P \mathbf{J}_n^T)(\mathbf{J}_n \hat{\mathbf{S}}_n^Q \mathbf{J}_n^H + \mathbf{J}_n \hat{\mathbf{S}}_n^P \mathbf{J}_n^T + \mathbf{J}_n^* (\hat{\mathbf{S}}_n^Q)^* \mathbf{J}_n^T + \mathbf{J}_n^* (\hat{\mathbf{S}}_n^P)^* \mathbf{J}_n^H + \mathbf{R})^{-1} (\mathbf{J}_n \hat{\mathbf{S}}_n^P + \mathbf{J}_n^* (\hat{\mathbf{S}}_n^Q)^*), \quad (4.11)$$

$$\mathbf{G}_n = (\mathbf{S}_n^Q \mathbf{J}_n^H + \mathbf{S}_n^P \mathbf{J}_n^T) \mathbf{R}^{-1}, \quad (4.12)$$

$$\mathbf{b}_n = \hat{\mathbf{b}}_n + \mathbf{G}_n (\mathbf{I}_n - \gamma |\hat{\mathbf{a}}_n|^2). \quad (4.13)$$

The size of $\mathbf{S}_n^Q$ or $\mathbf{S}_n^P$ is N^2 , where N is the total number of the pixels in the image. Thus, the covariance matrix dominates the memory requirements. The inversion of the covariance matrix has a computational complexity of $\mathcal{O}(N^3)$ in each step. Both the storage requirement and computational burden make the above update algorithm impractical for real applications. Here we make some mild assumptions and derivations, resulting in a low-complexity algorithm with reduced storage requirement. After some derivations (see more in Appendices B and C), we prove Lemma 4.1 as well as Theorems 4.1 and 4.2. Theorem 4.1 is derived from the ACEKF update Eqs. (4.8)-(4.11). It shows that if the covariance matrix at step $n-1$ has the form $\mathbf{S}_{n-1}^Q = \mathbf{Q}_{n-1}$ and $\mathbf{S}_{n-1}^P = \mathbf{P}_{n-1} \mathbf{E}$, where $\mathbf{Q}_{n-1}$ and $\mathbf{P}_{n-1}$ are diagonal, then the covariance matrix at step n has the same form as that of step $n-1$ (see Eqs. (4.20)-(4.21)). Therefore, once the first covariance matrix is initialized as $\mathbf{S}_0^Q = \mathbf{Q}_0$ and $\mathbf{S}_0^P = \mathbf{P}_0 \mathbf{E}$, then the subsequent matrices will keep the same form. Since the matrices in Theorem 4.1 are diagonal, the computational complexity in Theorem 4.1 is $\mathcal{O}(N)$. Theorem 4.2, derived from Eqs. (4.12)-(4.13), provides a new Kalman gain and updates formula using the diagonal matrices $\mathbf{Q}_n$ and $\mathbf{P}_n$.

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Lemma 4.1 *If a matrix $\mathbf{M}$ is diagonal and its diagonal entries are rotationally symmetric in 2-D, then $\mathbf{E}\mathbf{M}\mathbf{E} = \mathbf{M}$, where $\mathbf{E} = \mathbf{K}\mathbf{K}^T$, and $\mathbf{K}$ is the Discrete Fourier Transform Matrix. ■*

Theorem 4.1 *If*

$$\mathbf{S}_{n-1}^Q = \mathbf{Q}_{n-1} \quad (4.14)$$

$$\mathbf{S}_{n-1}^P = \mathbf{P}_{n-1}\mathbf{E}, \quad (4.15)$$

where $\mathbf{Q}_{n-1}$ and $\mathbf{P}_{n-1}$ are diagonal, then we derive from the ACEKF update Eqs. (4.8)-(4.13) that the covariance matrix can be updated as follows

Predict:

$$\hat{\mathbf{Q}}_n = \mathbf{Q}_{n-1} \quad (4.16)$$

$$\hat{\mathbf{P}}_n = \mathbf{H}\mathbf{P}_{n-1}\mathbf{H}. \quad (4.17)$$

Update:

$$\mathbf{Q}_n = \hat{\mathbf{Q}}_n - (\hat{\mathbf{Q}}_n + \hat{\mathbf{P}}_n)(\hat{\mathbf{Q}}_n + \hat{\mathbf{P}}_n + (\hat{\mathbf{Q}}_n)^* + (\hat{\mathbf{P}}_n)^* + qI)^{-1}(\hat{\mathbf{Q}}_n + (\hat{\mathbf{P}}_n)^*) \quad (4.18)$$

$$\mathbf{P}_n = \hat{\mathbf{P}}_n - (\hat{\mathbf{Q}}_n + \hat{\mathbf{P}}_n)(\hat{\mathbf{Q}}_n + \hat{\mathbf{P}}_n + (\hat{\mathbf{Q}}_n)^* + (\hat{\mathbf{P}}_n)^* + qI)^{-1}(\hat{\mathbf{P}}_n + (\hat{\mathbf{Q}}_n)^*) \quad (4.19)$$

$$\mathbf{S}_n^Q = \mathbf{Q}_n \quad (4.20)$$

$$\mathbf{S}_n^P = \mathbf{P}_n\mathbf{E}, \quad (4.21)$$

where $\mathbf{Q}_n$ and $\mathbf{P}_n$ are diagonal, and $q = \frac{1}{\gamma}$. ■

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Theorem 4.2 *The Kalman gain and update formula for the state are*

$$G_n = (\mathbf{S}_n^{\mathbf{Q}} \mathbf{J}_n^H + \mathbf{S}_n^{\mathbf{P}} \mathbf{J}_n^T) \mathbf{R}^{-1} = (\mathbf{Q}_n + \mathbf{P}_n) (\mathbf{J}_n)^{-1} q^{-1}. \quad (4.22)$$

$$\mathbf{b}_n = \hat{\mathbf{b}}_n + \mathbf{G}_n (\mathbf{I}_n - \gamma |\hat{\mathbf{a}}_n|^2). \quad (4.23)$$

■

Table 4.1: Sparse augmented complex extended Kalman filter for estimating a wave field.

(1) Initialization $\mathbf{b}_0$, $\mathbf{Q}_0$ and $\mathbf{P}_0$.	
(2) Prediction:	
	$\hat{\mathbf{b}}_n = \mathbf{H} \mathbf{b}_{n-1} \quad (4.24)$
	$\hat{\mathbf{Q}}_n = \mathbf{Q}_{n-1} \quad (4.25)$
	$\hat{\mathbf{P}}_n = \mathbf{H} \mathbf{P}_{n-1} \mathbf{H} \quad (4.26)$
(3) Update:	
	$\hat{\mathbf{a}}_n = \mathbf{K}^H \hat{\mathbf{b}}_n \quad (4.27)$
	$\mathbf{Q}_n = \hat{\mathbf{Q}}_n - (\hat{\mathbf{Q}}_n + \hat{\mathbf{P}}_n) (\hat{\mathbf{Q}}_n + \hat{\mathbf{P}}_n + (\hat{\mathbf{Q}}_n)^* + (\hat{\mathbf{P}}_n)^* + q\mathbf{I})^{-1} (\hat{\mathbf{Q}}_n + (\hat{\mathbf{P}}_n)^*) \quad (4.28)$
	$\mathbf{P}_n = \hat{\mathbf{P}}_n - (\hat{\mathbf{Q}}_n + \hat{\mathbf{P}}_n) (\hat{\mathbf{Q}}_n + \hat{\mathbf{P}}_n + (\hat{\mathbf{Q}}_n)^* + (\hat{\mathbf{P}}_n)^* + q\mathbf{I})^{-1} (\hat{\mathbf{P}}_n + (\hat{\mathbf{Q}}_n)^*) \quad (4.29)$
	$\mathbf{b}_n = \hat{\mathbf{b}}_n + (\mathbf{Q}_n + \mathbf{P}_n) (\mathbf{J}_n)^{-1} q^{-1} (\mathbf{I}_n - \gamma \hat{\mathbf{a}}_n ^2). \quad (4.30)$

The resulting algorithm, referred to as the sparse ACEKF, is summarized in Table 4.1. Matrices $\mathbf{Q}_n$ and $\mathbf{P}_n$ are diagonal, and hence they can be stored as two vectors. The storage burden of Eqs. (4.10)-(4.11) in the update step is reduced from N^2 to N . The inverse of $\mathbf{J}_n$ in Eq. (4.30) can be computed by Fast Fourier Transform (FFT), which has a computational complexity of $\mathcal{O}(N \log(N))$. Since $\mathbf{Q}_n$ and $\mathbf{P}_n$ are diagonal, the matrix multiplications and inversions in Eqs. (4.28)-(4.29) have a computational complexity of $\mathcal{O}(N)$. The overall computational complexity of the sparse ACEKF is

$\mathcal{O}(N_z N \log(N))$, limited by the complexity of FFT.

4.4 Analysis of the convergence

The convergence of ACEKF, for the complex state space model, has not been well analyzed in the literature. However, the convergence and stability of the extended Kalman filter (EKF) for the real state is well studied [59–61]. Thus, we first convert the ACEKF state space model into its equivalent dual form as a real state space model (EKF), then we use existing methods to analyze the convergence of the dual form.

We follow [56] to derive the dual real form of the ACEKF state space model (4.4)-(4.5). Define

$$\mathbf{M} = \frac{1}{2} \begin{bmatrix} \mathbf{U} & \mathbf{U} \\ -j\mathbf{U} & j\mathbf{U} \end{bmatrix}, \quad (4.31)$$

where $\mathbf{U}$ is an identity matrix. When multiplied by $\mathbf{M}$, a complex variable is converted to its corresponding real form:

$$\begin{bmatrix} \text{Re}(\mathbf{b}_n) \\ \text{Im}(\mathbf{b}_n) \end{bmatrix} = \mathbf{M} \begin{bmatrix} \mathbf{b}_n \\ \mathbf{b}_n^* \end{bmatrix}, \quad (4.32)$$

where $\text{Re}(\mathbf{b}_n)$ and $\text{Im}(\mathbf{b}_n)$ are the real and imaginary parts of $\mathbf{b}_n$, respectively. The

complex model (4.4)-(4.5) becomes a real-valued model:

$$\text{state: } \begin{bmatrix} \text{Re}(\mathbf{b}_n) \\ \text{Im}(\mathbf{b}_n) \end{bmatrix} = \mathbf{A}_n \begin{bmatrix} \text{Re}(\mathbf{b}_{n-1}) \\ \text{Im}(\mathbf{b}_{n-1}) \end{bmatrix}, \quad (4.33)$$

$$\text{observation: } \mathbf{I}_n = \mathbf{C}_n \begin{bmatrix} \text{Re}(\mathbf{b}_n) \\ \text{Im}(\mathbf{b}_n) \end{bmatrix} - \gamma |\hat{\mathbf{a}}_n|^2 + \mathbf{v}, \quad (4.34)$$

where

$$\mathbf{A}_n = \mathbf{M} \begin{bmatrix} \mathbf{H} & 0 \\ 0 & \mathbf{H}^* \end{bmatrix} \mathbf{M}^{-1}, \quad (4.35)$$

$$\mathbf{C}_n = \begin{bmatrix} \mathbf{J}_n & \mathbf{J}_n^* \end{bmatrix} \mathbf{M}^{-1}. \quad (4.36)$$

By applying the theory of EKF convergence in [59] to our real-valued model, we obtain Theorem 4.3 which provides the convergence and stability of the model.

Theorem 4.3 *The estimation error of the EKF algorithm in Eqs. (4.33)-(4.34) is bounded, and hence also the estimation error of ACEKF algorithm for Eqs. (4.4)-(4.5) is bounded, when the initial estimation error and the noise are small enough, and the EKF model satisfies the following conditions [59]:*

1. There exist positive numbers $\bar{a}, \bar{c}, \bar{s}, \underline{s}, \underline{v} > 0$, such that for every $n \geq 0$:

$$\|\mathbf{A}_n\| \leq \bar{a}, \quad (4.37)$$

$$\|\mathbf{C}_n\| \leq \bar{c}, \quad (4.38)$$

$$\underline{s}\mathbf{U} \leq \mathbf{S}_n \leq \bar{s}\mathbf{U}, \quad (4.39)$$

$$\underline{v}\mathbf{U} \leq \mathbf{v}. \quad (4.40)$$

2. $\mathbf{A}_n$ is non-singular for every n .

3. The linearization at Eq. (4.3) has a bounded error. ■

In Theorem 4.3, $\|\cdot\|$ denotes the spectral norm of matrices. Assuming the initial estimation error and the noise are small enough, let us check each condition of Theorem 4.3. From the definition, the propagation matrix $\mathbf{H}$ is non-singular and determined by the propagation distance Δz . Since $\mathbf{M}$ is full rank, the matrix $\mathbf{A}_n$ given in Eq. (4.35) is bounded and non-singular. Therefore, the inequality (4.37) and the second condition of Theorem 4.3 are satisfied. The linearization in Eq. (4.3) is a first-order truncation of Taylor series expansion of a quadratic function. Therefore, the linearization has a bounded error and the real observation matrix $\mathbf{C}_n$ of Eq. (4.34) is bounded as well, as required by the inequality (4.38) and the third condition of Theorem 4.3. The matrix $\mathbf{R}$ is the covariance matrix of the Poisson noise in Eq. (4.2), and it is bounded as the amplitude of the state is bounded.

The inequality (4.39) requires the covariance matrix to be bounded for every n . In [59], it is shown that the boundedness of the covariance matrix is closely related to observability and detectability properties of the EKF model. However, it is difficult to prove the observability of the model directly, because $\mathbf{A}_n$ and $\mathbf{C}_n$ are based on the

observed data at each step. We calculate the rank of the observability matrix and the bound on the covariance matrix by testing our algorithm on the synthetic data (see Data Set 2 in section 4.5). We initialize the covariance matrix $\mathbf{Q}_0$ and $\mathbf{P}_0$ in Table 4.1 with 30 different values. The matrix $\mathbf{Q}_0$ is initialized as $q\mathbf{U}$ ($\mathbf{U}$ is identity matrix), with q ranging from 70 to 7000, and $\mathbf{P}_0$ is initialized as $p\mathbf{U}$, with p ranging from 50 to 5000. Figure 4.1 shows that the minimum singular value of the observability matrix is larger than zero, so the observability matrix is full rank at each step. Figures 4.2 and 4.3 show the maximum and minimum singular value of the covariance matrix at each step with different initializations. The covariance matrix is bounded, as required by inequality (4.39).

Figure 4.1: Minimum singular value of observability matrix with 30 different initializations of the covariance matrix $\mathbf{Q}_0$ and $\mathbf{P}_0$. The matrix $\mathbf{Q}_0$ is initialized as $q\mathbf{U}$, with q ranging from 70 to 7000, and $\mathbf{P}_0$ is initialized as $p\mathbf{U}$, with p ranging from 50 to 5000.

4.5 Experimental results

We consider three sets of data to assess the performance the augmented Kalman filter.

Data Set 1 consists of 100 images of size 100×100 pixels artificially generated to

Figure 4.2: Maximum singular value of covariance matrix with 30 different initializations of p and q in the covariance matrix.

Figure 4.3: Minimum singular value of covariance matrix with 30 different initializations of p and q in the covariance matrix.

simulate a complex field propagating from focus in $0.5 \mu m$ steps over a distance of $50 \mu m$ with illumination wavelength of $532 nm$. Pixels are corrupted by Poisson noise so that, on average, each pixel detects $\gamma = 0.998$ photons. **Data Set 2** comprises 50 images of size 150×150 pixels acquired by a microscope. The wavelength was again $532 nm$, and the defocused intensity images were captured by moving the camera axially with a step size of $2 \mu m$ over a distance of $100 \mu m$. **Data Set 3** has 101 images of size 492×656 pixels acquired by a microscope. The light source is partially coherent (both spatially and temporally), and filtered by a narrow-band color filter of

center wavelength $633nm$. The images were captured by moving the camera axially with a step size of $2\mu m$. Figure 4.4 shows the images of synthetic data (Data Set 1) and experimental data (Data Set 2 and Data Set 3).

Figure 4.4: (a) Data Set 1: synthetic images with strong noise (100×100 pixels with size of $1\mu m \times 1\mu m$). (b) Data Set 2: experimental data acquired by a microscope (150×150 pixels with size of $2\mu m \times 2\mu m$). (c) Data Set 3: experimental data of large size (492×656 pixels with size of $0.74\mu m \times 0.74\mu m$) obtained by a microscope.

4.5.1 Synthetic data

Table 4.2 summarizes the results of Data Set 1 using three methods: ACEKF (augmented complex extended Kalman filter) [51], diagonalized CEKF [58], and the proposed method sparse ACEKF. The ACEKF method has a high computational complexity of $\mathcal{O}(N_z N^3)$ and storage requirement of $\mathcal{O}(N^2)$. In order to alleviate the computational burden of ACEKF, the images are divided into independent blocks of size 50×50 , but it still takes 1.4×10^4 seconds by a standard CPU. On the other

hand, the computational complexity of the sparse ACEKF is $\mathcal{O}(N_z N \log N)$, and it takes 0.40 seconds to process the 100 (full) images, thus giving a speedup factor of 35000x.

