Thesis to get the degree of a Master of Science

Title of the thesis

Subtitle

Avina Chetana Kalle

Date (optional)

Universität Hamburg
Faculty of Mathematics, Informatics and Natural Sciences
Department of Mathematics

Supervisor
Prof. Dr. Christina Brandt

Reviewers
Prof. Dr. aaa bbb
Prof. Dr. xxx yyy

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2. Pre-requisite Concepts

2.1. Fourier Transformation

Define the following notations in continuous and discrete spaces:

	Continuous variable/ operation	Discrete equivalent
Time coordinate	$x \in \mathbb{R}$	$n\Delta x \in \mathbb{R}, n \in \mathbb{Z}$
Frequency coordinate	$\omega \in \mathbb{R}$	$m\Delta\omega \in \mathbb{R}, m \in \mathbb{Z}$
Fourier transform	$\mathcal{F}$	$\mathbb{F}$
Inverse Fourier transform	$\mathcal{F}^{-1}$	$\mathbb{F}^{-1}$

Table 2.1.: Continuous and discrete variables and operations

Definition 2.1. (Fourier Transform) Consider the function $f(x)$. The continuous Fourier transform (FT) of $f(x)$ is defined by

$$\begin{gathered} \mathcal{F} : \mathbb{C}^N \to \mathbb{C}^N \\ \mathcal{F}[f(x)] = F(\omega) = \tfrac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} f(x) \exp(-i\omega x)\, dx \end{gathered} \tag{2.1}$$

Definition 2.2. (Fourier Transform) Similarly, the continuous inverse Fourier transform (IFT) of $F(x)$ is defined by

$$\begin{gathered} \mathcal{F} : \mathbb{C}^N \to \mathbb{C}^N \\ \mathcal{F}^{-1}[F(x)] = f(\omega) = \tfrac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} F(x) \exp(i\omega x)\, d\omega \end{gathered} \tag{2.2}$$

Definition 2.3. (Discrete Fourier Transform) Consider a vector $\mathbf{z} = [z_0, z_1, ..., z_{N-1}] \in \mathbb{C}^N$. The discrete Fourier transform (DFT) of $\mathbf{z}$ is $\mathbf{Z} := [Z_0, Z_1, ..., Z_{N-1}]$ and is defined by

$$\begin{aligned} &\mathbb{F} : \mathbb{C}^N \to \mathbb{C}^N \\ &\mathbb{F}(\mathbf{z}) = \mathbf{Z}; \qquad Z_k = \textstyle\sum_{n=0}^{N-1} z_n \exp\left(-i\frac{2\pi}{N}kn\right) \end{aligned} \tag{2.3}$$

Definition 2.4. Similarly, the discrete inverse Fourier transform (DIFT) is defined as

$$\begin{aligned} &\mathbb{F}^{-1} : \mathbb{C}^N \to \mathbb{C}^N \\ &\mathbb{F}^{-1}(\mathbf{Z}) = \mathbf{z}; \qquad z_k = \tfrac{1}{N} \textstyle\sum_{n=0}^{N-1} Z_n \exp\left(i\frac{2\pi}{N}kn\right) \end{aligned} \tag{2.4}$$

Remark 2.1. The discrete spacing of the real/ time space (i.e., Δx) and the discrete spacing of the reciprocal/ frequency space (i.e., $\Delta\omega$) is inversely related as follows:

$$\Delta x = \frac{1}{\Delta\omega}.\frac{2\pi}{N} \tag{2.5}$$

Proof. As a consequence of the definitions of continuous and discrete Fourier transform (2.1 and 2.3), the exponential functions must be equal:

$$\begin{aligned}&\exp\left(-i\omega x\right) = \exp\left(im\Delta\omega\cdot n\Delta x\right) = \exp\left(-i\tfrac{2\pi}{N}mn\right)\\&\implies im\Delta\omega\cdot n\Delta x = \tfrac{2\pi}{N}mn\\&\therefore \Delta\omega\Delta x = \tfrac{2\pi}{N}\end{aligned}$$

□

2.2. Some useful functions and their Fourier transforms

In the course of this project, there are some important functions that will be used.

