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OPTIMIZATION OF ZONAL WAVEFRONT ESTIMATION
AND
CURVATURE MEASUREMENTS

by

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A dissertation submitted in partial fulfillment of the requirements
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Major Professor: Jannick P. Rolland
ABSTRACT

Optical testing in adverse environments, ophthalmology and applications where characterization by curvature is leveraged all have a common goal: accurately estimate wavefront shape. This dissertation investigates wavefront sensing techniques as applied to optical testing based on gradient and curvature measurements. Wavefront sensing involves the ability to accurately estimate shape over any aperture geometry, which requires establishing a sampling grid and estimation scheme, quantifying estimation errors caused by measurement noise propagation, and designing an instrument with sufficient accuracy and sensitivity for the application.

Starting with gradient-based wavefront sensing, a zonal least-squares wavefront estimation algorithm for any irregular pupil shape and size is presented, for which the normal matrix equation sets share a pre-defined matrix. A Gerchberg–Saxton iterative method is employed to reduce the deviation errors in the estimated wavefront caused by the pre-defined matrix across discontinuous boundary. The results show that the RMS deviation error of the estimated wavefront from the original wavefront can be less than $\lambda/130 \approx \lambda/150$ (for $\lambda$ equals 632.8nm) after about twelve iterations and less than $\lambda/100$ after as few as four iterations. The presented approach to handling irregular pupil shapes applies equally well to wavefront estimation from curvature data.

A defining characteristic for a wavefront estimation algorithm is its error propagation behavior. The error propagation coefficient can be formulated as a function of the eigenvalues of the wavefront estimation-related matrices, and such functions are established for each of the basic estimation geometries (i.e. Fried, Hudgin and Southwell) with a serial numbering scheme,
where a square sampling grid array is sequentially indexed row by row. The results show that with the wavefront piston-value fixed, the odd-number grid sizes yield lower error propagation than the even-number grid sizes for all geometries. The Fried geometry either allows sub-sized wavefront estimations within the testing domain or yields a two-rank deficient estimation matrix over the full aperture; but the latter usually suffers from high error propagation and the waffle mode problem. Hudgin geometry offers an error propagator between those of the Southwell and the Fried geometries. For both wavefront gradient-based and wavefront difference-based estimations, the Southwell geometry is shown to offer the lowest error propagation with the minimum-norm least-squares solution. Noll’s theoretical result, which was extensively used as a reference in the previous literature for error propagation estimate, corresponds to the Southwell geometry with an odd-number grid size.

For curvature-based wavefront sensing, a concept for a differential Shack-Hartmann (DSH) curvature sensor is proposed. This curvature sensor is derived from the basic Shack-Hartmann sensor with the collimated beam split into three output channels, along each of which a lenslet array is located. Three Hartmann grid arrays are generated by three lenslet arrays. Two of the lenslets shear in two perpendicular directions relative to the third one. By quantitatively comparing the Shack-Hartmann grid coordinates of the three channels, the differentials of the wavefront slope at each Shack-Hartmann grid point can be obtained, so the Laplacian curvatures and twist terms will be available. The acquisition of the twist terms using a Hartmann-based sensor allows us to uniquely determine the principal curvatures and directions more accurately than prior methods. Measurement of local curvatures as opposed to slopes is unique because curvature is intrinsic to the wavefront under test, and it is an absolute as opposed to a relative measurement. A zonal least-squares-based wavefront estimation algorithm was developed to
estimate the wavefront shape from the Laplacian curvature data, and validated. An implementation of the DSH curvature sensor is proposed and an experimental system for this implementation was initiated.

The DSH curvature sensor shares the important features of both the Shack-Hartmann slope sensor and Roddier’s curvature sensor. It is a two-dimensional parallel curvature sensor. Because it is a curvature sensor, it provides absolute measurements which are thus insensitive to vibrations, tip/tilts, and whole body movements. Because it is a two-dimensional sensor, it does not suffer from other sources of errors, such as scanning noise. Combined with sufficient sampling and a zonal wavefront estimation algorithm, both low and mid frequencies of the wavefront may be recovered. Notice that the DSH curvature sensor operates at the pupil of the system under test, therefore the difficulty associated with operation close to the caustic zone is avoided. Finally, the DSH-curvature-sensor-based wavefront estimation does not suffer from the $2\pi$-ambiguity problem, so potentially both small and large aberrations may be measured.
To my parents, who have been patiently supporting me for my studying since my young age!

To my grandparents, who love me so much as always!

To my sisters, who love me and encourage me all the time!
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TABLE OF CONTENTS

LIST OF FIGURES ......................................................................................................................... i

LIST OF TABLES ........................................................................................................................... i

LIST OF ACRONYMS/ABBREVIATIONS .................................................................................. i

CHAPTER ONE: INTRODUCTION ............................................................................................. 3

1.1 Historical review of optical testing ....................................................................................... 3

1.1.1 Hartmann test ................................................................................................................. 4

1.1.2 Shack-Hartmann sensor and Pyramid wavefront sensor ............................................... 6

1.1.3 Interferometric tests ..................................................................................................... 10

1.2 Recovery of the mid-spatial frequency: Modal or Zonal? .................................................. 12

1.3 Vibrational effects ............................................................................................................... 15

1.4 Motivation ........................................................................................................................... 16

1.5 Dissertation outline ............................................................................................................. 17

CHAPTER TWO: REVIEW OF CURVATURE SENSING ..................................................... 20

2.1 Roddier’s wavefront curvature sensor ................................................................................20

2.1.1 Methodology evolution .............................................................................................. 22

2.1.2 Implementations .......................................................................................................... 25

2.1.3 Advantages and disadvantages .................................................................................... 26

2.2 Special wavefront curvature sensors ................................................................................. 27

2.2.1 CGS wavefront curvature sensor ................................................................................. 28

2.2.2 Hybrid wavefront curvature sensor ............................................................................. 31

2.2.3 Curvature profiling technique ...................................................................................... 32
2.3 Summary ............................................................................................................................. 35

CHAPTER THREE: REVIEW OF WAVEFRONT ESTIMATION TECHNIQUES .................. 36

3.1 Neumann boundary problem in wavefront estimation .................................................. 36

3.2 Slope-based wavefront estimations .............................................................................. 39

3.2.1 Zonal slope-based wavefront estimation ................................................................. 40

3.2.1.1 Least-squares fitting method ................................................................................. 42

3.2.1.2 Fourier transform method ..................................................................................... 44

3.2.2 Modal slope-based wavefront estimation ................................................................. 46

3.2.2.3 Least-squares based modal estimation .................................................................. 48

3.2.2.4 Fourier transform-based modal estimation ........................................................... 51

3.2.3 Radon transform-based modal estimation ................................................................. 53

3.3 Curvature-based wavefront estimations ....................................................................... 54

3.3.1 Zonal curvature-based wavefront estimation ............................................................ 55

3.3.1.1 Least-squares-based zonal estimation ................................................................. 56

3.3.1.2 Fourier transform-based zonal estimation ............................................................ 56

3.3.2 Modal curvature-based wavefront estimation ......................................................... 58

3.4 Phase retrieval techniques ............................................................................................. 61

3.4.1 Gerchberg-Saxton and Misell methods .................................................................... 63

3.4.1.1 Gerchberg-Saxton method .................................................................................. 63

3.4.1.2 Misell algorithm .................................................................................................. 65

3.4.2 Phase diversity technique ......................................................................................... 67

3.5 Comparisons and Summary .......................................................................................... 69

3.5.1 Phase diversity technique and the S-H sensor ........................................................ 69
3.5.2 Phase diversity technique and Roddier’s curvature sensor ........................................ 70
3.5.3 Summary .................................................................................................................... 71

CHAPTER FOUR: ITERATIVE SLOPE-BASED WAVEFRONT ESTIMATION FOR ANY
SHAPED PUPILS .................................................................................................................... 72

4.1 Proposed wavefront estimation algorithm for any size and pupil shape ..................... 73
  4.1.1 Pre-defined matrix equation for wavefront estimation ............................................. 73
  4.1.2 Wavefront slope computations .............................................................................. 78
    4.1.2.1 Wavefront y-slope computation ................................................................. 78
    4.1.2.2 Wavefront z-slope computation ................................................................. 80
  4.1.3 Least-squares -based Gerchberg-Saxton iterative algorithm .................................. 82

4.2 Examples and Results ............................................................................................... 85
  4.2.1 Case 1: Circular pupil without central obscuration ................................................ 86
  4.2.2 Case 2: Circular pupil with a 10% central obscuration .......................................... 87
  4.2.3 Algorithm convergence ....................................................................................... 89

4.3 Computational complexity ....................................................................................... 90
  4.3.1 Computational complexity of the proposed iterative algorithm ............................ 90
    4.3.1.1 Spatial complexity ..................................................................................... 91
    4.3.1.2 Time complexity (Impact on computation time) ......................................... 91
  4.3.2 Complexity comparison with the FFT-based iterative algorithms ......................... 93
    4.3.2.1 Comparison of time complexity ................................................................. 93
    4.3.2.2 Comparison of spatial complexity ............................................................. 94

4.4 Error propagation estimation .................................................................................... 95

4.5 Summary .................................................................................................................... 99
LIST OF FIGURES

Figure 1.1 Hartmann test (Adopted from D. Malacara) ................................................................. 5

Figure 1.2 (a) The concept of the S-H sensor and (b) a sampling grid ....................................... 7

Figure 1.3 The spot centroiding in a quad cell in a CCD target ................................................... 8

Figure 1.4 Quad cell in S-H WFS versus quadrant in pyramid WFS (Adopted from Bauman) .... 9

Figure 2.1 The illustration of Roddier’s curvature sensing (from Malacara) ......................... 21

Figure 2.2 Schematic for a reflection CGS curvature sensor (Adopted from Kolawa) ............ 29

Figure 2.3 The principle of a CSG curvature sensor (from Kolawa, et al) ............................... 30

Figure 2.4 The foci in the hybrid wavefront curvature sensor ................................................. 32

Figure 2.5 The differential measurement of slope (Adopted from Glenn) ............................... 33

Figure 2.6 Schematic layout of the curvature profiling instrument (Adopted from Glenn) ...... 34

Figure 3.1 The testing aperture for wavefront estimation .......................................................... 37

Figure 3.2 Sampling geometries for wavefront estimation ..................................................... 39

Figure 3.3 Five-point stencil ....................................................................................................... 40

Figure 3.4 The flow chart of Gerchberg’s fringe extrapolation algorithm. (from Roddier & Roddier 1987) ................................................................. 45

Figure 3.5 An example of interferogram extrapolation (from Roddier & Roddier 1987) (a) Interferogram before fringe extrapolation (b) Interferogram after fringe extrapolation .... 45

Figure 3.6 Flow Chart for the iterative FT-based wavefront estimation from slope data (from Roddier & Roddier 1991) ................................................................. 46

Figure 3.7 Flow Chart of iterative FT-based wavefront estimation from curvature data (from Roddier & Roddier) ................................................................. 57
Figure 3.8  Gerchberg-Saxton algorithm (Adopted from Chanan)................................. 64
Figure 3.9  Misell algorithm ............................................................................................... 66
Figure 3.10  Optical layout of a phase diversity system (from Paxman et al)....................... 67
Figure 4.1  The double sampling grid systems illustrated in the y-direction.......................... 74
Figure 4.2  The domain extension for an irregular-shaped pupil.......................................... 75
Figure 4.3  Non-iterative wavefront estimation with pre-defined matrix.............................. 77
Figure 4.4  Flow chart of the least-squares-based Gerchberg-Saxton-type iterative wavefront
estimation algorithm ........................................................................................................ 84
Figure 4.5 (a) A 30-mm diameter circular pupil within the extended domain \( \Omega_f \). (b) The ground-
truth wavefront within the circular pupil \( \Omega_o \) on a vertical scale of \( \pm 1 \mu \text{m} \)................. 86
Figure 4.6 Wavefront deviation error (on scale of \( \pm 1 \mu \text{m} \)) for a 30 mm-diameter circular pupil
with iterations \( i=0, 1, 2, 3, 4, \) and 13, respectively (\( \lambda=632.8 \text{nm} \)).................................. 87
Figure 4.7 (a). A 30-mm diameter circular pupil with a 10% central obscuration. (b). A ground-
truth wavefront at this pupil \( \Omega_o \) on a vertical scale of \( \pm 1 \mu \text{m} \) (right). ......................... 88
Figure 4.8 Wavefront deviation error (on scale of \( \pm 1 \mu \text{m} \)) for a 30 mm-diameter circular pupil
with a 10% central obscuration through iterations \( i=0, 1, 2, 3, 4, 10, \) respectively
(\( \lambda=632.8 \text{nm} \)).................................................................................................................. 88
Figure 4.9  Plot of RMS deviation errors as a function of the number of iterations............... 89
Figure 4.10 The condition number of normal estimation matrix versus grid dimension size..... 98
Figure 5.1 Previous results on error propagation.................................................................. 104
Figure 5.2 Grid array with serial numbering scheme .......................................................... 108
Figure 5.3 WFD-based error propagators for the Hudgin geometry ................................... 112
Figure 5.4 WFD-based error propagators for the Southwell geometry ........................................ 115
Figure 5.5 WFD-based error propagators for the Fried geometry ............................................... 118
Figure 5.6 Comparison of the WDF-based error propagators .................................................... 120
Figure 5.7 Comparison of the slope-based error propagators ..................................................... 124
Figure 6.1: The x- and y-differential shears of the Hartmann grid ............................................. 129
Figure 6.2: An implementation of the DSH curvature sensor without calibration path ............... 131
Figure 6.3 Optical layout of the experimental system for the DSH curvature sensor ................... 134
Figure 6.4 Picture of the experimental system for the DSH curvature sensor ............................ 135
Figure 6.5 GUI of the DSH sensor experimental setup .............................................................. 136
Figure 6.6 A 52-point S-H Grid ................................................................................................. 138
Figure 6.7 The edge points ........................................................................................................ 139
Figure 6.8 The corner points ..................................................................................................... 140
Figure 7.1 Wavefront estimation with an 8x8 grid array ........................................................... 149
Figure 7.2 Wavefront estimation with 30x30 grid array .......................................................... 151
Figure 7.3 Wavefront deviation errors and the defocus values ................................................ 152
Figure 7.4 Wavefront discretization error versus discretization grid size ............................... 153
LIST OF TABLES

Table 3.1  The Zernike polynomials and their 1\textsuperscript{st} to 2\textsuperscript{nd} derivatives................................. 58

Table 5. 1 Qualitative comparisons of the WFD-based error propagators ................................. 121
LIST OF ACRONYMS/ABBREVIATIONS

CGS  Coherent Gradient Sensor
CCD  Coupled Charge Devices
CRLB  Crame´r–Rao Lower Bound
DFT  Discrete Fourier Transform
DIMM  Differential Image Motion Monitor
DSH  Differential Shack-Hartmann
ESO  European Southern Observatory
FFT  Fast Fourier Transform
FLOPS  Floating-Point Operations
GUI  Graphic User Interface
ITE  Irradiance Transport Equation
LACS  Large Area Curvature Scanning
LSMN  Least-Squares solution with Minimum Norm
NTT  New Technology Telescope
OPD  Optical Path Difference
OTF  Optical Transfer Function
1-D  One-Dimensional
PDE  Partial Differential Equation
PSD  Power Spectral Density
PSF  Point Spread Function
PSI  Phase Shifting Interferometry
P-V
Peak to Valley

PWFS
Pyramid Wavefront Sensor

S-H
Shack-Hartmann

SOR
Successive Over-Relaxation

SNS
Serial Numbering Scheme

SVD
Singular Value Decomposition

2-D
Two-Dimensional

WFD
Wavefront Difference

WFS
Wavefront Sensor

“^”
Denote a value of an estimate

“*”
Denote the operation of convolution
CHAPTER ONE: INTRODUCTION

In the introductory part of this dissertation, a brief history of optical testing techniques will be reviewed with an emphasis on quantitative wavefront testing. The research motivation will then be given, and the outline of the dissertation will be summarized.

1.1 Historical review of optical testing

In modern optics, optical testing refers to the optical measurement of surface errors or optical system aberrations. The testing accuracy sets the limit of the working accuracy. An optical element or surface, especially an aspheric surface, can only be made as good as it can be tested. In most cases the goal is to determine the optical path differences (OPD) of the wavefront that either passed through the optical system under test or reflected from the optical surface under test. The shape of the optical surfaces under test can be either flat, spherical, conic, and aspheric or free form, among which aspheric and free form surface tests are typically more complex. Wavefront measurement is becoming more and more demanding today, because it is not only a key technique in measuring optical surfaces and optical systems, but also one of the main parts in active/adaptive optics, ophthalmology, and laser wavefront and media turbulence characterizations.

The history of optical testing can be dated back to at least the 17th century when Galileo Galilei (1564-1642, Italy) tried to make telescopes for viewing celestial bodies. The optical testing problem that he faced at that time remains the challenge for the telescope makers today. One of the oldest optical testing method is the Knife-edge test, which was invented by Foucault
(1852, France).\(^1,2,3\) It is a Schlieren method that tests the wavefront aberrations by examining the shadow or intensity distribution in the Schlieren field. The advantages of the Knife-edge test are its high sensitivity and simplicity both in apparatus and in qualitative interpretation (Ojeda-Castaneda 1992).\(^4\) It was the primary technique for testing mirror surface errors before the invention of the quantitative methods, and it is still an important test in amateur optical workshop today. The Schlieren tests also include the Caustic test (Platzeck & Gaviola 1939),\(^5,6,7\) and the Ronchi test (Ronchi 1923)\(^1\).

Instead of the qualitative Schlieren tests, the Hartmann test is an important quantitative method (Hartmann 1900).\(^1\) In the reminder part of this chapter, we will first review the Hartmann test followed by the Shack-Hartmann wavefront sensor and pyramidal wavefront sensor. Then we will briefly review interferometric tests with a focus on shearing interferometry and phase shifting interferometry.

### 1.1.1 Hartmann test

As shown in Figure 1.1,\(^1\) a Hartmann screen is a screen with many holes, which is put at the pupil or a location that conjugates to the pupil of an optical system under test or over the major surface under test. The light passing through the screen holes will generate an array of dots on the image plane, whose position distribution is affected by the system aberrations. The Hartmann test measures transverse aberrations and it is not sensitive to the piston error. The relationship between wavefront aberrations \(W(x, y)\) and the ray aberrations \((\delta_x, \delta_y)\) at the image plane can be expressed as\(^8\)

\[
\delta_x = \frac{\partial W(x, y)}{\partial x} L \quad (1.1a)
\]
\[ \delta_y = \frac{\partial W(x, y)}{\partial y} L \]  

where \( L \) is the distance from the exit pupil to the image plane. A wavefront integration algorithm is needed to integrate these measurements in the \( x \)- and \( y \)-directions. The distribution patterns of the holes on the Hartmann screen comes in many varieties, such as the classical radial pattern, a helical pattern and a square-array pattern. Due to its uniformity in data sampling and convenience in wavefront estimation, the Hartmann screen with a square-array pattern is the most common. With the advent of CCD camera, which is essentially an array of quadrant detectors, the traditional Hartmann test is improved and becoming an increasingly popular quantitative method for optical testing.

Because the holes on the Hartmann screen are small, the focused Hartmann spots are affected by diffraction. Historically, it has been time-consuming to measure the focused spot centroid. However, the natural rectangular grid of the CCD camera can be matched to the screen-hole pattern to yield rapid data acquisition.
1.1.2 Shack-Hartmann sensor and Pyramid wavefront sensor

Roland Shack and Ben Platt expanded the concept of the Hartmann test by re-imaging the aperture onto a lenslet array located at the exit pupil (Shack and Platt 1971), yielding a popular wavefront sensor known as the Shack-Hartmann (S-H) sensor. The concept of the S-H sensor and a Hartmann grid array are illustrated in Figure 1.2. Comparing with the classical Hartmann test, a lenslet array replaces the traditional Hartmann screen to concentrate the light energy inside each hole to form an array of focused Hartmann grid points, which dramatically improves the spot position measurement accuracy. Shifts in the positions of the grid points can be shown to be proportional to the mean wavefront gradient over each sub-pupil. With a CCD detector in the image plane as the photon detector to replace the traditional photographic plate, the Hartmann spot centroiding accuracy and the speed of the data sampling are dramatically increased.

Shack and Platt proposed the S-H sensor while working on a classified laser project for the U.S. Air Force in an attempt to improve satellite images blurred by atmospheric turbulence. Equipped with a modern computer to process the sampled data and with a wavefront estimator, the S-H sensor has become a real-time wavefront sensor for optical shop testing, active/adaptive optics, and ophthalmic diagnoses.

Compared with the Hartmann test, the S-H wavefront sensor has the following merits: (1) It offers better photon efficiency; (2) The position of a S-H grid point is only proportional to the average wavefront slope over each sub-aperture, and it is thus independent of higher-order aberrations and intensity profile variations; (3) The Shack-Hartman sensor is a real-time, parallel wavefront sensor; (4) Its working wavelength range varies from infrared band to ultraviolet band.
Figure 1.2  (a) The concept of the S-H sensor and (b) a sampling grid

Usually a reference wavefront is needed for the S-H sensor to calibrate the wavefront measurement, as illustrated in Figure 1.2(a). Quantitatively comparing the coordinates of each S-H grid point from the measurement beam with that from the reference beam yields wavefront slopes in x- and y- directions as
\[ \frac{\partial W}{\partial x} = \frac{x_{\text{mea}} - x_{\text{ref}}}{f}, \quad \frac{\partial W}{\partial y} = \frac{y_{\text{mea}} - y_{\text{ref}}}{f}, \]  

\[ (1.2) \]

where \((x_{\text{ref}}^i, y_{\text{ref}}^i)\) \((i = 1, 2, \ldots, m, m \times t\) is the total number of grid points) is the Hartmann grid coordinates of the reference beam, \((x_{\text{mea}}^i, y_{\text{mea}}^i)\) is the Hartmann grid coordinates of the measurement beam, and \(f\) is the focal length of the lenslet array.

![The spot centroiding in a quad cell in a CCD target](image)

**Figure 1.3** The spot centroiding in a quad cell in a CCD target

The centroiding of the S-H spot on the CCD camera can be simulated with a model of quad-cell, as shown in Figure 1.3. Given a Hartmann spot with diameter \(d\), its centroid coordinate in a quad cell can be computed by

\[
\begin{aligned}
\begin{cases}
  x = \left( \frac{d}{2} \right) \frac{I_1 - I_2 - I_3 + I_4}{I_1 + I_2 + I_3 + I_4} \\
  y = \left( \frac{d}{2} \right) \frac{I_1 + I_2 - I_3 - I_4}{I_1 + I_2 + I_3 + I_4}
\end{cases}
\end{aligned}
\]

\[ (1.3) \]

where \(I_i (i = 1, 2, 3, 4)\) is the intensity of each quarter area of the quad cell as shown in Figure 1.3.
A recent variation of the S-H sensor is the pyramid wavefront sensor (PWFS), which was invented by R. Ragazzoni (Ragazzoni 1996). A four-faceted pyramidal prism is used in the nominal focal plane of the optical system to divide the focal image into four quadrants, which is analogous to using a quad cell to divide a S-H spot in the CCD camera, except for the order reverse of the optical element layouts between the two sensors (Bauman 2003). As shown in Figure 1.4, the circle indicates the beam footprint on the wavefront sensor. For a S-H sensor each sub-aperture on the CCD camera is a quad cell, while in a pyramid wavefront sensor each pixel in each of the four pupils represents a quadrant of the quad cell. The pyramid wavefront sensor uses a circular scan of the image to increase the measurement dynamic range, while in a S-H sensor an increase of dynamic range can be achieved by employing a sub-aperture that is larger than a quad cell to measure each S-H spot centroid. It was shown that the pyramid sensor has a higher sensitivity with respect to a S-H sensor for the scenario of small wavefront...
aberrations (Ragazzoni & Farinato 1999). However, fabricating the pyramidal prism for the pyramid wavefront sensor has proven to be difficult.

1.1.3 Interferometric tests

Modern interferometry can be dated from the Michelson interferometer, which was invented by Albert Abraham Michelson (1887). The classical interferometric tests in many cases provide direct measurement of the optical path difference (OPD). Interferometry needs at least two coherent wavefronts to interfere each other to generate an interferogram that records the wavefront deformations. The two wavefronts could be either the reference wavefront and the wavefront under test, or the wavefront under test and its duplicated wavefront with an offset (shear).

For the first kind of interferometric tests, the reference wavefront is usually a perfectly spherical or flat wavefront. The difference between the wavefront from the surface/system under test and the reference wavefront is the wavefront OPD, which is a direct measure of the wavefront error of the optical system under test. A perfect reference wavefront is quite important for the first kind of interferometric tests, and the generation of a perfect reference wavefront is difficult.

Shearing interferometry provides an alternate solution to this problem by using a copy of the wavefront under test to replace the reference wavefront. The relative dimensions or orientation of the reference wavefront must be changed (sheared) in some way with respect to the wavefront under test. As such, an interferogram can be obtained from the interference of the two sheared wavefronts. The most popular one is the lateral shearing interferometer, in which
the duplicated wavefront is laterally displaced with respect to the original one. This relation suggests that the parameters being directly measured are wavefront differences (WFD) in the shearing directions of the wavefront, from which we can infer everything of the wavefront except the piston term.\textsuperscript{19, 20, 21} The disadvantage of shearing interferometry is that it requires phase unwrapping and integration, and it requires separate x and y channels with a narrow wavelength band.