As illustrated in Table 4.2, the computational complexity of the diagonalized CEKF is lower than that of ACEKF. However, the latter yields better results in terms of phase error. In order to reduce the error of the diagonalized CEKF, forward and backward sweeps (iterations) are applied in [58]. However, the iteration increases the computational complexity linearly, and makes the method no longer recursive. The sparse ACEKF method has an intensity error of 0.0071, and a phase error of 0.0143 (radian). Compared with the diagonalized CEKF, the sparse ACEKF has the same computational complexity and storage requirement, but returns more accurate images.

We assess the quality of reconstruction by root mean square error (RMSE). The proposed sparse ACEKF has an error near to that of ACEKF, while the recovered phase and intensity images of the sparse ACEKF in Fig. 4.5 might look better. The images recovered by ACEKF exhibit a block effect as straight lines crossing the images, whereas the result of sparse ACEKF is free of such block effect. The sparse ACEKF has a much lower complexity, which avoids the need of dividing the images into independent blocks. The images recovered by ACEKF and the diagonalized CEKF contain traces of phase in the intensity images due to errors. However, the trace of phase is mostly removed in the estimated intensity image from the sparse ACEKF.

Table 4.2: Comparison of different methods. Each image is divided into 4 blocks of size 50×50 for ACEKF, while the proposed sparse ACEKF and the diagonalized CEKF processes the images without separating into blocks.

	Complexity	Time[s]	Storage	Intensity error	Phase error [radians]
ACEKF	$\mathcal{O}(N_z N^3)$	1.3×10^4	$\mathcal{O}(N^2)$	0.0091	0.0139
Diagonalized CEKF	$\mathcal{O}(N_z N \log N)$	0.30	$\mathcal{O}(N)$	0.0079	0.0166
Sparse ACEKF	$\mathcal{O}(N_z N \log N)$	0.40	$\mathcal{O}(N)$	0.0071	0.0143

Figure 4.5: Recovered intensity and phase [radian] images from synthetic Data Set 1 by ACEKF, diagonalized CEKF, and the proposed sparse ACEKF.

4.5.2 Experimental data

In Fig. 4.6, we compare the estimated intensity and phase images of Data Set 2 using the ACEKF, the diagonalized CEKF, and the sparse ACEKF. Stripes in the phase image recovered by the diagonalized CEKF look darker, while the stripes in the recovered phase image of the sparse ACEKF method have stronger contrast. In Fig. 4.7(a), we show the recovered phase of the Data Set 3 by ACEKF, the diagonalized CEKF, and the sparse ACEKF. The real depth of the sample in Data Set 3 is around $75 \pm 5nm$. The proposed method takes 20.24 seconds to process 101

images of size 492×656 . However, the ACEKF method takes 54.15 hours and each image is separated into 117 pieces of 50×50 blocks. In Fig. 4.7(b), we compare the depth across the black line of the recovered phase in Fig. 4.7(a). The sparse ACEKF method shows a result much closer to the true value, compared to the ACEKF and the diagonalized CEKF. However, the reconstructed phase image obtained by sparse ACEKF contains low-frequency noise, especially at the edges. This shadow effect may be attributed to the partial coherence of the light, which is not incorporated into our model (we assume full coherence). The low frequency issue may be alleviated through a nonlinear diffusion filter, which we will explore in future work.

Figure 4.6: Estimated intensity and phase [radians] of Data Set 2 by ACEKF, diagonalized CEKF, and the proposed sparse ACEKF.

(a)

(b)

Figure 4.7: (a) Estimated height [nm] for Data Set 3 by ACEKF, diagonalized CEKF, and the proposed sparse ACEKF. (b) Depth along the black line in (a).

4.6 Conclusions

The proposed method efficiently recovers phase and amplitude from a series of noisy defocused images. Although a constant defocus step size is used for the through-focal series in this chapter, it can be generalized to cases of non-constant step-size. The method can directly deal with large data sets and high-resolution images because of its low computational complexity and storage requirement. It can process the images recursively in real-time after the data has been captured, or even during the capture sequence. For example, with further work, this method could form the basis for an adaptive phase imaging method, in which the current estimate of the phase informs the choice of the next measurement plane (defocus distance). Since the optimal measurement planes will depend on the object itself [22], real-time estimation during capture could lead to optimization not only of the processing, but also optimization of the measurement scheme itself. Furthermore, due to the scalability of the wave equations and the simplicity of the measurement technique, this method could find use in phase imaging beyond optical wavelengths (for example, X-ray or neutron imaging), where high-quality images are difficult to obtain and noise is significant and unavoidable.

Chapter 5

Transport of Intensity phase imaging by intensity spectrum fitting of exponentially spaced defocus planes

5.1 Introduction

In Chapter 3 and Chapter 4, we proposed Kalman filtering methods to deal with the noise issue in the intensity measurements. In this chapter, we consider the Transport of Intensity Equation (TIE) phase recovery methods, which have advantages of much less sensitive to illumination coherence [27] and no need of phase unwrapping. As reviewed in Section 2.2, the TIE methods [31, 32, 62] performs fittings on defocused intensity images vs. z in order to estimate the axial intensity derivative. We propose in this chapter a new TIE phase recovery method in which we perform through-focus fitting of the data, except we do the fitting in Fourier space, rather than in real space. The advantage of this method can be understood from Fig. 5.1. On the left, we show

a stack of through-focus intensity images, with a few example plots of the intensity vs. z behavior. These are the curves that would be fit to polynomials in higher order TIE [32]. It is easy to see that they do not conform to any particular functional form. On the right side of Fig. 5.1, we take 2D Fourier transforms of the intensity images at each of the defocus steps (showing here only the real part), then plot the intensity spectrum vs. z plots for a few example spatial frequencies. In contrast to the real space plots, these curves display a distinct sinusoidal behavior which can be predicted by the Contrast Transfer Function [20, 63, 64]. By using this a priori information of how light propagates in spatial frequency space, we can simultaneously deal with nonlinearity and noise in order to obtain a better derivative estimate.

Figure 5.1: Intensity evolution in frequency space is more predictable than in real space, demonstrating approximately sinusoidal behavior. (Top) Intensity images through-focus and their corresponding Fourier spectra's real part, from simulated data with $dz = 1\mu m$, size $200\mu m \times 200\mu m$ using the object in Fig. 5.5. (Bottom left) Intensity variations over z for 4 sample pixels (x, y) denoted as dots above. (Bottom right) Real part of intensity spectrum over z for 4 spatial frequency (u, v) values denoted as dots above.

Here, we propose to fit the spectral data with Gaussian process (GP) regression [65].

GP regression does not require that the inputs are equally spaced and can suppress the unwanted high-frequency components in the fitted function by using the squared exponential covariance function (see details in Appendix D.1). The curves in Fig. 5.1 follow sinusoidal trajectories, but actual behavior may deviate from this model due to breaking of the small phase approximation or unmodeled coherence effects. GP regression is able to flexibly fit the data to variations in the model using the Contrast Transfer Function as a priori information to set a threshold for suppressing the unwanted high frequency components in the fitted function. In this way, the over-fitting to noise is avoided without knowing or fitting to the precise function of a sinusoid.

In studying the frequency behavior for through-focus images, we find that equally spaced defocus steps in z are not ideal. Previous methods generally use images equally spaced in z , though higher order TIE can accommodate arbitrary z steps [62]. In a recent study [66], an exponentially-growing measurement scheme is proposed to deal with the regularization problem. Here, we show that exponentially spaced defocus steps can provide a large reduction in the number of images required for a high quality phase result. We suggest an efficient scheme for choosing the z plane distances (within the limits of the motion stage), from the perspective of efficiently transferring phase information to intensity images, and show how our method can achieve high quality phase results with far fewer images than equally spaced schemes.

The rest of the chapter is structured as follows. In Section 5.2, we apply GP regression to TIE phase recovery and propose an exponential spacing measurement scheme. In Section 5.3, we compare the error performance of the proposed algorithm with traditional TIE methods. In Section 5.4, we discuss the experimental results. We offer concluding remarks in Section 5.5.

5.2 Theory

5.2.1 Intensity spectrum fitting

We consider the intensity derivative estimation problem from the spatial frequency domain. When the phase $\phi(x, y)$ is small, the variations of intensity over z can be approximated in frequency space by the Contrast Transfer Function [20, 63, 64]:

$$\mathcal{I}(u, v, z) = \delta(u, v) - 2U(u, v) \cos[\pi\lambda(u^2 + v^2)z] - 2\Phi(u, v) \sin[\pi\lambda(u^2 + v^2)z], \quad (5.1)$$

where $\delta(u, v)$ denotes Dirac delta function, and $\mathcal{I}(u, v, z)$, $U(u, v)$, and $\Phi(u, v)$ are Fourier transforms of $I(x, y, z)$, $-\frac{1}{2} \ln I(x, y, 0)$, and $\phi(x, y)$, respectively. For each spatial frequency (u_m, v_n) , $\mathcal{I}(u_m, v_n, z)$ follows a sinusoidal pattern that oscillates with frequency $\pi\lambda(u_m^2 + v_n^2)$. Thus, instead of fitting the intensity curves in real space to polynomials (as in higher order TIE [32]), we use the sinusoids in the intensity spectra through-focus as prior in the fitting.

5.2.2 TIE using Gaussian process regression

To fit the data to our model, we employ Gaussian process regression. We estimate the derivative of the intensity spectrum with respect to defocus $\left. \frac{\partial \mathcal{I}(u, v, z)}{\partial z} \right|_{z=0}$ from $\mathcal{I}(u, v, z_1), \dots, \mathcal{I}(u, v, z_N)$, which are the 2D Fourier transforms of the measured intensity images. For each spatial frequency (u_m, v_n) , $\left. \frac{\partial \mathcal{I}(u_m, v_n, z)}{\partial z} \right|_{z=0}$ can be obtained from the continuous function fitted from the discrete data points $\mathcal{I}(u_m, v_n, z_1), \dots, \mathcal{I}(u_m, v_n, z_N)$.

GP regression is a suitable fitting method that allows us to fit the discrete points $\mathcal{I}(u_m, v_n, z_1), \dots, \mathcal{I}(u_m, v_n, z_N)$ to a continuous sinusoidal function (see details in Ap-

pendix D.1). In the fitted function, frequency components of the axial oscillation that are higher than a threshold s_c can be suppressed by initializing appropriate hyper-parameters in the regression (see details in Appendix D.2). From the Contrast Transfer Function (Eq. (5.1)), $\mathcal{I}(u_m, v_n, z)$, as a function of z , does not contain frequency components higher than $\pi\lambda(u_m^2 + v_n^2)$. Therefore, the threshold can be set just above $\pi\lambda(u_m^2 + v_n^2)$ in order to eliminate high-frequency noise while fitting over the inputs $\mathcal{I}(u_m, v_n, z_1), \dots, \mathcal{I}(u_m, v_n, z_N)$. Although the Contrast Transfer Function is derived under the weak phase assumption, it only serves as a guideline to pick a frequency threshold, above which variations are treated as noise. Thus, large phase variations can still be recovered, beyond the small phase approximation. Furthermore, by using GP regression, other prior knowledge about the sinusoidal pattern could be incorporated into the regression - for example, coherence effects of the illumination could be modeled in the Contrast Transfer Function as a product term, since reduced spatial coherence blurs defocused images and thus reduces the amplitude of the oscillations away from the focus plane.

Table 5.1: Algorithm of GP TIE.

<p>For each frequency v_m, v_n:</p> <p>(1) Inputs are N data points $\mathcal{I}(v_m, v_n, z_1), \mathcal{I}(v_m, v_n, z_2), \dots, \mathcal{I}(v_m, v_n, z_N)$.</p> <p>(2) Set $s_c = \gamma\pi\lambda(u_m^2 + v_n^2)$, with $\gamma = 1.1 \sim 1.2$.</p> <p>(3) Initialize the hyper-parameters in GP regression, in order to suppress the frequency components higher than s_c.</p> <p>(4) Output is obtained by calculating $\left. \frac{\partial \mathcal{I}(v_m, v_n, z)}{\partial z} \right _{z=0}$ through Eq. (D.12).</p>
--

The resulting algorithm of GP TIE is summarized in Table 5.1. The scaling factor γ in Step (2) of the table allows a trade-off between accuracy and noise filtering. Since the computational complexity of GP regression is proportional to the cubic of the number of measurements [65], the algorithm has a computational complexity of

$\mathcal{O}(N(N_z)^3)$, where N is the number of pixels in one image, and N_z is the number of measurements. This algorithm is very amenable to parallel processing and can be implemented with Graphics Processing Units (GPUs) for near real-time performance, in conjunction with GPU-based TIE solvers [67]. Further, GP regression does not require the measuring positions $z_1, z_2, \dots, z_N$ to be equally spaced, so any set of measurement positions along the axial dimension can be used as input. We show in the next session why this is not only convenient, but also leads to better phase recovery.

5.2.3 Exponential spacing measurement scheme

Looking at this problem from Fourier space, we see that equally spaced z steps are not the ideal measurement scheme. The choice of z distances is crucial, since it defines how much phase information from the object is transferred into intensity contrast in the defocused images [22]. Each z distance measurement can be thought of as having its own phase to intensity transfer function, with its own set of preferred spatial frequencies. The low-frequency information of phase is particularly poorly represented, as seen in the Laplacian inversion (see Eq. (2.20)). To better capture this low frequency phase information, images with large z are required, ideally out to the maximum range of the axial motion stage. However, the high-frequency components favor a small z and are important for recovering fine detail in the phase result. We would like to capture images *both* at the minimum z possible as well as at the maximum z possible. For linearly spaced schemes, this will require excessive data capture in between. To avoid this, we introduce an unequally spaced measurement scheme that balances these concerns. Since diffraction goes as $(\Delta x)^2/\lambda z$ [29], with Δx relating to the object size, we expect the ideal spacing to follow a nonlinear trajectory.

To derive an ideal z sampling scheme, we start with Eq. (5.1) and extract the phase transfer function, $g(u, v, z)$:

$$g(u, v, z) = \sin[\pi\lambda(u^2 + v^2)z]. \quad (5.2)$$

This equation tells us how much phase information for a given spatial frequency is converted into intensity contrast, and thus relates to the signal-to-noise ratio (SNR) of the measurement. For a given position z , the phase transfer function is a sine function of $\pi\lambda(u^2 + v^2)$ that will be maximized for particular spatial frequencies, as shown in Fig. 5.2. Since each object contains a different mix of spatial frequencies in its phase information, the theoretically optimal measurement planes are object-dependent [22]. So it is not possible to determine them without knowing the object itself. Thus, we do not aim for the absolute optimal set of measurements, but rather for the optimal coverage of sensitivity across all spatial frequencies that pass through the imaging system, treating each equally.

Consider the goal of selecting a set of z planes such that the maximum phase measurement sensitivity (set by the value of the transfer function) is at least α for the largest range of spatial frequencies possible. In the following, we demonstrate an exponential spacing measurement scheme that achieves this goal with the least number of measurement required. The highest frequency that can be recovered is set by the diffraction limit as NA/λ , where NA is the numerical aperture of the imaging system. This will define the minimum defocus distance from which we can capture relevant information. We define $f = \pi\lambda(u^2 + v^2)$ and $f \leq \pi\lambda(\frac{\text{NA}}{\lambda})^2$. First, we select the minimum defocus distance z_1 such that the sensitivity $g(u, v, z_1)$ is α at frequencies corresponding to the maximum frequency allowed $f_1 = \pi\lambda(\frac{\text{NA}}{\lambda})^2$, the solution of which is $z_1 = \frac{\pi - \arcsin(\alpha)}{\pi(\text{NA})^2}\lambda$. Defocus steps smaller than z_1 will not provide useful infor-

mation and are thus unnecessary, though in practice the minimum z step size may be set by the axial motion stage. As shown by the blue curve in Fig. 5.2, the sensitivity remains above α until $f_2 = \frac{\arcsin(\alpha)\pi(NA)^2}{\lambda[\pi-\arcsin(\alpha)]}$. Next, we select the second defocus distance $z_2 = \beta z_1$, where $\beta = \frac{\pi-\arcsin(\alpha)}{\arcsin(\alpha)} > 1$, such that the sensitivity $g(u, v, z_2)$ is α at f_2 , and will remain at least α for a range of frequencies, as illustrated by the green curve in Fig. 5.2. By induction, the optimal measurement scheme that satisfies a minimum phase measurement sensitivity α should satisfy the following exponential relation for the defocus distances

$$z_{n+1} = \beta z_n. \quad (5.3)$$

The exponential spacing implies that a large z can be reached with far fewer measurements as compared to the equal-spacing measurement schemes. Large z images are crucial for transferring low-frequency phase information, and the exponential spacing scheme enables us to reach this without taking an excessive number of measurements or trading off high-frequency information. The larger the maximum z , the better the low-frequency result, and we desire to keep the minimum z as small as possible in order to maintain diffraction-limited phase resolution, both extremes being limited by the motion stage axial range. Accuracy can be traded off against number of images through the choice of α . Larger values results in more accurate phase retrieval, at the cost of requiring more images.