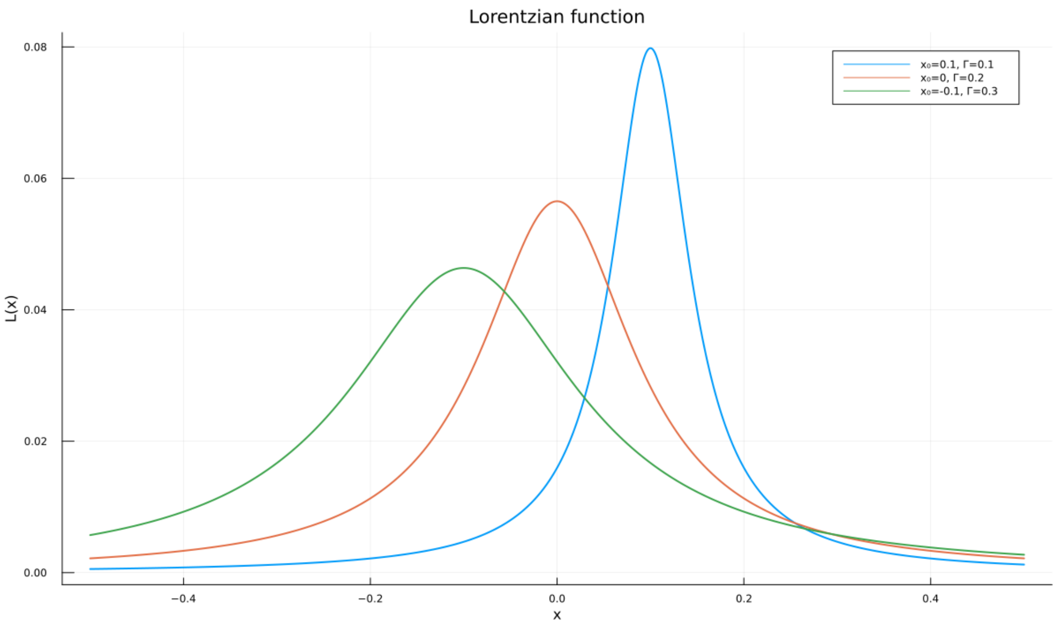

Figure 2.1.: Lorentzian function

Definition 2.5. (Lorentzian function) [Wei]: For $x \in \mathbb{R}$, the Lorentzian function is defined by

$$\begin{aligned}L &: \mathbb{R} \to \mathbb{R}\\L(x) &= \frac{1}{\pi}\frac{\frac{1}{2}\Gamma}{(x-x_0)^2+\left(\frac{1}{2}\Gamma\right)}\end{aligned} \tag{2.6}$$

where $x_0 \in \mathbb{R}$ is the centre and $\Gamma \in \mathbb{R}^+$ is a parameter specifying the width of the function. It is normalized such that $\int_{-\infty}^{\infty} L(x) = 1$. Figure 2.1 shows the Gaussian function.

The Fourier transform of the Lorentzian function is

$$\mathcal{F}\left[L\right](k) = \exp\left(-2\pi i k x_0 - \Gamma\pi\left|k\right|\right) \tag{2.7}$$