Phase shifting interferometry (PSI), also known as phase measuring interferometry, fringe scanning interferometry, real-time interferometry, AC interferometry and heterodyne interferometry, is not a specific optical interferometry configuration, but rather a data collection and analysis method that can be applied in a variety of interferometric testing scenarios (Greivenkamp and Bruning, 1992).\textsuperscript{22} It was initiated by Carre in 1966 and later developed for optical testing in the early 1970s (Crane 1969, Bruning et al 1974, and Wyant 1975),\textsuperscript{22, 23, 24, 25} PSI estimates the wavefront phase at each point of a sampling grid array from the intensities measured from a series of interferograms with introduced reference phase shifts, such as 90\textdegree-optical phase changes of 0, π/2, π, 3π/2 for the four-step-algorithm. The problem of finding the fringe centers and reading the order of the fringes as done in the traditional interferometric testing is avoided; as a result the PSI precision is much better than the precision of a static fringe analysis.\textsuperscript{1} Here the accuracy is independent of the fringe pattern and the fringe frequency in the interferogram.\textsuperscript{22} Usually phase shifting is achieved in steps or in a continuous manner by moving the reference mirror along the axis of wavefront propagation. As proved by Kafri, if everything else is perfect, a short coherence length and a long sampling time will improve the accuracy (Kafri 1989).\textsuperscript{26} However, both a short coherence length and a long sampling time make
the interferometer more sensitive to mechanical vibrations and external changes. Therefore PSI
is not useful for testing systems in the presence of vibrations or turbulence.

It is to be noticed that the difficulty associated with the standard interferometric
measurements as well as the slope-based wavefront measurements, such as the S-H test, is their
sensitivity to rigid body rotations and displacements of the surface under test, and thus such
techniques are well-known to be vibration sensitive.

1.2 Recovery of the mid-spatial frequency: Modal or Zonal?

The shape of the wavefront error can be thought to be a combined contribution from the
errors of the following groups of spatial frequencies: the low spatial frequencies, which
contribute to the figure of wavefront; the mid-spatial frequencies, which contribute to the
“waviness” of wavefront; and the high spatial frequencies, which contribute to the roughness of
wavefront.27,28 The low spatial frequencies characterize wavefront errors of less than 6 cycles
per aperture, the mid-spatial frequencies characterize wavefront errors of more than 6 cycles but
less than 20 cycles per aperture and the high-spatial frequencies characterize wavefront errors of
more than 20 cycles per aperture. Among them, the recovery of the wavefront mid-spatial
frequency errors is more interesting because it can help bringing the accuracy of wavefront
estimation to the next stage of the art, given that the low-spatial-frequency-based wavefront
estimations have been investigated extensively.

Wavefront errors can be quantitatively characterized by the power spectral density (PSD)
function of the wavefront, which is defined as the ensemble average of the squared modulus of
the wavefront function in the spatial domain.29 The PSD function quantifies the spectral power
of each spatial frequency in the pupil, which is actually a weight function for different spatial frequency errors. As we will detail in Chapter 3, the wavefront values can be either evaluated at each local point by zonal estimation or estimated as a set of orthogonal polynomials over the whole test pupil by modal estimation. If a wavefront function is modal estimated with Zernike polynomials, its PSD function can be computed by the following formula (Levine et al 1998)\(^{30}\)

\[
PSD(f) = \sum_{n} |a_n(f)|^2
\]  

(1.4)

Where \(f\) is the spatial frequency in the Fourier domain, and \(a_n(f)\) is the Fourier transform of a Zernike polynomial coefficient.

In this dissertation, a characteristic frequency is defined as the average of the peak PSD frequency values of a number of aberration realizations represented in the Zernike basis for a given Zernike order, where the Zernike coefficients are generated by a Gaussian distribution for each case.\(^{31}\) The characteristic frequency for a Zernike-based function of a given order is a target aberration spatial-frequency (i.e. the dominant spatial frequency) that one may match to a given Zernike order in unit of cycles per aperture.\(^{31}\) A numerical simulation suggests that the characteristic frequency can be expressed as a linear function of the Zernike order as (Dean & Bowers)\(^{31}\)

\[
f_{\text{char}} = 0.1787Z_{\text{order}} + 1.64.
\]  

(1.5)

For a given Zernike order \(N\), the total number of terms of the Zernike polynomials is given by \((N+1)(N+2)/2\). For the mid-spatial-frequency wavefront errors of 6-20 cycles per aperture, the Zernike order needed for representing such wavefront errors is 25 to 103 according to Eq.(1.5), which corresponds to 351 to 5460 terms of the Zernike polynomials! Therefore, the recovery of
the mid to high spatial frequencies with a modal approach becomes impractical given that such a
modal estimation requires solving for thousands of aberration basis coefficients.

Typically modal methods are good for the recovery of low spatial frequencies. One of the
advantages of the modal estimations is that the wavefront can be conveniently expressed as a set
of orthogonal polynomials, such as the Zernike polynomials, which individual term represents a
specific optical aberration. As a disadvantage, the orthogonality requirement of the Zernike
polynomials over the sampling geometry is a problem. Strictly speaking, the Zernike
polynomials are not orthogonal over a discrete set of sampling points inside a circular pupil, or a
pupil with central obscuration. Nevertheless, the tolerance on the pupil obscuration can be taken
up to thirty percent for example, without much effect on the Zernike coefficients. However, the
orthogonality of the Zernike polynomials can be seriously affected by the radial non-symmetry
of the pupil.

A higher-order modal decomposition can be thought to provide a better approximation to
the wavefront estimation, but this improvement is limited due to the fact that high frequencies or
‘‘spiky’’ phase data cannot be accurately represented by a Zernike basis (or any other basis) for a
fixed number of data values across the pupil. Dean & Bowers showed that for modal fitting of a
deformable mirror with Zernike polynomials, the Zernike order needs to go up to 50 (i.e.1326
terms!) for the RMS fit error to reaches \( \lambda /100 \) with a mid-spatial frequency wavefront error of 10
cycles/ aperture. \(^{31}\)

The alternate to modal estimation is zonal estimation, which is advantageous to move
wavefront estimation to the next level of accuracy. With zonal estimation, more sampling points
are also required for the retrieval of the mid-spatial frequencies. However, the slope/curvature
data sampling can be made as dense as needed without much computational burden for zonal
wavefront estimation, because the zonal method estimates the wavefront locally instead of globally across the pupil in a modal method. For the zonal methods, the finite difference method can be adopted for numerically solving a Poisson equation. With the finite difference method, a wavefront value is a direct weighted average of its neighboring wavefront values corrected by the increments gained from the neighboring slope measurements as we will detail in Chapter 3. With curvature measurements, we will show in Chapter 6 that the zonal wavefront estimation becomes very simple and elegant. Besides, there is no orthogonality requirement for zonal wavefront estimation, thus any irregular pupil shapes may be considered as long as the boundary conditions are satisfied. For these reasons mentioned above, we will focus on the zonal wavefront estimation in this dissertation.

1.3 Vibrational effects

Mechanical vibrations (harmonic and nonharmonic) are often the principal source of image degradation. Image motion or image blur caused by vibrations is common when the imaging systems are located on a moving vehicle. Generally random vibrational motions are a combination of many complex motions, including linear, quadratic and exponential motions, and the intensity of each kind can be characterized by the power spectrum of the vibrations. In airborne and terrestrial reconnaissance, astronomy, robotics, machine vision, and computer vision systems, this motion degradation is generally much more severe than that from electronics and optics.

Vibrations degrade the image of optical systems, so does misalignment. They are often the main error sources in optical testing, such as in a S-H sensor. The effect of misalignment
errors on the RMS wavefront error measured in a S-H sensor are detailed in a recent paper (Curatu & Curatu and Rolland 2006).\textsuperscript{36}

The impact of vibrations on optical testing is especially severe in the PSI technique, in which the required data acquisitions at different phase steps make the PSI measurements more vulnerable to vibration errors, and the accuracy of the PSI method is mainly restricted by the vibrations during the measurements.\textsuperscript{37} Various efforts have been made to depress the vibrations and improve the measurement accuracy. The methods that have been proposed for suppressing the vibrations include (1) taking the measurements fast enough to essentially freeze out vibrations (Wizinowich 1990);\textsuperscript{38} (2) reducing the sensitivity of PSI to external vibrations by simultaneously acquiring two complementary interferograms (Deck 1996);\textsuperscript{39} (3) using a filter-based deconvolution to restore vibration-degraded video imagery (Barnard et al 1999);\textsuperscript{40} (4) adopting longer sampling windows and higher frame rates (Ruiz et al 2001);\textsuperscript{41} (5) realizing the required phase shift by quarter-wave plates and polarizers to avoid motion errors (Ngoi et al 2001);\textsuperscript{42} (6) using an active control loop to compensate for effects of vibrations (Zhao & Burge 2001);\textsuperscript{43} (7) data postprocessing (Huntley 1998),\textsuperscript{44} and (8) numerical optimization method (Milman 2002).\textsuperscript{45}

1.4 Motivation

Application requirements across various disciplines are always the original motivation to move the technology of shape sensing forward. Questions fermented in applications for wavefront testing technique include: How should one (1) handle the wavefront apertures that are not round or square? (2) estimate wavefronts with a sampling geometry or methodology that has
the lowest noise propagation? (3) move wavefront testing to next level of accuracy? (4) recover of the mid-spatial frequency error and (5) remove or reduce the effect of vibration and misalignments?

In this dissertation, our research is focused on how to optimize wavefront estimation with the above mentioned concerns. A zonal wavefront estimation algorithm without any required apriori knowledge of the pupil shape is developed, which provides a solution for wavefront estimation with irregular pupil shape. In order to reduce the wavefront estimation error, the error propagations in wavefront estimation with different geometries are studied, and the lowest error propagator for wavefront estimation is explored.

Considering a surface with a regular mesh, the slope measurement at each mesh location is a linear approximation of the surface with a tangential plane, while the local curvature is a quadratic approximation to the surface with an osculating quadric spherical surface.\textsuperscript{46} As a consequence, the local curvature measurements are believed to yield a better recovery of the mid-spatial-frequency errors than from the local gradient data.\textsuperscript{27} The principal curvatures and their directions, which can be computed from the local Laplacian curvatures and the twist curvature terms, provide a better characterization of wavefront local shape. In addition, a curvature sensor as opposite to a slope sensor yields vibration-insensitive measurements. For these reasons, a new sensor called differential Shack-Hartmann curvature sensor is proposed and developed in this dissertation.

1.5 Dissertation outline

The remainder of the dissertation will be arranged as follow:
Chapter 2 summarizes the previous related work performed on curvature measurements, which includes Roddier’s curvature sensor, the hybrid wavefront curvature sensor, and the curvature profiling technique.

Chapter 3 reviews previous wavefront estimation techniques, which include wavefront estimation algorithms from slope or curvature data based on the least-squares or Fourier transform method. The wavefront phase retrievals from wavefront irradiance measurements are also reviewed, which include the Gerchberg-Saxton method, Misell method, and phase diversity techniques.

Chapter 4 describes a new least-squares-based wavefront estimation algorithm from slope data for any irregular pupil shape. The mathematical framework for a pre-defined wavefront estimation matrix without knowledge of the pupil shape is given, and examples for two different pupil shapes are illustrated.

Chapter 5 quantitatively investigates error propagation in wavefront estimation. The functions that depict the error propagation behavior for different estimation geometries are established based on the matrix eigenvalue technique.

In Chapter 6, a new wavefront curvature sensor is proposed, called differential Shack-Hartmann (DSH) curvature sensor. The algorithm for zonal wavefront estimation from curvature measurements is given, and the mathematical framework for evaluating the principal curvatures is presented.

Chapter 7 provides a validation of the proposed zonal curvature-based wavefront estimation algorithm. An Error analysis of the experimental system for the DSH curvature sensor is also given.
Chapter 8 summarizes the contributions of the research presented in this dissertation and discusses future directions.
CHAPTER TWO: REVIEW OF CURVATURE SENSING

In this chapter, we will focus on the popular quantitative wavefront sensors that are based on measurement of wavefront curvature, the second derivative of wavefront. Wavefront curvature is an intrinsic parameter of wavefront. Unlike the slopes (gradients or the first order derivatives of shape), which vary with the surface orientation change, the surface normal curvature is insensitive to tip/tilt or orientation change of the surface.

In this chapter, the curvature sensing techniques will be briefly reviewed, which include Roddier’s wavefront curvature sensor, the Coherent Gradient Sensing method, a hybrid wavefront curvature sensor, and the curvature profiling technique.

2.1 Roddier’s wavefront curvature sensor

Considering a surface with a regular mesh, and given two arbitrary but orthogonal directions referred to the x- and y- directions, the local curvatures of the wavefront surface $W(x,y)$ along the x- and y- directions $c_x$ and $c_y$ are given by

\[
\begin{align*}
    c_x &= \frac{\partial^2 W(x,y)}{\partial x^2}, \\
    c_y &= \frac{\partial^2 W(x,y)}{\partial y^2},
\end{align*}
\]  

(2.1)

and the Laplacian of the wavefront is defined by

\[
\nabla^2 W(x,y) = \frac{\partial^2 W(x,y)}{\partial x^2} + \frac{\partial^2 W(x,y)}{\partial y^2}.
\]  

(2.2)
In 1988, Francois Roddier proposed a method to measure the local curvature of a wavefront surface by measuring the difference in illumination at the two planes located before and after the focal point (Roddier 1988).\textsuperscript{47} The principle of this sensor is illustrated in Figure 2.1.\textsuperscript{48} Later, this method was extended to wavefront sensing with an extended reference source by comparing the Fourier transforms of two oppositely defocused images instead of measuring the difference in illumination (Kupke, Roddier and Mickey 1998).\textsuperscript{49, 50}

Figure 2.1 The illustration of Roddier’s curvature sensing (from Malacara)
2.1.1 Methodology evolution

In the early 1980s, Teaque’s (Teaque 1982, 1983)\textsuperscript{51,52} and Steible’s (1984)\textsuperscript{53} work established how to retrieve phase information from a focused image and a defocused image formed by a non-coherent imaging system. They showed that if a diffracting aperture is much larger than the wavelength, a paraxial beam (monochromatic or incoherent) propagating along the z-axis can be written as a differential equation as 48

\[ \nabla^2 E(x,y,z) + 2k^2 E(x,y,z) + 2i\frac{\partial E(x,y,z)}{\partial z} = 0, \]  

(2.3)

where \( k = \frac{2\pi}{\lambda} \) is the wave number. One solution to this equation is of the form

\[ E(x,y,z) = \left\{ I(x,y;z) \right\}^{1/2} \exp(ikW(x,y;z)), \]  

(2.4)

where \( I(x, y; z) \) is the distribution of the illumination at a location \( z \) along the beam, and \( W(x, y; z) \) is the wavefront at a distance \( z \) from the origin. Substituting \( E(x,y,z) \) of Eq.(2.4) into Eq.(2.3), and equating real and imaginary parts to zero separately, yields\textsuperscript{52}

\[ \frac{\partial W}{\partial z} = I + \frac{I}{4k^2 I} \nabla^2 I - \frac{1}{2} \left\{ \nabla W \right\}^2 - \frac{1}{8k^2 I^2} \left\{ \nabla I \right\}^2 \]  

(2.5)

and\textsuperscript{52}

\[ \frac{\partial I}{\partial z} + \nabla I \nabla W + \nabla^2 W = 0 \]  

(2.6)

where \( \nabla = \frac{\partial}{\partial x} \hat{x} + \frac{\partial}{\partial y} \hat{y} \) is the gradient operator. Eq.(2.5) is the wavefront transport equation, and Eq.(2.6) is the irradiance transport equation. The \( \nabla I \nabla W \) term in Eq.(2.6) is called the prism term, representing the irradiance variation caused by a transverse shift of the beam due to the local tilt of the wavefront, and the term \( \nabla^2 W \) is called the lens term, which can be interpreted as the irradiance variation caused by the convergence or divergence of the beam, whose local
curvature is proportional to $\nabla^2 W$. Eq. (2.6) was originally derived for coherent light, but it is also valid for an incoherent extended light source when the source is uniform and symmetric.\textsuperscript{53}

Solutions to Eq.(2.6) are available. A Fourier transform-based phase retrieval method was reported by Ichikawa et al (1988).\textsuperscript{54} Teaque (1983) provided a solution based on a Green’s function, whose boundary value is constrained to be zero at the edge.\textsuperscript{54} By the use of the Neumann boundary condition, another Green’s function-based solution was given by Woods and Greenaway (2003).\textsuperscript{55}

The irradiance transport equation shows that one can estimate the wavefront local curvature by measuring the axial irradiance. If we assume that the illumination over the pupil plane is uniformly equal to $I_0$ ($\nabla I = 0$) everywhere but at the pupil edge, we have the boundary condition

$$ \nabla I = -I_0 n \delta_c $$ \hspace{1cm} (2.7)

where $\delta_c$ is a linear Dirac distribution around the pupil edge, and $n$ is a unit vector perpendicular to the edge and pointing outward.

Combining Eq.(2.6) and Eq.(2.7) yields (Roddier 1990)\textsuperscript{56}

$$ \frac{\partial I}{\partial z} = I_0 \frac{\partial W}{\partial n} \delta_c - I_0 P \nabla^2 W $$ \hspace{1cm} (2.8)

where $\nabla W / \partial n = n \cdot \nabla W$, and $P(x, y)$ is defined as the pupil function, whose value is one inside the pupil and zero outside. The irradiances at two defocused pupil images are given as

$$ \begin{cases} I_1 = I_0 + \frac{\partial I}{\partial z} \Delta z \\ I_2 = I_0 - \frac{\partial I}{\partial z} \Delta z \end{cases} $$ \hspace{1cm} (2.9)

Therefore,
\[
\frac{I_1 - I_2}{I_1 + I_2} = \frac{1}{I_0} \frac{\partial I}{\partial z} \Delta z \tag{2.10}
\]

By combining Eq.(2.10) with Eq.(2.8), Roddier obtained

\[
\frac{I_1 - I_2}{I_1 + I_2} = \left( \frac{\partial W}{\partial n} \delta_e - PV^2 W \right) \Delta z, \tag{2.11}
\]

where \( \Delta z \) is the distance from the pupil plane to the defocused plane \( P_1 \) or \( P_2 \) viewed from the object space. A plane at a distance \( \Delta z \) from the pupil can be Fourier transformed to a plane at a distance from the focus. Roddier proved that (1993)\(^{57}\)

\[
\Delta z = \frac{f(f - l)}{l}, \tag{2.12}
\]

where \( f \) is the system focal length and \( l \) is the defocus distance of the defocused plane. Then he obtained the well-known equation for curvature sensing given by

\[
\frac{I_1 - I_2}{I_1 + I_2} = \frac{f(f - l)}{l} \left( \frac{\partial W}{\partial n} \delta_e - PV^2 W \right). \tag{2.13a}
\]

Specifically,

\[
\frac{I_1(\vec{r}) - I_2(-\vec{r})}{I_1(\vec{r}) + I_2(-\vec{r})} = \frac{f(f - l)}{l} \left[ \frac{\partial W(f/\vec{r})}{\partial n} \delta_e - PV^2 W(f/\vec{r}) \right] \tag{2.13b}
\]

As pointed by D. Malacara et al., the operations on the irradiances in the two measured images must correspond to the same point on the pupil plane (Malacara 1998).\(^{48}\) As such, one of the defocused image is rotated 180\(^0\) with respect to the other. The above derivation is based on geometrical approximation, which is valid only when the irradiance measurements are made close to the pupil.\(^ {47, 58}\) Chanan obtained an equation that is the same as Eq.(2.11) by making an
integration on the focal plane based on the method of stationary phase provided by Born & Wolf (Chanan 2000). 59, 60

### 2.1.2 Implementations

In principle, the two out-of-focus images should be measured simultaneously, or within a time interval much shorter than the expected wavefront evolution time. In optical testing applications, this time constant is determined by the vibrational environment that is to be overcome. One implementation of curvature sensing is to employ two beam splitter prisms and one right angle prism to separate out the two extra-focal images and direct them on one detector array. 61 The advantage of this approach is that both images are detected at the same time, and this approach involves no moving parts, therefore it is very stable. This approach may suffer, however, from chromatic and geometric aberrations (spherical and astigmatism) introduced by prisms if it is not properly configured.

Another implementation is to employ a variable curvature membrane mirror driven acoustically at 7 kHz to switch between the re-imaging of the two defocused beam cross sections onto a detector. 62, 63 This oscillating membrane is located at the focus of the optical transfer lens. When the membrane mirror is flat, the light reflected from this mirror will re-image the telescope pupil onto the detector; when the mirror is inflated, the pupil image will be defocused on the detector in either direction. Because the distance to the focus changes continuously as the membrane vibrates, a stroboscopic technique or a fiber-optic LED transmitter is used to freeze the position of the mirror when the membrane vibrates back and forth. In one cycle of the membrane oscillation, the detector needs to record both intra focal and extra focal distributions
of the light beam. This process usually makes the system quite noisy, and to-date this implementation has not been very successful.

Besides the above configurations, Ervin Goldfain proposed a curvature sensor with a single-detector/single-image setup with partially coherent light (Goldfain 1998), in which the twin images were computed from the mutual intensity in the paraxial image plane according to the propagation laws of mutual intensity along the optical axis.

### 2.1.3 Advantages and disadvantages

The advantage of the curvature sensing method given by Roddier is its opto-mechanical simplicity and the fact that no lenslet arrays or re-imaging systems are needed. Also the sensitivity of the curvature sensor is comparable to that of the S-H test, and it can be changed continuously by varying the defocus distance \( l \). The most impressive advantage of such a curvature sensor is that the signal from the curvature sensor can be amplified and directly applied to the mirror actuator in a deformable mirror system without any wavefront estimation process.

The potential disadvantage of Roddier’s curvature sensing method as it is applied to optical testing is the error propagation in the wavefront estimation algorithm (Roddier 1990). Its performance is limited not only by the quality of the detector used for irradiance measurements but also by the separation between measurement planes used for the calculation of the axial derivative of intensity (Soto, Acosta & Ríos 2003). From the finite difference point of view, if the separation between measurement planes is small, the axial derivative should be more precise, but the spatial resolution of the sampling is low. On the other hand, if the distance
between the planes is large, the spatial resolution of the sampling will be increased, but the calculation of the derivative is less precise. Therefore, there exists an optimum separation distance between the intensity measurement planes.

The determination of the defocus distance is also affected by seeing blur and the caustic zone. The defocus image diameter should be twice as large of the seeing blur, and the defocused image planes should be taken outside the caustic zone, because inside the caustic zone the rays coming from different sample pupil points intersect. Unfortunately the size of the caustic zone depends on the aberrations of the optics under test, and the evaluation of an optimum position for the defocused measurement planes depends on the apriori knowledge of the phase to be measured. Besides the difficulty in determining the defocused distance, the exact position of the optical focus can be hard to determine, especially for slow \( f \)-ratios. Therefore, the distances of the measurement interfaces to the focus and their sizes may not be identical. As discussed above, how to determine the twin measurement interfaces is critical to the proper operation of Roddier’s curvature sensor. In 2003 a formula was presented by Soto et al. for determining the ideal defocused measurement planes when only a minimum knowledge of the phase is available. In 2003, a derivative of Roddier’s curvature sensor, which consists in directly measuring the Zernike components of an aberrated wavefront, was introduced (Neil, Booth & Wilson 2000).

### 2.2 Special wavefront curvature sensors

In this section, we briefly review other special curvature sensing techniques, the Coherent Gradient Sensing method and a hybrid technique for wavefront curvature sensing.
2.2.1 CGS wavefront curvature sensor

Coherent Gradient Sensing (CGS) is a diffraction-based, full-field, real-time, wavefront sensing approach for measuring wavefront curvature (Tippur 1992). CGS is especially useful for measuring curvatures of micro-mechanical structures and thin films in electronic devices and for studying the properties of materials and the stress distribution. CGS yields curvature data over the entire surface area of interest and it is insensitive to rotation or displacement of the object under test. A reflection-mode CGS setup is shown schematically in Figure (2.2). The coherent collimated laser beam is directed to the surface under test and reflected. The beam then passes through two identical Ronchi gratings (40 lines/mm) separated by a distance \( \Delta \), and the interference between two wavefronts sheared in a distance \( \omega \) takes place. A lens is used to image the wavefront fringes on the image plane, while focusing the diffracted light to form distinct diffraction spots on a filter plane. A filtering aperture is used in the filter plane to select a diffraction order of interest and block the other orders. A video camera is used to receive the fringe map, which is a contour plot of the wavefront gradient field. The video image is digitized and processed to extract information on the curvature of the surface under test.