5.3 Simulations

We compare the performance of various phase recovery methods that use equal spacing and exponential spacing. In the simulation, the illumination wavelength is set

Figure 5.2: Rationale for exponential spacing measurement scheme. Plot shows phase transfer functions for exponentially spaced z steps, which ensure a minimum sensitivity of α across a range of frequencies. $g(u, v, z_1)$, $g(u, v, z_2)$, and $g(u, v, z_3)$ are the phase transfer functions at z_1 , z_2 , and z_3 , respectively. The minimum sensitivity plot shows the frequencies which are transferred at the sensitivity higher than α by choosing z_1 , z_2 , and z_3 . Larger z brings more low-frequency sensitivity.

as $632.8nm$, and each image has 100×100 pixels (pixel size $2\mu m \times 2\mu m$). **Equally Spaced Stack** has 9 intensity images simulated with a constant defocus step size of $5\mu m$. **Exponentially Spaced Stack** also has 9 images; however, they are exponentially spaced, at z positions around focus of $\pm 5\mu m$, $\pm 20\mu m$, $\pm 80\mu m$ and $\pm 320\mu m$ (see Fig. 5.3). Although both data sets use the same number of images, the exponentially spaced data set contains more information about the low-frequency phase information because it has a higher z range.

Figure 5.3: Simulated data sets for equal and exponential spacing of z steps. (a) Equally Spaced Stack: images equally spaced by $5\mu m$. (b) Exponentially Spaced Stack: images exponentially spaced, with z of $\pm 5\mu m$, $\pm 20\mu m$, $\pm 80\mu m$, and $\pm 320\mu m$. The exponential spacing data contains more low-frequency phase information due to the larger range of z steps.

In order to assess the error performance, the intensity images of the equally and exponentially spaced stacks are corrupted by white noise with SNR ranging from 18.5 to 8 dB (noise variance from 0 to 0.02). Fig. 5.4 shows the average mean square error (MSE) of the recovered phase over 50 trials as SNR decreases. For the Equally Spaced Stack, higher order TIE performs significantly worse than SGDF TIE, and GP TIE is slightly better than SGDF TIE. For the Exponentially Spaced Stack, we show the results for two possible choices of Higher order TIE: $m = 9$, which performs better in low noise, and $m = 5$, which performs better in high noise. GP TIE with exponential spacing clearly exhibits the lowest MSE. This can be explained by the fact that the exponentially spaced data contains more low-frequency phase content in the measurements than the equally spaced data, and there is no trade-off between noise and nonlinearity. Figure 5.5 gives an example of the recovered phase at SNR of 11.1dB.

Figure 5.4: Comparison of mean square error (MSE) in phase results for various methods as noise level increases. GP TIE with exponential spacing yields the best error performance.

Figure 5.5: Phase images recovered from simulated data with SNR of 11.1dB. (Top) Results of the Equally Spaced Stack, using higher order TIE ($m=5$, MSE 0.1194 in radian), SGDF TIE (0.0295), and the proposed GP TIE (0.0279). (Bottom) Results for Exponentially Spaced Stack, using Higher order TIE ($m=5$, MSE 0.0237) and GP TIE (0.0065). GP TIE using exponential spacing provides the best phase result.

5.4 Experimental results

We tested our method experimentally in a microscope (magnification 20x, NA=0.5) with filtered white light illumination (center wavelength 650nm, 10nm bandwidth). **Data Set 1** comprises 129 images of human cheek cells, equally spaced by a constant small step size $dz = 4\mu m$ over a large defocus range $[-252\mu m$ to $252\mu m]$ (Fig. 5.7(a)). In Fig. 5.6, the GP fitted intensity spatial frequency variations along the propagation direction z for 3 different (u, v) values are shown. Both the measured and fitted curves follow nearly sinusoidal patterns, as predicted by Eq. (5.1). Note that the delay of each sinusoid is dependent on the absorption of the object at the corresponding spatial frequency. When the frequency (u, v) is high, the intensity spectrum variations diminish for large defocus distance (see plot of (u_{60}, v_{60}) in Fig. 5.6). This is due to the effect of partially coherent illumination, which will be the subject of future work.

Figure 5.6: (Left) GP regression of the intensity spectrum's real part over z for three sample frequency points (u, v) (Data Set 1). (Right) The frequency (u, v) of the three components depicted on real part of the recovered spectrum of phase (the image size is 945×888 but only the central part of the spectrum is shown for clarity). According to Eq. (5.1), the values for $\pi\lambda(u^2 + v^2)$ are $0.029 \times 10^4 m^{-1}$, $4.145 \times 10^4 m^{-1}$, and $17.299 \times 10^4 m^{-1}$, respectively.

With our exponentially spaced measurement scheme, GP TIE requires fewer images to be captured in order to obtain a high quality phase result. To demonstrate this, we compare the recovered phase by GP TIE from different subsets of Data Set 1 (Fig. 5.7) by sampling the image stack along z using various strategies. Figure 5.7(b) uses data subsets with equally spaced z -planes. First, we show the best possible phase result, when all 129 images are used. With equally spaced planes, we have two possibilities for reducing the number of images: we can either reduce the defocus range (keeping the step size small) or increase the step size (reducing the defocus range). If we reduce the defocus range, the recovered phase becomes susceptible to low-frequency noise (see the middle of Fig. 5.7(b)). This is due to the fact that the low-frequency information of phase is not well captured at small defocus distances. If we instead increase the step size (keeping the defocus range large), high-frequency components are lost due to nonlinearity (see the right of Fig. 5.7(b)). In order to accurately capture both high and low-frequency information with the same reduced number of images,

Figure 5.7: Exponentially spaced defocus steps with GP TIE provide accurate phase results using less images. (a) Data Set 1: equally spaced $dz = 4\mu m$, from $-256\mu m$ to $256\mu m$. Each image has 945×888 pixels with effective size $0.31\mu m \times 0.31\mu m$. (b) Phase recovered with equally spaced z steps: (left) with all 129 images [$-256\mu m$ to $256\mu m$, $dz = 4\mu m$]; (middle) subset of 15 images using minimum z step size [$-28\mu m$ to $28\mu m$, $dz = 4\mu m$]; and (right) subset of 15 images using maximum z range [$-252\mu m$ to $252\mu m$, $dz = 36\mu m$]. With equal spacing, there is a forced trade-off between low-frequency noise and high-frequency blurring, such that many images are required for good quality phase results. (c) Phase recovered with exponentially spaced z steps: (left) subset of 15 images ($\beta = 2$), and (right) subset of 9 images ($\beta = 4$). The minimum and maximum defocus distances are fixed at $\pm 4\mu m$ and $\pm 256\mu m$, respectively.

we need nonlinearly spaced measurements. Near the focus, the step size should be small, yet a large focus range can still be covered with only a few measurements in our exponentially spaced scheme. In Fig. 5.7(c), we extract images from Data Set 1 according to the exponential spacing scheme described in Section 5.2.3. As can be seen from Fig. 5.7(c), the phase results are free of low-frequency noise and also have high resolution. Even after further reducing the dataset to only 9 exponentially spaced images, we obtain a similar result to that with all 129 images. Thus, we have reduced the data capture requirement by more than an order of magnitude, without sacrificing quality.

Having shown that exponential spacing is advantageous, we now compare GP TIE with Higher order TIE, both of which are capable of using unequally spaced data. **Data Set 2** comprises 9 images of human cheek cells, exponentially spaced about focus at $\pm 5.7\mu m$, $\pm 11.4\mu m$, $\pm 22.8\mu m$, and $\pm 45.6\mu m$ (Fig. 5.8(a)). The imaging system has 10x magnification and NA of 0.5. Each image has 350×360 pixels of size $0.62\mu m \times 0.62\mu m$. Figure 5.8(b) shows the recovered phase of Data Set 2 obtained by Higher order TIE and GP TIE. We show the results for higher order TIE with the order of polynomial fitting m equal to 2, 3, and 4. The phase images of $m = 2$ and 3 have small low-frequency noise but appear blurred. The phase of $m = 4$ has strong contrast in some regions, but contains low-frequency noise. In contrast, GP TIE does not suffer from this tradeoff, so the phase recovered has less low-frequency noise and also exhibits high contrast. We can see details inside cells in the phase image recovered by GP TIE.

Figure 5.8: (a) Data Set 2: exponentially spaced, with z of $\pm 5.7\mu m$, $\pm 11.4\mu m$, $\pm 22.8\mu m$, and $\pm 45.6\mu m$. Each image has 350×360 pixels of size $0.62\mu m \times 0.62\mu m$. (b) Phase images of Data Set 2 by Higher order TIE ($m = 2, 3$, and 4) and GP TIE.

5.5 Conclusions

In this chapter, we proposed a TIE phase recovery method that exploits prior knowledge of spatial frequency variations of the intensity in order to yield more accurate phase images from exponentially spaced images through-focus. Our proposed method estimates the intensity derivative by means of GP regression. It is robust and stable with noise, while incorporating the a priori knowledge of the sinusoidal patterns predicted when fitting spectrum variations over z . We derived an exponentially spaced measurement scheme which guarantees a minimum phase measurement sensitivity across the full range of available spatial frequencies with the least possible number of images required. In future work, we will extend the current technique to add more a priori information, such as partial coherence of the illumination and large phase effects. With the freedom to choose nonlinearly spaced measurement positions, we can develop new strategies to optimize measurements if any prior knowledge of the

phase spectrum is known.

It should be noted that improving the TIE result by incorporating prior knowledge has been previously considered in [68–70]. The difference is that the previous approach considers priors over the phase [68, 69] or refractive index distribution [70]. In these work, the phase distribution or its gradient is assumed to be sparse, so a l_1 regularization could be applied in the phase recovery. However, in this chapter we use a prior on intensity spectral evolution, which is directly obtained from wave propagation, to improve the intensity derivative estimate. We expect the approach considered here should have wide application as it not only can be directly apply to the special cases in [68–70], but also to more general situations without constraints on the phase distribution.

Chapter 6

Partially coherent phase imaging with unknown source shapes

6.1 Introduction

We have mainly considered the phase recovery from defocused intensity images illuminated with coherent source in previous chapters. We use a Kalman filtering approach [51], which provides the theoretically near-optimal phase solution, even in severe noise. The method represents a hybrid between iterative methods and TIE, in that it uses a nonlinear forward model (as in iterative methods), but updates the phase estimate according to a linearization at each step (as in TIE). Thus, we get the benefits of using a large range of defocus distances, with good convergence. The main benefit of the Kalman filter method is that it provides a pixel-by-pixel adaptive noise filtering by estimating pixel-wise noise covariance. Unfortunately, this means that one must store and manipulate a 4D covariance matrix of size N^2 , where N is the total number of pixels in each image, becoming prohibitive in computation. We recently solved this problem by proving that the covariance matrix should be sparse [71], reducing the computational complexity by many orders of magnitude and achieving nearly real-time computation. With the sparse Kalman filter, we achieve

nanometer level phase sensitivity with a fast algorithm that converges reliably and is extremely robust to noise.

This chapter focuses on an important extension to our Kalman filter method which enables partially coherent illumination [72]. This topic has been discussed extensively in the context of TIE, since coherence plays an important role in propagation [27]. The TIE method is often cited as being robust to partial coherence [27], but only if the defocus distance is small and the source is circular [25, 73]. When non-circular sources are used, the phase result is incorrect [74], so coherence effects must be explicitly incorporated [75, 76]. However, as propagation distances increase beyond the ‘small defocus’ regime allowed in TIE methods, partial coherence becomes more problematic [77, 78]. We seek here to explicitly account for illumination coherence in our phase retrieval, without extra measurements.

Most imaging systems have incoherent sources (e.g. light bulbs, LEDs) in Köhler geometry (the source is the Fourier plane of the sample), resulting in spatially homogeneous illumination at the sample. In this setup, illumination coherence is controlled by the shape of the source according to the Van Cittert-Zernike theorem. Smaller sources produce more coherent illumination, generally achieved by closing the condenser aperture and blocking much of the light. Thus, less coherent illumination is desired because it provides larger photon flux, as well as immunity to speckle noise and improved resolution (up to twice the coherent band-limit). Further, some applications do not have the option of controlling the coherence, or require non-traditional sources to support the required resolution (e.g. lithography [13]).

Here, we show that coherence effects through-focus can be modeled by a convolution model, resulting in a simple modification to our Kalman filter method that allows us to solve for phase accurately from partially coherent intensity images with any

arbitrary source shape. In addition, we show here that, with an added optimization procedure and some assumptions on the source shape, we can also recover the source size (coherence) itself, meaning that one need not know it a priori.

The rest of the chapter is structured as follows. In Section 6.2 we develop a sparse Kalman filtering method for partially coherent phase recovery. In Section 6.3 we propose a method to recover phase and source shape parameters. In Section 6.4, we validate our methods with data measured from a commercial microscope. Section 6.5 offers conclusions.

6.2 Partially coherent phase recovery

Our method is based upon the Kalman filter presented in [51, 71], which we refer to here as the ‘coherent Kalman filter’. Previous work made an inherent assumption that the illumination was spatially coherent, but this breaks down in the case of a large or non-circular source, introducing phase errors (Fig. 6.2). Here, we modify our algorithm to account for illumination coherence explicitly, assuming an incoherent source of arbitrary shape in the Köhler configuration (Fig. 6.1). We note that the phase we solve for is that of the sample, not the illumination [79]. Generally, modeling spatial coherence for a 2D beam requires a 4D function, which is difficult to know or measure a priori [80]. Since the source is in Fourier space, the Van Cittert-Zernike theorem shows that we can model coherence with a much simpler 2D function describing the source shape. We can therefore treat the forward model as a coherent situation with an extra convolution step due to the source shape at each defocus position. We formulate a state-space model for propagation of partially coherent light and develop a sparse Kalman filtering algorithm for phase recovery.

Figure 6.1: We compute phase and coherence from a stack of images taken through-focus with an arbitrary source in Köhler configuration (Fourier space). (Left) Our brightfield microscope with z axis motion stage attached and an extra camera and lens for imaging the source plane. (Right) Through-focus stack of intensity images, which are used to recover the 2D phase and amplitude of the sample (human cheek cell) as well as the source shape.

The intensity $I(x, y, z)$ defocused by z can be written as a convolution between the intensity that would have been measured with coherent illumination $|A(x, y, z)|^2$ and a scaled source distribution $S(x, y)$ [73, 81]:

$$I(x, y, z) = |A(x, y, z)|^2 \otimes S\left(-\frac{f}{z}x, -\frac{f}{z}y\right), \quad (6.1)$$

where f is the focal length of the condenser lens.

In order to fit into the framework of our state-space model, we first discretize the continuous model. We denote the 2D continuous $x - y$ plane $A(x, y, z)$ with a column vector $\mathbf{a}_n$ and the Fourier transform of $A(x, y, z)$ with $\mathbf{b}_n$. Propagation in Fourier domain is written as:

$$\mathbf{b}_{n-1} = \mathbf{K}\mathbf{a}_{n-1}, \quad (6.2)$$

$$\mathbf{b}_n = \mathbf{H}\mathbf{b}_{n-1}, \quad (6.3)$$

where $\mathbf{K}$ is the discrete Fourier transform (DFT) matrix, and $\mathbf{H}$ is a diagonal matrix describing propagation.

Assuming that the intensity measurement is polluted by Gaussian noise [71], Equation (6.1) is discretized as:

$$\mathbf{I}_n = \mathbf{C}_n |\mathbf{a}_n|^2 + \mathbf{v}, \quad (6.4)$$

where $\mathbf{v}$ is Gaussian vector noise with zero mean and covariance $\mathbf{R}_n = \text{diag}(\mathbf{C}_n |\mathbf{a}_n|^2)$, and $\mathbf{C}_n$ is a circulant matrix describing the convolution of $S(-\frac{f}{z_n}x, -\frac{f}{z_m}y)$. From the eigenvalue decomposition property of circulant matrix, $\mathbf{C}_n = \mathbf{K}^H \mathbf{S}_n \mathbf{K}$. Here $\mathbf{S}_n$ is a diagonal matrix with its diagonal entries equal to the Fourier transform of the scaled source $S(-\frac{f}{z_n}x, -\frac{f}{z_n}y)$.

The nonlinear observation model is further linearized:

$$\begin{aligned} \mathbf{I}_n = & \mathbf{C}_n |\hat{\mathbf{a}}_n|^2 + \mathbf{C}_n \text{diag}(\hat{\mathbf{a}}_n^*) (\mathbf{a}_n - \hat{\mathbf{a}}_n) + \\ & \mathbf{C}_n \text{diag}(\hat{\mathbf{a}}_n) (\mathbf{a}_n^* - \hat{\mathbf{a}}_n^*) + \mathbf{v}, \end{aligned} \quad (6.5)$$

where $\hat{\mathbf{a}}_n$ is the state predicted from the previous $n - 1$ observations, and Eq. (6.5) is the first order Taylor series expansion of Eq. (6.4) with respect to $\hat{\mathbf{a}}_n$. Here $\mathbf{a}_n^*$ denotes the complex conjugate of $\mathbf{a}_n$, and $\text{diag}(\mathbf{a}_n^*)$ is a diagonal matrix with its corresponding diagonal entries equal to the elements in the vector $\mathbf{a}_n^*$.