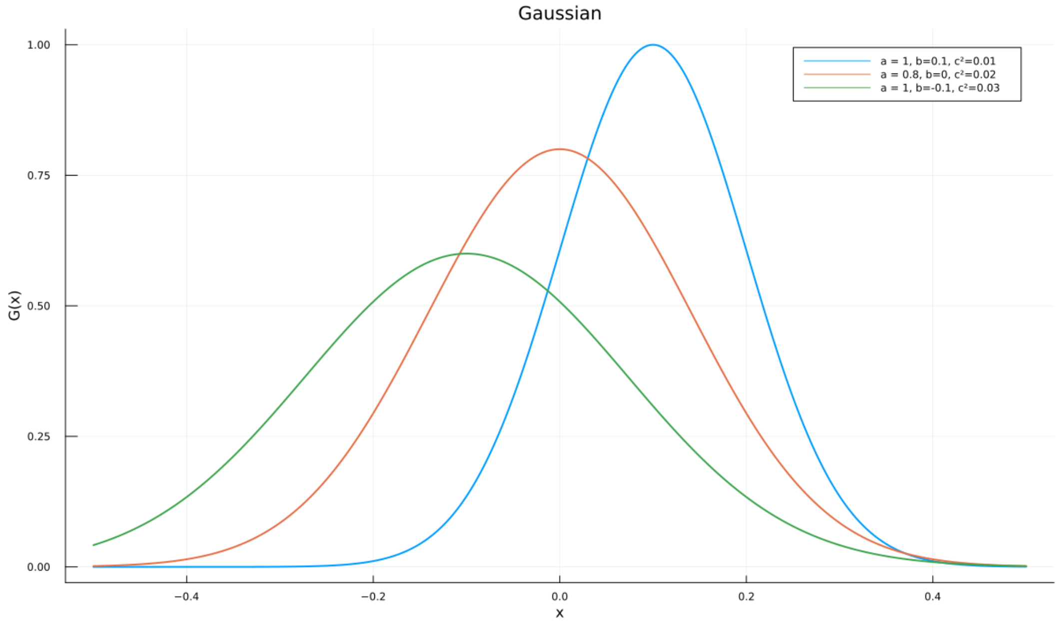

Figure 2.2.: Gaussian function

Definition 2.6. (Gaussian function) [Wik22]: For $x \in \mathbb{R}$, the Gaussian function is defined by

$$\begin{aligned} G &: \mathbb{R} \to \mathbb{R} \\ G(x) &= a \exp\left(-\frac{(x-b)^2}{2c^2}\right) \end{aligned} \tag{2.8}$$

where $a \in \mathbb{R}^+$ is the height of the peak, $b \in \mathbb{R}$ is the centre of the peak and $c \in \mathbb{R}^+$ specifies the width of the curve. Figure 2.2 shows the Gaussian function.

The Fourier transform of a simple Gaussian function $G_s(x) = a \exp\left(-\frac{x^2}{2c^2}\right)$ is

$$\mathcal{F}\left[G\right](k) = ac\sqrt{2\pi}\exp\left(-2\pi^2 k^2 c^2\right) \tag{2.9}$$

Definition 2.7. Schur (or Hadamard) product [Mil07]: Let $M_{m\times n}$ be the set of matrices of dimension $m \times n$. For $A, B \in M_{m\times n}$, the Schur product $A \circ B$ is defined to be:

$$\begin{aligned} \circ &: M_{m\times n} \to M_{m\times n} \\ (A \circ B)_{ij} &= (B \circ A)_{ij} = (A)_{ij}\,(B)_{ij} \end{aligned} \tag{2.10}$$

3. Nuclear Phase Retrival Spectroscopy

3.1. Experimental Set-up

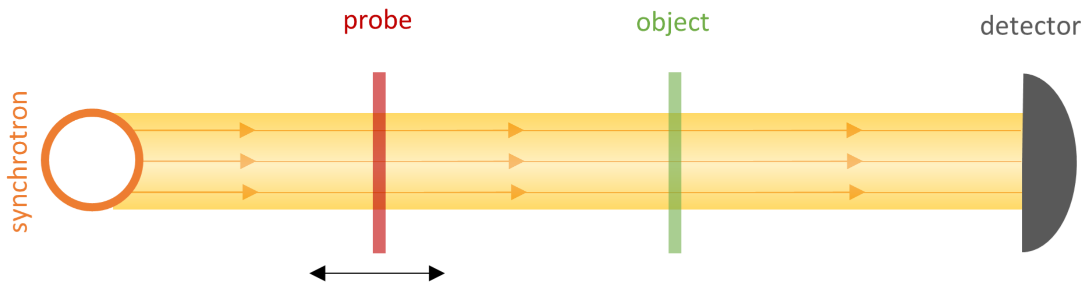

Figure 3.1.: Schematic of the Nuclear Phase Retrival Spectroscopy set-up

A schematic of the Nuclear Phase Retrieval Spectroscopy (NPRS) is shown in Figure 3.1. A synchrotron source emits synchrotron radiation (SR). SR has high spectral brightness and can be easily focus on to small objects (at the micrometre scale). [BG19]

This radiation is initially scattered by the probe (which may be of known properties) and then scattered by the target/ object. The scattered light's intensity is, then, measured by the detector.

The probe is shifted forwards and backwards to create multiple detected data. These data and the mathematical model are used to retrieval the complex energy response of the sample.

3.2. Mathematical Formulation

Let us define the following notations:

1. Energy range: Discretize the energy (frequency) range as $[-M\omega, M\omega]$ with a step-size of $\Delta\omega \in \mathbb{R}$ and $2M+1$ is the number of elements in the range. Each element is denoted by ω_j where $j \in [1, 2M+1] \subset \mathbb{Z}^+$.

2. Time range: Discretize the time (space) range as $[-N\Delta x, N\Delta x]$ with a step-size of $\Delta x \in \mathbb{R}$ whose value is given by Equation 2.5 and $2N+1$ is the number of elements in the range. Each element is denoted by ω_j where $j \in [1, 2N+1] \subset \mathbb{Z}^+$.