If the Ronchi grating lines are oriented along the \( x_1 \) axis, the working principle of the CSG curvature sensor is illustrated in Figure 2.3. The incident beam on the primary grating \( G_1 \) is diffracted into several wavefronts denoted as \( E_0, E_1, E_{-1}, E_2, E_{-2}, \) etc, which are further diffracted by grating \( G_2 \). Various sets of parallel diffracted beams are combined by the filtering lens to form diffraction spots \( D_1, D_0, \) and \( D_{-1}, \) etc. An aperture pupil is placed on the filter plane to select the order of interest.
Figure 2.2  Schematic for a reflection CGS curvature sensor (Adopted from Kolawa)

The constructive interference maybe expressed as

\[ W(x_1, x_2 + \omega) - W(x_1, x_2) = n^{(2)} \lambda, \quad n^{(2)} = 0, \pm 1, \pm 2, \cdots \quad (2.14) \]

where \( n^{(2)} \) represents the integer identifying fringes observed for shearing along the \( x_2 \) direction. And \( \omega = \theta \Delta \), where \( \Delta \) is the interval between two gratings; \( \theta = \lambda / p \) is small, where \( p \) is the grating period. For sufficiently small \( \omega \), the authors obtained

\[ \frac{\partial W(x_1, x_2)}{\partial x_2} = \frac{W(x_1, x_2 + \omega) - W(x_1, x_2)}{\omega} = \frac{n^{(2)} \lambda}{\omega} = \frac{n^{(2)} p}{\Delta}, \quad n^{(2)} = 0, \pm 1, \pm 2, \cdots \quad (2.15) \]
This equation shows that the wavefront slopes in the $x_2$ direction are obtained. By rotating the two gratings in $90^\circ$, we can obtain the wavefront slopes in $x_1$ direction. Generally, in the $x_1$ or $x_2$ directions, we have

$$\frac{\partial W(x_1,x_2)}{\partial x_\alpha} = \frac{n^{(\alpha)} p}{\Delta}, \quad n^{(\alpha)} = 0, \pm 1, \pm 2, \cdots \text{ and } \alpha = \{1, 2\}. \quad (2.16)$$

A detailed Fourier optics analysis proved that the image plane of a CGS sensor is a gradient field of the wavefront under test\textsuperscript{70}, from which the curvature information can be extracted by a finite difference method. For small curvatures, $|\nabla^2 W| << 1$, a curvature tensor $\kappa_{\alpha\beta}$ along the unit tangent vectors $a_1$ and $a_2$ can be approximated as\textsuperscript{70}

$$\kappa_{\alpha\beta}(x_1,x_2) \approx \frac{\partial^2 W(x_1,x_2)}{\partial x_\alpha \partial x_\beta} \approx \frac{p}{\Delta} \left( \frac{\partial n^{(\alpha)}(x_1,x_2)}{\partial x_\beta} \right) n^{(\alpha)} = 0, \pm 1, \pm 2, \cdots \alpha, \beta = \{1, 2\}. \quad (2.17)$$
where $\kappa_{\alpha\beta}$ is the symmetric curvature tensor, whose component $\kappa_{11}$ and $\kappa_{22}$ are termed as normal curvatures, and $\kappa_{12} = \kappa_{21}$ as twist curvature terms.

### 2.2.2 Hybrid wavefront curvature sensor

The hybrid wavefront curvature sensor to be described here measures the curvatures and gradients of the wavefront using a configuration that resembles a Shack–Hartmann sensor (Paterson & Dainty 2000). An array of astigmatic lenslets is used to generate an array of foci on a single detector plane. The shape of each focused spot is related to the local wavefront curvature as shown in Figure 2.4, and a quad-cell detector is used to measure each spot.

When a parallel wavefront (i.e. there is no wavefront curvature) is incident on a lenslet, the focus is shown in Figure (2.4a). If the incident wavefront has curvature, the balance between the two diagonal cells is broken. The normalized difference between the sums of the signal intensities from diagonal elements of the quad cell yields an estimation of the local wavefront Laplacian, which is given as

$$
\frac{s_c}{s_1 + s_2 + s_3 + s_4}.
$$

The normalized difference between the right and left half (or upper and lower) of the quad cell yields a measure of the wavefront gradient given by

$$
\begin{align*}
    s_x &= \frac{s_1 + s_2 - s_3 - s_4}{s_1 + s_2 + s_3 + s_4}, \\
    s_y &= \frac{s_1 - s_2 - s_3 + s_4}{s_1 + s_2 + s_3 + s_4}.
\end{align*}
$$

(2.19)
Figure 2.4  The foci in the hybrid wavefront curvature sensor

The foci were generated by a single astigmatic lenslet with (a) an un-aberrated wavefront, (b) a negative-curvature wavefront and (c) a positive-curvature wavefront; (d) shows the labeling convention of the quad-cell element. (Adopted from Paterson & Dainty)

2.2.3 Curvature profiling technique

A non-contact 1-D curvature profiling technique that measures test surface curvature on a point-by-point basis was proposed and implemented (Glenn 1990). It simultaneously measures the local slopes at two slightly displaced surface locations with optical probes to obtain the surface slope differentials. This technique was further developed by Weingaertner and Schulz et al as the Large Area Curvature Scanning (LACS) method, which uses an extended-area optical probe to replace the point-sized optical probe. By scanning the test surface, a profile of curvature was built, and the height profile could be deduced.
The optical schematic for the differential measurement of slope is shown in Figure 2.5.\textsuperscript{27} A calcite plate was used to produce two parallel beams with opposite linear polarization, and a polarizing beam splitter was placed in the reflected path from the test piece to separate the two measurement beams before they were focused by the collimation lens onto two separate detectors. The “zero” curvature positions on the two detectors could be calibrated beforehand, and the difference between sensed positions on the detectors, which is proportional to the difference of the test piece slopes at the two measurement locations, were used to calculate the curvature at each test point. The schematic layout of the curvature profiling instrument is shown in Figure 2.6,\textsuperscript{27} where the steering mirror is used for scanning the test surface, and the movable detector is used to accommodate the focused spots on the centers of the two detectors.
Figure 2.6 Schematic layout of the curvature profiling instrument

(Adopted from Glenn)

The curvature profiling instrument measures the mid-frequency surface errors, whose spatial periods span from a fraction of a millimeter to a hundred or more millimeters. Curvature is an intrinsic property of the test piece which is independent of its position and angular orientation, and such property makes this approach fundamentally insensitive to all types of vibration and drift in both surface height and surface slope. It is a self-reference test where no reference surface is needed. The slope detectors can be two dimensional in order to measure both the normal curvature (longitudinal or lateral) and the twist curvature term.

The disadvantages of this approach are listed below. (1) It is a one-dimensional point-by-point measurement, which limits the temporal working bandwidth. (2) To reach the highest performance, it is necessary to calibrate the steering mirror intrinsic curvature and the calcite residual power, which is a complex problem since the steering mirror rotates in two dimensions. (3) This approach measures the curvature of the test surface only, which corresponds to the mid-spatial frequency errors, and it loses the information about the low spatial frequency errors, such as spherical aberration and astigmatism. This technique demonstrates sub-angstrom accuracy and
\( \lambda/1000 \) sensitivity with the differential distance of 0.3mm and a sample spacing of 10 \( \mu \)m on a test piece of 10mm.\(^7\)

### 2.3 Summary

Curvature is intrinsic and absolute parameter of wavefront and the curvature measurements is usually vibration insensitive. In this chapter, we reviewed four curvature sensing techniques, the Roddier curvature sensor, the CGS wavefront curvature sensor, a hybrid curvature sensor, and a 1-D curvature profiling technique. Of all these sensors the 1-D curvature profiling technique measures the second derivatives only, Roddier’s curvature measurements include both wavefront Laplacian inside the pupil and wavefront gradient around the boundary, and the others measure both the second derivatives and the first derivatives of the wavefront. Currently Roddier’s curvature sensor is mainly applied in astronomy for adaptive optics system to take the advantage of the analog nature of its sensor signal to the deformation of the deformable mirror. The curvature profiling technique is used as a unique instrument in profilometry which is immune to vibrations. So far the CGS and the hybrid wavefront curvature sensors have not been widely used in applications. More features of curvature sensing will be explored as a new wavefront curvature is proposed and implemented in Chapter 6.
In this chapter, we will first review wavefront estimation techniques that are based on wavefront parameter measurements, specifically the first and second derivative measurements (i.e. wavefront slope (gradient) and curvature measurements). Wavefront estimation converts the wavefront parameter measurements into wavefront OPD, or wavefront phase by multiplying the OPD by the optical wave number $2\pi/\lambda$. Mathematically it is a Neumann boundary problem of Poisson’s equation. 11

The wavefront phase retrieval methods that are based on the irradiance measurements are also reviewed. The phase retrieval methods include Gerchberg-Saxton and Misell methods, and the phase diversity technique, all of which employ phase deconvolution algorithms with iterative Fourier transform operations. The phase retrieval algorithms are usually computational intensive.

3.1 Neumann boundary problem in wavefront estimation

Consider that the measured gradient function of a wavefront is $g(x,y)$, which includes the real wavefront gradient $\nabla W$ and the random additive measurement noise $n(x,y)$, i.e.

$$g(x,y) = \nabla W(x,y) + n(x,y),$$ (3.1)

where $W$ is the wavefront under estimation, and $\nabla$ is the gradient operator. In a least-squares sense, the task of wavefront estimation is to find a wavefront $W(x,y)$ that minimizes the difference between $\nabla W$ and $g(x,y)$, which is equivalent to minimize the functional integral
\[ J = \iint_{\Omega} \left[ (\nabla W(x,y) - g(x,y))^2 \right] \, dxdy, \]  

(3.2)

where \( \Omega \) is the wavefront testing area, either a composite field or a simply connected field, in \( \mathbb{R}^2 \) with boundary \( \partial \Omega = C_0 + \bigcup_{i=1}^{n} C_i \) and closure \( \bar{\Omega} = \partial \Omega \cup \Omega \) as shown in Figure 3.1. In the following part we will show that wavefront estimation is a functional extremum problem in the calculus of variations.\(^60\)

![Figure 3.1 The testing aperture for wavefront estimation](image)

Let \( C^2(\bar{\Omega}) \) denote the space of all functions \( W : \bar{\Omega} \to \mathbb{R} \), such that \( W \) has continuous derivatives of second order, and let’s define a functional

\[ F(x,y,W_x,W_y) = \left[ \nabla W(x,y) - g(x,y) \right]^2 = \left[ W_x \, \dd{\bar{x}} + W_y \, \dd{\bar{y}} - g(x,y) \right]^2, \quad (3.3) \]

where \( W_x = \partial W / \partial x \), and \( W_y = \partial W / \partial y \). If \( F \) is a smooth function of \( x, y, W_x \) and \( W_y \), then the functional integral becomes \( J : C^2(\bar{\Omega}) \to \mathbb{R} \) with the form

\[ J[W(x,y)] = \iint_{\Omega} F(x,y,W_x,W_y) \, dxdy. \quad (3.4) \]

For the slope or Laplacian curvature-based wavefront estimations, the Neumann boundary conditions should be satisfied. Therefore, the permissible function set for the solutions to this problem is
\[ S = \left\{ W \mid W \in C^2(\overline{\Omega}), \left. \frac{\partial W}{\partial n} \right|_{\partial \Omega} = g_o(x,y) \right\}. \quad (3.5) \]

To obtain an extremum for the function \( J[W(x,y)] \) in Eq. (3.4), the Euler-Lagrange equation should be satisfied, \(^{79}\) i.e.

\[ \frac{\partial}{\partial x} \left( \frac{\partial F}{\partial W_y} \right) + \frac{\partial}{\partial y} \left( \frac{\partial F}{\partial W_y} \right) = 0. \quad (3.6) \]

Applying Equation (3.3) in Equation (3.6) yields

\[ \frac{\partial^2 W}{\partial x^2} + \frac{\partial^2 W}{\partial y^2} = \frac{\partial g}{\partial x} \bar{x} + \frac{\partial g}{\partial y} \bar{y}, \quad (3.7) \]

or

\[ \nabla^2 W = \nabla \cdot g(x,y) = f(x,y), \quad (3.8) \]

which is a Poisson equation. The wavefront estimation problem can then be described as a Neumann boundary problem of the Poisson’s equation stated as \(^{11}\)

\[ \begin{cases} \nabla^2 W = f(x,y) \\ \left. \frac{\partial W}{\partial n} \right|_{\partial \Omega} = g_o(x,y) \quad (x,y) \in \overline{\Omega} \end{cases}. \quad (3.9) \]

We have supposed that the wavefront function \( W \) has at least second order derivatives that are continuous on a closed region \( \overline{\Omega} \), so the solution to the Neumann boundary problem exists and is unique, except for an additive constant.

As implied by Eq.(3.9), we can estimate the wavefront by measuring either the wavefront gradient \( g(x,y) \) or wavefront curvature \( f(x,y) \), but it is difficult to find an analytic solution for this problem, so a numerical solution is sought in practice. By employing a finite difference method, the wavefront testing domain can be discretized into a regular mesh grid. We can either
evaluate the wavefront value at each local point that best fits the measurement data (i.e. the zonal wavefront estimation) or evaluate the estimated wavefront as a set of orthogonal polynomials over the whole pupil under test (i.e. the wavefront modal estimation).

### 3.2 Slope-based wavefront estimations

As we discussed in Chapter 1, a zonal estimation is advantageous in mid-spatial frequency recovery, and it is also convenient for accommodating irregular pupil shapes. Basically, there are three sampling geometries available for wavefront estimation from slope data: the Hudgin geometry, the Southwell geometry, and the Fried geometry as shown in Figure 3.2, where the small circles symbolize the wavefront values and the small arrows are wavefront slope measurements in the x- and y-directions.

![Sampling geometries for wavefront estimation](image)

Figure 3.2  Sampling geometries for wavefront estimation

(1) Hudgin geometry (2) Southwell geometry (3) Fried geometry.

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\(^\text{a}\) In recent literature, Hudgin was published as Hutchins
3.2.1 Zonal slope-based wavefront estimation

The zonal slope-based wavefront estimation can be performed either by a least-squares fitting method or by a Fourier transform method. The zonal least-squares estimation is usually a numerical solution to Poisson’s equation with the finite difference method. The Poisson’s equation can be expressed by a system of difference equations defined on the sampling grid. Since a partial derivative is an ordinary derivative taken with respect to one variable while the other variable is held fixed, we can write

$$\frac{\partial^2 W}{\partial x^2}(x_i, y_j) \approx \frac{W(x_{i-1}, y_j) - 2W(x_i, y_j) + W(x_{i+1}, y_j)}{a^2}, \quad (3.10)$$

where $a$ is the grid interval. Similarly for the $y$-derivative we can write,

$$\frac{\partial^2 W}{\partial y^2}(x_i, y_j) \approx \frac{W(x_i, y_{j-1}) - 2W(x_i, y_j) + W(x_i, y_{j+1})}{a^2}. \quad (3.11)$$

![Figure 3.3 Five-point stencil](image-url)
Substituting Eqs. (3.10) and (3.11) into Eq. (3.9), we obtain a discretization approximation to Poisson’s equation with a precision order of \( O(a^2) \),

\[
W(x_{i-1}, y_j) + W(x_{i+1}, y_j) - 4W(x_i, y_j) + W(x_{i-1}, y_{j-1}) + W(x_{i+1}, y_{j+1}) = a^2 f(x_i, y_j).
\]  

(3.12)

Each equation involves five unknown wavefront values, whose relative locations represent the weights with which the five unknowns are combined as shown in Figure 3.3. This geometry is called the five-point stencil in the finite difference method, which can be used for approximating the Poisson’s equation.\(^{11,80}\) The right side of this equation is wavefront curvature, which can either be obtained from direct measurements or numerically estimated from the slope measurements.

Fourier transforms of the slopes of a wavefront, for example in the x-direction, can be given as

\[
FT\left\{ \frac{\partial W(x,y)}{\partial x} \right\}(\xi) = i2\pi \xi \cdot FT\{W(x,y)\},
\]

(3.13)

where \( \xi \) is the spatial frequency associated to the x-dimension. Similarly, we can obtain the Fourier transform of slopes in the y-direction as

\[
FT\left\{ \frac{\partial W(x,y)}{\partial y} \right\}(\eta) = i2\pi \eta \cdot FT\{W(x,y)\},
\]

(3.14)

where \( \eta \) is the spatial frequency associated with the y-dimension. We then obtain the Fourier transform-based formula for wavefront estimation from slope data as\(^48\)

\[
W(x,y) = -\frac{i}{2\pi} \cdot FT^{-1}\left\{ \frac{\xi \cdot FT\left[ \frac{\partial W(x,y)}{\partial x} \right] + \eta \cdot FT\left[ \frac{\partial W(x,y)}{\partial y} \right]}{\xi^2 + \eta^2} \right\}.
\]

(3.15)
3.2.1.1 **Least-squares fitting method**

The zonal wavefront estimation technique can be traced back to 1974 when Rimmer formulated to estimate the wavefront from static shearing interferograms sampled on a rectangular array of points (Rimmer 1974). The estimation geometry Rimmer adopted was actually known later on as the so-called Hudgin geometry (Hudgin 1977), in which the wavefronts are evaluated at each grid point while the WFDs are measured between two neighboring grid points. The wavefront estimation matrix was established using a least-squares fitting method. An iterative relaxation method was employed to solve this equation. With the Hudgin geometry, a real-time wavefront reconstructor for adaptive optics was built (Hardy, Lefebvre & Koliopoulos 1977). J. Wyant showed that the wavefront measurement accuracy of this geometry depends only on the radiance of the shearing light source and not upon the angular subtense of the source (Wyant 1975).

For the Fried geometry, the wavefront value at each grid point is evaluated while the slopes (or WFDs) at the center of each grid cell are measured (Fried 1977). The slope data between each pair of neighboring grid points is estimated as an average of two slope data at the centers of the two neighboring grid cells. Given a generalized square array of the sampling grid, Hunt formulated the wavefront estimation matrix equation for the Hudgin and Fried geometries (Hunt 1979). Hunt, Hudgin and Fried all found that the error propagation in the estimation shared the form of $\alpha \ln(N) + \beta$, where $N$ is the number of the sampling grid size, and $\alpha$ and $\beta$ are constants that depend on the sampling geometry adopted. Noll revealed that the logarithmic behavior of the error is a fundamental property of the Green’s function for a Neumann boundary problem of a Poisson’s equation, and that the offset of the results from Hudgin and Fried is
caused by neglecting the contribution from the boundary condition (Noll 1978). We will show in Chapter 5 that parity of the sampling array dimension also contributes to the error propagation in wavefront estimation.

The Southwell geometry is characterized by taking the wavefront slope measurements and wavefront values estimation at the same nodes (Southwell 1980). The wavefront slope data at the midpoint between each pair of neighboring points is estimated as an average of the slope data at these two neighboring points. Southwell formulated the error propagation for zonal wavefront estimation and showed its superiority over other geometries. However, Wallner formulated a different opinion regarding the performance between different wavefront estimation geometries (Wallner 1983). In Chapter 5, we will discuss error propagation for different wavefront estimation geometries in detail.

Hudgin, Hardy et al, Fried, Hunt, Southwell, and Su et al all showed that a least-squares based estimation scheme of a wavefront value \( W_i \) can be expressed as

\[
W_i = \frac{1}{G}(A + B + C + D + a - b - c + d),
\]

where \( A, B, C \) and \( D \) are the wavefront values at the four adjacent nodes of \( W_i \); \( a, b, c \) and \( d \) are the adjacent WFDs between \( W_i \) and its adjacent nodes. \( G \) will be 4 if \( W_i \) is an interior node, and 3 and 2 if \( W_i \) is an edge or corner node, respectively. The wavefront inside the pupil is the average of its four nearest neighbors plus the average of the four connecting WFDs with the appropriate signs in the WFDs. This is actually the discretized approximation of Poisson’s equation, a general form for slope-based least-squares wavefront estimation.

Herrmann formulated the matrix equations for wavefront estimation for Hudgin and Fried geometries and showed that the ranks of the estimation matrices for the two geometries are \( m-1 \)
and \( m-2 \), respectively (Herrmann 1980), where \( m \) is the total number of wavefront grid points. Since the estimation matrix is rank-deficient, Herrmann suggested using singular value decomposition (SVD) to obtain the Moore-Penrose inverse of the estimation matrix, which is a least-squares solution with the minimum norm (LSMN). Besides the LSMN solution, he suggested to set a “zero point” for the wavefront to make the estimation matrices full-rank, at which the wavefront value is assigned to zero or other constant. Herrmann’s method of evaluating the LSMN solution by forcing the wavefront mean value to be zero is limited, because a wavefront that has a minimum norm does not necessarily have a zero mean value.

The Fried geometry perfectly matches with the lenslet array of the S-H sensor and actuator array of a deformable mirror, yielding currently the most popular configuration in adaptive optics. But wavefront estimation with the Fried geometry suffers from waffle mode (or checkerboard mode), which will be further detailed in Chapter 5.

### 3.2.1.2 Fourier transform method

A Fourier transform-based algorithm for wavefront estimation from slopes was proposed (Roddier & Roddier 1991). In order to remove the boundary effect in the Fourier transform process due to the limited size and shape of the pupil function, Gerchberg-Saxton iterations were used to extrapolate the fringes outside of the test pupil (Roddier & Roddier 1987). The Gerchberg-Saxton algorithm is an iterative irradiance-based wavefront estimation method that is widely used in phase retrieval, which will be further detailed in Section 3.4. The flow chart of the Gerchberg’s fringe extrapolation algorithm is illustrated in Figures 3.4, and Figure 3.5 shows a comparison between the interferograms before and after the extrapolation of the fringes. Based
on Gerchberg’s extrapolation, an iterative Fourier transform-based wavefront estimation from slope data can be performed, whose flow chart is illustrated in Figure 3.6.

Figure 3.4 The flow chart of Gerchberg’s fringe extrapolation algorithm.
(from Roddier & Roddier 1987)

Figure 3.5 An example of interferogram extrapolation (from Roddier & Roddier 1987)
(a) Interferogram before fringe extrapolation (b) Interferogram after fringe extrapolation
3.2.2 Modal slope-based wavefront estimation

In modal estimation, a wavefront is decomposed into a linear combination of whole-aperture basis functions, such as Zernike polynomials, Karhunen-Loeve functions, Legendre polynomials, Fourier Series, etc. Thus a wavefront can be expressed as

\[ W(x, y) = \sum_{k=0}^{M} a_k Z_k(x, y) \]  

(3.17)

where \( a_k \) are the coefficients to be determined, and \( Z_k(x, y) \) are two-dimensional functions that are orthogonal over the discretely sampled aperture. The Zernike circle polynomials are such a
set of orthogonal functions over a unit circle, which was first introduced by Zernike (Zernike 1934) and was later studied by Brinkman, Nijber, Bhatia and Wolf, Mahajan, et al. In a polar system, the modified Zernike circle polynomials given by Noll can be written as.

\[ Z_k(\rho, \theta) = \begin{cases} \sqrt{2(n+1)} R_n^m(\rho) \cos(m\theta) & k \text{ even, } m \neq 0 \\ \sqrt{2(n+1)} R_n^m(\rho) \sin(m\theta) & k \text{ odd, } m \neq 0 \\ \sqrt{(n+1)} R_n^m(\rho) & m = 0 \end{cases} \]  

where \( 0 \leq \rho \leq 1 \) and \( 0 \leq \theta \leq 2\pi \). The radial degree \( n \) and the azimuthal frequency \( m \) should satisfy \( m \leq n \) and \( m - n \) even. The index \( k = 1, 2, 3 \ldots \) is a mode ordering number, and \( k = n(n + m)/2 + m \). Born and Wolf showed that

\[ R_n^m(\rho) = \sum_{s=0}^{(n-m)/2} \frac{(-1)^s (n-s)!}{s!(n+m)/2-s!(n-m)/2-s!} \rho^{n-2s}. \]

Therefore the modified Zernike polynomial can be written in the following form

\[ Z_k(\rho, \theta) = 1 + 2\rho \cos \theta + 2\rho \sin \theta + \sqrt{3(2\rho^2 - 1)} + \sqrt{6\rho^2 - 1} \cos 2\theta + \sqrt{6\rho^2 - 1} \sin 2\theta + \sqrt{8(3\rho^2 - 2\rho) \sin \theta} + \sqrt{8(3\rho^2 - 2\rho) \cos \theta} + \sqrt{8\rho^2 \sin 3\theta} + \sqrt{8\rho^2 \cos 3\theta} \ldots \]

According to Mahajan, the Zernike circular polynomials (3.18) can be written in a simpler form as

\[ Z_k(\rho, \theta) = (n+1)^{1/2} R_n^m(\rho) \exp(im\theta). \]

The orthogonality of the Zernike polynomials means that the inner product of any Zernike polynomials is zero when the inner product is performed over a unit circle, which is

\[ \frac{1}{\pi} \int_0^{2\pi} \int_0^1 Z_k(\rho, \theta) Z_l^*(\rho, \theta) \rho d\rho d\theta = \delta_{kl}, \]

where \( \delta_{kl} \) is zero for \( k \neq l \) and 1 for \( k = l \).
The merit of the Zernike polynomials is that each term represents a specific wavefront aberration. For example, the constant 1 represents the piston error, terms \( \rho \sin \theta \) and \( \rho \cos \theta \) are wavefront tip/tilt, and term \( \rho^2 \sin 2\theta \) and \( \rho^2 \cos 2\theta \) are astigmatism, etc. Furthermore, the Zernike polynomials are orthogonal to each other over a unitary (i.e. normalized to 1) circular pupil without central obscuration. Then the variance of the wavefront is given by the sum of the squared aberration coefficients.\(^{106}\)

3.2.2.3 Least-squares based modal estimation

If a wavefront is given by Eq. (3.17), then the derivatives of the wavefront are given by

\[
\nabla W(x, y) = \sum_{k=1}^{M} a_k \nabla Z_k(x, y). \tag{3.23}
\]

By matching the gradient data measured in wavefront sensing at each discrete node

\[
G = (g_1, \ldots, g_N)^T, \text{ where } g_i = \left. \frac{\partial W}{\partial x} \right|_i + \left. \frac{\partial W}{\partial y} \right|_i, i = 1, 2, \ldots, N,
\]

we have a matrix equation

\[
DA = G, \tag{3.24}
\]

where \( D \) is the gradient matrix, and \( A = (a_1, \ldots, a_M)^T \) is the coefficient vector to be determined. In the least-squares sense, both Cubalchini (1979)\(^ {107}\) and Jan Herrmann (1981) derived the corresponding normal equation as\(^ {108}\)

\[
D^T DA = D^T G. \tag{3.25}
\]

If matrix \( D \) has its full column rank, then the least-squares solution is\(^ {109}\)

\[
A = (D^T D)^{-1} D^T G. \tag{3.26}
\]
The Zernike polynomials are orthogonal only on a unit disk. They are not orthogonal over an irregular shaped pupil, such as a pupil with a central obscuration which is a common case for an astronomical telescope. Furthermore, the Zernike polynomials are not strictly orthogonal over discrete points in a unit circle disk, and all of the derivatives of the Zernike polynomials are not orthogonal. Therefore, it is not proper to estimate the mode coefficients directly from the slope data or curvature data by least-squares estimations.