Summarizing, the augmented model is then:

$$\text{state: } \begin{bmatrix} \mathbf{b}_n \\ \mathbf{b}_n^* \end{bmatrix} = \begin{bmatrix} \mathbf{H} & 0 \\ 0 & \mathbf{H}^* \end{bmatrix} \begin{bmatrix} \mathbf{b}_{n-1} \\ \mathbf{b}_{n-1}^* \end{bmatrix} \quad (6.6)$$

$$\text{observation: } \mathbf{I}_n = \begin{bmatrix} \mathbf{J}_n & \mathbf{J}_n^* \end{bmatrix} \begin{bmatrix} \mathbf{b}_n \\ \mathbf{b}_n^* \end{bmatrix} - \mathbf{C}_n |\hat{\mathbf{a}}_n|^2 + \mathbf{v}, \quad (6.7)$$

where $\mathbf{v}$ is white Gaussian noise with variance of $\mathbf{R}_n$,

$$\mathbf{R}_n = \text{diag}(\mathbf{C}_n |\hat{\mathbf{a}}_n|^2), \text{ and } \mathbf{J}_n = \mathbf{C}_n \text{diag}(\hat{\mathbf{a}}_n^*) \mathbf{K}^H. \quad (6.8)$$

Table 6.1: Sparse Kalman filter method for partially coherent phase recovery.

(1) Initialization $\mathbf{b}_0$, $\mathbf{Q}_0$ and $\mathbf{P}_0$.
(2) Prediction: $\hat{\mathbf{b}}_n = \mathbf{H}\mathbf{b}_{n-1}$; $\hat{\mathbf{Q}}_n = \mathbf{Q}_{n-1}$; $\hat{\mathbf{P}}_n = \mathbf{H}\mathbf{P}_{n-1}\mathbf{H}$
(3) Update:
$\hat{\mathbf{a}}_n = \mathbf{K}^H \hat{\mathbf{b}}_n$ (6.9)
$\mathbf{Q}_n = \hat{\mathbf{Q}}_n - (\hat{\mathbf{Q}}_n + \hat{\mathbf{P}}_n)(\hat{\mathbf{Q}}_n + \hat{\mathbf{P}}_n + (\hat{\mathbf{Q}}_n)^* + (\hat{\mathbf{P}}_n)^* + \mathbf{S}_n^{-2})^{-1}(\hat{\mathbf{Q}}_n + (\hat{\mathbf{P}}_n)^*)$ (6.10)
$\mathbf{P}_n = \hat{\mathbf{P}}_n - (\hat{\mathbf{Q}}_n + \hat{\mathbf{P}}_n)(\hat{\mathbf{Q}}_n + \hat{\mathbf{P}}_n + (\hat{\mathbf{Q}}_n)^* + (\hat{\mathbf{P}}_n)^* + \mathbf{S}_n^{-2})^{-1}(\hat{\mathbf{P}}_n + (\hat{\mathbf{Q}}_n)^*)$ (6.11)
$\mathbf{b}_n = \hat{\mathbf{b}}_n + (\mathbf{Q}_n + \mathbf{P}_n)\mathbf{K}\text{diag}(\hat{\mathbf{a}}_n)\mathbf{C}_n\mathbf{R}_n^{-1}(\mathbf{I}_n - \mathbf{C}_n \hat{\mathbf{a}}_n ^2).$ (6.12)

From the state space Eqs (6.6)- (6.7), we derive a sparse extended Kalman filter as in [71] (see Appendix E). The resulting sparse Kalman filter algorithm for partially

coherent phase recovery is summarized in Table 6.1. The computational complexity of the sparse algorithm is $\mathcal{O}(N \log N)$, compared to $\mathcal{O}(N^3)$ in the standard extended Kalman filter. Because the matrices $\mathbf{H}$, $\mathbf{S}_n$, $\mathbf{Q}_n$, and $\mathbf{P}_n$ Eqs. (6.10)-(6.12) are diagonal, the computational complexity of matrix multiplication in the algorithm is reduced to be linear in the size N of image.

6.3 Phase recovery with unknown source shape

The partially coherent phase recovery algorithm only works when the source shape $S(x, y)$ is known. Any errors in measuring or estimating the source shape will result in errors in the recovered phase. Thus, we further extend our method to the case where the source shape is unknown. Because the same phase and amplitude information of the sample are imprinted on each of the coherent modes (source points), the resulting through-focus intensity stack contains sufficient information. For example, one can consider a blind deconvolution process for recovering the coherent intensity stack from the partially coherent intensity stack, then running a coherent phase retrieval algorithm. Here, we aim to solve for both simultaneously.

Consider the source size estimation for the simplified case that the complex field $\mathbf{a}_0$ is known already and the source $S(x, y)$ is a circle, with θ denoting its radius. The problem is to estimate θ from the measured partially coherent intensity $\mathbf{I}_n$. The estimation of θ can be formulated as a nonlinear optimization problem:

$$\operatorname{argmin}_{\theta} \sum_{n=1}^N (\mathbf{I}_n - \mathbf{C}_n(\theta) |\mathbf{a}_n|^2)^T (\mathbf{I}_n - \mathbf{C}_n(\theta) |\mathbf{a}_n|^2), \quad (6.13)$$

where $|\mathbf{a}_n|^2$ can be obtained by defocusing $\mathbf{a}_0$. The optimization problem finds an

optimal θ to minimize the squared error between measurements $\mathbf{I}_n$ and the estimation $\mathbf{C}_n(\theta)|\mathbf{a}_n|^2$.

Table 6.2: Partially coherent phase recovery with unknown source shape parameters.

- (1) For the first iteration $i = 0$, initialize $\mathbf{a}_0^{(i=0)}$ and $\theta^{(i=0)}$.
- (2) With the current estimated parameters $\theta^{(i)}$, recover the complex field $\mathbf{a}_0^{(i+1)}$ by the sparse Kalman filter algorithm of partially coherent phase recovery in Table 6.1.
- (3) Using the complex field $\mathbf{a}_0^{(i+1)}$ estimated in the step 2, find the optimal $\theta^{(i+1)}$ by Eq. (6.13).
- (4) If stopping criteria is not met, go back to step 2.

To estimate both the complex field $\mathbf{a}_0$ and θ simultaneously, we propose an iterative update to $\mathbf{a}_0^{(i)}$ and $\theta^{(i)}$ in Table 6.2. By iterating between the step (2) and step (3), the error keeps reducing, and the estimation of the complex field and the source shape parameters are updated gradually until convergence is reached.

6.4 Experimental results

We tested our method experimentally in a Nikon TE300 microscope (see Fig. 6.1) with a white light source filtered to be centered around wavelength 550 nm. We took intensity focal stacks of cheek cells with different condenser apertures to vary the coherence of the illumination (see top row of Fig. 6.2). The first three shapes were obtained by progressively increasing the size of the condenser aperture. The ring shape in the fourth case is obtained by choosing the annular diaphragm of the Ph1 condenser. The images of the source were taken by adding a $2f$ system at the side port

Figure 6.2: Comparison of experimental results by coherent Kalman filter and partially coherent Kalman filter with known and unknown sources. (Top) Source shapes measured by imaging the condenser aperture onto a second camera. The red line shows the estimated source size (NA) by the partially coherent Kalman filter with unknown source size. (Second row) The recovered phase by the coherent Kalman filter is blurred for less coherent sources. (Third row) Recovered phase by the sparse partially coherent Kalman filter (with known source size). (Bottom) Recovered phase by the partially coherent Kalman filter with unknown source size.

of the microscope. The measured numerical apertures (NA) of the first three circles are 0.040, 0.122 and 0.213, respectively. The Ph1 source has inner circle corresponding to NA of 0.165 and outer NA of 0.197. For each shape, the sample was defocused symmetrically about the focus at 9 z-planes from $1\mu m$ to $16\mu m$, exponentially spaced as in [82].

The second row of Fig. 6.2 shows the phase images recovered by the coherent Kalman filter [71]. In the case of Size 1, the light source can be approximately viewed as coherent since the source size is small. The coherent Kalman filter thus recovers an accurate phase result. As the size of light source increases, however, the level of coherence reduces and the recovered phase becomes more blurred, degrading the phase result. Next, we test our sparse Kalman filter method for partially coherent phase recovery (Table 6.1), showing that it can recover an accurate phase result for each of the cases of arbitrary source size or shape. Its recovered phase images do not suffer from blurring and contain fine details for all source shapes, as shown by the third row of Fig. 6.2. In fact, the less coherent phase results have slightly better resolution than the coherent case, due to the partial coherence of the illumination.

Finally, we show results for our algorithm with unknown source size (Table 6.2). The recovered NA of the source is similar to the measured values (see Table 6.3) and we can see in Fig. 6.3 that the estimated NA converges to the correct value after a few iterations. The recovered phase images also show good fidelity (bottom row of Fig. 6.2) and in fact contain somewhat better details than those with a known source shape, suggesting that the recovered source shapes are more accurate than the measured ones.

Table 6.3: Recovered NA.

	Size 1	Size 2	Size 3	Ph1
Measured NA	0.040	0.122	0.213	0.197, 0.165
Estimated NA	0.045	0.124	0.203	0.197, 0.151

Figure 6.3: Convergence of NA estimation.

6.5 Conclusion

In this chapter, we demonstrated new methods to recover phase and illumination spatial coherence from a stack of defocused intensity images with arbitrary source shape. Our algorithm can either incorporate a known or unknown source size of arbitrary shape. This embedded calibration step is particularly helpful in making our algorithm more general and easy to implement. We expect that it will find use not only in biological microscopes, but also in X-ray and TEM imaging, where coherent illumination is rare. In the lithography industry, for example, current trends towards source-mask optimization (SMO) mean that non-traditional source shapes are becoming the norm. Thus, the ability to work with partially coherent illumination, along with the simplicity of phase-from-defocus techniques, opens up new application areas.

Chapter 7

Conclusion and future work

This thesis has studied computational methods to recover phase from a stack of defocused intensity images. We have explored various aspects: phase recovery techniques (diagonalized CEKF, sparse ACKEF and GP TIE), intensity measurement scheme and phase imaging with partially coherent illumination. The contributions of this thesis could be summarized as:

- We proposed the diagonalized complex extended Kalman filter (CEKF) to recover phase. It is fast and recursive. It allows to trade-off between the accuracy and computational complexity.
- We developed the sparse augmented complex extended Kalman filter (ACKEF) which has computational complexity and storage requirement linear to the number of pixels in one image. It provides a full description of the second order statistical properties of the complex variable due to the augmentation in the state-space model. It is efficient, robust, and may be applied in real-time high resolution phase imaging.
- We proposed the exponential spacing measurement scheme. It measures least number of intensity images and guarantees a minimum transferring sensitivity for the full range of available spatial frequencies of the phase.

- We proposed GP TIE for phase recovery. By using Gaussian process regression in the TIE intensity axial derivative estimation, it incorporates the a priori knowledge of the intensity spectrum variation in the intensity fitting. It reduces the nonlinearity error and improves the stability with noise in the measurement.
- We demonstrated methods to recover not only phase but also illumination spatial coherence from a stack of defocused intensity images with arbitrary source shape in Köhler geometry.

We have considered the issues of noise in the intensity measurement and the effect of partially coherent illumination. It is worth to mention that we validate our methods with experimental measured from a bright field microscopy, in which the sample is assumed to be 2D by ignoring the 3D effect. We expect that our methods could find use in phase imaging where high-quality intensity images are difficult to obtain or the coherent illumination is seldom used, for example X-ray, transmission electron microscopy (TEM) and neutron imaging.

There are several aspects which are interesting to study in future work. Since the optimal measurement defocus position is object-dependent [22], a better measurement scheme could be explored if any prior knowledge of the object is known. The GP TIE method in Chapter 5 could also be extended to the phase recovery of partially coherent illumination by incorporating the knowledge of the partially coherent intensity variation in the regression. In Chapter 6, we only explored the partially coherent source shape in Köhler geometry. However, a full description of the partial coherence in 2D field requires a 4D mutual intensity function. The problem of recovering the mutual intensity function from defocus stack is interesting to study in future work. The source estimation in Chapter 6 only recovers the source shape which is described

by several parameters, such radius. This limitation can be broken through if the algorithm is extended to recover arbitrary source shape. In the thesis, we only consider recovering 2D quantitative phase. A possible extension is to recover 3D phase tomography of the defocused stack using coded illumination patterns (*e.g.* Led array illumination microscopy). An interesting problem to consider is whether the similar algorithm/idea can be applied to reconstruct a 3D distribution of fluorophores in fluorescent microscopy. The future work mentioned here is difficult to be realized by simply adapting the proposed methods in the thesis. The forward (measurement) model of each work needs to be carefully considered, and the algorithm to solve the inverse problem should also be designed according to the specific problem.

Author's publications

Journal Papers

1. **Z. Jingshan**, J. Dauwels, M. A. Vázquez, and L. Waller, “Sparse ACEKF for phase reconstruction,” *Opt. Express* **21**, 18125–18137 (2013).
2. **Z. Jingshan**, R. A. Claus, J. Dauwels, L. Tian, and L. Waller, “Transport of intensity phase imaging by intensity spectrum fitting of exponentially spaced defocus planes,” *Opt. Express* **22**, 10661–10674 (2014).
3. **Z. Jingshan**, L. Tian, R. A. Claus, J. Dauwels, and L. Waller, “Partially coherent phase imaging with simultaneous source recovery,” *Biomed. Opt. Express* (6), 257-265 (2015).

Conference Papers

1. **Z. Jingshan**, J. Dauwels, M. A. Vázquez, and L. Waller, “Efficient Gaussian inference algorithms for phase imaging,” in “Acoustics, Speech and Signal Processing (ICASSP), 2012 IEEE International Conference on,” (IEEE, 2012), pp. 617–620.
2. **Z. Jingshan**, J. Dauwels, M. Vazquez, and L. Waller, “Low-complexity noise-resilient recovery of phase and amplitude from defocused intensity images,” in

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- “Computational Optical Sensing and Imaging,” (Optical Society of America, 2012), pp. CTu4B–1.
3. **Z. Jingshan**, L. Tian, R. A. Claus, J. Dauwels, and L. Waller, “Partially coherent phase recovery by Kalman filtering,” in “Frontiers in Optics,” (Optical Society of America, 2013), pp. FW6A–9.
 4. **Z. Jingshan**, R. A. Claus, J. Dauwels, L. Tian, and L. Waller, “Non–uniform sampling and gaussian process regression in transport of intensity phase imaging,” in “Acoustics, Speech and Signal Processing (ICASSP), 2014 IEEE International Conference on,” (IEEE, 2014), pp. 7784–7788.
 5. **Z. Jingshan**, L. Tian, J. Dauwels, and L. Waller, “Partially coherent phase microscopy with arbitrary illumination source shape,” in “Computational Optical Sensing and Imaging,” (Optical Society of America, 2014), pp. CTu1C–5.

Patents

1. J. Dauwels, **Z. Jingshan**, Methods and apparatus for recovering phase and amplitude from intensity images, Patent Provisional App. US 13/760,790 (2013).
2. **Z. Jingshan**, L. Tian, J. Dauwels, L. Waller, Partially coherent phase recovery by Kalman filtering, US Patent Provisional App. US 61/949,420 (2014).

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Appendix A

Proof for the diagonalized CEKF algorithm

Lemma 3.1 *If $\mathbf{M}_{n-1}$ is diagonal, then $\hat{\mathbf{M}}_n = \mathbf{H}\mathbf{M}_{n-1}\mathbf{H}^H = \mathbf{M}_{n-1}$.* ■

Proof: From the definition in Eq. 3.6, the matrix $\mathbf{H}$ is unitary and diagonal. Since $\mathbf{M}_{n-1}$ is diagonal, it commutes with $\mathbf{H}$, and consequently $\hat{\mathbf{M}}_n = \mathbf{M}_{n-1}\mathbf{H}\mathbf{H}^H = \mathbf{M}_{n-1}$. ■

Lemma 3.2 $\mathbf{R} = (4\gamma)^{-1}\mathbf{J}\mathbf{J}^H$. ■

Proof: From the definition of $\mathbf{J}$ in Eq. (3.11) we have:

$$\begin{aligned}\mathbf{J}\mathbf{J}^H &= 4\gamma^2 \text{diag}(\hat{\mathbf{a}}_n^*) \mathbf{K}^H \mathbf{K} \text{diag}(\hat{\mathbf{a}}_n) \\ &= 4\gamma^2 \text{diag}(\hat{\mathbf{a}}_n^*) \text{diag}(\hat{\mathbf{a}}_n) \\ &= 4\gamma \mathbf{R}.\end{aligned}\tag{A.1}$$

Theorem 3.1 *If $\mathbf{M}_0 = \alpha_0 \mathbf{U}$, then $\mathbf{M}_n = \alpha_n \mathbf{U}$ with $\alpha_n = \frac{\alpha_{n-1}}{(4\gamma)\alpha_{n-1}+1}$.* ■

Proof: We prove this theorem by induction. From the Kalman update Eqs. (3.12)-(3.14), and Lemma 3.2 it follows:

$$\begin{aligned}
 \mathbf{M}_n &= \hat{\mathbf{M}}_n - \hat{\mathbf{M}}_n \mathbf{J}^H (\mathbf{J} \hat{\mathbf{M}}_n \mathbf{J}^H + (4\gamma)^{-1} \mathbf{J} \mathbf{J}^H)^{-1} \mathbf{J} \hat{\mathbf{M}}_n \\
 &= \hat{\mathbf{M}}_n - \hat{\mathbf{M}}_n \mathbf{J}^H (\mathbf{J} (\hat{\mathbf{M}}_n + (4\gamma)^{-1} \mathbf{U}) \mathbf{J}^H)^{-1} \mathbf{J} \hat{\mathbf{M}}_n \\
 &= \hat{\mathbf{M}}_n - \hat{\mathbf{M}}_n \mathbf{J}^H (\mathbf{J}^H)^{-1} (\hat{\mathbf{M}}_n + (4\gamma)^{-1} \mathbf{U})^{-1} (\mathbf{J})^{-1} \mathbf{J} \hat{\mathbf{M}}_n \\
 &= \hat{\mathbf{M}}_n - \hat{\mathbf{M}}_n (\hat{\mathbf{M}}_n + (4\gamma)^{-1} \mathbf{U})^{-1} \hat{\mathbf{M}}_n.
 \end{aligned} \tag{A.2}$$

If we initialize $\mathbf{M}_0 = \alpha_0 \mathbf{U}$, then we have $\hat{\mathbf{M}}_1 = \mathbf{M}_0 = \alpha_0 \mathbf{U}$, and hence we can write

$$\mathbf{M}_1 = \hat{\mathbf{M}}_1 - \hat{\mathbf{M}}_1 (\hat{\mathbf{M}}_1 + (4\gamma)^{-1} \mathbf{U})^{-1} \hat{\mathbf{M}}_1 \tag{A.3}$$

$$= \alpha_0 \mathbf{U} - \alpha_0 (\alpha_0 + (4\gamma)^{-1})^{-1} \alpha_0 \mathbf{U} \tag{A.4}$$

$$= \frac{\alpha_0}{(4\gamma)\alpha_0 + 1} \mathbf{U}. \tag{A.5}$$

Therefore, $\mathbf{M}_1$ has the same form as $\mathbf{M}_0$ (diagonal matrix). We proceed now to the induction step: if $\mathbf{M}_{n-1} = \alpha_{n-1} \mathbf{U}$, then we have

$$\mathbf{M}_n = \hat{\mathbf{M}}_n - \hat{\mathbf{M}}_n (\hat{\mathbf{M}}_n + (4\gamma)^{-1} \mathbf{U})^{-1} \hat{\mathbf{M}}_n \tag{A.6}$$

$$= \frac{\alpha_{n-1}}{(4\gamma)\alpha_{n-1} + 1} \mathbf{U} = \alpha_n \mathbf{U}. \tag{A.7}$$

■

The previous theorem allows for the easy update of the covariance matrix $\mathbf{M}_n$. Now, in order to find a simplified expression for $\mathbf{b}_n$, we will make use of another theorem.