3. Response function of the object: $\mathcal{O}(\omega)$. Discretized, this is the vector

$$\boldsymbol{O} = (\mathcal{O}(-\omega_{max}), \mathcal{O}(-\omega_{max} - \Delta\omega), ..., \mathcal{O}(\omega), \mathcal{O}(\Delta\omega), ..., \mathcal{O}(\omega_{max})) \quad (3.1)$$

4. Response function of the probe: $\mathcal{P}_{\tilde{m}}(\omega + \tilde{m}\Delta\omega)$. Here, $\tilde{m} \in [-\tilde{m}_{max}, \tilde{m}_{max}] \subset \mathbb{Z}$ represents the shift in the probe to create multiple data intensities. Discretized, this is the vector

$$\boldsymbol{P}_{\tilde{m}} = (\mathcal{P}((\tilde{m} - M)\Delta\omega), ..., \mathcal{P}(\tilde{m}\Delta\omega), ..., \mathcal{P}((m + M)\Delta\omega)) \quad (3.2)$$

5. Measured intensities : $I_{\tilde{m}}(x)$ is a sequence of measurements.

$$\begin{aligned} &I : (\boldsymbol{O}, \boldsymbol{P}_{\tilde{m}}) \rightarrow \mathbb{R}^{2N+1} \\ &I_{\tilde{m}}(x) = |\mathbb{F}[\boldsymbol{O} \circ \boldsymbol{P}_{\tilde{m}}]|^2 \end{aligned} \quad (3.3)$$

3.3. Ptychographic Iterative Engines

Ptychographic iterative engines (PIEs) are algorithms that use an initial object guess, the measured intensities and an iterative update function to calculate the unknown object's phase and modulus.

3.3.1. Rodenburg-Faulkner PIE

One of the PIEs that shall be explored in this thesis was described by Rodenburg and Faulkner, in 2004.[RF04] It is described by the following algorithm:

1. Create an initial object function (which is guessed): $O_{g,n}(\omega)$ where g represents that it is guessed and n represents the iteration number.

2. Take the probe at a shift $\tilde{m}(P(\omega + \tilde{m}\Delta\omega))$and multiple it with the guessed object to create:

$$\psi_{g,n}(\omega, \tilde{m}) = O_{g,n}(\omega) \circ P(\omega + \tilde{m}\Delta\omega) \quad (3.4)$$

3. Fourier transform the above function $\psi_{g,n}$ to find the function in the time domain: $\Psi_{g,n}(x, \tilde{m})$. This can also be rewritten in terms of its amplitude ($|\Psi_{g,n}(x, \tilde{m})|$) and phase ($\theta_{g,n}(x, \tilde{m})$).

$$\Psi_{g,n}(x, \tilde{m}) = \mathcal{F}[\psi_{g,n}(\omega, \tilde{m})] = |\Psi_{g,n}(x, \tilde{m})| \exp(i\theta_{g,n}(x, \tilde{m})) \quad (3.5)$$

4. Replace the modulus of the above function with the corresponding known value (from the intensity measurements, $I_{\tilde{m}}(x) = |\Psi_{k,n}(x,\tilde{m})|^2$).

$$\Psi_{k,n}(x,\tilde{m}) = |\Psi_{k,n}(x,\tilde{m})| \exp\left(i\theta_{g,n}(x,\tilde{m})\right) \tag{3.6}$$

5. Inverse fourier transfrom the above back to the energy space to create a new guessed version.

$$\psi_{k,n}(\omega,\tilde{m}) = \mathcal{F}^{-1}\left[\Psi_{k,n}(x,\tilde{m})\right] \tag{3.7}$$

6. Using an update function, calculate the new guessed object function, where α and β are chosen parameters.

$$\begin{aligned} O_{g,n+1}(\omega) = O_{g,n}(\omega) + \frac{|P(\omega+\tilde{m}\Delta\omega)|}{|P_{max}(\omega+\tilde{m}\Delta\omega)|}\frac{P^{*}(\omega+\tilde{m}\Delta\omega)}{(|P(\omega+\tilde{m}\Delta\omega)|^2+\alpha)} \\ \times \beta\left(\psi_{k,n}(\omega,\tilde{m}) - \psi_{g,n}(\omega,\tilde{m})\right) \end{aligned} \tag{3.8}$$