Cubalchini studied the effect of cross correlation between the modal estimates as a result of the non-orthogonality of the derivatives of the Zernike polynomials (Cubalchini 1979). He showed that the modal estimation is sensitive to the number of slope measurements used and their sampling geometry adopted. Although the set of basis functions needs not to be necessarily orthogonal to each other, they should be independent (Hardy 1998). Jan Herrmann further pointed out that the aberration cross coupling problem, caused by the lack of linear independence of the column vectors of the matrix $\mathbf{D}$, can be avoided if a least-squares estimate is performed with an increased number of modes (Hermann 1981). To make a polynomial orthogonal, a process called Gram-Schmidt orthogonalization can be employed (Wang and Silva 1980). With the Gram-Schmidt orthogonalization, the Zernike orthogonal polynomials over circular apertures can be extended to an annular aperture, or an hexagonal aperture, or other general-shape apertures.

Gavrielides first proposed to construct polynomials that are orthogonal to the gradient of the Zernike polynomials for modal estimation (Gavrielides 1982). Given that the constructed polynomials $V_i^*(\rho, \theta)$ and the gradient of the Zernike polynomials $\nabla Z_k(\rho, \theta)$ are orthogonal to each other, their inner product satisfies
\[ \nabla Z_k(\rho, \theta) \cdot \mathbf{V}_k^*(\rho, \theta) = \delta_{kl}. \]  

(3.27)

If the gradient data measured is \( \mathbf{G}(\rho, \theta) \), then the Zernike coefficients can be computed by

\[ a_k = \mathbf{G}(\rho, \theta) \cdot \mathbf{V}_k^*(\rho, \theta). \]  

(3.28)

The constructed polynomials \( \mathbf{V}_k(\rho, \theta) \) were given by an integral of a product of the gradient of a Green function defined on the unit circle and a Zernike polynomial. 114

Alternate to Gavrielides’ method, Acosta et al proposed to introduce an auxiliary vector function \( \mathbf{F}_k(r) \) whose gradient is orthogonal to the basis function (Acosta, Bara, Rama and Rios, 1995) 115, which is

\[ \nabla \cdot \mathbf{F}_k(r) = \psi^*_k(r), \]  

(3.29)

where \( \psi_k(r) \) is a basis function. Then the modal expansion coefficients of a wavefront \( W \) can be computed in terms of a weighted integral of the wavefront slopes. Therefore, if \( W \mathbf{F}_k \) is continuously differential in \( \sigma \) and its boundary \( C \), according to the divergence theorem, then

\[
\begin{align*}
    a_k &= \frac{1}{\|\psi_k\|} \iint_{\sigma} \psi^*_k W d\sigma \\
    &= \frac{1}{\|\psi_k\|} \iint_{\sigma} (\nabla \cdot \mathbf{F}_k) W d\sigma \\
    &= \frac{1}{\|\psi_k\|} \left( \int_C \nabla \cdot (W \mathbf{F}_k) dC - \iint_{\sigma} (\nabla W) \cdot \mathbf{F}_k d\sigma \right) \\
    &= \frac{1}{\|\psi_k\|} \left( \int_C W \mathbf{F}_k \cdot dC - \iint_{\sigma} (\nabla W) \cdot \mathbf{F}_k d\sigma \right). 
\end{align*}
\]  

(3.30)

By carefully choosing \( \mathbf{F}_k \) the integral along boundary \( C \) in the above equation can be made to vanish. Then

\[ a_k = \frac{-1}{\|\psi_k\|} \iint_{\sigma} (\nabla W) \cdot \mathbf{F}_k d\sigma, \]  

(3.31)
where $\nabla W$ is the wavefront gradient. As a result, the value of $a_k$ can be obtained by a numerical evaluation of this integral. More studies on this topic by Solomon et al can be found (Solomon et al 2001). \footnote{116}

Southwell adopted the Legendre polynomials to expand a phase function\footnote{88}

$$\phi(x, y) = \sum_{k=0}^{M} a_k n_k L_k(x, y)$$

(3.32)

where $a_k$ are the coefficients to be determined, $n_k$ are the normalized constants, and $L_k(x, y)$ are the orthogonal basis functions over the discretely sampled aperture, which are constructed from production of the Legendre polynomials. The slope function is obtained by differentiating Eq.(3.32), whose terms turned out to be another Legendre polynomials thus are still orthogonal. Based on the Legendre polynomials, Grediac proposed a method that can be used for wavefront estimation for slope or curvature measurements over a rectangular area (Grediac 1997). \footnote{117}

3.2.2.4 \textbf{Fourier transform-based modal estimation}

Freischlad and Koliopoulos proposed a Fourier transform-based modal wavefront estimation method (Freischlad & Koliopoulos 1985, 1986). \footnote{118, 119} A set of complex exponential basis functions with

$$Z_{pq}(m,n) = \frac{1}{N} \exp \left[ \frac{2\pi i}{N} (pm + qn) \right], \quad 1 \leq m,n \leq N, 0 \leq p,q \leq N-1,$$

(3.33)

were adopted. They are orthogonal over a square discrete data array, so are their derivatives. Expanded in complex exponential basis functions, the wavefront is the inverse discrete Fourier transforms (DFT$^{-1}$) of the expansion coefficients $a_{pq}$, i.e.
\[ W(m,n) = \sum_{p,q=0}^{N-1} a_{pq} Z_{pq}(m,n) = DFT^{-1}(a_{pq}). \] (3.34)

Then the expansion coefficients \( a_{pq} \) are the discrete Fourier transform (DFT) of the wavefront \( W(m,n) \), i.e.

\[ a_{pq} = \sum_{m,n=1}^{N} W(m,n) Z^*_{pq}(m,n) = DFT[W(m,n)] \] (3.35)

where the asterisk \( * \) denotes the complex conjugate.

In order to obtain the coefficients \( a_{pq} \), Eq.(3.34) is differentiated, yielding

\[ \nabla W(m,n) = \sum_{p,q=0}^{N-1} a_{pq} \nabla Z_{pq}(m,n), \] (3.36)

where the discrete gradient can be obtained by the noisy measurements, i.e. \( S = \nabla W + n \), and \( n \) is the measurement noise.

For the Hudgin geometry,

\[ \nabla Z_{pq}(m,n) = \begin{pmatrix} Z_{x,pq}^d \\ Z_{y,pq}^d \end{pmatrix} = \begin{pmatrix} e^{\frac{2\pi n}{N}} - 1 \\ e^{\frac{2\pi q}{N}} - 1 \end{pmatrix} Z_{pq}(m,n). \] (3.37)

Matching the measured slope data \( S(m,n) \) in the x-and y-directions with Eqs.(3.36) and (3.37) provides

\[
\begin{align*}
S_x(m,n) &= \sum_{p,q=0}^{N-1} a_{pq} \left( e^{\frac{2\pi n}{N}} - 1 \right) Z_{pq}(m,n) = DFT^{-1} \left[ a_{pq} \left( e^{\frac{2\pi n}{N}} - 1 \right) \right], \\
S_y(m,n) &= \sum_{p,q=0}^{N-1} a_{pq} \left( e^{\frac{2\pi q}{N}} - 1 \right) Z_{pq}(m,n) = DFT^{-1} \left[ a_{pq} \left( e^{\frac{2\pi q}{N}} - 1 \right) \right].
\end{align*}
\] (3.38)

Solving this equation in a least-squares sense, we obtain the estimate of coefficients \( a_{pq} \) as
\[
\hat{a}_{pq} = \begin{cases} 
0, & \text{(if } p = q = 0) \\
(e^{\frac{2\pi i p}{N}} - 1)DFT(S_x) + (e^{\frac{2\pi i q}{N}} - 1)DFT(S_y) \\
\frac{4}{N^2} \left( \sin^2 \left( \frac{\pi}{N} p \right) + \sin^2 \left( \frac{\pi}{N} q \right) \right) & \text{(otherwise)}
\end{cases}
\] (3.39)

Applying the obtained coefficients into Eq.(3.34), the wavefront estimate is then available.

The error propagation of modal estimation is comparable to that of the zonal estimation, except that most of the error occurs in sharp peaks at the edges and corners in the modal estimation, because a N×N array has only (N-1)×N gradient data for the Hudgin geometry. To generate the missing data, a periodicity requirement is assumed. The average difference of each row or column should be zero. This method can be easily extended to rectangular sampling arrays, but it is difficult to generalize it to irregular arrays over which the complex exponentials are not orthogonal. The Fourier transform-based modal estimation algorithm is efficient; and its computational complexity is approximately proportional to the number of grid points \(N^2\).

In order to handle the irregular pupil shaped applications, Freischlad extended this algorithm for general pupil shapes (Freischlad 1992). In Freischlad’s method, additional least-squares matrix equations were required for generating the missing slope data to extend an irregular shaped pupil to a square shaped domain. The condition of integrability was used for generating the missing WFDs outside of the original pupil, which satisfies the condition that summation of the WFDs around each grid cell should be zero.

### 3.2.3 Radon transform-based modal estimation

Aksenov and Isaev proposed a modal wavefront phase estimation method based on the Radon transform (Aksenov & Isaev 1992). If the wavefront slope in the x- and in y- directions
are $\mu(x,y) = \frac{\partial W(x,y)}{\partial x}$ and $\nu(x,y) = \frac{\partial W(x,y)}{\partial y}$, then according to the inverse Radon transform the wavefront phase can be expressed as\(^{121}\)

$$W(x,y) = \frac{1}{2\pi} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \frac{I}{(x-x')^2 - (y-y')^2} \left[ (x-x')\mu(x',y') + (y-y')\nu(x',y') \right] dx'dy'. \hspace{1cm} (3.40)$$

If the wavefront phase in a circular pupil can be expressed as a sum of the Zernike polynomials

$$W(x,y) = \sum_{k} a_k \psi_k(x,y), \hspace{1cm} (3.41)$$

then $a_k$ can be defined as\(^{121}\)

$$a_k = \frac{\langle W, \psi_k \rangle}{\|\psi_k\|} = \sqrt{\frac{\pi R^2}{n+1}} \int_{0}^{2\pi} \int_{0}^{R} W(\rho,\varphi) \psi_k(\rho,\varphi) \rho d\rho. \hspace{1cm} (3.42)$$

Computing the above integration yields the coefficients of the Zernike polynomials. More simulation studies on Radon transform-based wave front estimation were presented (Dam and Lane 2002).\(^{122}\)

### 3.3 Curvature-based wavefront estimations

Curvature-based wavefront estimation was not reported in the previous literature until recently, because the wavefront curvature sensing was not popular before F. Roddier invented a curvature sensor based on axial differential irradiance measurements.\(^{47}\) Since then, curvature-based wavefront estimation has become an active topic of research in wavefront sensing. Curvature is a characteristic parameter of wavefront, and the curvature-based wavefront sensing is vibration insensitive, which is an important feature for in-situ wavefront sensing and optical workshop testing.
3.3.1 Zonal curvature-based wavefront estimation

As discussed in Section 3.1, curvature-based zonal wavefront estimation is a numerical solution to the Poisson’s equation with Neumann boundary. It is a particular type of elliptical partial differential equation (PDE) with a non-unique solution. Curvature-based zonal wavefront estimation can be performed with either a least-square method or with a Fourier-transform-based method.

For the curvature-based zonal wavefront estimation with a least-squares method, a finite-difference solution to the PDE may be obtained by replacing the curvature terms \( f(x_j, y_j) \) in Eq.(3.12) with direct curvature measurements.

For the curvature-based zonal wavefront estimation with a Fourier-transform based method, the wavefront Laplacian is given as

\[
\nabla^2 W(x, y) = \frac{\partial^2 W(x,y)}{\partial x^2} + \frac{\partial^2 W(x,y)}{\partial y^2}, \quad (3.43)
\]

and the Fourier transforms of Laplacian curvatures are given by

\[
FT\left( \frac{\partial^2 W(x,y)}{\partial x^2} \right)(\xi) = -4\pi^2 \xi^2 \cdot FT\{W(x,y)\}, \quad (3.44)
\]
\[
FT\left( \frac{\partial^2 W(x,y)}{\partial y^2} \right)(\eta) = -4\pi^2 \eta^2 \cdot FT\{W(x,y)\}. \quad (3.45)
\]

Therefore, the Fourier transform of the wavefront Laplacian is

\[
FT\{\nabla^2 W(x,y)\}(\xi, \eta) = -4\pi^2 (\xi^2 + \eta^2) \cdot FT\{W(x,y)\}. \quad (3.46)
\]

Following this method, Roddier and Roddier obtained the curvature (Laplacian)-based wavefront estimation formula as\(^92\)
\[
W(x, y) = -\frac{1}{4\pi^2} \cdot FT^{-1} \left\{ \frac{FT\left[\nabla^2 W(x, y)\right]}{\xi^2 + \eta^2} \right\}.
\] (3.47)

3.3.1.1 Least-squares-based zonal estimation

On the basis of the finite difference method, N. Roddier presented an iterative least-squares-based algorithm for wavefront estimation from curvature data (N Roddier 1991). To speed up the solution convergence, N Roddier employed the successive over-relaxation (SOR) method in the iterative algorithm for all the points inside the pupil area. Since the test pupil has central obscuration, the boundary condition given at the outer edge was applied for wavefront estimation, and no boundary condition was needed for the inner edge. The wavefront values inside the central obscuration were estimated with zero curvature by algorithm interpolations.

3.3.1.2 Fourier transform-based zonal estimation

Roddier and Roddier proposed a curvature-based algorithm for zonal wavefront estimation with Roddier’s curvature sensor (Roddier & Roddier 1991). This algorithm starts with the curvature data sampled inside the test domain and the curvature set to zero outside of the domain. The wavefront Laplacians are estimated by taking the difference between the illuminations in symmetrically defocused planes. The radial derivatives are forced to zero within a narrow band surrounding the boundaries, while the inner slopes are forced to be equal to the edge signal. Then a Fast Fourier Transform (FFT) is applied and an iterative process is performed as shown in Figure 3.7.
For Roddier's curvature sensor, the wavefront estimation from curvature data is valid only for small magnitude of the aberrations and it becomes inaccurate for large aberrations\textsuperscript{47,57}. To improve the estimation accuracy for a wavefront with large aberrations, an iterative process can be employed by compensating the effect of the estimated aberrations on the defocused images as a simulation of an active optics control loop. The residual wavefront estimated in each iteration is added to the estimated wavefront in the 1\textsuperscript{st} iteration until the noise level is reached.\textsuperscript{57}
3.3.2 Modal curvature-based wavefront estimation

In curvature-based modal estimation, the wavefront aberrations are represented by a linear combination of a set of orthogonal basis functions, such as the Zernike polynomials. To evaluate the modal coefficients, the first- and second-order derivatives of the Zernike polynomials must be employed to fit the slope data at the boundary and the curvature data inside the test pupil. The problem lies in that the first- and second-order derivatives of the Zernike polynomials are not orthogonal, and the modal estimation is not unique.

Table 3.1 The Zernike polynomials and their 1st to 2nd derivatives

<table>
<thead>
<tr>
<th>k</th>
<th>Z_k</th>
<th>( \frac{\partial Z_k}{\partial \rho} )</th>
<th>( \nabla^2 Z_k )</th>
</tr>
</thead>
<tbody>
<tr>
<td>2</td>
<td>( \rho \cos \theta )</td>
<td>( \cos \theta )</td>
<td>0</td>
</tr>
<tr>
<td>3</td>
<td>( \rho \sin \theta )</td>
<td>( \sin \theta )</td>
<td>0</td>
</tr>
<tr>
<td>4</td>
<td>( 2\rho^2 - 1 )</td>
<td>( 4\rho )</td>
<td>8</td>
</tr>
<tr>
<td>5</td>
<td>( \rho^2 \cos 2\theta )</td>
<td>( 2\rho \cos 2\theta )</td>
<td>0</td>
</tr>
<tr>
<td>6</td>
<td>( \rho^2 \sin 2\theta )</td>
<td>( 2\rho \sin 2\theta )</td>
<td>0</td>
</tr>
<tr>
<td>7</td>
<td>( (3\rho^3 - 2\rho) \cos \theta )</td>
<td>( (9\rho^2 - 2) \cos \theta )</td>
<td>24\rho \cos \theta</td>
</tr>
<tr>
<td>8</td>
<td>( (3\rho^3 - 2\rho) \sin \theta )</td>
<td>( (9\rho^2 - 2) \sin \theta )</td>
<td>24\rho \sin \theta</td>
</tr>
<tr>
<td>9</td>
<td>( \rho^3 \cos 3\theta )</td>
<td>( 3\rho^2 \cos 3\theta )</td>
<td>0</td>
</tr>
<tr>
<td>10</td>
<td>( \rho^3 \sin 3\theta )</td>
<td>( 3\rho^2 \sin 3\theta )</td>
<td>0</td>
</tr>
<tr>
<td>11</td>
<td>( 6\rho^4 - 6\rho^2 + 1 )</td>
<td>( 24\rho^3 - 12\rho )</td>
<td>24(4\rho^2 - 1)</td>
</tr>
<tr>
<td>12</td>
<td>( (4\rho^4 - 3\rho^2) \cos 2\theta )</td>
<td>( (16\rho^3 - 6\rho) \cos 2\theta )</td>
<td>48\rho^3 \cos 2\theta</td>
</tr>
<tr>
<td>13</td>
<td>( (4\rho^4 - 3\rho^2) \sin 2\theta )</td>
<td>( (16\rho^3 - 6\rho) \sin 2\theta )</td>
<td>48\rho^3 \sin 2\theta</td>
</tr>
<tr>
<td>14</td>
<td>( \rho^4 \cos 4\theta )</td>
<td>( 4\rho^3 \cos 4\theta )</td>
<td>0</td>
</tr>
<tr>
<td>15</td>
<td>( \rho^4 \sin 4\theta )</td>
<td>( 4\rho^3 \sin 4\theta )</td>
<td>0</td>
</tr>
<tr>
<td>16</td>
<td>( (10\rho^5 - 12\rho^3 + 3\rho) \cos \theta )</td>
<td>( (50\rho^4 - 36\rho^2 + 3) \cos \theta )</td>
<td>48(5\rho^3 - 2\rho) \cos \theta</td>
</tr>
<tr>
<td>17</td>
<td>( (10\rho^5 - 12\rho^3 + 3\rho) \sin \theta )</td>
<td>( (50\rho^4 - 36\rho^2 + 3) \sin \theta )</td>
<td>48(5\rho^3 - 2\rho) \sin \theta</td>
</tr>
<tr>
<td>18</td>
<td>( (5\rho^5 - 4\rho^3) \cos 3\theta )</td>
<td>( (25\rho^4 - 12\rho^2) \cos 3\theta )</td>
<td>80\rho^3 \cos 3\theta</td>
</tr>
<tr>
<td>19</td>
<td>( (5\rho^5 - 4\rho^3) \sin 3\theta )</td>
<td>( (25\rho^4 - 12\rho^2) \sin 3\theta )</td>
<td>80\rho^3 \sin 3\theta</td>
</tr>
<tr>
<td>20</td>
<td>( \rho^5 \cos 5\theta )</td>
<td>( 5\rho^4 \cos 5\theta )</td>
<td>0</td>
</tr>
<tr>
<td>21</td>
<td>( \rho^5 \sin 5\theta )</td>
<td>( 5\rho^4 \sin 5\theta )</td>
<td>0</td>
</tr>
<tr>
<td>22</td>
<td>( 20\rho^6 - 30\rho^4 + 12\rho^2 - 1 )</td>
<td>( 120\rho^5 - 120\rho^3 + 24\rho )</td>
<td>48(15\rho^4 - 10\rho^2 + 1)</td>
</tr>
</tbody>
</table>
Han proposed to estimate the wavefront without solving the Poisson equation for the curvature signal (Han 1995).\textsuperscript{124} As shown in Table 3.1, the Laplacian of some Zernike polynomials are zero.\textsuperscript{124} Han named the polynomials that have zero Laplacian as B-mode terms, and the others terms as L-mode terms.\textsuperscript{124} Therefore, the Laplacian region, which is the inside of the test pupil, does not contain any information about the B-mode terms whose information is only contained in the boundary region. Han estimated the L-mode terms from the Laplacian region co-aligned with the B-mode terms from the boundary region. As pointed by Han, the problems lying in this algorithm are the non-orthogonality of the L-mode terms and the difficulty in separating the boundary region from the Laplacian region.\textsuperscript{124}

Similar to Han’s work, Gureyev et al decomposed the wavefront phase expressed by the Zernike polynomials into two orthogonal parts. One part was composed of the diagonal Zernike polynomials (i.e. $m=n$) whose Laplacian are zero, and the other part was composed of the non-diagonal Zernike polynomials (i.e. $m \neq n$) whose Laplacian are nonzero (Gureyev, Roberts and Nugent 1995).\textsuperscript{125} They showed that the wavefront phase of the diagonal terms depends on the wavefront slopes at the boundary and the boundary values of the non-diagonal terms, while the wavefront phase of the non-diagonal terms depends only on the nonzero wavefront curvature inside the aperture. Both the wavefront phase and the wavefront curvature could be expanded into a series of Zernike polynomials, and a matrix was found to convert the coefficients of the wavefront phase into the coefficients of the wavefront curvature. The modal phase retrieval could be performed with the matrix method over a circular aperture.

As we introduced in Sect.3.2.2, Gavrielides first proposed in 1982 to construct a set of polynomials that are orthogonal to the gradient of the Zernike polynomials in modal estimation.\textsuperscript{114} Then the modal coefficient is the inner product of the auxiliary function and the
differential measurements over the testing area. Voitsekhovich similarly proposed to introduce an auxiliary set of polynomials that are orthogonal to some differentials of the wavefront (such as the 2nd derivatives) for Roddier’s curvature sensing (Voitsekhovich 1995). Following the work on the slope-based modal estimation given by Acosta et al., which was to introduce an auxiliary vector function whose gradient is orthogonal to the basis function, Rios et al proposed to introduce an auxiliary set of basis functions $\xi_k (k = 1,2,\cdots,m)$ whose Laplacians are orthogonal to basis functions such as the Zernike polynomials $\psi_k (k = 1,2,\cdots,m)$ over the testing domain $\sigma$ (Acosta, Bara, Rama, and Rios1995). The auxiliary function is chosen in such a way that it satisfies the following equation set

$$\begin{cases}
\nabla^2 \xi_k (r) = \psi_k (r) \quad \text{for } r \in \sigma \\
\frac{\partial \xi_k (r)}{\partial n} = 0 \quad \text{for } r \in c
\end{cases},$$

(3.48)

where $\sigma$ is the test pupil and $c$ is its boundary. Then they obtained the modal coefficients by employing Green's second identity as

$$a_k = c_k^{-1} \left\{ \int_c \xi_k \frac{\partial W}{\partial n} dl + \int_\sigma \xi_k \nabla^2 W d\sigma \right\}.$$

(3.49)

In order to evaluate the above multiple integrals, a numerical integration method called Albrecht’s cubature was adopted for the integral within the pupil region $\sigma$, combining with a composite trapezoidal rule for the integral along the pupil boundary (Bara, Rios & Acosta 1996). This method provides a more accurate result with smaller number of measurements than those of other usual integration routine, such as the Gauss-Legendre, Simpson’s rule and the composite trapezoidal rule. Nevertheless, the problem in this algorithm is that the Zernike polynomials are not strictly orthogonal over the discrete set of sampling points.
3.4 Phase retrieval techniques

The amplitude-based wavefront sensing, usually called the phase retrieval problem, is an old problem in optics. It estimates the wavefront by measuring the irradiances at the pupil or image plane, and find applications from Fourier transform spectroscopy, x-ray crystallography, particle scattering and electron microscopy to optical imaging. The earliest report in the literature can be dated back to the beginning of the 1960s (Wolf 1962, O’Neill and Walther 1962, Walther 1962, Dialetis and Wolf 1967, and Greenaway 1977). For coherent imaging, the advent of the laser and the technique of off-axis holography pioneered by Leith and Upatnieks solved this problem (Leith & Upatnieks 1962, Wolf 1970). For incoherent imaging, Gerchberg and Saxton proposed a Fourier transform-based iterative algorithm for the evaluation of the amplitude and phase from the irradiance measurements at the pupil and image planes (Gerchberg & Saxton 1971, 1972), which became a first practical method for phase retrieval in optics. The Gerchberg-Saxton algorithm involves iterative Fourier transform back and forth between the object and the Fourier domain, while applying the measured data or known constraints in each domain. Later on Fienup modified the Gerchberg-Saxton algorithm to speed up the convergence and developed an algorithm called the input-output approach (Fienup 1974).