Theorem 3.2 *The update formula for state is*

$$\mathbf{b}_n = (1 - 4\alpha_n\gamma)\hat{\mathbf{b}}_n + 4\alpha_n\gamma\mathbf{J}^{-1}\mathbf{I}_n.$$

■

Proof: Another common expression for the Kalman gain is $\mathbf{G}_n = \mathbf{M}_n\mathbf{J}^H\mathbf{R}^{-1}$. Then, from Lemma 3.2 it follows

$$\begin{aligned}\mathbf{G}_n &= \mathbf{M}_n\mathbf{J}^H\mathbf{R}^{-1} \\ &= 4\alpha_n\gamma\mathbf{J}^H\mathbf{J}^{-H}\mathbf{J}^{-1} \\ &= 4\alpha_n\gamma\mathbf{J}^{-1},\end{aligned}\tag{A.8}$$

and substituting Eq. (A.8) in Eq. (3.13) we arrive at

$$\begin{aligned}\mathbf{b}_n &= \hat{\mathbf{b}}_n + 4\alpha_n\gamma\mathbf{J}^{-1}(\mathbf{I}_n - \mathbf{J}\hat{\mathbf{b}}_n) \\ &= (1 - 4\alpha_n\gamma)\hat{\mathbf{b}}_n + 4\alpha_n\gamma\mathbf{J}^{-1}\mathbf{I}_n.\end{aligned}\tag{A.9}$$

■

Appendix B

Derivation of Lemma 4.1

Lemma 4.1 *If a matrix $\mathbf{M}$ is diagonal and its diagonal entries are rotationally symmetric in 2-D, then $\mathbf{E}\mathbf{M}\mathbf{E} = \mathbf{M}$, where $\mathbf{E} = \mathbf{K}\mathbf{K}^T$, and $\mathbf{K}$ is the Discrete Fourier Transform Matrix.* ■

Proof: We separate the proof into two steps. First, it is to prove that $\mathbf{E}$ is a permutation matrix. Second, it is to prove that $\mathbf{E}\mathbf{H}\mathbf{E} = \mathbf{H}$.

The formula of 2-D Discrete Fourier Transform is:

$$F(u, v) = \sum_{m=0}^{M-1} \sum_{n=0}^{N-1} f(m, n) \exp \left[-i2\pi \left(\frac{mu}{M} + \frac{nv}{N} \right) \right]. \quad (\text{B.1})$$

We can express the formula with multiplication of two vectors by introducing matrix $\mathbf{W}(u, v)$. The entry of $\mathbf{W}(u, v)$ at location (m, n)

$$\mathbf{W}(u, v)_{mn} = \exp \left[-i2\pi \left(\frac{mu}{M} + \frac{nv}{N} \right) \right]. \quad (\text{B.2})$$

Then we reshape the 2-D spatial-domain data of $f(m, n)$ into row vector $\mathbf{f}$, and reshape the matrix $\mathbf{W}(u, v)$ into row vector $\mathbf{a}(u, v)$. We can express the DFT formula

with these two vectors $\mathbf{f}$ and $\mathbf{a}(u, v)$:

$$F(u, v) = \mathbf{a}(u, v) \mathbf{f}^T. \quad (\text{B.3})$$

We can express the 2-D DFT matrix with the row vector $\mathbf{a}(u, v)$:

$$\mathbf{K} = \begin{bmatrix} \mathbf{a}(0, 0) \\ \mathbf{a}(0, 1) \\ \vdots \\ \mathbf{a}(0, N-1) \\ \mathbf{a}(1, 0) \\ \mathbf{a}(1, 1) \\ \vdots \\ \mathbf{a}(M-1, N-1) \end{bmatrix}. \quad (\text{B.4})$$

From the definition $\mathbf{E} = \mathbf{K} \mathbf{K}^T$, the entry of $\mathbf{E}$ at (i, j)

$$\mathbf{E}_{ij} = \mathbf{a}(u_i, v_i) \mathbf{a}(u_j, v_j)^T = \sum_{m=0}^{M-1} \sum_{n=0}^{N-1} \exp \left[-i2\pi \left(\frac{mu_i}{M} + \frac{nv_i}{N} \right) \right] \exp \left[-i2\pi \left(\frac{mu_j}{M} + \frac{nv_j}{N} \right) \right] \quad (\text{B.5})$$

$$= \sum_{m=0}^{M-1} \sum_{n=0}^{N-1} \exp \left[-i2\pi \left(\frac{m(u_i + u_j)}{M} + \frac{n(v_i + v_j)}{N} \right) \right]. \quad (\text{B.6})$$

From equation (B.6), when it satisfies both $\{u_i + u_j = 0 \text{ or } M\}$ and $\{v_i + v_j = 0 \text{ or } N\}$,

$\mathbf{E}_{ij} = MN$; When in other cases, $\mathbf{E}_{ij} = 0$.

Define

$$\mathbf{P}_N = \begin{bmatrix} 1 & 0 & \cdots & 0 & 0 \\ 0 & 0 & \cdots & 0 & 1 \\ 0 & 0 & \cdots & 1 & 0 \\ \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 1 & \cdots & 0 & 0 \end{bmatrix}. \quad (\text{B.7})$$

Thus after normalization

$$\mathbf{E} = \begin{bmatrix} \mathbf{P}_N & 0 & \cdots & 0 & 0 \\ 0 & 0 & \cdots & 0 & \mathbf{P}_N \\ 0 & 0 & \cdots & \mathbf{P}_N & 0 \\ \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & \mathbf{P}_N & \cdots & 0 & 0 \end{bmatrix}. \quad (\text{B.8})$$

It is already known that the matrix $\mathbf{H}$ is diagonal and the diagonal entries of $\mathbf{H}$ is rotationally symmetric.

Define

$$\mathbf{H}_2 = \mathbf{EHE}. \quad (\text{B.9})$$

We can reshape the diagonal entries of $\mathbf{H}$ into matrix $\mathbf{A}$ ($M \times N$), and reshape the diagonal entries of $\mathbf{H}_2$ into matrix $\mathbf{B}$ ($M \times N$). Fig. B.1 shows the relation between $\mathbf{A}$ and $\mathbf{B}$. $\mathbf{B}$ can be gotten from $\mathbf{A}$ after rotation. When $\mathbf{A}$ is rotationally symmetric, we can have that $\mathbf{B} = \mathbf{A}$. Therefore, it proves $\mathbf{EHE} = \mathbf{H}$.

■

Figure B.1: Relation between **A** and **B** .

Appendix C

Derivations of Theorem 4.1 and 4.2

C.1 Derivation of theorem 4.1

Theorem 4.1 *If*

$$\begin{aligned} \mathbf{S}_{n-1}^Q &= \mathbf{Q}_{n-1} \\ \mathbf{S}_{n-1}^P &= \mathbf{P}_{n-1} \mathbf{E}, \end{aligned}$$

where $\mathbf{Q}_{n-1}$ and $\mathbf{P}_{n-1}$ are diagonal, then we derive from the ACEKF update Eqs. (4.8)-(4.13) that the covariance matrix can be updated as follows

Predict:

$$\begin{aligned} \hat{\mathbf{Q}}_n &= \mathbf{Q}_{n-1} \\ \hat{\mathbf{P}}_n &= \mathbf{H} \mathbf{P}_{n-1} \mathbf{H}. \end{aligned}$$

Update:

$$\begin{aligned}\mathbf{Q}_n &= \hat{\mathbf{Q}}_n - (\hat{\mathbf{Q}}_n + \hat{\mathbf{P}}_n)(\hat{\mathbf{Q}}_n + \hat{\mathbf{P}}_n + (\hat{\mathbf{Q}}_n)^* + (\hat{\mathbf{P}}_n)^* + qI)^{-1}(\hat{\mathbf{Q}}_n + (\hat{\mathbf{P}}_n)^*) \\ \mathbf{P}_n &= \hat{\mathbf{P}}_n - (\hat{\mathbf{Q}}_n + \hat{\mathbf{P}}_n)(\hat{\mathbf{Q}}_n + \hat{\mathbf{P}}_n + (\hat{\mathbf{Q}}_n)^* + (\hat{\mathbf{P}}_n)^* + qI)^{-1}(\hat{\mathbf{P}}_n + (\hat{\mathbf{Q}}_n)^*) \\ \mathbf{S}_n^Q &= \mathbf{Q}_n \\ \mathbf{S}_n^P &= \mathbf{P}_n \mathbf{E},\end{aligned}$$

where $\mathbf{Q}_n$ and $\mathbf{P}_n$ are diagonal, and $q = \frac{1}{\gamma}$. ■

Proof:

Predict step:

If $\mathbf{Q}_{n-1}$ and $\mathbf{P}_{n-1}$ are diagonal, from the fact that the propagation matrix $\mathbf{H}$ is diagonal (see Eq. (3.6)) it follows:

$$\hat{\mathbf{P}}_n = \mathbf{H} \mathbf{P}_{n-1} \mathbf{H} \tag{C.1}$$

$$\hat{\mathbf{Q}}_n = \mathbf{H} \mathbf{Q}_{n-1} \mathbf{H}^H = \mathbf{Q}_{n-1}. \tag{C.2}$$

Since the propagation matrix $\mathbf{H}$ is diagonal and its diagonal entries are rotationally symmetric, from Eq. (4.8)-(4.9) and Lemma 4.1, it follows:

$$\hat{\mathbf{S}}_n^Q = \mathbf{H} \mathbf{S}_{n-1}^Q \mathbf{H}^H = \mathbf{H} \mathbf{Q}_{n-1} \mathbf{H}^H = \hat{\mathbf{Q}}_n \tag{C.3}$$

$$\hat{\mathbf{S}}_n^P = \mathbf{H} \mathbf{S}_{n-1}^P \mathbf{H} = \mathbf{H} \mathbf{P}_{n-1} \mathbf{E} \mathbf{H} = \mathbf{H} \mathbf{P}_{n-1} \mathbf{H} \mathbf{E} = \hat{\mathbf{P}}_n \mathbf{E}. \tag{C.4}$$

Update step:

From the update formula in Eqs. (4.10)-(4.11), we have

$$\begin{aligned} \mathbf{S}_n^Q = & \hat{\mathbf{S}}_n^Q - (\hat{\mathbf{S}}_n^Q \mathbf{J}_n^H + \hat{\mathbf{S}}_n^P \mathbf{J}_n^T)(\mathbf{J}_n \hat{\mathbf{S}}_n^Q \mathbf{J}_n^H + \mathbf{J}_n \hat{\mathbf{S}}_n^P \mathbf{J}_n^T + \mathbf{J}_n^* (\hat{\mathbf{S}}_n^Q)^* \mathbf{J}_n^T + \mathbf{J}_n^* (\hat{\mathbf{S}}_n^P)^* \mathbf{J}_n^H + \\ & \mathbf{R})^{-1} (\mathbf{J}_n \hat{\mathbf{S}}_n^Q + \mathbf{J}_n^* (\hat{\mathbf{S}}_n^P)^*). \end{aligned} \quad (\text{C.5})$$

From Eq. (4.6), $\mathbf{J}_n = \gamma \text{diag}(\hat{\mathbf{a}}_n^*) \mathbf{K}^H$. Let us define $\mathbf{D} = \gamma \text{diag}(\hat{\mathbf{a}}_n^*)$, so that $\mathbf{J}_n = \mathbf{D} \mathbf{K}^H$. It follows:

$$\begin{aligned} \mathbf{S}_n^Q = & \hat{\mathbf{S}}_n^Q - (\hat{\mathbf{S}}_n^Q \mathbf{K} \mathbf{D}^H + \hat{\mathbf{S}}_n^P \mathbf{K}^* \mathbf{D}^T)(\mathbf{D} \mathbf{K}^H \hat{\mathbf{S}}_n^Q \mathbf{K} \mathbf{D}^H + \mathbf{D} \mathbf{K}^H \hat{\mathbf{S}}_n^P \mathbf{K}^* \mathbf{D}^T + \mathbf{D}^* \mathbf{K}^T (\hat{\mathbf{S}}_n^Q)^* \mathbf{K}^* \mathbf{D}^T \\ & + \mathbf{D}^* \mathbf{K}^T (\hat{\mathbf{S}}_n^P)^* \mathbf{K} \mathbf{D}^H + q \mathbf{D} \mathbf{K}^H \mathbf{K} \mathbf{D}^H)^{-1} (\mathbf{D} \mathbf{K}^H \hat{\mathbf{S}}_n^Q + \mathbf{D}^* \mathbf{K}^T (\hat{\mathbf{S}}_n^P)^*), \end{aligned} \quad (\text{C.6})$$

where $q = \frac{1}{\gamma}$.