7. Measure the sum squared error (SSE) and check if it adequately small (i.e., if it is smaller than a certain ϵ).

$$\mathrm{SSE} = \frac{\left(|\Psi_{k,n}(x,\tilde{m})|^2 - |\Psi_{g,n}(x,\tilde{m})|^2\right)^2}{2N+1} \tag{3.9}$$

8. If the SSE is not small enough, repeat the steps 2 to 7 until it is.

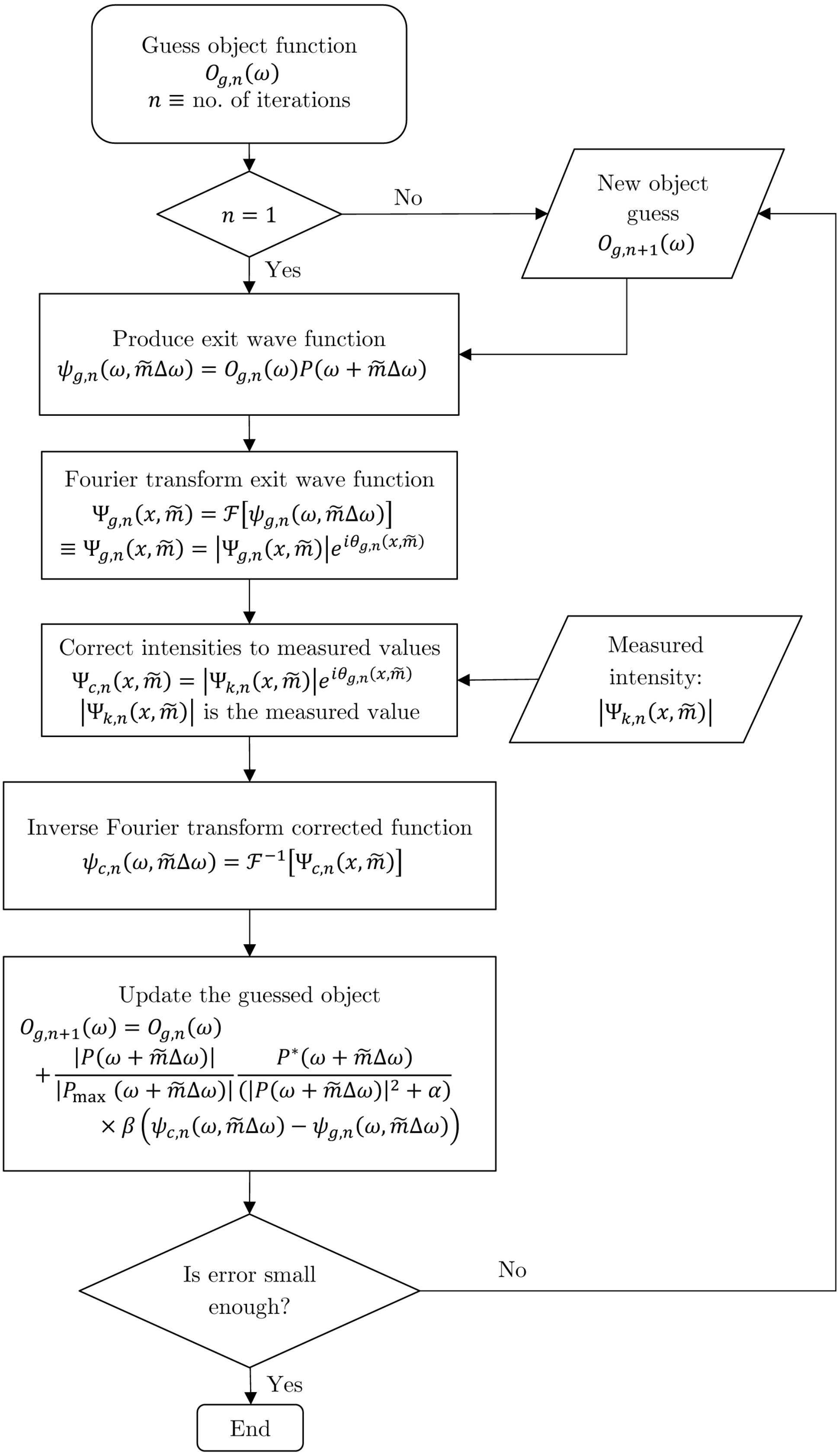

Figure 3.2.: Rodenburg-Faulkner Ptychographic Iterative Engine

A. Appendix

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