As an alternate to the Gerchberg-Saxton algorithm, the wavefront phase can also be estimated from the irradiance measurement of a single image. When the measurement is made at the image plane, the irradiance distribution should be related to the complex pupil function through a Fourier transform. By comparing the computed image irradiance with the measured image irradiance, the wavefront phase at the pupil can be identified. As a metric to search for the
solution, a merit function can be defined as a mean squared sum of the difference between the computed and the measured irradiance values. Given that the detector noise is Gaussian, the wavefront phase retrieval problem is how to search a solution that minimizes this merit function in the sense of the maximum-likelihood. This method was independently proposed by Gonsalves and Southwell (Gonsalves 1976, Southwell 1977).

At this point, the phase retrieval problem became a numerical computational problem rather than an optics problem. It is generally computationally intensive. The numerical method, such as the steepest decent gradient method, can be applied in the solution search. Usually, the phase retrieval is valid for small aberrations only, unless one can constrain the numerical solution in a limited space, because there is a $2\pi$-phase ambiguity for the large aberrations.

The phase diversity method was actually initiated by Misell (Misell 1973), when Misell proposed an iterative phase retrieval algorithm from the irradiance measurements of the images taken at two different defocused values. The iterative scheme, which is closely related to the Gerchberg-Saxton algorithm, was established between the two images by convolution. Because the irradiance measurements were performed in the image space, and the knowledge of the amplitude function in the pupil is not required, the Misell algorithm is more convenient than the Gerchberg-Saxton algorithm for phase retrieval in practice. Roddier & Roddier modified the Misell algorithm by taking the irradiance measurements of image at three different defocus values to improve the convergence, while minimizing the effect of misalignment errors on the CCD camera in the analysis of the imaging capability of the Hubble Space Telescope (Roddier & Roddier 1993).

However, the phase diversity method is nowadays referred to as another phase deconvolution technique that was proposed by R. A. Gonsalves (Gonsalves 1979).
phase diversity technique can provide a joint estimation of object and phase aberrations by collecting two incoherent images: one is the traditional paraxial image, and another is an image with given quadratic defocus error. This method is good for both point and extended objects. Extensive simulation studies including noise effect were performed by Paxman et al., and some simulation and experimental investigations, including closed-loop adaptive optics experimental demonstration was presented by Kendrick and Jeffries et al.

3.4.1 Gerchberg-Saxton and Misell methods

In this section, we first review the Gerchberg-Saxton method and then briefly review the Misell algorithm, which is much related to the Gerchberg-Saxton method.

3.4.1.1 Gerchberg-Saxton method

The Gerchberg-Saxton method evaluates the wavefront phase by an iterative procedure that constrains the wavefront amplitudes to the irradiance measurements in both the image and the pupil planes that form a Fourier transform pair. Given that the wavefront amplitude is proportional to the square root of the measured wavefront intensity, detectors are needed to record the irradiances at the image plane and pupil plane in the Gerchberg-Saxton method.

The principle of the Gerchberg-Saxton method is shown in Figure 3.8. An array of random numbers are generated between $-\pi$ and $+\pi$ as the initial phase values at the image plane. These are combined with the sampled image amplitudes to synthesize a complex discrete function. By employing the FFT algorithm given by Cooley and Tukey (Cooley & Tukey
this complex function is Fourier transformed into the pupil plane. The computed phases at the sample points are combined with the sampled pupil amplitude function to form a new estimate of the complex function in the pupil plane. The iteration then continues until it converges to a solution when the complex function of the Fourier transform pair satisfies the irradiance measurements in both pupil and image planes. The Gerchberg-Saxton algorithm is the basic algorithm for a variety of phase retrieval methods.

The Gerchberg-Saxton algorithm is paraxial imaging-based, which can be generalized to accommodate for both paraxial and non-paraxial imaging systems (Yang et al 1994). This method is easy to implement, and it is sensitive to piston errors. However, it is nonlinear, computationally intensive, and requires the wavelength band to be narrow. The uniqueness of the solution can also be a problem. Adding an arbitrary but constant phase to any function whose irradiance in the image and pupil planes are the same as the measured irradiance will yield a new complex function that still satisfies the Fourier transform between the image plane and the pupil.
plane. It also has a $2\pi$-phase ambiguity problem. The dynamic range of the phase measurements is limited between $-\pi$ and $+\pi$, and the method fails if the dynamic range exceeds $2\pi$. Finally, as pointed by Fienup, the convergence of the Gerchberg-Saxton algorithm is slow.

### 3.4.1.2 Misell algorithm

Instead of employing an iterative scheme between the image and pupil planes as in the Gerchberg-Saxton algorithm, Misell established an iterative scheme between the focused image and a given defocused image. The Misell algorithm is shown in Figure 3.9, and the iterative procedures are shown as follows:

1. The complex wave function $\psi_1(r)$ at the focused image plane is formed with its amplitude obtained from measurement and its phase values randomly assigned between $-\pi$ and $+\pi$.

2. Evaluate the convolution $\psi'_2(r) = \psi_1(r) * G(r)$ to obtain a wave function $\psi'_2(r)$ at the defocused image plane. The quadratic defocus phase term $G(r)$ is defined by

$$G(r) = FT^{-1}\left\{\exp\left(-i\frac{1}{2}k_0\Delta f\nu^2\lambda_0^2\right)\right\},$$  \hspace{1cm} (3. 50)

where $k_0 = 2\pi/\lambda_0$, $\lambda_0$ is the wavelength of the light source, $\Delta f$ is the defocus value between the two images, and $\nu = (\nu_x, \nu_y)$ is the spatial frequency in the Fourier domain.

3. Compare the computed amplitude of $\psi'_2(r)$ with the actual image amplitudes from measurement. If the difference is not acceptable, replace the computed amplitude with the measurement and retain the phase terms to form a new wave function $\psi_2(r)$. 

4. Evaluate another convolution $\psi'_1(\mathbf{r}) = \psi'_2(\mathbf{r}) \ast G'(\mathbf{r})$ to obtain a new function $\psi'_1(\mathbf{r})$ at the focused image plane, where the quadratic defocus phase term $G'(\mathbf{r})$ is defined by

$$G'(\mathbf{r}) = FT^{-1}\left\{\exp\left[i\frac{1}{2}k_0\Delta\hat{v}^2\hat{z}^2\right]\right\}. \quad (3.51)$$

5. Compare the computed amplitudes of $\psi'_1(\mathbf{r})$ with the measured amplitudes at the focused image plane. If the difference is appreciable, then a new wave function $\psi'_2(\mathbf{r})$ at the focused image plane is formed with the amplitude of $\psi'_1(\mathbf{r})$ replaced with the measurement and the phase term retained. Then going to Step 2, and the iteration continues.

The iteration is completed when a specified small difference between the computed and the measured amplitudes is satisfied. In this algorithm the absolute defocus values are not required, only the relative defocus value between images is measured.
3.4.2 Phase diversity technique

As initiated by Misell, phase diversity is a phase-retrieval algorithm that uses a pair of intensity images at different defocused values: One image can be the conventional focal-plane image \( I_1(x, y) \), and another one can be the image with a known defocused value \( I_2(x, y) \). The optical layout of a phase diversity system is shown in Figure 3.10.\(^{151}\)

![Figure 3.10 Optical layout of a phase diversity system (from. Paxman et al)](image)

For an extended object, the images at different defocus planes are

\[
I_i(x, y) = O(x, y) * P_i(x, y) + n_i(x, y), \quad i = 1, 2. \tag{3.52}
\]

where \( O(x, y) \) is the incoherent object under estimation, \( P_i(x, y) \) is the PSF of having a diversity, which is the squared modulus of the Fourier transform of the corresponding complex pupil function, and \( n_i(x, y) \) is the measurement noise. The complex pupil function in Fourier space can be written as

\[
\psi_i(u, v) = A(u, v) \exp(i \varphi(u, v) + i \theta_i(u, v)), \tag{3.53}
\]

where \( A(u, v) \) is the zero-one pupil function, \( \varphi(u, v) \) is the phase function under estimate, and
\( \theta_i(u,v) \) is the given quadratic defocus phase term, which is zero for the focused image.

Gonsalves introduced an error metric as

\[
E = \sum_1^2 \iint [I_i(x,y) - \hat{O}(x,y)^* \hat{P}_i(x,y)]^2 dxdy
\]  

(3.54)

where \( \hat{O}(x,y) \) and \( \hat{P}_i(x,y) \) are the estimates of the object function and the PSF for different defocus values. Now the phase retrieval becomes how to find a solution \( \phi(u,v) \) that minimizes the \( E \)-metric in Eq. (3.54), which is identical to the solution search in the phase retrieval with one image observation.\textsuperscript{142,143,149} Paxman et al showed that this is equivalent to the maximum-likelihood estimate.\textsuperscript{151} According to Parseval’s theorem, the \( E \)-metric can be computed in the spatial frequency domain and the Fourier transform of \( \hat{O}(x,y) \) should satisfy

\[
\hat{O}(u,v) = \frac{\sum_{i=1}^2 \hat{P}_i^*(u,v) I_i(u,v)}{\sum_{i=1}^2 |\hat{P}_i(u,v)|^2}.
\]  

(3.55)

Then applying Eq.(3.55) in Eq. (3.54), the \( E \)-metric becomes

\[
E = \iint \frac{\left[ I_1(u,v) \hat{P}_2(u,v) - I_2(u,v) \hat{P}_1(u,v) \right]^2}{\left| \hat{P}_1(u,v) \right|^2 + \left| \hat{P}_2(u,v) \right|^2} dudv
\]  

(3.56)

Extensive studies on the optimal diversity selection were given by Dean and Bowers\textsuperscript{31} and Dolne et al.\textsuperscript{157} By making the maximum contrast of the defocused PSF image, Dean and Bowers showed that the optimal diversity defocus value can be determined by

\[
\hat{a}_{\text{max}} = \pm \frac{v_o^2}{4(2n + 1)}n = 0,1,2,3,\ldots,
\]  

(3.57)

where \( v_o \) is the dominant spatial frequency of the wavefront under test. We should avoid the diversity defocus values that yield minimum contrast of the defocused PSF image, which are
determined by\textsuperscript{31}

\[ \hat{a}_{\text{min}} = \frac{\pm \nu^2}{8n}, \quad n = 0,1,2,3,\cdots, \]

They showed that the phase retrieval convergence is relatively quick for small defocus values, but the large-defocused phase retrieval is more accurate, which is advantageous for the recovery of higher-spatial-frequency phase aberrations.\textsuperscript{31}

Brady and Fienup proposed a phase retrieval algorithm for any arbitrary desired plane,\textsuperscript{158} and more extensive studies on the phase diversity by many authors can be found in recent literatures.\textsuperscript{159,160,161,162,163,164,165,166,167,168,169,170,171,172}

### 3.5 Comparisons and Summary

In this section, we compare the phase retrieval and the phase diversity techniques with the S-H slope sensor and Roddier’s curvature sensor.

#### 3.5.1 Phase diversity technique and the S-H sensor

The phase diversity technique employs two or more channels of diversity data to determine the phase aberrations, which provides information that makes the phase aberrations more uniquely identified than would a standard single channel of conventional image data.\textsuperscript{173}

In summary, except for its intensive computation, the phase diversity method has the following practical advantages over standard techniques such as the S-H slope sensor: (1) The phase diversity method requires minimum of optics, and (2) the phase diversity method is vibration-insensitive. (3) The spatial scales on the aberrations sensed can be easily changed. (4) The phase
diversity method can be used for phase retrieval with both point or extended sources. (5) The phase diversity method can work for phase retrieval with a discontinuous wavefront, such as in a segmented mirror figure testing.

3.5.2 Phase diversity technique and Roddier’s curvature sensor

Roddier’s curvature sensor measures the irradiance of the wavefront near the focus for estimating curvature information, which belongs to amplitude-based wavefront sensing. Campbell, et al asserted that if the two intensity measurements are taken symmetrically about the system input pupil (or equivalently about the image focal plane), the phase diversity method becomes a curvature-sensing algorithm (Campbell, et al 2004).174

However, because the wavefront estimation for Roddier’s curvature sensor is directly based on wavefront curvature not on wavefront amplitude, Roddier’s curvature sensor and the phase diversity method are different in principle.175 (1) Their wavefront estimation algorithms are different. The phase diversity method provides a joint estimate of the object and the wavefront aberrations, whereas the Roddier curvature sensor yields the estimate of wavefront aberrations only. (2) Their data measurements are performed at different distances from the focal plane. The plane of phase diversity measurement is only several wavelengths away from the focal plane, which is inside of the caustic zone, but Roddier’s curvature sensor measures data symmetrically in two planes which are at least several hundreds of wavelengths away from the focal plane to keep away from the caustic zone. (3) The phase diversity requires no apriori knowledge of the object and works well with extended objects, whereas the Roddier curvature sensor requires the object to be a point source. (4) The phase diversity can work with a continuous or discontinuous
wavefront, but Roddier’s curvature sensor works with continuous wavefront only. (5) Roddier’s curvature sensor works well with both monochromatic light and broadband light, whereas the phase diversity works with monochromatic light. The expansion to broadband would require further investigations.175

Whenever a parameter is being estimated by using random data, the accuracy of the estimate is fundamentally limited by the randomness of the data. This is intuitive and quantified by the Cramér–Rao theorem.176 The smallest possible unbiased estimator variance for a given estimation problem is given as the Cramér–Rao lower bound (CRLB).177,178,179 Fienup showed that by applying the CRLB the measurements of the phase diversity inherently possesses more information on phase aberrations than Roddier’s curvature sensor,175 which works on a large defocus. Therefore, the wavefront estimation with phase diversity can achieve a higher accuracy.

3.5.3 Summary

Wavefront phase retrieval methods are based on irradiance measurements, which employ phase deconvolution algorithms with iterative Fourier transform operations. The intensive computation for phase retrieval from image irradiance measurements is the main disadvantage of the phase diversity technique. However, with the developments of computing technology and the phase retrieval technique, there is potential for the phase diversity technique to yield a real-time wavefront sensing technique.
CHAPTER FOUR: ITERATIVE SLOPE-BASED WAVEFRONT ESTIMATION FOR ANY SHAPED PUPILS

Various methods and algorithms for wavefront estimation have been reviewed in Chapter 3. Of most interest among them are those that can handle general pupil shapes. Such algorithms can be categorized into either FT-based algorithms or linear least-squares-based algorithms. For FT-based algorithms, Gerchberg and Saxton in 1972 proposed iterative phase retrievals from amplitude measurements in the aperture and the image planes.\textsuperscript{137} Freischlad and Koliopoulos in 1985 proposed a DFT-based modal estimation from wavefront slope measurements for square-shaped pupils.\textsuperscript{118,119} Later on, Freischlad extended this algorithm to handle general pupil shapes by introducing additional least-squares equations for creating the missing slope data outside of the original pupil to make a square one.\textsuperscript{120} Roddier & Roddier proposed a FFT-based algorithm for irregular shaped pupils by extrapolating the wavefront slopes outside the pupil using the Gerchberg-Saxton method.\textsuperscript{92,93} Zou and Zhang established a pre-defined linear least-squares-based matrix equation for any pupil shape by setting the slope data outside the original pupil to zero (Zou & Zhang 2000),\textsuperscript{11} but this method introduces large deviation errors in the estimated wavefront (i.e. up to $\lambda/4$ peak-to-valley), which may not be acceptable for most optical tests.

Usually, changes in the pupil shape or size will cause changes in the wavefront estimation matrix and require a new setup of the wavefront estimation process for each new size or shape, which can be time-consuming in optical testing, especially when the grid size is large. Thus, a mathematical formulation that can automatize the wavefront estimation for any size and shape pupil would not only improve the efficiency of the testing process but also minimize potential errors necessarily associated in setting up a new wavefront estimation matrix.
While the Zou and Zhang’s least-squares algorithm suffers from large deviation errors due to the discontinuity across the original pupil boundaries, its strength is that it creates a pre-defined matrix for wavefront estimation, and provides an immediate basis function for effective wavefront estimation from slope measurements for any pupil shape or size. By adding a Gerchberg-Saxton iterative process, in this chapter we propose to develop an iterative algorithm for wavefront estimation based on the pre-defined matrix equation. This process will enable extrapolating the slope data outside the pupil, and thereby satisfy the continuity of the wavefront slope inside the extended domain, which is required by Neumann boundary problem.

### 4.1 Proposed wavefront estimation algorithm for any size and pupil shape

The pre-defined wavefront estimation matrix established by Zou and Zhang\textsuperscript{11} will be used in this chapter for wavefront estimation in the proposed method. The Southwell sampling geometry will be adopted because of its superiority over other geometries in error propagation as we will discussed in Chapter 5. As illustrated in Figure 3.2, the Southwell geometry is characterized by taking the wavefront slope measurements and wavefront values estimation at the same nodes.

#### 4.1.1 Pre-defined matrix equation for wavefront estimation

In a problem with discrete slope measurements as a starting point, a 2-D array of discrete values \( w_i (i=1, 2, 3, \ldots t \times t) \) was used to map the estimated wavefront values. An interlaced array of \( j \) nodes was introduced to facilitate the estimation of wavefront slopes at the midpoints
between wavefront nodes. Figure 4.1 shows the geometry in one direction (e.g. the y-direction) with both the nodes \(i\) and the interlaced nodes \(j\). The slope data between two neighboring points is assumed to change linearly with distance, which allows performing linear interpolation to estimate the slope between nodes.

Figure 4.1 The double sampling grid systems illustrated in the y-direction

Suppose the wavefront travels in the x-direction, the wavefront slopes at the nodes \(i\) in the y and z directions are denoted as \(s_{yi}\) and \(s_{zi}\) \((i=1, 2, 3... t \times t-1, i \neq t)\), respectively. The slope at node \(j\) in the y-direction is then estimated as an average of the slopes at nodes \(i\) and \(i+1\) by

\[
s_{yi} = \frac{1}{2} \left( s_{yi} + s_{yi+1} \right), \tag{4.1}
\]

where the slope \(s_{yi}\) could also be expressed as a quotient of the wavefront value difference at nodes \(i\) and \(i+1\) and their separation \(a\), so that

\[
s_{yi} = \frac{w_{i+1} - w_i}{a}. \tag{4.2}
\]

By combining Eq.(4.1) and Eq.(4.2) the relationship between the wavefront slopes and the wavefront values at \(i+1\) and \(i\) is established as
\[ w_{i+1} - W_i = \frac{a}{2} (s_{y_i} + s_{y_{i+1}}). \] (4.3)

Similarly in the z direction, according to the sign convention shown in Figure 4.1, the relationship follows

\[ w_i - W_{i+1} = \frac{a}{2} (s_{z_i} + s_{z_{i+1}}). \] (4.4)

Figure 4.2 The domain extension for an irregular-shaped pupil

The pre-defined wavefront estimation model of Zou and Zhang follows these steps:\textsuperscript{11}

1. Without loss of generality, the regular square net has a \( t \times t = m \) grid points.

2. Furthermore, the original sampling domain \( \Omega_0 \) (i.e. exit pupil, simply connected domain or multiple connected domains) is embedded into a regular square domain \( \Omega_1 \) that contains the sampling domain \( \Omega_0 \). Then the square domain \( \Omega_1 \) can be thought as being composed of two parts: the real part \( \Omega_0 \) and the imaginary part \( \Omega_1 \backslash \Omega_0 \), both shown in Figure 4.2.
3. The grid points in $\Omega_1$ are indexed sequentially from 1 to $m$ row by row (the grid points could also be indexed equivalently column by column as an alternative). This numbering mode is referred to as the serial number scheme (SNS).

4. The slopes were set to zero in the imaginary part $\Omega_1 \setminus \Omega_0$.

With such a numbering mode, Eq. (4.3) and Eq.(4.4) can be written in matrix form as

$$\begin{bmatrix}
-w_1 & -1 & 1 & 0 & \cdots & 0 & -1 \\
-w_2 & -1 & 1 & 0 & \cdots & 0 & -1 \\
\vdots & \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\
-w_t & -1 & 1 & 0 & \cdots & 0 & -1 \\
\end{bmatrix} \begin{bmatrix}
w_{t+1} \\
w_{t+2} \\
\vdots \\
w_{m-2t+1} \\
w_{m-2t+2} \\
\vdots \\
w_{m-t} \\
w_{m-t+1} \\
w_{m-1} \\
w_m \\
\end{bmatrix} = \begin{bmatrix}
c_{2,1} \\
c_{3,2} \\
\vdots \\
c_{t+1,t-1} \\
c_{t+2,t+1} \\
\vdots \\
c_{m-1,m} \\
d_{t+1,t} \\
d_{t+2,t} \\
\vdots \\
d_{m-1,m-t} \\
d_{m,m-t} \\
\end{bmatrix}, \quad (4.5a)$$

or

$$CW = S, \quad (4.5b)$$

where $c_{i+1,i}$ and $d_{i+1,i}$ are defined as

$$\begin{align*}
  c_{i+1,i} &= \frac{a}{2} \left( s_{y_{i+1,t}} + s_{y_i} \right), \\
  d_{i+1,i} &= \frac{a}{2} \left( s_{z_{i+1,t}} + s_{z_i} \right). \quad (4.6)
\end{align*}$$

The corresponding normal equation set can be written as
The original test pupil is embedded into a larger square domain to obtain the pre-defined matrix that is good for any test pupil shape. After the “zero point” of the estimated wavefront is determined, the matrix equation becomes positive. The Cholesky decomposition method can be employed in solving the normal matrix equation. However, results are limited by up to $\lambda/4$ peak-to-valley deviation errors, which are shown in Figure 4.3.

Figure 4.3 Non-iterative wavefront estimation with pre-defined matrix
(a) Ground-truth or original wavefront (b) Wavefront estimated by the non-iterative pre-defined matrix equation (c) Wavefront deviation error map as the difference between (a) and (b)

In Figure 4.3 (a), the original wavefront is an estimated wavefront that is considered to represent ground truth for wavefront estimation as will be further explained in Section 4.2. The estimated wavefront from slope data with the pre-defined matrix equation is shown in Figure 4.3 (b). The difference between the estimated and the original wavefronts is shown in Figure 4.3(c), which represents the deviation errors associated with the domain extension made across the boundary. Therefore, while the domain extension technique is quite useful for developing a regular pre-defined estimation matrix for any irregular pupil shapes, the challenge lies in how to
remove the deviation errors in the estimated wavefront. A least-squares-based Gerchberg-Saxton iterative process will be established to make a smooth slope extrapolation and thereby minimize the deviation error in the estimated wavefront.

4.1.2 Wavefront slope computations

The proposed algorithm will first require calculating slope data in the extended domain from the estimated wavefront in iteration in order to enable an iterative process. Such computations will be first presented.

Slope computation from a given wavefront could be thought simply as the inverse problem of wavefront estimation from slope data. In this case, one would inverse the equations established in Section 4.1.1 to obtain a matrix equation set for slope computation. However, such a resultant matrix is rank-deficient, which is intrinsically linked to the Southwell geometry chosen for the problem. The Southwell geometry is optimal in terms of noise propagation and thus will be conserved in the algorithm. Therefore, additional independent equations will be needed for slope extractions from a given wavefront. Such equations are chosen to be established based on curvature estimates. We shall first describe the matrix formulation for the wavefront slope computations in the y-direction, and then provide the matrix formulation for the z-direction computation.