Because $\mathbf{D}$ is diagonal matrix, it has $\mathbf{D}^T = \mathbf{D}$ and $\mathbf{D}^H = \mathbf{D}^*$.

$$\begin{aligned} \mathbf{S}_n^Q = & \hat{\mathbf{S}}_n^Q - (\hat{\mathbf{S}}_n^Q \mathbf{K} + \hat{\mathbf{S}}_n^P \mathbf{K}^* \mathbf{D} (\mathbf{D}^*)^{-1})(\mathbf{K}^H \hat{\mathbf{S}}_n^Q \mathbf{K} + \mathbf{K}^H \hat{\mathbf{S}}_n^P \mathbf{K}^* \mathbf{D} (\mathbf{D}^*)^{-1} + \mathbf{D}^{-1} \mathbf{D}^* \mathbf{K}^T (\hat{\mathbf{S}}_n^Q)^* \\ & \mathbf{K}^* \mathbf{D} (\mathbf{D}^*)^{-1} + \mathbf{D}^{-1} \mathbf{D}^* \mathbf{K}^T (\hat{\mathbf{S}}_n^P)^* \mathbf{K} + q \mathbf{K}^H \mathbf{K})^{-1} (\mathbf{K}^H \hat{\mathbf{S}}_n^Q + \mathbf{D}^{-1} \mathbf{D}^* \mathbf{K}^T (\hat{\mathbf{S}}_n^P)^*). \end{aligned} \quad (\text{C.7})$$

Since in our phase recovery problem the value of phase is small, here we consider the approximation $\mathbf{D}^* \mathbf{D}^{-1} \approx \mathbf{I}$. Future research will explore the influence of large phase values.

$$\begin{aligned} \mathbf{S}_n^Q = & \hat{\mathbf{S}}_n^Q - (\hat{\mathbf{S}}_n^Q \mathbf{K} + \hat{\mathbf{S}}_n^P \mathbf{K}^*)(\mathbf{K}^H \hat{\mathbf{S}}_n^Q \mathbf{K} + \mathbf{K}^H \hat{\mathbf{S}}_n^P \mathbf{K}^* + \mathbf{K}^T (\hat{\mathbf{S}}_n^Q)^* \mathbf{K}^* \\ & + \mathbf{K}^T (\hat{\mathbf{S}}_n^P)^* \mathbf{K} + q \mathbf{K}^H \mathbf{K})^{-1} (\mathbf{K}^H \hat{\mathbf{S}}_n^Q + \mathbf{K}^T (\hat{\mathbf{S}}_n^P)^*). \end{aligned} \quad (\text{C.8})$$

Taking $\mathbf{K}^H$ and $\mathbf{K}$ out of the inverse term yields

$$\begin{aligned} \mathbf{S}_n^Q &= \hat{\mathbf{S}}_n^Q - (\hat{\mathbf{S}}_n^Q \mathbf{K} + \hat{\mathbf{S}}_n^P \mathbf{K}^*)(\mathbf{K}^H (\hat{\mathbf{S}}_n^Q + \hat{\mathbf{S}}_n^P \mathbf{K}^* \mathbf{K}^H + \mathbf{K} \mathbf{K}^T (\hat{\mathbf{S}}_n^Q)^* \mathbf{K}^* \mathbf{K}^H \\ &\quad + \mathbf{K} \mathbf{K}^T (\hat{\mathbf{S}}_n^P)^* + qI) \mathbf{K})^{-1} (\mathbf{K}^H \hat{\mathbf{S}}_n^Q + \mathbf{K}^T (\hat{\mathbf{S}}_n^P)^*). \end{aligned} \quad (\text{C.9})$$

It follows:

$$\begin{aligned} \mathbf{S}_n^Q &= \hat{\mathbf{S}}_n^Q - (\hat{\mathbf{S}}_n^Q + \hat{\mathbf{S}}_n^P \mathbf{K}^* \mathbf{K}^H) (\hat{\mathbf{S}}_n^Q + \hat{\mathbf{S}}_n^P \mathbf{K}^* \mathbf{K}^H + \mathbf{K} \mathbf{K}^T (\hat{\mathbf{S}}_n^Q)^* \mathbf{K}^* \mathbf{K}^H + \mathbf{K} \mathbf{K}^T (\hat{\mathbf{S}}_n^P)^* + qI)^{-1} \\ &\quad (\hat{\mathbf{S}}_n^Q + \mathbf{K} \mathbf{K}^T (\hat{\mathbf{S}}_n^P)^*). \end{aligned} \quad (\text{C.10})$$

Likewise, we can derive a similar expression for the update of $\mathbf{S}_n^P$:

$$\begin{aligned} \mathbf{S}_n^P &= \hat{\mathbf{S}}_n^P - (\hat{\mathbf{S}}_n^Q + \hat{\mathbf{S}}_n^P \mathbf{K}^* \mathbf{K}^H) (\hat{\mathbf{S}}_n^Q + \hat{\mathbf{S}}_n^P \mathbf{K}^* \mathbf{K}^H + \mathbf{K} \mathbf{K}^T (\hat{\mathbf{S}}_n^Q)^* \mathbf{K}^* \mathbf{K}^H + \mathbf{K} \mathbf{K}^T (\hat{\mathbf{S}}_n^P)^* + qI)^{-1} \\ &\quad (\hat{\mathbf{S}}_n^P + \mathbf{K} \mathbf{K}^T (\hat{\mathbf{S}}_n^Q)^*). \end{aligned} \quad (\text{C.11})$$

From Lemma 1 and Eqs. (C.3)-(C.4), we obtain:

$$\begin{aligned} \mathbf{S}_n^Q &= \hat{\mathbf{Q}}_n - (\hat{\mathbf{Q}}_n + \hat{\mathbf{P}}_n \mathbf{E} \mathbf{E}) (\hat{\mathbf{Q}}_n + \hat{\mathbf{P}}_n \mathbf{E} \mathbf{E} + \mathbf{E} (\hat{\mathbf{Q}}_n)^* \mathbf{E} + \mathbf{E} (\hat{\mathbf{P}}_n)^* \mathbf{E} + qI)^{-1} \\ &\quad (\hat{\mathbf{Q}}_n + \mathbf{E} (\hat{\mathbf{P}}_n)^* \mathbf{E}) \end{aligned} \quad (\text{C.12})$$

$$\begin{aligned} \mathbf{S}_n^P &= \hat{\mathbf{P}}_n \mathbf{E} - (\hat{\mathbf{Q}}_n + \hat{\mathbf{P}}_n \mathbf{E} \mathbf{E}) (\hat{\mathbf{Q}}_n + \hat{\mathbf{P}}_n \mathbf{E} \mathbf{E} + \mathbf{E} (\hat{\mathbf{Q}}_n)^* \mathbf{E} + \mathbf{E} (\hat{\mathbf{P}}_n)^* \mathbf{E} + qI)^{-1} \\ &\quad (\hat{\mathbf{P}}_n \mathbf{E} + \mathbf{E} (\hat{\mathbf{Q}}_n)^* \mathbf{E} \mathbf{E}). \end{aligned} \quad (\text{C.13})$$

We initialize $\mathbf{Q}_0$ and $\mathbf{P}_0$ as a scalar times the identity matrix. From Eqs. (C.1)-(C.2) and (C.12)-(C.13), the covariance matrices remain rotationally symmetric during the

update. From Lemma 4.1, it follows:

$$\mathbf{S}_n^Q = \hat{\mathbf{Q}}_n - (\hat{\mathbf{Q}}_n + \hat{\mathbf{P}}_n)(\hat{\mathbf{Q}}_n + \hat{\mathbf{P}}_n + (\hat{\mathbf{Q}}_n)^* + (\hat{\mathbf{P}}_n)^* + qI)^{-1}(\hat{\mathbf{Q}}_n + (\hat{\mathbf{P}}_n)^*) \quad (\text{C.14})$$

$$\begin{aligned} \mathbf{S}_n^P &= \hat{\mathbf{P}}_n \mathbf{E} - (\hat{\mathbf{Q}}_n + \hat{\mathbf{P}}_n)(\hat{\mathbf{Q}}_n + \hat{\mathbf{P}}_n + (\hat{\mathbf{Q}}_n)^* + (\hat{\mathbf{P}}_n)^* + qI)^{-1}(\hat{\mathbf{P}}_n \mathbf{E} + (\hat{\mathbf{Q}}_n)^* \mathbf{E}) \\ &= (\hat{\mathbf{P}}_n - (\hat{\mathbf{Q}}_n + \hat{\mathbf{P}}_n)(\hat{\mathbf{Q}}_n + \hat{\mathbf{P}}_n + (\hat{\mathbf{Q}}_n)^* + (\hat{\mathbf{P}}_n)^* + qI)^{-1}(\hat{\mathbf{P}}_n + (\hat{\mathbf{Q}}_n)^*)) \mathbf{E}. \end{aligned} \quad (\text{C.15})$$

■

C.2 Derivation of Theorem 4.2

Theorem 4.2 *The Kalman gain and update formula for the state are*

$$\begin{aligned} G_n &= (\mathbf{S}_n^Q \mathbf{J}_n^H + \mathbf{S}_n^P \mathbf{J}_n^T) \mathbf{R}^{-1} = (\mathbf{Q}_n + \mathbf{P}_n) (\mathbf{J}_n)^{-1} q^{-1}. \\ \mathbf{b}_n &= \hat{\mathbf{b}}_n + \mathbf{G}_n (\mathbf{I}_n - \gamma |\hat{\mathbf{a}}_n|^2). \end{aligned}$$

■

Proof: In Eq. (4.12), the Kalman gain for the augmented Kalman filter is given as:

$$\begin{aligned} G_n &= (\mathbf{S}_n^Q \mathbf{J}_n^H + \mathbf{S}_n^P \mathbf{J}_n^T) \mathbf{R}^{-1} \\ &= (\mathbf{S}_n^Q \mathbf{J}_n^H + \mathbf{S}_n^P \mathbf{J}_n^T) (\mathbf{J}_n^H)^{-1} (\mathbf{J}_n)^{-1} q^{-1} \\ &= (\mathbf{S}_n^Q + \mathbf{S}_n^P \mathbf{E}) (\mathbf{J}_n)^{-1} q^{-1} \\ &= (\mathbf{Q}_n + \mathbf{P}_n) (\mathbf{J}_n)^{-1} q^{-1}. \end{aligned} \quad (\text{C.16})$$

■

Appendix D

Appendix for the GP TIE

D.1 An introduction to Gaussian process regression

We review the basics of Gaussian process regression [65]. Consider the problem of 2-D regression: given input/output pairs (z_n, f_n) , where $n = 1, \dots, N$, we would like to estimate $f(z)$ at arbitrary position z . Under the Gaussian process assumption, the outputs f_n are drawn from the zero-mean Gaussian distribution with the covariance as a function of z_n :

$$(f_1, f_2, \dots, f_N | z_1, z_2, \dots, z_N) \sim \mathcal{N}(\mathbf{0}, \mathbf{K}(\mathbf{Z}, \mathbf{Z}) + \sigma_n \mathbf{I}), \quad (\text{D.1})$$

where $\mathbf{K}(\mathbf{Z}, \mathbf{Z})$ is the covariance matrix of the outputs given the input set $\mathbf{Z}$, and σ_n is the variance of additive Gaussian noise in outputs. Generally, the squared exponential covariance function is used to model the covariance matrix:

$$\mathbf{K}_{ij} = \sigma_f^2 \exp\left[-\frac{1}{2\ell^2}(z_i - z_j)^2\right], \quad (\text{D.2})$$

where $\mathbf{K}_{ij}$ is the element at coordinate (i, j) of the matrix $\mathbf{K}(\mathbf{Z}, \mathbf{Z})$. The parameters σ_f , ℓ , and σ_n in Eq. (D.1) are defined as the hyper-parameters of the GP model. We can write the joint distribution of the observed input/output pairs with the unknown value of $f(z)$ at z as:

$$\begin{bmatrix} \mathbf{f} \\ f(z) \end{bmatrix} \sim \mathcal{N} \left(\mathbf{0}, \begin{bmatrix} \mathbf{K}(\mathbf{Z}, \mathbf{Z}) + \sigma_n \mathbf{I} & \mathbf{K}(\mathbf{Z}, z) \\ \mathbf{K}(z, \mathbf{Z}) & \mathbf{K}(z, z) \end{bmatrix} \right), \quad (\text{D.3})$$

where $\mathbf{f} = [f_1, f_2, \dots, f_N]^T$. The conditional distribution of the unknown output $f(z)$ at z is calculated as:

$$(f(z) | f_1, f_2, \dots, f_N, z_1, z_2, \dots, z_N, z) \sim \mathcal{N}(\bar{f}(z), \bar{\mathbf{K}}), \quad (\text{D.4})$$

where

$$\bar{f}(z) = \mathbf{K}(z, \mathbf{Z})(\mathbf{K}(\mathbf{Z}, \mathbf{Z}) + \sigma_n \mathbf{I})^{-1} \mathbf{f}, \quad (\text{D.5})$$

$$\bar{\mathbf{K}} = \mathbf{K}(z, z) - \mathbf{K}(z, \mathbf{Z})(\mathbf{K}(\mathbf{Z}, \mathbf{Z}) + \sigma_n \mathbf{I})^{-1} \mathbf{K}(\mathbf{Z}, z). \quad (\text{D.6})$$

For convenience, we can define a vector of functions $\mathbf{h}(z)$:

$$\mathbf{h}(z)^T = \mathbf{K}(z, \mathbf{Z})(\mathbf{K}(\mathbf{Z}, \mathbf{Z}) + \sigma_n \mathbf{I})^{-1}. \quad (\text{D.7})$$

Thus we have

$$\bar{f}(z) = \mathbf{h}(z)^T \mathbf{f}. \quad (\text{D.8})$$

The predicted function $\bar{f}(z)$ can be understood as a weighted combination of the shifted equivalent kernel $h(z)$ [65, 83]. In [83], the Fourier transform of the equivalent kernel $h(z)$ for the squared exponential covariance function is given as:

$$\tilde{h}_{SE}(\mathbf{s}) = \frac{1}{1 + b \exp(2\pi^2 \ell^2 |\mathbf{s}|^2)}, \quad (\text{D.9})$$

where $b = \sigma_n^2 / \rho (2\pi \ell^2)^{1/2}$ and ρ is the average number of observations per unit (for example length). When b is small, $\tilde{h}_{SE}(\mathbf{s})$ is approximated by a step function. The rapid change from 1 to 0 happens at the point when

$$s_c^2 = \log(1/b) / (2\pi^2 \ell^2). \quad (\text{D.10})$$

Therefore, the frequency components above the threshold s_c in the fitted function $\bar{f}(z)$ are suppressed. From Eq. (D.10), we can set the desired threshold s_c by changing the hyper-parameters. The property of suppressing the unwanted high frequency components in the fitted function is applied in the regression of the intensity images in TIE.

D.2 Derivation of GP TIE

We have a 3D stack $\mathcal{I}(u, v, z_1), \dots, \mathcal{I}(u, v, z_N)$, which are the 2D Fourier transforms of the measured intensity images. Our goal is to use regression to estimate the first derivative of the intensity spectrum at $z = 0$, $\left. \frac{\partial \mathcal{I}(u, v, z)}{\partial z} \right|_{z=0}$. Instead of doing 3D regression, we perform GP regression for each lateral spatial frequency (u_m, v_n) on N data points $\mathcal{I}(u_m, v_n, z_1), \mathcal{I}(u_m, v_n, z_2), \dots, \mathcal{I}(u_m, v_n, z_N)$. It is easy to observe that $\mathcal{I}(u_m, v_n, z)$ is taken from $\mathcal{I}(u, v, z)$ at the same frequency coordinates (u_m, v_n) .

From Eq. (5.1), $\mathcal{I}(u_m, v_n, z)$ follows a sinusoidal pattern with frequency $\pi\lambda(u_m^2 + v_n^2)$. The sinusoids prior is incorporated into the GP regression by setting the frequency threshold s_c as $\pi\lambda(u_m^2 + v_n^2)$. This is realized by setting appropriate hyper-parameters σ_f, σ_n , and ℓ in the regression. The hyper-parameters σ_f and σ_n are initialized to keep b in Eq. (D.9) small. Next, the parameter ℓ is solved from Eq. (D.10) with s_c and σ_f, σ_n already known. The frequency threshold s_c can be larger than $\pi\lambda(u_m^2 + v_n^2)$ to allow trade-offs between accuracy and noise filtering.

Define $\left. \frac{\partial \mathcal{I}(u_m, v_n, z)}{\partial z} \right|_{z=0}$ as the element of $\left. \frac{\partial \mathcal{I}(u, v, z)}{\partial z} \right|_{z=0}$ at the coordinate (u_m, v_n) . From Eqs. (D.5)(D.7), the function $\bar{\mathcal{I}}(u_m, v_n, z)$ fitted by GP regression is expressed as:

$$\bar{\mathcal{I}}(u_m, v_n, z) = \mathbf{h}(u_m, v_n, z)^T \mathbf{I}_{mn}, \quad (\text{D.11})$$

where $\mathbf{I}_{mn} = [\mathcal{I}(u_m, v_n, z_1), \mathcal{I}(u_m, v_n, z_2), \dots, \mathcal{I}(u_m, v_n, z_N)]^T$ and $\mathbf{h}(u_m, v_n, z)$ can be obtained from Eq. (D.7). The fitted function $\bar{\mathcal{I}}(u_m, v_n, z)$ is a function of the single variable z . Therefore, its first derivative at $z = 0$, $\left. \frac{\partial \mathcal{I}(u_m, v_n, z)}{\partial z} \right|_{z=0}$, is approximated by:

$$\left. \frac{\partial \mathcal{I}(u_m, v_n, z)}{\partial z} \right|_{z=0} = \left. \frac{\partial \mathbf{h}(u_m, v_n, z)^T}{\partial z} \right|_{z=0} \mathbf{I}_{mn}, \quad (\text{D.12})$$

where

$$\begin{aligned} \frac{\partial \mathbf{h}(u_m, v_n, z)^T}{\partial z} &= \left[-\frac{\sigma_f^2}{\ell^2}(z - z_1) \exp\left[-\frac{1}{2\ell^2}(z - z_1)^2\right], \dots, -\frac{\sigma_f^2}{\ell^2}(z - z_N) \exp\left[-\frac{1}{2\ell^2}(z - z_N)^2\right] \right] \\ &\cdot (\mathbf{K}(\mathbf{Z}, \mathbf{Z}) + \sigma_n \mathbf{I})^{-1}. \end{aligned} \quad (\text{D.13})$$

In Eq. (D.12), the vector $\mathbf{I}_{mn}$ is known from the measurements, and the vector

$\left. \frac{\partial \mathbf{h}(u_m, v_n, z)^T}{\partial z} \right|_{z=0}$ can be derived from the GP regression with hyper-parameters already known. Therefore, $\left. \frac{\partial \mathcal{I}(u_m, v_n, z)}{\partial z} \right|_{z=0}$ is estimated by performing GP regression over data points $\mathcal{I}(u_m, v_n, z_1), \mathcal{I}(u_m, v_n, z_2), \dots, \mathcal{I}(u_m, v_n, z_N)$.

By repeating the same process, we can obtain all of the frequency components for the first derivative of intensity spectrum at focus $\left. \frac{\partial \mathcal{I}(u, v, z)}{\partial z} \right|_{z=0}$, then the phase is recovered with the Laplacian inversion in Eq. (2.18)(2.20). Because the computational complexity of GP regression is proportional to the cubic of the number of measurements [65], the algorithm has a computational complexity of $\mathcal{O}(N(N_z)^3)$, where N is the number of pixels in one image, and N_z is the number of measurements. In order to save computational time, the frequency components which have similar $u_m^2 + v_n^2$ values can share the same hyper-parameters and hence the same $\left. \frac{\partial \mathbf{h}(u_m, v_n, z)^T}{\partial z} \right|_{z=0}$.