4.1.2.1 Wavefront y-slope computation

For the slope at the midpoint between the nodes \( i \) and \( i+1 \), Eq. (4.3) may be written as
\[ s_{y_{i+1}} + s_{y_i} = e_j , \]  
\text{(4.8)}

where

\[ e_j = \frac{2}{a} \left( w_{i+1} - w_i \right), i=1, 2 \ldots m-1, \text{ but } i \neq t, 2t, 3t, \ldots m. \]  
\text{(4.9)}

In matrix form, Eq. (4.8) may be written as

\[ A_s y = E , \]  
\text{(4.10)}

which is not a full-rank matrix equation set. Curvature-based equations are then considered to determine a unique solution for slope computation. As illustrated in Figure 4.1, the curvature at a midpoint node \( j+1 \) is proportional to the slope difference between adjacent points \( i+1 \) and \( i+2 \). According to Figure 4.1, we have

\[ s_{y_{i+2}} - s_{y_{i+1}} = f_{j+1} , \]  
\text{(4.11)}

where

\[ f_{j+1} = \frac{1}{2a} \left( w_{i+3} - w_{i+2} - w_{i+1} + w_i \right) \]  
\text{(4.12)}

If Eq. (4.12) is divided by the grid separation \( a \), it will actually be a discrete approximation of the wavefront curvature at node \( j+1 \), which is of \( O(a^3) \) precision as shown in Eq. (A12) in APPENDIX. In matrix form, Eq. (4.11) may be expressed as

\[ A_2 S_y = F . \]  
\text{(4.13)}

Combining Eq. (4.10) and Eq. (4.13), a matrix-form equation set may be written as

\[ A S_y = U , \]  
\text{(4.14)}

where

\[ A = \begin{bmatrix} A_1 \\ A_2 \end{bmatrix} , \]  
\text{(4.15)}
\[ \mathbf{S}_y = \begin{bmatrix} s_{y1} & s_{y2} & \cdots & s_{ym} \end{bmatrix}^T, \quad (4.16) \]

\[ \mathbf{U} = \begin{bmatrix} \mathbf{E} \\ \mathbf{F} \end{bmatrix}, \quad (4.17) \]

with

\[ \mathbf{A}_1 = \text{diag}(\mathbf{D}_1, \mathbf{D}_1, \cdots, \mathbf{D}_1), \quad (4.18) \]

\[ \mathbf{A}_2 = \text{diag}(\mathbf{D}_2, \mathbf{D}_2, \cdots, \mathbf{D}_2), \quad (4.19) \]

where

\[ \mathbf{D}_1 = \begin{bmatrix} 1 & 1 \\ & 1 & 1 \\ & & \ddots & \ddots \\ & & & 1 & 1 \end{bmatrix}, \quad (4.20) \]

and

\[ \mathbf{D}_2 = \begin{bmatrix} -1 & 1 \\ & -1 & 1 \\ & & \ddots & \ddots \\ & & & -1 & 1 \\ & & & & -1 & 1 \end{bmatrix}. \quad (4.21) \]

Then the normal equation set for wavefront slope extraction in the y-direction can be written as

\[ \mathbf{A}^T \mathbf{A} \mathbf{S}_y = \mathbf{A}^T \mathbf{U}. \quad (4.22) \]

### 4.1.2.2 Wavefront z-slope computation

Similarly, the slope-based equations along the z-direction are given by

\[ s_{z_{1i}} + s_{z_{2i}} = g_j, \quad i=1, 2, \ldots, m-t, \quad (4.23) \]
where

\[ g_j = \frac{2}{a} (w_j - w_{i_1}) \]  \hspace{1cm} (4.24)

In matrix form, Eq. (4.23) may be written as

\[ \mathbf{B}_i \mathbf{s}_z = \mathbf{G} \]  \hspace{1cm} (4.25)

which is not a full-rank matrix equation. To get a full-rank equation set, the curvature-based equations can be added

\[ s_{z,i} - s_{z,i+2t} = h_{j+t}, \]  \hspace{1cm} (4.26)

where

\[ h_{j+t} = \frac{1}{2a} \left( w_i - w_{i+t} - w_{i+2t} + w_{i+3t} \right), \]  \hspace{1cm} (4.27)

and \( i=1,2,\ldots t, t+1, t+2, \ldots 2t-3,\ldots, m-3t \). The derivation of Eq. (4.27) is given as Eq.(A14) in APPENDIX. In matrix form, Eq.(4.26) becomes

\[ \mathbf{B}_s \mathbf{s}_z = \mathbf{H} \]  \hspace{1cm} (4.28)

Combining Eqs. (4.25) and (4.28) in a matrix-form equation set, we obtain

\[ \mathbf{B} \mathbf{S}_z = \mathbf{V}, \]  \hspace{1cm} (4.29)

where

\[ \mathbf{B} = \begin{bmatrix} \mathbf{B}_1 \\ \mathbf{B}_2 \end{bmatrix}, \]  \hspace{1cm} (4.30)

\[ \mathbf{S}_z = \begin{bmatrix} s_{z1} & s_{z2} & \cdots & s_{zm} \end{bmatrix}^T, \]  \hspace{1cm} (4.31)

\[ \mathbf{V} = \begin{bmatrix} \mathbf{G} \\ \mathbf{H} \end{bmatrix}, \]  \hspace{1cm} (4.32)

and
Then the normal equation set for the z-direction slope extraction may be written as

\[ \mathbf{B}^T \mathbf{B} \mathbf{s}_z = \mathbf{B}^T \mathbf{v}. \]  

(4.36)

### 4.1.3 Least-squares-based Gerchberg-Saxton iterative algorithm

Given the pre-defined linear least-squares matrix equation sets established for wavefront slope computation and wavefront estimation, we shall now detail the least-squares-based Gerchberg-Saxton iterative wavefront estimation algorithm, which is illustrated in the flow chart in Figure 4.4 (Zou and Rolland 2005). Using Eq. (4.7), as shown in Figure 4.2, the wavefront values are first estimated from the slope data in \( \Omega_1 \), which are the original slope measurements inside the original pupil and zero outside it. The matrix equation sets given by Eqs. (4.22) and (4.36) then serve to compute the slopes in the y- and z-directions from the estimated wavefront.
in \( \Omega_j \). The computed slopes are compared with the original slope data within \( \Omega_o \). If the differences are negligible (i.e. less than a termination criterion), the estimated wavefront over \( \Omega_j \) is output, where only the wavefront within \( \Omega_o \) is of interest. Otherwise, the computed slope data in \( \Omega_o \) are replaced with the original measured slope data, while the computed slope data in the extended area \( \Omega_j \setminus \Omega_o \) (i.e. outside \( \Omega_o \) but within \( \Omega_j \)) are kept unchanged. Based on the updated slope data, the wavefront estimation for the next iteration is performed. The iterative process continues until the established termination criterion is reached.

Such an iterative process is referred to as a Gerchberg-Saxton-type iteration, because the iterative process bears analogy to the Gerchberg-Saxton algorithm, which consists of substituting the computed amplitude of a complex function with the sampled amplitude across iterations until both amplitude and phase converge to a solution. The iterative algorithm presented in this dissertation substitutes the computed slope data in the test pupil with the sampled raw slope data iteratively until the estimated wavefront converges to a solution.

The algorithm proposed here bears similarity to the algorithm proposed by Roddier and Roddier (1991) in the sense that both algorithms use Gerchberg-Saxton-type iterations to extrapolate the wavefront slope function outside the boundary. The basic difference between the two algorithms lies in that the Roddier and Roddier’s algorithm is based on the Fourier transform, which is also the case of the Gerchberg-Saxton algorithm, but the algorithm proposed here is based on the linear least-squares equations. Therefore, a significant advantage of the algorithm proposed here is that it does not suffer from the \( 2\pi \)-phase ambiguity, while the Fourier transform-based algorithms do.
Figure 4.4 Flow chart of the least-squares-based Gerchberg-Saxton-type iterative wavefront estimation algorithm

Without the iterative process, the slope data crossing the original pupil boundaries between the original pupil $\Omega_0$ and the extended domain $\Omega_1 \setminus \Omega_0$ are not continuous, and such discontinuity yields severe errors in the wavefront estimation not only close to the edge of the pupil $\Omega_0$ but also within the pupil $\Omega_0$, as shown in Figure 4.3. The iterative process enables a continuous practical extrapolation of the slope data outside the original pupil $\Omega_0$, while it does
not interfere with the internal region of $\Omega_0$. The iterative algorithm converges quickly to an unbiased solution, while at the same time the smoother the wavefront surface under construction the smaller the residue deviation error as expected, and the fewer iterations needed. The deviation error of this unique solution will decrease to zero in theory, but the measurement noise prohibits it from reaching zero, so it staggers to its minimum.

4.2 Examples and Results

Two examples are presented for validating and assessing the capability of the proposed algorithm across irregular shaped pupils: one with a circular 30-mm-diameter pupil, and another with the same size pupil but with a 10% central obscuration inside. Both data sets were acquired from a previous experiment reported in a previous paper.\textsuperscript{11} The sampling grids for both cases had a pitch area of 2×2mm\textsuperscript{2}. They were located at the pupil position, which was conjugated to a 500-mm diameter mirror under test. The wavefront with 10% central obscuration was obtained by considering the slope data within the unobstructed part of the pupil only.

In order to establish the ground truth for each example, we estimated the wavefront from the same set of slope data without domain extension but with the conventional iterative or direct solution methods, such as the Jacobi iterative method, the Gauss elimination method, or the Cholesky decomposition method, etc.\textsuperscript{11, 181} All these methods yield exactly the same estimated wavefront, which we thus consider to represent the ground truth (i.e. the original wavefront, for example in Figure 4.3: (a)), against which the proposed iterative wavefront estimation algorithm could be assessed.
4.2.1 Case 1: Circular pupil without central obscuration

A circular pupil without obscuration is a simply connected domain. The considered 30-mm diameter pupil with an array of 161 S-H grid points is shown in Figure 4.5. The grid points outside the circular pupil in the square domain are the imaginary points. The ground-truth wavefront is shown in Figure 4.5(b).

The deviation error maps of the wavefront estimated by the proposed Gerchberg-Saxton-type iterative algorithm through several iterations (i.e. $i=0, 1, 2, 3, 4, 13$) are shown in Figure 4.6. Results show that for $\lambda=632.8\text{nm}$, the RMS deviation errors were reduced from $\lambda/16$ to $\lambda/129$ after 13 iterations, where it reaches its minimum. The residual deviation error is 12% of its original value and 88% of the deviation error was removed.

![Figure 4.5](image)

(a) A 30-mm diameter circular pupil within the extended domain $\Omega_j$. (b) The ground-truth wavefront within the circular pupil $\Omega_0$ on a vertical scale of $\pm1\mu$m.
Figure 4.6 Wavefront deviation error (on scale of ±1µm) for a 30 mm-diameter circular pupil with iterations i=0, 1, 2, 3, 4, and 13, respectively (λ=632.8nm).

4.2.2 Case 2: Circular pupil with a 10% central obscuration

A 30-mm circular pupil with a 10% central obscuration is shown in Figure 4.7. Such a percent of obscuration is common for astronomical telescope mirrors. The deviation error maps of the wavefront values estimated by the proposed Gerchberg-Saxton-type iterative algorithm through several iterations (i.e. i=0, 1, 3, 5, 7, 10) are shown in Figure 4.8. Results show that for λ= 632.8nm the RMS deviation errors were reduced from λ/14 to λ/154 after 10 iterations, where it reaches its minimum. The residual deviation error is 9% of its original value, and 91% of the deviation error was removed.
Figure 4.7 (a). A 30-mm diameter circular pupil with a 10\% central obscuration.

(b). A ground-truth wavefront at this pupil $\Omega_p$ on a vertical scale of $\pm 1\mu m$ (right).

$i=0$, rms=$\lambda/14$ 

$i=1$, rms=$\lambda/26$ 

$i=3$, rms=$\lambda/63$

$i=5$, rms=$\lambda/107$ 

$i=7$, rms=$\lambda/135$ 

$i=10$, rms=$\lambda/154$

Figure 4.8 Wavefront deviation error (on scale of $\pm 1\mu m$) for a 30 mm-diameter circular pupil with a 10\% central obscuration through iterations $i=0$, 1, 2, 3, 4, 10, respectively ($\lambda=632.8$nm).
4.2.3 Algorithm convergence

The deviation error reduction through Gerchberg-Saxton-type iterations was found to be efficient. Specifically, the final deviation errors after a maximum of 4 iterations for the two examples considered are less than $\lambda/100$ for $\lambda$ equal to 632.8nm, as shown in Figures 4.6 and 4.8. The convergence indicated by the RMS wavefront error in units of wavelength as a function of the number of iterations is plotted in Figure 4.9. Such a finding is high performance for optical testing, and the algorithm can be said to be very efficient.

![Figure 4.9 Plot of RMS deviation errors as a function of the number of iterations](image)

Figure 4.9 Plot of RMS deviation errors as a function of the number of iterations
4.3 Computational complexity

In the proposed iterative wavefront estimation algorithm, there are three linear matrix equation sets that need to be solved at each iteration: One is the matrix equation set for wavefront estimation from the slope data, and the other two are the matrix equation sets for y-slope and z-slope computations from the estimated wavefront across iterations. The three matrix equation sets are highly sparse. If we define a fill-in factor, an indicator of matrix sparseness, as the quotient of the number of nonzero elements to the total number of the matrix elements, then the fill-in factor of the wavefront estimation matrix $C^T C$ is $(5t - 4)/t^3$, and the fill-in factors of the slope computation matrices $A^T A$ and $B^T B$ are both $(t + 4)/t^3$. For example, the fill-in factors of the wavefront estimation matrix and the slope computation matrices are 4.6% and 1.4% respectively for $t=10$, and they decrease to 0.05% and 0.01% at $t=100$. Besides their high sparsity, all three matrices are symmetrical, positive and banded, once the wavefront “zero-point” has been determined for the wavefront estimation.

4.3.1 Computational complexity of the proposed iterative algorithm

The computational complexity includes the spatial complexity and the time complexity. The spatial complexity is a measure of memory needed for computation when the algorithm runs, whereas the time complexity measures how much computation (thereby computation time) is needed for the algorithm to converge to the solution.
4.3.1.1 **Spatial complexity**

The extremely regular and symmetrical banded matrices of the three linear equation sets allow mapping the estimation matrix as a function of the index number of the matrix rows and columns, because the nonzero elements in these matrices are regularly patterned with the numbers 4,3,2,1,-1 only. Thus the problem of matrix storage is avoided in solving each equation except for about $t^3$ elements memory space reserved for the banded Cholesky decomposition of $C^TC$, which is a much smaller part in comparison with the $t^4/2$ element space needed for a conventional Cholesky decomposition. Naturally, a memory space of $3t^2$ elements is necessary in each linear equation for storing the slope data and the wavefront values.

4.3.1.2 **Time complexity (Impact on computation time)**

Before we discuss the computational complexity of our algorithm, we shall introduce “FLOPS”, an abbreviation of “Floating-Point Operations”, to denote the arithmetic operations that a computer performs, such as multiplications, additions (or subtractions). 

The positive definite slope-extraction matrices $A^TA$ and $B^TB$ are banded diagonal matrices with their semi-bandwidths of 2 and $t$, respectively. In computing the slope data from a given wavefront, it is an advantage to employ a direct solution method, such as the Cholesky method, because we can decompose the matrices $A^TA$ or $B^TB$ into two unique triangular matrices once and for all by several steps of derivation. Therefore no more Cholesky decompositions are needed in computation. The computations needed in solving the two systems of equations are substitutions, and the corresponding arithmetic cost is approximately a product of $4m$ with the
bandwidth,\textsuperscript{182} which yields $8t^2$ FLOPS for $A^T A$ and $4t^3$ FLOPS for $B^T B$. As a comparison, the computational cost needed for substitutions in solving an equation without exploiting the band structure is $2t^4$ FLOPS.\textsuperscript{182}

To solve the matrix equation set for wavefront estimation, we need to set a “zero-point” for the wavefront under estimation to make the matrix $C^T C$ positive and definite so that we can make Cholesky decomposition with $C^T C$, which is a banded sparse matrix with a bandwidth of $2t$. An algorithm for solving the wavefront estimation equations based on the banded Cholesky decomposition needs about $t^4 + 4t^3$ FLOPS in total, where $t^4$ FLOPS is used for decomposition and $4t^3$ FLOPS for substitutions.\textsuperscript{182} As a comparison, a solving algorithm based on the conventional Cholesky decomposition without exploiting the band structure of the matrix yields about $\frac{1}{3} t^6$ FLOPS for decomposition and $2t^4$ FLOPS for substitutions.

Other direct solution methods are also available in solving the above three equation sets, such as Gaussian Elimination and SVD methods, but such methods are more computationally intensive. Generally, the conventional Gaussian Elimination method has a cost of about $\frac{2}{3} t^6$ FLOPS, and the SVD method needs about $12t^6$ FLOPS.\textsuperscript{183} Because the SVD method yields a unique LSMN for a rank deficient least-squares problem, it is a good method in practice if the computational complexity is not a constraint.

An alternative to solving the matrix equation set is to use iterative methods, such as the SOR method, which is said to be one of the most efficient among the classical iterative methods. The convergence rate of the SOR method is closely related to the problem model, the discretization mesh size, the relaxation factor, and the grid indexing orders. However, the iterations needed for
the optimal SOR method to converge to a solution within a precision of $10^{-8}$ can be estimated by

$$R_{\text{orb}} = -8\left(\frac{\log_{10}(1 - \frac{2\pi}{t - 1})}{t - 1}\right)^{-1} \approx 2.94(t + 1) \approx 3t.$$ (4.37)

So if it requires approximately $5t^2$ FLOPS operations in iteration, the computational cost needed for solving Eq. (4.7) with the optimal SOR method is about $15t^3$ FLOPS.

Comparing with the banded Cholesky decomposition method, which needs $t^4 + 4t^3$ FLOPS of cost for solving Eq. (4.7), the SOR method is computationally more intensive for a small grid size ($t<11$), and less intensive for a large grid size ($t>11$). The complexity of the optimal SOR method increases as a cubic curve, whereas the complexity of the banded Cholesky method increases with a quartic curve.

### 4.3.2 Complexity comparison with the FFT-based iterative algorithms

#### 4.3.2.1 Comparison of time complexity

The fast Fourier transform (FFT) of a data set of length $m = 2^q$ ($q$ is a positive integer) requires about $m\log_2(m)$ complex multiplications, which is equivalent to $5m\log_2(m)$ FLOPS of arithmetic operations according to a detailed analysis (Brigham 1988). The FFT-based iterative algorithm proposed by Roddier and Roddier(1991) needs to compute two FFTs besides the computations of the y- and the z-slopes from the wavefront at each iteration. Therefore, if we suppose that the computation of the slope extractions takes the same computational cost in
both algorithms and we ignore this cost, the computational cost needed in one iteration of the FFT-based iterative algorithm is about \((20\log_2(t) + 7)t^2\) FLOPS, which is usually much smaller than that of the optimal SOR-based (i.e. \(15t^3\) FLOPS) iterative algorithm. Thus, based on the computational complexity evaluation of one iteration, the FFT-based algorithm is superior in performance to the proposed algorithm, which could be significant for large values of grid-array size \(t (t \times t = m)\).

At the same time, the required number of iterations for each algorithm will significantly affect the overall computational time. The number of iterations is a factor of the overall grid-array size and measurement noise levels, etc. The FFT-based algorithms usually converge slowly; for example, the Gerchberg-Saxton algorithm needs at least tens to hundreds or even thousands of iterations to converge to a solution, while we found that the algorithm proposed in this paper converges to less than \(\lambda/100\) deviation error with only four iterations.

### 4.3.2.2 Comparison of spatial complexity

It has been established that the space complexity required for a Fast Fourier Transform (FFT) is \(O(t^4)\), which is used for the storage of complex matrix arrays. As a comparison, the spatial complexity for the Gerchberg-Saxton-type iterative algorithm we have proposed with the banded Cholesky solution method is only \(O(t^3)\).

Some relatively subtle difference between the Roddier & Roddier (1991) algorithm and the algorithm proposed here is the fact that in performing FFTs, the square array matrix satisfies \(m = 2^q\), and therefore \(m\) must be even. In the case of the proposed algorithm, there is no such...
requirement, and we have shown that odd matrix sizes yield lower error propagation than even matrix sizes.

4.4 Error propagation estimation

If we ignore the perturbations introduced by the computer rounding errors, wavefront errors may occur from two sources: the algorithm discretization errors, which depend on the basic estimation scheme adopted, and the wavefront sensor measurement error such as the CCD centroiding error. The discretization errors of the wavefront estimation scheme adopted were discussed in a previous literature. In this section, we qualitatively study the propagation of the wavefront measurement error in wavefront estimation by evaluating the condition number of the wavefront estimation matrix. The quantitative analysis of the error propagation in wavefront estimation will be detailed in Chapter 5.

The condition number of a wavefront estimation matrix is an amplification factor for the error propagation in wavefront estimation. Regarding the pre-defined wavefront estimation matrix equation in Eq. (4.7), the condition number of $C^T C$ can be defined as

$$
\text{cond}(C^T C) := \text{lb}_2(C^T C) \text{lb}_2\left[(C^T C)^{-1}\right],
$$

(4.38)

where $\text{lb}_2(\cdot)$ is a matrix norm defined (for example, for matrix $C$) by

$$
\text{lb}_2(C) = \max_{X \neq 0} \left( \frac{X^T C^T C X}{X^T X} \right)^{1/2} = \left[ \rho(C^T C) \right]^{1/2},
$$

(4.39)

which is a corresponding matrix norm of the Euclidian norm of a vector $X$ $\|X\|_2 = \left( X^T X \right)^{1/2}$. Then we have

95
\[ \text{cond}(C^T C) = \rho(C^T C) \rho[(C^T C)^{-1}], \quad (4.40) \]

where \( \rho(C^T C) \) is the spectral radius of \( C^T C \). Since \( \rho(C^T C) = |\lambda_{\text{max}}| \), then \( \rho[(C^T C)^{-1}] = |\lambda_{\text{min}}|^{-1} \), where \( \lambda_{\text{max}} \) and \( \lambda_{\text{min}} \) are the maximum and minimum eigenvalues of the matrix \( C^T C \), respectively. Therefore the condition number of \( C^T C \) can be written as

\[ \text{cond}(C^T C) = \frac{|\lambda_{\text{max}}|}{|\lambda_{\text{min}}|}. \quad (4.41) \]

If matrix \( C^T C \) is invertible, the wavefront estimation error \( \Delta W = (\Delta w_1, \Delta w_2, \ldots, \Delta w_m)^T \) can be estimated by

\[ \Delta W = (C^T C)^{-1} C^T \Delta S_{\text{WFD}}, \quad (4.42) \]

where \( \Delta S_{\text{WFD}} \) is the WFD measurement error vector. Applying Euclidian norm on both sides of Eq. (4.42) yields\(^{181, 11, 186}\)

\[ \|\Delta W\|_2 \leq \frac{\text{cond}(C^T C)^{\frac{1}{2}}}{\text{lub}_2(C)} \|\Delta S_{\text{WFD}}\|_2. \quad (4.43) \]

In Chapter 5, we will show that \( \Delta S_{\text{WFD}} = \frac{1}{2} a C_s \Delta S \) for the Southwell geometry, where \( a \) is the pitch size of the sampling grid array, \( \Delta S = (\Delta s_1, \Delta s_2, \ldots, \Delta s_m)^T \) is the wavefront slope error vector, and \( C_s \) is a matrix used to convert a slope vector to a WFD vector. Therefore

\[ \|\Delta W\|_2 \leq \frac{1}{2} a [\text{cond}(C^T C)]^{\frac{1}{2}} \left[ \frac{\text{lub}_2(C_s)}{\text{lub}_2(C)} \right]^{\frac{1}{2}} \|\Delta S\|_2 = \frac{1}{2} a \frac{\lambda_{\text{max}}}{\lambda_{\text{min}}} \|\Delta S\|_2, \quad (4.44) \]

where \( \lambda_{\text{max}} \) is the maximum eigenvalue of matrix \( C_s^T C_s \).

If the wavefront slope errors are independent and have the same variance \( \sigma_s^2 \), then
\[
\|\mathbf{AW}\|_2 = \sqrt{m} \left( \frac{1}{m} \sum_{i=1}^{m} |A_{wi}|^2 \right)^{1/2} = t\sigma_w',
\]

and

\[
\|\mathbf{AS}\|_2 = \sqrt{m} \left( \frac{1}{m} \sum_{i=1}^{m} |A_{si}|^2 \right)^{1/2} = t\sigma_s',
\]

where $\sigma_w'$ is the RMS value of the estimated wavefront error, and $\sigma_s'$ is the RMS value of the wavefront slope measurement error. Applying Eqs. (4.45) and (4.46) in Eq. (4.44) yields

\[
\sigma_w' \leq \frac{1}{2} \left[ \frac{\lambda_{s_{\text{max}}}}{\lambda'_{\text{min}}} \right]^{1/3} \sigma_s'.
\]

Eq. (4.44) and Eq. (4.47) provide estimations of the wavefront error, which can be expressed by the matrix eigenvalues. The condition number of the estimation matrix is an indicator of error propagation. When the condition number is large (i.e. it is an ill-conditioned problem), a small error in the slope measurements can cause a large error in the estimated wavefront.

Since the normal equation matrix is symmetric, the classical Jacobi method can be employed to compute the eigenvalues.\(^{187}\) For the wavefront estimation matrix in Eq. (4.7), the eigenvalues of this matrix are sensitive to the variation of the wavefront “zero-point” position, the matrix dimension size, and even the number parity of the matrix dimension. As shown in Figure 4.10, when the “zero point” is fixed at the center of wavefront, a curve of the condition number can be obtained by computing the matrix eigenvalues. By making a least-squares fitting of this curve, a formula for the condition number of the wavefront estimation matrix is available:
\[
\text{cond}(C^T C) = \begin{cases} 
-243.44 + 150.87 e^{\frac{t}{0.52}}, & \text{t is odd} \\
-355.16 + 223.75 e^{\frac{t}{0.33}}, & \text{t is even}
\end{cases}
\] (4.48)

where \( t \) is the matrix dimension number \((t \times t = m)\). Results show that the wavefront estimation has a better performance in error propagation when the dimension number of the estimation matrix is odd. Therefore, an odd-number sampling grid array is preferable in wavefront estimation. When the matrix dimension becomes larger, the Jacobi method converges slowly. It takes about 68000 iterations to obtain the eigenvalues with \(10^{-7}\) accuracy for the case of \(t=15\).

![Figure 4.10 The condition number of normal estimation matrix versus grid dimension size.](image)

The above analysis is also applicable to the error propagation of slope computation provided by Eqs. (4.22) and (4.36). The eigenvalues of the two slope-computation matrices in
Eqs.(4.22) and (4.36) are found to be $2 - \sqrt{2}$, $2 + \sqrt{2}$ and 4 when $t > 4$, and the eigenvalues are $2 - \sqrt{2}$ and $2 + \sqrt{2}$ only for $t = 4$. Thus the condition numbers of these two matrices are both $4/(2 - \sqrt{2}) \approx 6.83$ for $t > 4$, and $(2 + \sqrt{2})/(2 - \sqrt{2}) \approx 5.83$ for $t = 4$. Therefore, such condition numbers indicate that the error propagation in the $y$- (or equivalently $z$-) slope computation is very stable and very slow.

### 4.5 Summary

Klaus Freischlad in 1992 pointed out that a wavefront estimation algorithm that is suitable for practical optical testing must have the following characteristics: 1. The wavefront estimates must be unbiased; 2. The error propagation coefficient must be slow; 3. The computation must be efficient, especially for large datasets; 4. The necessary memory space should be small enough to be applicable in the laboratory; Finally, 5. the algorithm should be easily adaptable to various pupil shapes. In this chapter with the domain extension technique, a pre-defined wavefront estimation matrix and the associated pre-defined slope-computation matrices for any pupil shape or size were obtained. A Gerchberg-Saxton-type iterative process based on the linear least-squares estimation has been implemented to obtain a practical unbiased wavefront estimation algorithm for any pupil shape, which combines the accuracy of the Gerchberg-Saxton-type iterative wavefront slope extrapolation technique with the efficiency of linear sparse matrix.

In summary, the proposed iterative algorithm has the following features: 1. To our knowledge it is the first time that the Gerchberg-Saxton iterations were implemented by linear
least-squares matrix estimations. (2) It does not have the $2\pi$-phase ambiguity problem that all FT-based Gerchberg-Saxton algorithms suffer from, so it is good for phase retrieval with large aberrations. (3) It provides a once-for-all pre-defined wavefront estimation matrix that is good for any pupil size without apriori knowledge of the pupil shape. (4) It is a fast-converging iterative algorithm, which was demonstrated with some examples, that converges much faster than the FT-based Gerchberg Saxton algorithm. (5) It has high estimation accuracy. The deviation error can be less than $\lambda/150$ as shown in the examples. (6) Its error propagation is slow in wavefront estimation. An analysis of error propagation showed that the wavefront estimation matrix is well-conditioned, yielding low propagation errors.

A U.S. patent has been filed in the United States of America regarding this iterative wavefront estimation algorithm.\textsuperscript{188}
CHAPTER FIVE: QUANTIFICATIONS OF ERROR PROPAGATION IN WAVEFRONT ESTIMATION

5.1 Introduction

As discussed in Chapter 3, the wavefront estimation is a numerical solution to the Neumann’s boundary problem of Poisson equation. Using a 2-D finite difference grid to cover the testing domain, one can discretize this problem, and evaluate the wavefront values at each grid point by solving a difference equation set defined on the grid. The matrix equation set for this problem, as shown in Eq. (4.5b), can be expressed as

\[ \mathbf{C} \mathbf{W} = \mathbf{S}, \quad (5.1) \]

where \( \mathbf{C} \) is the wavefront estimation matrix, \( \mathbf{W} \) is the vector of wavefront values, and \( \mathbf{S} \) is the vector of the WFD between the neighboring grid points, which can be converted from the wavefront slope vector \( \mathbf{G} \) by

\[ \mathbf{S} = \mu a \mathbf{M} \mathbf{G}, \quad (5.2) \]

where \( \mu \) is a constant related to the given geometry, \( a \) is the pitch size of the sampling grid, and \( \mathbf{M} \) is the conversion matrix for a given geometry.

Owing to the measurement noise, Eq.(5.1) has weak solutions only, and an unbiased least-squares approximation can be employed. The normal matrix equation for the least-squares solution is

\[ \mathbf{C}^T \mathbf{C} \mathbf{W} = \mathbf{C}^T \mathbf{S}, \quad (5.3) \]
which is a discretization form of the Poisson equation as shown in Eq. (3.8). It shall be noted that
the Tikhonov regularized least-squares solution, adopted widely in other applications such as
adaptive optics, provides a biased estimate that would not be desirable in optical testing.\textsuperscript{189}

The noisy WFD vector can be written as $S = S_0 + N$, where $S_0$ is the vector of the true
WFD values, and $N$ is the measurement noise of the WFD. If the induced wavefront error from
measurement noise $N$ is $\varepsilon$, then the estimated wavefront can be written as $W = W_0 + \varepsilon$, where
$W_0$ is the true wavefront values. The error propagation coefficient provides a quantitative metric
for evaluating wavefront estimation. As defined in the previous literature,\textsuperscript{87,88,120} the error
propagation coefficient $\eta$ is the ratio of the mean variance of the wavefront estimation error
$\sigma_w^2$ given by

$$\sigma_w^2 = \|\varepsilon\|_2^2 / m, \quad (5.4)$$

where $\| \|$ is the Euclidian norm and $m$ is the total number of grid points ($m = t \times t$ for a square
array, $t$ is the grid size), to the mean variance of the WFD measurement error $\sigma_n^2$, i.e.

$$\eta = \frac{\sigma_w^2}{\sigma_n^2}. \quad (5.5)$$

This definition is referred to as the WFD-based error propagation coefficient, which is a
quantitative indicator of the error propagator in the WFD-based wavefront estimation. In this
chapter, we present a general formulation for the WFD-based error propagation coefficient with
the matrix eigenvalue method (Zou and Rolland, 2004, 2006).\textsuperscript{190,191} With the serial numbering
wavefront estimation scheme introduced, the general error propagation formulation is
implemented for the Hudgin geometry, the Southwell geometry and the Fried geometry.\textsuperscript{190}

Based on the WFD-based error propagation coefficient formulation, the definition of the slope-
based error propagation coefficient is introduced and formulated for each of the basic estimation geometries.190

### 5.2 Brief review of previous work

Wavefront estimation can be performed on the three introduced geometries: the Hudgin geometry,82 the Southwell geometry,88 and the Fried geometry.85 As shown in Figure 3.2, the slope measurements (or alternatively the WFD measurements) are denoted by small arrows, and the grid points are denoted by small circles in each of the geometries. The slope measurements are performed at the mid-point between each pair of neighboring grid points in the Hudgin geometry, and at the center point circled by each four neighboring grid points in the Fried geometry. The Southwell geometry is characterized by taking the wavefront slope measurements and the wavefront value estimations at the same nodes. It was given by Southwell that this latter geometry has the lowest error propagation in wavefront estimation across relatively small grid sizes,88 as shown in Figure 5.1.

Let us focus the previous analysis of error propagation on the zonal wavefront estimation induced by the WFD measurements with different geometries. As shown in Figure 5.1, the error propagation coefficient was shown to be logarithmic dependent on the grid size \( t \).88,82,85 From Eq. (35) in Ref.85, we obtained the result given by Fried as

\[
\eta_{\text{Fried}} = 0.6558 + 0.3206 \ln(t)
\]  

and from Eq. (32) in Ref.82, we got the result given by Hudgin as

\[
\eta_{\text{Hudgin}} = 0.561 + 0.103 \ln(t).
\]
For the Southwell geometry, we least-squares fit our discrete coordinate measurements of curve A in Fig. 2 on page 1003 of Ref. 88 given by Southwell, and obtained

\[ \eta_{\text{Southwell}} = -0.10447 + 0.2963 \ln(t). \]  (5.8)

By using a general Green’s function and neglecting the boundary conditions, Noll analytically derived that the error propagation is a logarithmic dependent function of its grid size \( t \). For a square aperture with the phase value at the origin set to be zero, the coefficient was can be obtained by 87

\[ \eta_{\text{Noll}} = 0.1072 + 0.318 \ln(t). \]  (5.9)

Figure 5.1 Previous results on error propagation
In modal estimation with discrete Fourier transform, Freischlad and Koliopoulos also showed that the error propagation satisfies a logarithmic dependence of \( \eta_{HS,\text{modal}} = a + \frac{1}{\pi} \ln(t) \) for the Hudgin geometry and the Southwell geometry, and a logarithmic dependence of \( \eta_{F,\text{modal}} = a + \frac{3}{\pi} \ln(t - 1) \) for the Fried geometry. On the basis of the Hudgin geometry and a fast FT-based algorithm, which requires an even size, Freischlad confirmed that it is almost identical to Noll’s theoretical result with \[ \eta_{\text{Freischlad}} = 0.09753 + \frac{1}{\pi} \ln(t). \] (5.10)

Hunt extended Hudgin’s method for error coefficient prediction in terms of the discrete Fourier transform and obtained a result that shares the constant term with Noll and the logarithmic term with Fried and Hudgin, which yields little difference from both Noll’s and Freischlad’s results.

Figure 5.1 shows that the Southwell geometry is superior to all the other geometries regarding the error propagation when \( t \) is small, but the Hudgin geometry tends to be slightly superior to the Southwell geometry when the grid array size \( t \) becomes large (when \( t > 30 \)).

**5.3 Formulation of the error propagation with matrix method**

Given Eq.(5.1) and considering that in the case of zero noise Eq.(5.1) reduces to \( S_\theta = CW_\theta \), the WFD error \( N \) and the induced wavefront error \( \varepsilon \) should satisfy the equation

\[ C_\varepsilon = N. \] (5.11)

In a general case, the least-squares solution for Eq. (5.11) can be written as
\[ \epsilon = C^+ N, \] (5.12)

where \( C^+ \) is the Moore-Penrose pseudo-inverse of matrix \( C \). Given the relationship between the WFD vector and the wavefront slope vector provided by Eq. (5.2), similarly the WFD error \( N \) and the wavefront slope noise \( N' \) should satisfy

\[ N = \mu a M N'. \] (5.13)

Starting with the expression of the mean variance given by Eq. (5.4), the Euclidian norm for a statistical wavefront error vector is defined as

\[ \| \epsilon \|_2 = \left( \sum_{i=1}^{m} \langle \epsilon_i^2 \rangle \right)^{1/2} = \left( tr(\epsilon \epsilon^T) \right)^{1/2}, \] (5.14)

where the bracket \( \langle \cdot \rangle \) denotes the averaging operator, \( tr(\cdot) \) is the matrix trace. And

\[ \epsilon \epsilon^T = C^+ NN^T (C^+)^T = C^+ \mu a M N' N'^T M^T \mu a (C^+)^T, \] (5.15)

where \( N' N'^T \) is given by \(^{189}\)

\[ N' N'^T = \begin{bmatrix} n_1^2 & n_1n_2 & \cdots & n_1n_m \\ n_2n_1 & n_2^2 & \cdots & n_2n_m \\ \vdots & \vdots & \ddots & \vdots \\ n_mn_1 & n_mn_2 & \cdots & n_m^2 \end{bmatrix}. \] (5.16)

If we simply assume that the wavefront slope noise is random, independent, and has zero mean with the same variance \( \sigma_s^2 \), the ensemble statistical average of the slope errors yields

\[ \langle n_i n_j \rangle = \sigma_s^2 \delta_{ij} = \begin{cases} \sigma_s^2, & \text{when } i = j \\ 0, & \text{when } i \neq j \end{cases}. \] (5.17)

So the slope noise covariance matrix is given by
\[
\langle N'N'^\top \rangle = \sigma_s^2 I,
\] 
(5.18)

where \(I\) is the identity matrix. Therefore, Eq.(5.15) yields

\[
\langle \varepsilon\varepsilon^\top \rangle = \mu^2 a^2 \sigma_s^2 C^\top M M^\top (C^+)\,^\top.
\] 
(5.19)

Accordingly the mean variance of the wavefront estimation error \(\sigma_w^2\) is given by,

\[
\sigma_w^2 = \frac{1}{m} ||\varepsilon||_2^2 = \frac{1}{m} \text{tr}\{\langle \varepsilon\varepsilon^\top \rangle\} = \frac{\mu^2 a^2 \sigma_s^2}{m} \text{tr}\left[ C^\top M M^\top (C^+)\,^\top \right].
\] 
(5.20)

Similarly, the variance of the WFD measurement error \(\sigma_n^2\) is given by

\[
\sigma_n^2 = \frac{1}{m} ||N||_2^2 = \frac{1}{m} \text{tr}\{\langle NN^\top \rangle\} = \frac{\mu^2 a^2 \sigma_s^2}{m} \text{tr}\{M M^\top \}. \] 
(5.21)

With the definition of the error propagation coefficient given in Eq. (5.5), we can write

\[
\eta = \frac{\sigma_w^2}{\sigma_n^2} = \frac{\text{tr}\left[ C^\top M M^\top \right]}{\text{tr}\left[ M M^\top \right]}.
\] 
(5.22a)

This equation is useful for the computation of the error propagation coefficient. It can be noted that Eq.(5.22a) can also be written in the form of the Frobenius norm\(^{187}\) as

\[
\eta = \frac{||C^\top M||_F^2}{||M||_F^2}.
\] 
(5.22b)

Equations (5.22) provide a generalized expression for the error propagation coefficient in zonal wavefront estimation. This formula is good for either the slope measurements or the direct WFD measurements, because we can convert either the slope measurements or any other specific WFD measurements into the wavefront value difference between each pair of the neighboring grid points, which is actually the direct WFD measurement in the Hudgin geometry.
In next Section, the serial number scheme (SNS) will be adopted for wavefront estimation in studying the error propagation for each of the basic geometries. The SNS, as adopted in Chapter 4 and the previous literatures\textsuperscript{189,11}, makes wavefront estimation become a standardized process. Instead of numbering the estimation grid array with 2-D coordinates \((i, j)\) as previously provided,\textsuperscript{82,85,88,120} the grid array is indexed sequentially from 1 to \(m\) row by row as illustrated in Figure 5.2 for a square domain. With such a numbering mode, a regular and banded sparse estimation matrix is pre-defined, which resembles Hunt’s matrix formulation.\textsuperscript{11,86}

**5.4 Quantification of Wavefront difference-based error propagation**

In this section, the WFD-based error propagators for Hudgin, Southwell and Fried geometries are formulated and their behaviors compared. As alternative to the WFD-based definition, the wavefront slope-based error propagators are also defined, and the formulations for different geometries are derived.
5.4.1 Wavefront difference-based error propagators

For the WFD-based wavefront estimation, we apply the general formula of the error propagation coefficient we developed for the three basic estimation geometries: the Hudgin geometry, the Southwell geometry and the Fried geometry. With SNS the wavefront estimation matrix for each of the geometries is established, and the eigenvalues for each of the estimation-related matrix are numerically computed, from which the formulas of the WFD-based error propagation coefficients are obtained.

5.4.1.1 Hudgin Geometry

In the Hudgin geometry, the wavefront slopes are measured at the mid-point between two neighboring grid points, and the WFD between each pair of neighboring grid points in the x-and y-directions can be estimated as

\[
\begin{align*}
    s_{x,i+1,i} &= g_{x,i+1,i} a \\
    s_{y,i+1,i} &= g_{y,i+1,i} a,
\end{align*}
\]

where \( a \) is the pitch size of the sampling grid array, \( g_{x,i+1,i} \) is the wavefront slope in the x-direction at the midpoint between point \( i \) and point \( i+1 \), and \( g_{y,i+1,i} \) is the wavefront slope in the y-direction at the midpoint between point \( i+1 \) and point \( i \). With the SNS mode the wavefront estimation equations can be written in the x-direction as

\[
w_{i+1} - w_i = s_{x,i+1,i}, \quad i = 1,2,\ldots,m, \quad i \neq kt, \; k \text{ integer},
\]

and in the y-direction as

\[
w_i - w_{i+t} = s_{y,i+1,i}, \quad i = 1,2,\ldots,m-t.
\]
When written in matrix form, the estimation equation set for the Hudgin geometry is given by

\[ \mathbf{H} \mathbf{W} = \mathbf{S}, \quad (5.26) \]

where \( \mathbf{H} \) is the wavefront estimation matrix, \( \mathbf{S} = \alpha \mathbf{G} \) is the WFD vector, and \( \mathbf{G} \) is the wavefront slope vector. In comparison with Eq. (5.2), \( \mathbf{S} = \alpha \mathbf{G} \) yields \( \mu = 1 \) and \( \mathbf{M} = \mathbf{I} \), where \( \mathbf{I} \) is the identity matrix. According to Eqs. (5.22a) and (5.22b), where \( \mathbf{C} \) equals \( \mathbf{H} \) for the Hudgin geometry, \( \eta \) takes the form

\[ \eta_\mu = \frac{\text{tr}\left[ \mathbf{H}^+ \left( \mathbf{H}^+ \right)^T \right]}{\text{tr}[\mathbf{I}]} = \frac{1}{m} \text{tr}\left[ \left( \mathbf{H}^T \mathbf{H} \right)^+ \right] = \frac{1}{m} \| \mathbf{H}^+ \|_F^2. \quad (5.27) \]

In optical testing, it is the wavefront shape from a reference, not the absolute wavefront piston values, that is desirable. Thus it is common to set a point on the wavefront as the reference point, namely the “zero point”, at which the wavefront value is assigned to zero or other constant. Setting a “zero point” for the wavefront will not affect the estimated shape, as any piston value in the estimation can be subtracted.

The rank of matrix \( \mathbf{H}^T \mathbf{H} \) is \( \gamma = m - 1 \). Matrix \( \mathbf{H}^T \mathbf{H} \) will become of full rank (\( \gamma = m \)) if a “zero point” is set for the wavefront. If \( \mathbf{H}^T \mathbf{H} \) is of full rank in column, then its generalized inverse matrix is \( \mathbf{H}^+ = (\mathbf{H}^T \mathbf{H})^{-1} \mathbf{H}^T \), and \( \text{tr}\left[ \mathbf{H}^+ \left( \mathbf{H}^+ \right)^T \right] = \text{tr}\left[ (\mathbf{H}^T \mathbf{H})^{-1} \right] \). If the nonzero eigenvalues of matrix \( (\mathbf{H}^T \mathbf{H}) \) are \( \lambda_{\mathbf{H},i} > 0 \) \( (i = 1,2,..,\gamma) \), then the nonzero eigenvalues of matrix \( (\mathbf{H}^T \mathbf{H})^+ \) are \( \lambda_{\mathbf{H},i}^{-1} > 0 \) \( (i = 1,2,..,\gamma) \). The WFD-based error coefficient for the Hudgin geometry can be therefore expressed as

\[ \eta_\mu = \frac{1}{m} \text{tr}\left[ (\mathbf{H}^T \mathbf{H})^+ \right] = \frac{1}{m} \left( \sum_{i=1}^{\gamma} \lambda_{\mathbf{H},i}^{-1} \right). \quad (5.28) \]
This result is somewhat similar to the result obtained by Southwell for modal wavefront estimation. Southwell formulated the error propagation in the modal estimation, showing that the mean-square phase error is proportional to the trace of \((A^+A)^{-1}\).

The numerical methods, such as the Jacobi and the SVD methods, can be employed to evaluate the matrix eigenvalues. The Jacobi method approximates the eigenvalues of symmetric matrices by reducing the off-diagonal elements to zero, while the SVD method approaches the eigenvalues by decomposing the matrix into a diagonal matrix multiplied by an orthonormal matrix on each side.

The eigenvalues of matrix \(H^TH\) are sensitive with the position of the wavefront “zero point”, the matrix dimension size, and the number parity of the matrix dimension. In this problem, the “zero point” mentioned is located at the center point of the estimation grid array for all geometries, at which the matrix has its smallest condition number. Given that the coefficients in matrix \(H^TH\) are pre-defined, the eigenvalues of matrix \(H^TH\) for different grid sizes can be computed numerically. The simulation results are plotted in Figure 5.3.

Fitting the numerical results (up to \(t=50\)) in the least-squares sense, we obtain the error propagation coefficients for the Hudgin geometry as

\[
\eta_{H, odd} = 0.3797 + 0.3171 \ln(t - 0.6672) \approx 0.3222 + 0.3316 \ln(t), \ (t \ is \ odd)
\]  (5.29) 

and

\[
\eta_{H, even} = 0.3294 + 0.4795 \ln(t - 0.2136) \approx 0.3049 + 0.4856 \ln(t). \ (t \ is \ even)
\]  (5.30)

When no “zero point” is appointed, the rank of the matrix \(H^TH\) is \(\gamma = m - l\). The solution space for the matrix equation has one degree of freedom. With the Moore-Penrose pseudo-inverse of the matrix \(H^TH\), we obtained the LSMN solution, which is a least-squares solution
that holds the same wavefront shape as that with a set “zero point” but has the minimum Euclidian norm of the wavefront values. In that case, we computed the eigenvalues of the estimation matrix with SVD, and obtained the simulation results with data up to $t=50$ as

$$\eta_{H,LSMN} = 0.3252 + 0.1593 \ln(t - 1.1208) \approx 0.2605 + 0.1764 \ln(t). \quad (5.31)$$

Figure 5.3 WFD-based error propagators for the Hudgin geometry

Figure 5.3 confirms that the behavior of the error propagation is logarithmic dependent on the grid size as previously established in the literature. The error propagation curves for the SNS with the “zero point” given (curves 2 and 3) are higher than the curves of Noll’s result (Curve 0) and the Hudgin results (Curve 1). However, the error propagation curve for the SNS
with the LSMN solution (Curve 4) is the lowest of all, nevertheless, at the expense of extensive computations; moreover, it is approaching the Hudgin result when the grid size increases. For wavefront estimation with a “zero point” set, an odd-number grid size is preferable for the Hudgin geometry.

### 5.4.1.2 Southwell Geometry

In the Southwell geometry the slope measurements and the wavefront estimate are located at each grid point. As Southwell did, the average of the measured slopes over two neighboring grid points is adopted as an estimate of the slope at the mid-point. The wavefront estimation equation set can be obtained with the SNS in the x-and y-directions as

$$w_{i+1} - w_i = \frac{a}{2} (g_{x_i} + g_{x_{i+1}}), \quad (5.32)$$

where $i = 1, 2, \ldots, m-1$ (with $i \neq kt, k$ is an integer), and $g_{x_i}$ is the slope data in the x-direction, and

$$w_i - w_{i-t} = \frac{a}{2} (g_{y_i} + g_{y_{i+t}}), \quad (5.33)$$

where $i = 1, 2, \ldots, m - t$, and $g_{y_i}$ is the slope data in the y-direction. In matrix form,

$$\mathbf{HW} = \mathbf{S}_H, \quad (5.34)$$

where matrix $\mathbf{H}$ is the same wavefront estimation matrix as for the Hudgin geometry, and $\mathbf{S}_H$ is the WFD vector, which is given by $\mathbf{S}_H = \frac{I}{2} a \mathbf{C}_s \mathbf{G}$. Comparing $\mathbf{S}_H$ with Eq.(5.2), we obtain $\mu = 1/2$ and $\mathbf{M} = \mathbf{C}_s$. It should be noted that matrices $\mathbf{C}_s$ and $\mathbf{H}$ are closely related: matrix $\mathbf{C}_s$ can be obtained by changing the sign of the coefficient “-1” in matrix $\mathbf{H}$.
According to Eq. (5.22), we have

\[
\eta_s = \frac{\text{tr}\left[H^+ C_s \left(H^+ C_s\right)^T\right]}{\text{tr}\left[C_s^T H^+ C_s\right]} = \frac{\text{tr}\left[C_s^T \left(H^+ H^+\right)^T H^+ C_s\right]}{\text{tr}\left[H H^T\right]},
\]

(5.35)

where \(\text{tr}\left[H H^T\right] = 4(t - i) = 4(m - t)\). Given \(H^+ = \left(H^T H\right)^+ H^T\), \(^{192}\) then the WFD-based error propagation coefficient for the Southwell geometry is expressed as

\[
\eta_s = \frac{\text{tr}\left[C_s^T \left(H^+ H^+\right)^T H^+ C_s\right]}{4(m - t)}.
\]

(5.36)

Finally,

\[
\eta_s = \frac{1}{4(m - t)} \left(\sum_{i=1}^{\gamma} \lambda_{s,i}\right),
\]

(5.37)

where \(\lambda_{s,i}(i=1,2,\ldots, \gamma)\) are the nonzero eigenvalues of matrix \(C_s^T H \left[H^T H\right]^\beta H^T C_s\), and \(\gamma\) is the rank of this matrix.

When a “zero point” is set, \(H^T H\) is invertible, and we have \(\gamma = m\) and \(H^+ = \left(H^T H\right)^+ H^T\).