Appendix E

Derivations of partially coherent phase recovery by Kalman filtering

E.1 Sparse Kalman filter method for partially coherent phase recovery

Defines that the state covariance matrix of the augmented state has the form:

$$\mathbf{S}_n = \begin{bmatrix} \mathbf{S}_n^Q & \mathbf{S}_n^P \\ (\mathbf{S}_n^P)^* & (\mathbf{S}_n^Q)^* \end{bmatrix}. \quad (\text{E.1})$$

From the state space model (Eqs. (6.6) and (6.7)) and the update equations of ACEKF [51, 52], we have the following steps to update the state:

1. Initialize: b_0 , $\mathbf{S}_0^Q$, and $\mathbf{S}_0^P$.
2. Predict:

$$\hat{\mathbf{S}}_n^Q = \mathbf{H}\mathbf{S}_{n-1}^Q\mathbf{H}^H, \quad (\text{E.2})$$

$$\hat{\mathbf{S}}_n^P = \mathbf{H}\mathbf{S}_{n-1}^P\mathbf{H}. \quad (\text{E.3})$$

3. Update:

$$\mathbf{S}_n^Q = \hat{\mathbf{S}}_n^Q - (\hat{\mathbf{S}}_n^Q \mathbf{J}_n^H + \hat{\mathbf{S}}_n^P \mathbf{J}_n^T)(\mathbf{J}_n \hat{\mathbf{S}}_n^Q \mathbf{J}_n^H + \mathbf{J}_n \hat{\mathbf{S}}_n^P \mathbf{J}_n^T + \mathbf{J}_n^* (\hat{\mathbf{S}}_n^Q)^* \mathbf{J}_n^T + \mathbf{J}_n^* (\hat{\mathbf{S}}_n^P)^* \mathbf{J}_n^H + \mathbf{R}_n)^{-1} (\mathbf{J}_n \hat{\mathbf{S}}_n^Q + \mathbf{J}_n^* (\hat{\mathbf{S}}_n^P)^*), \quad (\text{E.4})$$

$$\mathbf{S}_n^P = \hat{\mathbf{S}}_n^P - (\hat{\mathbf{S}}_n^Q \mathbf{J}_n^H + \hat{\mathbf{S}}_n^P \mathbf{J}_n^T)(\mathbf{J}_n \hat{\mathbf{S}}_n^Q \mathbf{J}_n^H + \mathbf{J}_n \hat{\mathbf{S}}_n^P \mathbf{J}_n^T + \mathbf{J}_n^* (\hat{\mathbf{S}}_n^Q)^* \mathbf{J}_n^T + \mathbf{J}_n^* (\hat{\mathbf{S}}_n^P)^* \mathbf{J}_n^H + \mathbf{R}_n)^{-1} (\mathbf{J}_n \hat{\mathbf{S}}_n^P + \mathbf{J}_n^* (\hat{\mathbf{S}}_n^Q)^*), \quad (\text{E.5})$$

$$\mathbf{G}_n = (\mathbf{S}_n^Q \mathbf{J}_n^H + \mathbf{S}_n^P \mathbf{J}_n^T) \mathbf{R}_n^{-1}, \quad (\text{E.6})$$

$$\mathbf{b}_n = \hat{\mathbf{b}}_n + \mathbf{G}_n (\mathbf{I}_n - \gamma \mathbf{C}_n |\hat{\mathbf{a}}_n|^2). \quad (\text{E.7})$$

However, the computational complexity of the ACEKF update equations (Eqs. (E.2) - (E.7)) is $\mathcal{O}(N^3)$, where N is the total number of the pixels in the image. In order to derive the sparse Kalman filter method for partially coherent phase recovery in Table 6.1, we introduce Theorems E.1 and E.2. We provide the derivations in Section E.2 and Section E.3.

Theorem E.1 *If*

$$\mathbf{S}_{n-1}^Q = \mathbf{Q}_{n-1}$$

$$\mathbf{S}_{n-1}^P = \mathbf{P}_{n-1} \mathbf{E},$$

where $\mathbf{Q}_{n-1}$ and $\mathbf{P}_{n-1}$ are diagonal, then we derive from the original ACEKF update

that the covariance matrix can be updated as follows

Predict:

$$\hat{\mathbf{Q}}_n = \mathbf{Q}_{n-1}$$

$$\hat{\mathbf{P}}_n = \mathbf{H} \mathbf{P}_{n-1} \mathbf{H}$$

Update:

$$\mathbf{Q}_n = \hat{\mathbf{Q}}_n - (\hat{\mathbf{Q}}_n + \hat{\mathbf{P}}_n)(\hat{\mathbf{Q}}_n + \hat{\mathbf{P}}_n + (\hat{\mathbf{Q}}_n)^* + (\hat{\mathbf{P}}_n)^* + \frac{1}{\gamma} \mathbf{S}_n^{-2})^{-1}(\hat{\mathbf{Q}}_n + (\hat{\mathbf{P}}_n)^*)$$

$$\mathbf{P}_n = \hat{\mathbf{P}}_n - (\hat{\mathbf{Q}}_n + \hat{\mathbf{P}}_n)(\hat{\mathbf{Q}}_n + \hat{\mathbf{P}}_n + (\hat{\mathbf{Q}}_n)^* + (\hat{\mathbf{P}}_n)^* + \frac{1}{\gamma} \mathbf{S}_n^{-2})^{-1}(\hat{\mathbf{P}}_n + (\hat{\mathbf{Q}}_n)^*)$$

$$\mathbf{S}_n^Q = \mathbf{Q}_n$$

$$\mathbf{S}_n^P = \mathbf{P}_n \mathbf{E},$$

where $\mathbf{Q}_n$ and $\mathbf{P}_n$ are diagonal.

■

Theorem E.2 The Kalman gain and update formula for the state are

$$\mathbf{G}_n = (\mathbf{S}_n^Q \mathbf{J}_n^H + \mathbf{S}_n^P \mathbf{J}_n^T) \mathbf{R}_n^{-1} \approx (\mathbf{Q}_n + \mathbf{P}_n) \mathbf{K} \text{diag}(\hat{\mathbf{a}}_n) \mathbf{C}_n \mathbf{R}_n^{-1}.$$

$$\mathbf{b}_n = \hat{\mathbf{b}}_n + \mathbf{G}_n (\mathbf{I}_n - \gamma \mathbf{C}_n |\hat{\mathbf{a}}_n|^2).$$

■

E.2 Proof of theorem E.1

Predict step:

The matrix $\mathbf{H}$ is a diagonal matrix for the wave prorogation in Fourier domain. From the Fresnel propagation, the diagonal entries of $\mathbf{H}$ only introduce phase changes. If $\mathbf{Q}_{n-1}$ and $\mathbf{P}_{n-1}$ are diagonal, it follows:

$$\hat{\mathbf{P}}_n = \mathbf{H}\mathbf{P}_{n-1}\mathbf{H} \quad (\text{E.8})$$

$$\hat{\mathbf{Q}}_n = \mathbf{H}\mathbf{Q}_{n-1}\mathbf{H}^H = \mathbf{Q}_{n-1}. \quad (\text{E.9})$$

Since the propagation matrix $\mathbf{H}$ is diagonal and its diagonal entries are rotationally symmetric, from Eqs. (E.2)-(E.3), Eqs. (E.8)-(E.9) and Lemma 4.1, it follows:

$$\hat{\mathbf{S}}_n^Q = \mathbf{H}\mathbf{S}_{n-1}^Q\mathbf{H}^H = \mathbf{H}\mathbf{Q}_{n-1}\mathbf{H}^H = \hat{\mathbf{Q}}_n \quad (\text{E.10})$$

$$\hat{\mathbf{S}}_n^P = \mathbf{H}\mathbf{S}_{n-1}^P\mathbf{H} = \mathbf{H}\mathbf{P}_{n-1}\mathbf{E}\mathbf{H} = \mathbf{H}\mathbf{P}_{n-1}\mathbf{H}\mathbf{E} = \hat{\mathbf{P}}_n\mathbf{E}. \quad (\text{E.11})$$

Update step:

From Eq. (E.4), we have

$$\begin{aligned} \mathbf{S}_n^Q &= \hat{\mathbf{S}}_n^Q - (\hat{\mathbf{S}}_n^Q\mathbf{J}_n^H + \hat{\mathbf{S}}_n^P\mathbf{J}_n^T)(\mathbf{J}_n\hat{\mathbf{S}}_n^Q\mathbf{J}_n^H + \mathbf{J}_n\hat{\mathbf{S}}_n^P\mathbf{J}_n^T + \mathbf{J}_n^*(\hat{\mathbf{S}}_n^Q)^*\mathbf{J}_n^T + \mathbf{J}_n^*(\hat{\mathbf{S}}_n^P)^*\mathbf{J}_n^H + \mathbf{R}_n)^{-1} \\ &\quad (\mathbf{J}_n\hat{\mathbf{S}}_n^Q + \mathbf{J}_n^*(\hat{\mathbf{S}}_n^P)^*). \end{aligned} \quad (\text{E.12})$$

From Eq. (6.8), $\mathbf{J}_n = \gamma \mathbf{C}_n \text{diag}(\hat{\mathbf{a}}_n^*) \mathbf{K}^H$. Define $\mathbf{D} = \gamma \text{diag}(\hat{\mathbf{a}}_n^*)$, so that $\mathbf{J}_n = \mathbf{C}_n \mathbf{D} \mathbf{K}^H$. It follows:

$$\begin{aligned} \mathbf{S}_n^Q &= \hat{\mathbf{S}}_n^Q - (\hat{\mathbf{S}}_n^Q \mathbf{K} \mathbf{D}^H \mathbf{C}_n^H + \hat{\mathbf{S}}_n^P \mathbf{K}^* \mathbf{D}^T \mathbf{C}_n^T) (\mathbf{C}_n \mathbf{D} \mathbf{K}^H \hat{\mathbf{S}}_n^Q \mathbf{K} \mathbf{D}^H \mathbf{C}_n^H + \mathbf{C}_n \mathbf{D} \mathbf{K}^H \hat{\mathbf{S}}_n^P \mathbf{K}^* \\ &\quad \mathbf{D}^T \mathbf{C}_n^T + \mathbf{C}_n^* \mathbf{D}^* \mathbf{K}^T (\hat{\mathbf{S}}_n^Q)^* \mathbf{K}^* \mathbf{D}^T \mathbf{C}_n^T + \mathbf{C}_n^* \mathbf{D}^* \mathbf{K}^T (\hat{\mathbf{S}}_n^P)^* \mathbf{K} \mathbf{D}^H \mathbf{C}_n^H + \mathbf{R}_n)^{-1} (\mathbf{C}_n \mathbf{D} \mathbf{K}^H \hat{\mathbf{S}}_n^Q + \\ &\quad \mathbf{C}_n^* \mathbf{D}^* \mathbf{K}^T (\hat{\mathbf{S}}_n^P)^*). \end{aligned} \quad (\text{E.13})$$

Since $\mathbf{C}_n$ is a real circulant matrix which describes the convolution of the scaled source, we have that $\mathbf{C}_n = \mathbf{C}_n^T = \mathbf{C}_n^* = \mathbf{C}_n^H$. We replace $\mathbf{C}_n^T$, $\mathbf{C}_n^*$, $\mathbf{C}_n^H$ in Eq. (E.13) with $\mathbf{C}_n$:

$$\begin{aligned} \mathbf{S}_n^Q &= \hat{\mathbf{S}}_n^Q - (\hat{\mathbf{S}}_n^Q \mathbf{K} \mathbf{D}^H \mathbf{C}_n + \hat{\mathbf{S}}_n^P \mathbf{K}^* \mathbf{D}^T \mathbf{C}_n) (\mathbf{C}_n \mathbf{D} \mathbf{K}^H \hat{\mathbf{S}}_n^Q \mathbf{K} \mathbf{D}^H \mathbf{C}_n + \mathbf{C}_n \mathbf{D} \mathbf{K}^H \hat{\mathbf{S}}_n^P \mathbf{K}^* \mathbf{D}^T \mathbf{C}_n + \\ &\quad \mathbf{C}_n \mathbf{D}^* \mathbf{K}^T (\hat{\mathbf{S}}_n^Q)^* \mathbf{K}^* \mathbf{D}^T \mathbf{C}_n + \mathbf{C}_n \mathbf{D}^* \mathbf{K}^T (\hat{\mathbf{S}}_n^P)^* \mathbf{K} \mathbf{D}^H \mathbf{C}_n + \mathbf{R}_n)^{-1} (\mathbf{C}_n \mathbf{D} \mathbf{K}^H \hat{\mathbf{S}}_n^Q + \mathbf{C}_n \mathbf{D}^* \mathbf{K}^T \\ &\quad (\hat{\mathbf{S}}_n^P)^*). \end{aligned} \quad (\text{E.14})$$

Cancel out $\mathbf{C}_n$ by taking it out of the inverse term, and it follows:

$$\begin{aligned} \mathbf{S}_n^Q &= \hat{\mathbf{S}}_n^Q - (\hat{\mathbf{S}}_n^Q \mathbf{K} \mathbf{D}^H + \hat{\mathbf{S}}_n^P \mathbf{K}^* \mathbf{D}^T) (\mathbf{D} \mathbf{K}^H \hat{\mathbf{S}}_n^Q \mathbf{K} \mathbf{D}^H + \mathbf{D} \mathbf{K}^H \hat{\mathbf{S}}_n^P \mathbf{K}^* \mathbf{D}^T + \mathbf{D}^* \mathbf{K}^T (\hat{\mathbf{S}}_n^Q)^* \mathbf{K}^* \\ &\quad \mathbf{D}^T + \mathbf{D}^* \mathbf{K}^T (\hat{\mathbf{S}}_n^P)^* \mathbf{K} \mathbf{D}^H + \mathbf{C}_n^{-1} \mathbf{R}_n \mathbf{C}_n^{-1})^{-1} (\mathbf{D} \mathbf{K}^H \hat{\mathbf{S}}_n^Q + \mathbf{D}^* \mathbf{K}^T (\hat{\mathbf{S}}_n^P)^*). \end{aligned} \quad (\text{E.15})$$

Because $\mathbf{D}$ is diagonal matrix, it has $\mathbf{D}^T = \mathbf{D}$ and $\mathbf{D}^H = \mathbf{D}^*$.

$$\begin{aligned} \mathbf{S}_n^Q &= \hat{\mathbf{S}}_n^Q - (\hat{\mathbf{S}}_n^Q \mathbf{K} + \hat{\mathbf{S}}_n^P \mathbf{K}^* \mathbf{D} (\mathbf{D}^*)^{-1}) (\mathbf{K}^H \hat{\mathbf{S}}_n^Q \mathbf{K} + \mathbf{K}^H \hat{\mathbf{S}}_n^P \mathbf{K}^* \mathbf{D} (\mathbf{D}^*)^{-1} + \mathbf{D}^{-1} \mathbf{D}^* \mathbf{K}^T (\hat{\mathbf{S}}_n^Q)^* \\ &\quad \mathbf{K}^* \mathbf{D} (\mathbf{D}^*)^{-1} + \mathbf{D}^{-1} \mathbf{D}^* \mathbf{K}^T (\hat{\mathbf{S}}_n^P)^* \mathbf{K} + \mathbf{D}^{-1} \mathbf{C}_n^{-1} \mathbf{R}_n \mathbf{C}_n^{-1} (\mathbf{D}^*)^{-1})^{-1} (\mathbf{K}^H \hat{\mathbf{S}}_n^Q + \mathbf{D}^{-1} \mathbf{D}^* \mathbf{K}^T \\ &\quad (\hat{\mathbf{S}}_n^P)^*). \end{aligned} \quad (\text{E.16})$$

We have following three steps. Firstly, we consider the approximation $\mathbf{D}^* \mathbf{D}^{-1} \approx \mathbf{I}$ by making assumption that the value of phase is small in our phase recovery problem.

$$\begin{aligned} \mathbf{S}_n^Q &= \hat{\mathbf{S}}_n^Q - (\hat{\mathbf{S}}_n^Q \mathbf{K} + \hat{\mathbf{S}}_n^P \mathbf{K}^*) (\mathbf{K}^H \hat{\mathbf{S}}_n^Q \mathbf{K} + \mathbf{K}^H \hat{\mathbf{S}}_n^P \mathbf{K}^* + \mathbf{K}^T (\hat{\mathbf{S}}_n^Q)^* \mathbf{K}^* + \mathbf{K}^T (\hat{\mathbf{S}}_n^P)^* \mathbf{K} + \\ &\mathbf{D}^{-1} \mathbf{C}_n^{-1} \mathbf{R}_n \mathbf{C}_n^{-1} (\mathbf{D}^*)^{-1})^{-1} (\mathbf{K}^H \hat{\mathbf{S}}_n^Q + \mathbf{K}^T (\hat{\mathbf{S}}_n^P)^*). \end{aligned} \quad (\text{E.17})$$

We take $\mathbf{K}^H$ and $\mathbf{K}$ out of the inverse term and use the property of DFT matrix $\mathbf{K} \mathbf{K}^H = \mathbf{I}$:

$$\begin{aligned} \mathbf{S}_n^Q &= \hat{\mathbf{S}}_n^Q - (\hat{\mathbf{S}}_n^Q \mathbf{K} + \hat{\mathbf{S}}_n^P \mathbf{K}^*) \{ \mathbf{K}^H (\hat{\mathbf{S}}_n^Q + \hat{\mathbf{S}}_n^P \mathbf{K}^* \mathbf{K}^H + \mathbf{K} \mathbf{K}^T (\hat{\mathbf{S}}_n^Q)^* \mathbf{K}^* \mathbf{K}^H + \mathbf{K} \mathbf{K}^T (\hat{\mathbf{S}}_n^P)^* \\ &+ \mathbf{K} \mathbf{D}^{-1} \mathbf{C}_n^{-1} \mathbf{R}_n \mathbf{C}_n^{-1} (\mathbf{D}^*)^{-1} \mathbf{K}^H) \mathbf{K} \}^{-1} (\mathbf{K}^H \hat{\mathbf{S}}_n^Q + \mathbf{K}^T (\hat{\mathbf{S}}_n^P)^*) \\ &= \hat{\mathbf{S}}_n^Q - (\hat{\mathbf{S}}_n^Q + \hat{\mathbf{S}}_n^P \mathbf{K}^* \mathbf{K}^H) \{ (\hat{\mathbf{S}}_n^Q + \hat{\mathbf{S}}_n^P \mathbf{K}^* \mathbf{K}^H + \mathbf{K} \mathbf{K}^T (\hat{\mathbf{S}}_n^Q)^* \mathbf{K}^* \mathbf{K}^H + \mathbf{K} \mathbf{K}^T (\hat{\mathbf{S}}_n^P)^* \\ &+ \mathbf{K} \mathbf{D}^{-1} \mathbf{C}_n^{-1} \mathbf{R}_n \mathbf{C}_n^{-1} (\mathbf{D}^*)^{-1} \mathbf{K}^H) \}^{-1} (\hat{\mathbf{S}}_n^Q + \mathbf{K} \mathbf{K}^T (\hat{\mathbf{S}}_n^P)^*). \end{aligned} \quad (\text{E.18})$$

Secondly, we show that the term inside the inversion in Eq. (E.18):

$$\mathbf{K} \mathbf{D}^{-1} \mathbf{C}_n^{-1} \mathbf{R}_n \mathbf{C}_n^{-1} (\mathbf{D}^*)^{-1} \mathbf{K}^H \approx q \mathbf{S}_n^{-2}. \quad (\text{E.19})$$

This term contains $\mathbf{R}_n$, so it is related to the level of noise. Since $\mathbf{C}_n$ is a real circulant matrix which describes the convolution of the scaled source, we have that $\mathbf{C}_n = \mathbf{K} \mathbf{S}_n \mathbf{K}^H$. The $\mathbf{S}_n$ here is a diagonal matrix whose diagonal entries are equal to Fourier transform of the scaled source $S(-\frac{f}{z_n}x, -\frac{f}{z_n}y)$. Since $\mathbf{K}$ is the DFT matrix,

$\mathbf{C}_n^{-1} = \mathbf{K}\mathbf{S}_n^{-1}\mathbf{K}^H$. We have

$$\begin{aligned}
& \mathbf{K}\mathbf{D}^{-1}\mathbf{C}_n^{-1}\mathbf{R}_n\mathbf{C}_n^{-1}(\mathbf{D}^*)^{-1}\mathbf{K}^H \\
&= \mathbf{K}\mathbf{D}^{-1}(\mathbf{K}\mathbf{S}_n^{-1}\mathbf{K}^H)\mathbf{R}_n(\mathbf{K}\mathbf{S}_n^{-1}\mathbf{K}^H)(\mathbf{D}^*)^{-1}\mathbf{K}^H \\
&= \mathbf{K}\mathbf{K} \{ \mathbf{K}^H\mathbf{D}^{-1}\mathbf{K} \} \mathbf{S}_n^{-1} \{ \mathbf{K}^H\mathbf{R}_n\mathbf{K} \} \mathbf{S}_n^{-1} \{ \mathbf{K}^H(\mathbf{D}^*)^{-1}\mathbf{K} \} \mathbf{K}^H\mathbf{K}^H \\
&= \mathbf{E} \{ \mathbf{K}^H\mathbf{D}^{-1}\mathbf{K} \} \mathbf{S}_n^{-1} \{ \mathbf{K}^H\mathbf{R}_n\mathbf{K} \} \mathbf{S}_n^{-1} \{ \mathbf{K}^H(\mathbf{D}^*)^{-1}\mathbf{K} \} \mathbf{E}. \tag{E.20}
\end{aligned}$$

Because $\mathbf{D}^{-1}$, $\mathbf{R}_n$, and $(\mathbf{D}^*)^{-1}$ are diagonal matrix and $\mathbf{K}$ is the DFT matrix, the multiplication $\{ \mathbf{K}^H\mathbf{D}^{-1}\mathbf{K} \}$, $\{ \mathbf{K}^H\mathbf{R}_n\mathbf{K} \}$ in Eq. (E.20) will result in circulant matrices, with the entries in each row of the circulant matrix obtaining by rotating from the Fourier transform of $\mathbf{D}^{-1}$, $\mathbf{R}_n$, and $(\mathbf{D}^*)^{-1}$. By taking the diagonal entries of these circulant matrix, $\{ \mathbf{K}^H(\mathbf{D}^*)^{-1}\mathbf{K} \}$ is approximated as diagonal matrix. Therefore, Eq. (E.20) is approximated as a multiplication of diagonal matrices, so we interchange the order of the matrix in the multiplication:

$$\begin{aligned}
& \mathbf{E} \{ \mathbf{K}^H\mathbf{D}^{-1}\mathbf{K} \} \mathbf{S}_n^{-1} \{ \mathbf{K}^H\mathbf{R}_n\mathbf{K} \} \mathbf{S}_n^{-1} \{ \mathbf{K}^H(\mathbf{D}^*)^{-1}\mathbf{K} \} \mathbf{E} \\
&\approx \mathbf{E} \{ \mathbf{K}^H\mathbf{D}^{-1}\mathbf{K} \} \{ \mathbf{K}^H\mathbf{R}_n\mathbf{K} \} \{ \mathbf{K}^H(\mathbf{D}^*)^{-1}\mathbf{K} \} \mathbf{S}_n^{-1}\mathbf{S}_n^{-1}\mathbf{E} \\
&= \mathbf{E} \{ \mathbf{K}^H\mathbf{D}^{-1}\mathbf{R}_n(\mathbf{D}^*)^{-1}\mathbf{K} \} \mathbf{S}_n^{-2}\mathbf{E}, \tag{E.21}
\end{aligned}$$

where $\mathbf{E} = \mathbf{K}\mathbf{K} = \mathbf{K}^H\mathbf{K}^H$ as shown by Lemma 4.1. We defined $\mathbf{R}_n = \gamma \text{diag}(\mathbf{C}_n|\hat{\mathbf{a}}_n|^2)$ (see Eq. (6.8)), and $\mathbf{D} = \gamma \text{diag}(\hat{\mathbf{a}}_n^*)$. Therefore, the multiplication $\mathbf{D}^{-1}\mathbf{R}_n(\mathbf{D}^*)^{-1} = \frac{1}{\gamma} \text{diag}(|\hat{\mathbf{a}}_n|^2)^{-1} \text{diag}(\mathbf{C}_n|\hat{\mathbf{a}}_n|^2)$. Since $\mathbf{C}_n$ is a circulant matrix for convolution, $\mathbf{C}_n|\hat{\mathbf{a}}_n|^2$ results in a blurred version of $|\hat{\mathbf{a}}_n|^2$. And hence, $\text{diag}(|\hat{\mathbf{a}}_n|^2)^{-1} \text{diag}(\mathbf{C}_n|\hat{\mathbf{a}}_n|^2) \approx \mathbf{I}$, and

then we have $\mathbf{D}^{-1}\mathbf{R}_n(\mathbf{D}^*)^{-1} \approx \frac{1}{\gamma}\mathbf{I}$. From Eq. (E.21) and Lemma 4.1, we have

$$\begin{aligned}
 & \mathbf{E} \left\{ \mathbf{K}^H \mathbf{D}^{-1} \mathbf{R}_n (\mathbf{D}^*)^{-1} \mathbf{K} \right\} \mathbf{S}_n^{-2} \mathbf{E} \\
 & \approx \mathbf{E} \left\{ \mathbf{K}^H \frac{1}{\gamma} \mathbf{K} \right\} \mathbf{S}_n^{-2} \mathbf{E} \\
 & = \frac{1}{\gamma} \mathbf{E} \mathbf{S}_n^{-1} \mathbf{S}_n^{-1} \mathbf{E} \\
 & = \frac{1}{\gamma} \mathbf{S}_n^{-2}.
 \end{aligned} \tag{E.22}$$

Finally, the computational burden in Eq. (E.18) can be further reduced by using the approximation $\mathbf{K} \mathbf{D}^{-1} \mathbf{C}_n^{-1} \mathbf{R}_n \mathbf{C}_n^{-1} (\mathbf{D}^*)^{-1} \mathbf{K}^H \approx \frac{1}{\gamma} \mathbf{S}_n^{-2}$. From Eq. (E.18), it follows:

$$\begin{aligned}
 \mathbf{S}_n^Q &= \hat{\mathbf{S}}_n^Q - (\hat{\mathbf{S}}_n^Q + \hat{\mathbf{S}}_n^P \mathbf{K}^* \mathbf{K}^H) (\hat{\mathbf{S}}_n^Q + \hat{\mathbf{S}}_n^P \mathbf{K}^* \mathbf{K}^H + \mathbf{K} \mathbf{K}^T (\hat{\mathbf{S}}_n^Q)^* \mathbf{K}^* \mathbf{K}^H + \mathbf{K} \mathbf{K}^T (\hat{\mathbf{S}}_n^P)^* + \\
 & \frac{1}{\gamma} \mathbf{S}_n^{-2})^{-1} (\hat{\mathbf{S}}_n^Q + \mathbf{K} \mathbf{K}^T (\hat{\mathbf{S}}_n^P)^*).
 \end{aligned} \tag{E.23}$$

Likewise, we can derive a similar expression for the update of $\mathbf{S}_n^P$:

$$\begin{aligned}
 \mathbf{S}_n^P &= \hat{\mathbf{S}}_n^P - (\hat{\mathbf{S}}_n^Q + \hat{\mathbf{S}}_n^P \mathbf{K}^* \mathbf{K}^H) (\hat{\mathbf{S}}_n^Q + \hat{\mathbf{S}}_n^P \mathbf{K}^* \mathbf{K}^H + \mathbf{K} \mathbf{K}^T (\hat{\mathbf{S}}_n^Q)^* \mathbf{K}^* \mathbf{K}^H + \mathbf{K} \mathbf{K}^T (\hat{\mathbf{S}}_n^P)^* + \\
 & \frac{1}{\gamma} \mathbf{S}_n^{-2})^{-1} (\hat{\mathbf{S}}_n^P + \mathbf{K} \mathbf{K}^T (\hat{\mathbf{S}}_n^Q)^*).
 \end{aligned} \tag{E.24}$$

From Lemma 4.1 and Eqs. (E.10)-(E.11), we obtain:

$$\begin{aligned}
 \mathbf{S}_n^Q &= \hat{\mathbf{Q}}_n - (\hat{\mathbf{Q}}_n + \hat{\mathbf{P}}_n \mathbf{E} \mathbf{E}) (\hat{\mathbf{Q}}_n + \hat{\mathbf{P}}_n \mathbf{E} \mathbf{E} + \mathbf{E} (\hat{\mathbf{Q}}_n)^* \mathbf{E} + \mathbf{E} (\hat{\mathbf{P}}_n)^* \mathbf{E} + \frac{1}{\gamma} \mathbf{S}_n^{-2})^{-1} (\hat{\mathbf{Q}}_n + \\
 & \mathbf{E} (\hat{\mathbf{P}}_n)^* \mathbf{E}),
 \end{aligned} \tag{E.25}$$

$$\begin{aligned}
 \mathbf{S}_n^P &= \hat{\mathbf{P}}_n \mathbf{E} - (\hat{\mathbf{Q}}_n + \hat{\mathbf{P}}_n \mathbf{E} \mathbf{E}) (\hat{\mathbf{Q}}_n + \hat{\mathbf{P}}_n \mathbf{E} \mathbf{E} + \mathbf{E} (\hat{\mathbf{Q}}_n)^* \mathbf{E} + \mathbf{E} (\hat{\mathbf{P}}_n)^* \mathbf{E} + \frac{1}{\gamma} \mathbf{S}_n^{-2})^{-1} (\hat{\mathbf{P}}_n \mathbf{E} \\
 & + \mathbf{E} (\hat{\mathbf{Q}}_n)^* \mathbf{E} \mathbf{E}).
 \end{aligned} \tag{E.26}$$

We initialize $\mathbf{Q}_0$ and $\mathbf{P}_0$ as a scalar times the identity matrix. From Eqs. (E.8)-(E.9) and (E.25)-(E.26), the covariance matrices remain rotationally symmetric during the update. From Lemma 4.1, it follows:

$$\mathbf{S}_n^Q = \hat{\mathbf{Q}}_n - (\hat{\mathbf{Q}}_n + \hat{\mathbf{P}}_n)(\hat{\mathbf{Q}}_n + \hat{\mathbf{P}}_n + (\hat{\mathbf{Q}}_n)^* + (\hat{\mathbf{P}}_n)^* + \frac{1}{\gamma}\mathbf{S}_n^{-2})^{-1}(\hat{\mathbf{Q}}_n + (\hat{\mathbf{P}}_n)^*), \quad (\text{E.27})$$

$$\begin{aligned} \mathbf{S}_n^P &= \hat{\mathbf{P}}_n \mathbf{E} - (\hat{\mathbf{Q}}_n + \hat{\mathbf{P}}_n)(\hat{\mathbf{Q}}_n + \hat{\mathbf{P}}_n + (\hat{\mathbf{Q}}_n)^* + (\hat{\mathbf{P}}_n)^* + \frac{1}{\gamma}\mathbf{S}_n^{-2})^{-1}(\hat{\mathbf{P}}_n \mathbf{E} + (\hat{\mathbf{Q}}_n)^* \mathbf{E}) \\ &= (\hat{\mathbf{P}}_n - (\hat{\mathbf{Q}}_n + \hat{\mathbf{P}}_n)(\hat{\mathbf{Q}}_n + \hat{\mathbf{P}}_n + (\hat{\mathbf{Q}}_n)^* + (\hat{\mathbf{P}}_n)^* + \frac{1}{\gamma}\mathbf{S}_n^{-2})^{-1}(\hat{\mathbf{P}}_n + (\hat{\mathbf{Q}}_n)^*)) \mathbf{E}. \end{aligned} \quad (\text{E.28})$$

E.3 Proof of theorem E.2

In Eq. (E.6), the Kalman gain for the augmented Kalman filter is given as:

$$\begin{aligned} G_n &= (\mathbf{S}_n^Q \mathbf{J}_n^H + \mathbf{S}_n^P \mathbf{J}_n^T) \mathbf{R}_n^{-1} \\ &= (\mathbf{S}_n^Q \mathbf{J}_n^H + \mathbf{S}_n^P \mathbf{J}_n^T) (\mathbf{J}_n^H)^{-1} \mathbf{J}_n^H \mathbf{R}_n^{-1} \\ &= (\mathbf{S}_n^Q + \mathbf{S}_n^P \mathbf{J}_n^T (\mathbf{J}_n^H)^{-1}) \mathbf{J}_n^H \mathbf{R}_n^{-1}. \end{aligned} \quad (\text{E.29})$$

Since $\mathbf{J}_n = \mathbf{C}_n \mathbf{D} \mathbf{K}^H$, we can have $\mathbf{J}_n^H = \mathbf{K} \mathbf{D}^H \mathbf{C}_n$ and $\mathbf{J}_n^T = \mathbf{K}^H \mathbf{D} \mathbf{C}_n$. Note that $\mathbf{C}_n$ is a real circulant matrix.

$$\begin{aligned} &(\mathbf{S}_n^Q + \mathbf{S}_n^P \mathbf{J}_n^T (\mathbf{J}_n^H)^{-1}) \mathbf{J}_n^H \mathbf{R}_n^{-1} \\ &= (\mathbf{S}_n^Q + \mathbf{S}_n^P \mathbf{K}^H \mathbf{D} \mathbf{C}_n \mathbf{C}_n^{-1} (\mathbf{D}^H)^{-1} \mathbf{K}^{-1}) \mathbf{K} \mathbf{D}^H \mathbf{C}_n \mathbf{R}_n^{-1}. \end{aligned} \quad (\text{E.30})$$

We have the small phase approximation $\mathbf{D}(\mathbf{D}^H)^{-1} \approx I$ and $\mathbf{K}^H \mathbf{K}^{-1} = \mathbf{K}^H \mathbf{K}^H = \mathbf{E}$.

$$\begin{aligned} & (\mathbf{S}_n^{\mathbf{Q}} + \mathbf{S}_n^{\mathbf{P}} \mathbf{E}) \mathbf{K} \mathbf{D}^H \mathbf{C}_n \mathbf{R}_n^{-1} \\ &= (\mathbf{Q}_n + \mathbf{P}_n) \mathbf{K} \text{diag}(\hat{\mathbf{a}}_n) \mathbf{C}_n \mathbf{R}_n^{-1}. \end{aligned} \tag{E.31}$$