The simulation results are shown in Figure 5.4. We least-squares fit the numerical results (up to \(t=50\)), and obtain the error propagation coefficients for the Southwell geometry as

\[
\eta_{S,odd} = 0.1489 + 0.2936 \ln(t - 0.06186) \approx 0.1428 + 0.2952 \ln(t), (t \text{ is odd })
\]

(5.38)

and

\[
\eta_{S,even} = 0.04941 + 0.4662 \ln(t + 2.7673) \approx 0.2861 + 0.41 \ln(t). (t \text{ is even})
\]

(5.39)

When no “zero point” is appointed, the LSMN solution is sought to make the Euclidian norm of the wavefront minimum. We computed the eigenvalues of the estimation matrix for this case by SVD up to \(t=50\), and obtained the error propagation coefficient as

\[
\eta_{S,LSMN} = 0.205 + 0.1487 \ln(t + 0.2562) \approx 0.217 + 0.1455 \ln(t)
\]

(5.40)
In Figure 5.4, when a wavefront “zero point” is assigned, the error propagation curve for the SNS is above the curve of Noll’s result (Curve 0) for the even-number grid sizes (Curve 3), and it is equivalent to (or slightly below) it for the odd-number grid sizes (Curve 2). Although both of the above mentioned two error propagators (Curve 2 and Curve 3) are shown to be worse than the Southwell’s result (Curve 1), the error propagator of the LSMN solution (Curve 4), when no “zero point” is set for the wavefront, is showed to be clearly better for the large grid size ($t>8$). Similar to the Hudgin geometry, an odd-number grid size is preferable for the Southwell geometry when a “zero point” is assigned.
5.4.1.3 Fried Geometry

In the Fried geometry, the grid for wavefront slope (or alternatively WFD) measurements and the grid for wavefront estimation are interleaved by a distance of \(a/2\) both in the x- and in the y-directions as shown in Figure 3.2. Fried proposed that the phase difference across the \((i, j)^{th}\) aperture element in the x-direction (or in the y-direction) can be estimated as the average of the phase differences along its two parallel borders in the x-direction (or in the y-direction). To compare the work in this dissertation with Fried’s result, a similar WFD estimation equation set as found in Fried’s work was established. For the Fried geometry with the SNS, we have

\[
\begin{align*}
    w_{i+1} - w_i + w_{i+1} - w_{i+1} &= 2s_x, \\
    w_i + w_{i+1} - w_{i+1} - w_{i+1} &= 2s_y,
\end{align*}
\]

where \(i = 1, 2, ..., m-t-1\), with \(i \neq kt\) (\(k\) is an integer); \(s_x = g_{xx} a\) and \(s_y = g_{yy} a\) are the WFDs in the x- and in the y- directions, and \(j = 1, 2, ..., (t-1)^2\), where \((t-1)^2\) is the total number of the measurement elements in the grid array. Writing them in matrix form, we obtain

\[
FW = S,
\]

where \(F\) is a pre-defined matrix for wavefront estimation for the Fried geometry, \(S = 2aG\) is the WFD vector, and \(G\) is the wavefront slope vector. As defined in Eq. (5.2), we obtain \(\mu = 2\), and \(M = I\), where \(I\) is the identity matrix. Given Eqs. (5.22), the WFD-based error propagation coefficient for the Fried geometry can be written as

\[
\eta_\nu = \frac{tr[F^+(F^+)^\top]}{tr[H^\top]} = \frac{1}{m} tr[(F^T F)^\top].
\]
Herrmann showed that the rank of the normal matrix $F^TF$ is $m-2$.\(^{91}\) If the nonzero eigenvalues of $F^TF$ are $\lambda_{F,i} > 0 (i=1, 2, \ldots, \gamma)$, where $\gamma$ is the rank of matrix $F^TF$, then

$$\eta_F = \frac{1}{m} \left( \sum_{i=1}^{\gamma} \lambda_{F,i}^{-1} \right).$$

(5.45)

When a grid point is frozen as the “zero point”, the rank of matrix $F^TF$ becomes $\gamma = m - 1$, and the piston value term of the estimated wavefront is defined. However, there is still one degree of freedom in the least-squares solution space, called the “waffle mode”, at which the wavefront at the estimation grid points can be pushed up and down with the same value in a checkerboard pattern, while it still satisfies the WFD estimation equation set defined in Eqs.(5.41) and (5.42). In other words, the Fried geometry can not sense the waffle mode error of the wavefront,\(^{193}\) which is not desirable in optical testing.

Given a “zero point” for the wavefront, the LSMN solution is to seek a least-squares solution in a one dimensional (1-D) solution space that makes the Euclidian norm of the wavefront shape minimum. While no “zero point” is assigned for the wavefront, we have $\gamma = m - 2$, and the LSMN solution is to seek a least-squares solution in a two-dimensional solution space (LSMN (2-D)) to minimize the Euclidian norm of the wavefront shape, which includes both the overall piston mode and the waffle mode errors. Theoretically, when the wavefront shape is flat, the LMSN solution can get rid of the waffle mode error. However, since the waffle mode error usually coexists with the wavefront shape, it is impossible to avoid the waffle mode error for the Fried geometry with the LMSN solution. The simulation results are shown in Figure 5.5.
For a wavefront with a “zero point” set, the matrix eigenvalues for the LSMN (1-D) solution are computed up to $t=50$, which yields the error propagation coefficients as

$$\eta_{F,\text{odd}} = 0.4461 + 0.2 \ln(t-0.8805) = 0.4146 + 0.207 \ln(t), \ (t \text{ is odd})$$

(5.46)

and

$$\eta_{F,\text{even}} = 0.4933 + 0.2866 \ln(t-0.6547) = 0.4338 + 0.3022 \ln(t). \ (t \text{ is even})$$

(5.47)

For wavefront with no “zero point” set, the matrix eigenvalues for the LSMN (2-D) solution are computed up to $t=50$, which yields the error propagation coefficients as

$$\eta_{F,\text{LSMN}} = 0.475 + 0.114 \ln(t-1.821) \approx 0.4076 + 0.1303 \ln(t).$$

(5.48)
Similar to the Hudgin and Southwell geometries, for a wavefront with a “zero point” set, an odd-number grid size is preferable for wavefront estimation. The LSMN(1-D) solution (Curves 2 and 3) offers error propagators better than Fried’s result (Curve 1); but the error propagator for the even-number grid sizes (Curve 3) is worse than Noll’s result (Curve 0), whereas the one for the large odd-number grid sizes (\( t > 16 \)) (Curve 2) is better than it. For a wavefront with no “zero point” set, the LSMN (2-D) solution offers the best error propagator for the Fried geometry.

It should be noticed that for wavefront estimation with the Fried geometry, it can either yield a LSMN solution on the full size of the estimation grid that suffers the waffle mode error, or yield a least-squares solution on a subsized estimation grid by discarding some of the wavefront boundary values (for example, the corner points). However, these solutions may not be acceptable in some optical testing cases.

**5.4.2 Comparisons of the error propagators**

To compare the error propagations in different wavefront estimation schemes, the simulation results for the Hudgin, Southwell and Fried geometries are plotted in Figure 5.6. The simulation results quantify how the error propagator depends on the parity of the wavefront estimation grid size, the wavefront estimation scheme, and the solution method used for solving the wavefront estimation.

Importantly, the odd-number grid sizes are shown to yield lower error propagation than the even-number grid sizes for all geometries. This can be explained by the following: If the grid size is odd, the “zero point” can be easily set at the geometrical center of the grid array so that the estimation scheme is symmetric and yields an estimation matrix with its minimum condition
number,\textsuperscript{11} which is steady and less sensitive to random noise disturbance. However, if the grid size is even, there is no direct way to set a “zero point” at the geometrical center of the sampling grid; therefore, the estimation scheme is typically non-symmetric, which is liable to be affected by random noise disturbance.

Figure 5.6 Comparison of the WDF-based error propagators

For wavefront estimation with a “zero point” set, the Fried geometry offers the best error propagator for the even-number grid sizes, and the Hudgin geometry offers the worst for both even- and odd-number grid sizes. For the odd-number grid size, the Southwell ($t<22$) and Fried...
Geometries offering the best error propagators, and the error curve of the Fried geometry almost overlaps that of the Southwell geometry, which well confirms both Noll’s and Freischlad’s results. It is interesting to notice that the error propagator for the Hudgin geometry with odd-number grid sizes is equivalent to that of the Fried geometry with even-number grid sizes. When no “zero point” is set for the wavefront, the error curves for Fried and Hudgin geometries superpose together, and the Southwell geometry still offers the best error propagator. The detailed qualitative comparisons are listed in Table 5.1

Table 5.1 Qualitative comparisons of the WFD-based error propagators
5.5 Quantification of wavefront slope-based error propagation

An alternative to Eq.(5.5) is to define the error propagation coefficient as the ratio of the mean variance of the wavefront estimation error to the variance of the wavefront slope error. From Eq.(5.20), we obtain

\[
\eta' = \frac{\sigma_w^2}{\sigma_s^2} = \frac{\mu^2 a^2}{m} \operatorname{tr}\left[C^\top C^\top \mu \mu^\top\right], \quad (5.49)
\]

or

\[
\eta' = K \eta, \quad (5.50)
\]

where \(\eta'\) is named as the slope-based error propagation coefficient, \(\eta\) is the WFD-based error propagation coefficient defined in Eq.(5.5), and

\[
K = \frac{\mu^2 A_0 \operatorname{tr}[M M^\top]}{m}, \quad (5.51)
\]

where \(A_0 = a^2\) is the pitch area of the sampling grid.

With this new definition, we can see the direct effect of the pitch area of the sampling grid on the error propagation. The larger the pitch area, the worse the error propagation. To compare the slope-based error propagators for different geometries, the slope-based error propagation coefficient is normalized with \(A_0 = 1\).

For the Hudgin geometry, it becomes

\[
\eta_{H'} = \frac{A_0}{m} \operatorname{tr}\left[H^\top H\right] = K_H \eta_H, \quad (5.52)
\]

where \(K_H = 1\), and \(\eta_H\) is the WFD-based error coefficient defined by Eq.(5.28).

For the Southwell geometry, it becomes
\[ \eta_S' = \frac{A_0}{4m} \text{tr} \left[ C_s^T \left( H^T \right)^T H^T C_s \right] = K_s \eta_S, \quad (5.53) \]

where \( K_s = \left( m - t \right) / m \), and \( \eta_s \) is the WFD-based error coefficient defined by Eq.(5.36).

For the Fried geometry, it becomes

\[ \eta_F = \frac{4 A_0}{m} \text{tr} \left[ \left( F^T F \right)^T \right] = K_F \eta_F. \quad (5.54) \]

where \( K_F = 4 \), and \( \eta_F \) is the WFD-based error coefficient defined by Eq.(5.44).

From the WFD-based definition to the slope-based definition, except for the effect of the pitch size, the error propagator remains the same for the Hudgin geometry, slightly improves for the Southwell geometry, and becomes four times worse for the Fried geometry. The slope-based coefficient may prove to be useful for the design of a slope-based optical testing system. Given the slope measurement noise and the wavefront error expected, for example, we can determine the pitch size required for the testing system.

The slope-based error propagators for the basic wavefront estimation geometries are plotted in Figure 5.7. The Southwell geometry is shown to be better than the Hudgin geometry, and the Fried geometry performs the worst. As previously found, the parity of the sampling grid size also affects the error propagator: A grid with an odd-number size is preferable to a grid with an even-number size. For wavefront estimation with no “zero point” set, the LSMN solution offers lower error propagators in comparison with the wavefront estimation with a “zero point” set for all geometries, among which the Southwell geometry offers the best.

Generally speaking, for a slope-based wavefront estimation in optical testing the Fried geometry is not preferred, because of its interlaced sampling scheme, which yields inadequate
slope information for estimating the wavefront over the entire sampling grid, and its high error propagation.

For both the slope-based and the WFD-based wavefront estimation, the Southwell geometry is preferred, because it offers the best error propagator for the wavefront estimation over the entire testing domain. The performance of the Southwell geometry can be explained by the noise-averaging effort in the WFD estimates. When slope data (or WFD) are estimated at the midpoint between the neighboring grid points, the estimated slope noise is reduced by the slope data averaging.

Figure 5.7 Comparison of the slope-based error propagators
5.6 Summary

In this chapter, the error propagation coefficient for the WFD-based wavefront estimation was derived with the matrix formulation. We established the functions to depict the error propagation behaviors for the three basic wavefront estimation geometries based on the wavefront estimation-related matrix eigenvalues.

The simulation results show that, for wavefront estimation with a “zero point”, the odd-number grid sizes are preferable to the even-number grid sizes. The Southwell geometry ($t<22$) and the Fried geometry ($t>22$) with the odd-number grid sizes offer the best error propagators if a “zero point” is set. The Southwell geometry offers the best error propagator for all grid sizes when no “zero point” is set.

Given the popularity of the slope-based wavefront sensors in optical testing, a slope-based error propagation coefficient is defined. The benefit of this metric is that, given the RMS noise in slope data, the RMS error in wavefront value can be directly estimated. Furthermore, this metric shows the direct dependence of the error propagation on the pitch size of the lenslet array. Using this metric, the Southwell geometry offers the best error propagators for wavefront estimation with and without a “zero point” set. Therefore, in optical testing the Southwell geometry is highly desirable. The Fried geometry is not recommended because of its high error propagation and the ambiguity in wavefront shape estimation. Not limited with the three basic geometries listed in this chapter, the generalized formulation presented here can be applied in any other estimation geometries for optical testing and wavefront control in adaptive optics; the corresponding formulas for the error propagation coefficients can be established with necessary numerical simulations.
CHAPTER SIX: DIFFERENTIAL SHACK-HARTMANN CURVATURE SENSOR

Curvature, the rate of the surface normal change, is an intrinsic parameter of optical surface. Unlike the slopes (gradients, or the first order derivatives of shape), which vary with changes in surface orientation, the surface normal curvature is insensitive to tip/tilt and whole body movement of the surface. Considering a surface with a regular mesh, the slope measurement at each local patch is a linear approximation of the surface with a tangential plane, while the curvature (the second derivative of shape) is a quadratic approximation of the surface with an osculating quadric spherical surface.\textsuperscript{46}

In this chapter, a Shack-Hartmann-based curvature sensor referred to as the DSH curvature sensor is presented for measuring the differentials of the wavefront slopes at each S-H grid point,\textsuperscript{194,195} and an experimental system is proposed to implement this concept. The DSH curvature sensor yields 2-D wavefront local curvature measurements at each Hartmann grid point in parallel. We show how wavefront curvature metrics, such as the Laplacian, mean, Gaussian, and importantly the principal curvatures and directions, are computed from wavefront slope differential measurements.

In the remainder of this Chapter, Section 6.1 introduces the concept of the differential Shack-Hartmann (DSH) curvature sensor, Section 6.2 describes an implementation of the differential Shack-Hartmann curvature sensor, and Section 6.3 presents the experimental system development. A least-squares-based zonal wavefront estimation algorithm is presented in Section 6.4, and in Section 6.5 we show the mathematical framework on how to compute the principal curvatures and directions.
6.1 Slope differential measurements

Wavefront local curvature is the local change in wavefront slope. While various definitions of curvature have been established in differential geometry, in the description of local shape the principal curvatures and their associated directions constitute the most concise elements among all. Within the mathematical framework, the principal curvatures are the eigenvalues of the matrix of the second fundamental form in differential geometry, and the principal directions are their corresponding eigenvectors. In the orthogonal principal directions, the curvatures of wavefront are simply the principal curvatures, and no twist curvature term exists. By diagonalizing the matrix of the second fundamental form, the principal curvatures can be computed from the normal curvatures in two arbitrary orthogonal directions together with the corresponding twist curvature terms.

Given a wavefront \( W(x, y) \) in a coordinate system with two arbitrary but orthogonal directions as the x- and y-axes, the S-H sensor provides the wavefront slopes by measuring the difference between the Hartmann grid coordinates of the measurement beam and the reference beam. The wavefront slopes in the x- and y-directions at each Hartmann grid point can be obtained by

\[
\begin{align*}
\frac{\partial W}{\partial x} & = \frac{y_{i}^{\text{mea}} - y_{i}^{\text{ref}}}{f} \\
\frac{\partial W}{\partial y} & = \frac{x_{i}^{\text{mea}} - x_{i}^{\text{ref}}}{f}
\end{align*}
\]  

(6.1)
where \((x_i^{\text{ref}}, y_i^{\text{ref}})\) (\(i=1,2,\ldots,m\), and \(m=t \times t\) is the total number of grid points) is the Hartmann grid coordinates of the reference beam, \((x_i^{\text{mea}}, y_i^{\text{mea}})\) is the Hartmann grid coordinates of the measurement beam, and \(f\) is the focal length of the lenslet array.

Now we shall focus on how to measure the Laplacian curvatures and the twist curvature terms. Measuring the differentials of the wavefront slopes along the x- or y-direction will yield the wavefront curvature along that direction, which can be implemented by measuring two slopes simultaneously over a given differential distance on wavefront. For the case of the S-H test, a wavefront slope differential in the x-direction can be obtained by extracting the S-H spot centroid coordinates of two differentially sheared Hartmann grid arrays along the x-direction, and the wavefront slope differential in the y-direction can also be similarly obtained. As shown in Figure 6.1,\(^{194}\) the coordinates of the x- and y-sheared grid points are denoted by \((x', y')\) and \((x'', y'')\), respectively. Therefore, the slope differentials in the x- and y-directions may be computed by

\[
c_x(i) = \frac{\partial^2 W}{\partial x^2} \bigg|_{i} = \frac{1}{s_x} \left( \frac{\partial W}{\partial x} \bigg|_{i} - \frac{\partial W}{\partial x} \bigg|_{i} \right) = \frac{1}{f} \left( \frac{x_i^{\text{mea}} - x_i^{\text{Ref}}}{s_x} \right) - c_{0,x}(i) \tag{6.2}
\]

\[
c_y(i) = \frac{\partial^2 W}{\partial y^2} \bigg|_{i} = \frac{1}{s_y} \left( \frac{\partial W}{\partial y} \bigg|_{i} - \frac{\partial W}{\partial y} \bigg|_{i} \right) = \frac{1}{f} \left( \frac{y_i^{\text{mea}} - y_i^{\text{Ref}}}{s_y} \right) - c_{0,y}(i)
\]

where \(s_x\) and \(s_y\) are the differential shears of the grids in the x- and y-directions, respectively, and the constants \(c_{0,x}(i)\) and \(c_{0,y}(i)\) are given by

\[
c_{0,x}(i) = \frac{1}{f} \left( \frac{x_i^{\text{Ref}} - x_i^{\text{Ref}}}{s_x} \right)
\]

\[
c_{0,y}(i) = \frac{1}{f} \left( \frac{y_i^{\text{Ref}} - y_i^{\text{Ref}}}{s_y} \right) \tag{6.3}
\]
Figure 6.1: The x- and y-differential shears of the Hartmann grid

Theoretically $c_{0,x}(i) = 1 / f$, because if the lenslet array moves a lateral distance $s_x$, such as in the x-direction, the reference S-H grid will move exactly the same distance $s_x$ in the x-direction accordingly, therefore, $x_i^{Ref} - x_i^{Ref} = s_x$. Similarly, $c_{0,y}(i) = 1 / f$. In practice, $c_{0,x}(i)$ and $c_{0,y}(i)$ must be calibrated as different CCD cameras are used in each measurement channel.

The slope differentials in the cross directions, referred to as the corresponding twist curvature terms, are given by

$$c_{xy}(i) = \frac{\partial^2 W}{\partial x \partial y} = \frac{1}{s_y} \left( \frac{\partial W}{\partial y} \bigg|_r - \frac{\partial W}{\partial x} \bigg|_r \right) = \frac{1}{f} \left( \frac{y_i^{\text{mea}} - y_i^{\text{mea}}}{s_x} \right) = c_{0,xy}(i),$$

$$c_{yx}(i) = \frac{\partial^2 W}{\partial y \partial x} = \frac{1}{s_y} \left( \frac{\partial W}{\partial x} \bigg|_r - \frac{\partial W}{\partial y} \bigg|_r \right) = \frac{1}{f} \left( \frac{x_i^{\text{mea}} - x_i^{\text{mea}}}{s_y} \right) = c_{0,yx}(i),$$

where $c_{0,xy}(i)$ and $c_{0,yx}(i)$ are constants given by
\[ c_{0,xy}(i) = \frac{I}{f} \left( \frac{y_i^{\text{Ref}} - y_i^{\text{Ref}}}{s_x} \right) \]

\[ c_{0,yx}(i) = \frac{I}{f} \left( \frac{x_i^{\text{Ref}} - x_i^{\text{Ref}}}{s_y} \right) \]

In Eqs. (6.2)-(6.5), \((x_i^{\text{mea}}, y_i^{\text{mea}}), (x_i^{\text{mea}}, y_i^{\text{mea}})\) and \((x_i^{\text{mea}}, y_i^{\text{mea}})(i=1,2,...,m)\) are the coordinates of the measurement beam at the original Hartmann grid, the x-sheared, and the y-sheared Hartmann grids, respectively; \((x_i^{\text{Ref}}, y_i^{\text{Ref}}), (x_i^{\text{Ref}}, y_i^{\text{Ref}})\) and \((x_i^{\text{Ref}}, y_i^{\text{Ref}})(i=1,2,...,m)\) are the corresponding coordinates of the reference beam.

Theoretically, \(c_{0,xy}(i)\) and \(c_{0,yx}(i)\) should be both zero for the first order approximation, but in practice \(c_{0,xy}(i)\) and \(c_{0,yx}(i)\) will need to be calibrated. In an experimental setup, a reference light beam would be introduced to generate the reference Hartmann grid arrays for the three channels, and Eqs. (6.3) and (6.5) could be used to compute the constants \(c_{0,xy}(i), c_{0,yx}(i), c_{i,xy}(i)\) and \(c_{i,yx}(i)\). To make the direction of the principal curvature unique, we suppose that the twist curvature terms are equal, i.e. \(c_{xy}(i) = c_{yx}(i)\).

6.2 Implementation of the DSH curvature sensor

The DSH curvature sensor can be implemented by modifying a conventional S-H sensor to yield three output channels. Suppose a collimated wavefront traveling in the z-direction is split into three channels along three directions perpendicular to each other, one still traveling in the z-direction, the others traveling in the x- and y-directions, separately. Lenslet arrays A, B and C are put in the three channels respectively to generate three separate S-H grid arrays. The
lenslets A and B are sheared laterally with respect to the lenslet C, by employing two micro-
screws to move lenslet A a lateral differential distance in the x-direction and move lenslet B a
lateral differential distance in the y-direction, independently. Each of the three lenslet arrays is
placed at an image position conjugated to the optical system entrance pupil, as shown in Figure
6.2. Three CCD cameras are used to record the beamlet centroid positions relative to the S-H
grid coordinates defined by the CCD pixel positions.

Other implementations are feasible, where the shearing elements can be replaced with
parallel glass plates (or other equivalences) instead of the micro-screws. For example, optical
parallel plates can be used to serve as both beam splitters to split the beam and shearing elements
to make differential shears among the three beams.

Figure 6.2: An implementation of the DSH curvature sensor without calibration path
In the implementation showed in Figure (6.2), the S-H grid coordinates of the three channels are recorded by three separate CCD cameras, therefore, calibrations are needed for the constant terms in Eqs.(6.2) and (6.4). With calibration, the discrepancies between the three image de-magnifying systems as well as the discrepancies between the two arms in different channels after the cube beam splitter can be canceled, and the residual aberrations in the collimation lens and the cube prisms eliminated. The error sources left are mainly from the beam splitters for reference and the measurement beam injections and the discrepancies between lenslets A, B, and C, which can be considered negligible given modern manufacturing technology for micro-lenslet arrays.

The idea of differential measurement was also exemplified by the technique called Differential Image Motion Monitor (DIMM), a well-known method for measuring atmospheric turbulence in astronomy.\textsuperscript{197, 198} Because DIMM measures the difference of the wavefront tilts over two sub-apertures some distance apart (i.e. a local wavefront curvature), it has advantage of being insensitive to vibration and tracking errors.

### 6.3 Experimental setup for the DSH curvature sensor

An experimental system for the DSH curvature sensor was developed in our laboratory.\textsuperscript{194} The optical layout of this experimental system is shown in Figure 6.3. A point light source $O_1$ was used to generate the measurement beam, and the point light source $O_2$ was used to generate the reference beam for calibration. Each of the two point light sources was made of a 15-micron diameter pinhole illuminated by a white light lamp (Krypton flashlight lamp 2.5volt, 430mA, brightness 0.6 CP). Once calibrated, no reference light beam was needed in this
system. In order to create a wavefront with a known aberration (i.e. spherical aberration) for demonstrating the ability of the system, a \(\lambda/4\)-quality (P-V) parabolic mirror with a diameter of 152.4mm and a focal length of 609.6mm was used, yielding a testing beam with \(f/8\) working focal ratio. A 25mm-diameter achromatic lens with a focal length of 120 mm was used to collimate the output beam. A 10×10 lenslet array (1790-90-s, Adaptive Optics Associates Inc.) with a 90mm focal length in common and a 1.79×1.79 mm\(^2\) area for each sub-aperture was used in each channel to generate the S-H sample.\(^{199}\) For this configuration, about 15mm diameter of the lenslet array area was illuminated, yielding 52 S-H grid points in an 8×8 square array used in testing. Two 25×25×25 mm\(^3\) beam splitter cubes (CVI, NCB-450-700-100, \(\lambda/4\)-quality (P-V)) were used to split the collimated beam into three channels—channel #0, channel #1 and channel #2. Another 25×25×25 mm\(^3\) cube was used to make a 90-degree image rotation in channel #2, so that a y-slope differential operation can be implemented in the horizontal plane. An optical demagnifying system with a reducing power of about 2.3:1 was used in each channel to image the S-H grid onto a CCD camera. As illustrated in Figure 6.3, two 45-degree tilted elliptical plate beam splitters (\(\lambda/4\) accuracy for both sides, 3-mm thickness, Bk7) were used for the testing wavefront feed, and they were deliberately put in two orthogonal orientations to reduce the astigmatism and coma induced by the beam splitters in the convergent beam. Given that the entrance angle (~22.5 degree) was small, this splitter generated small aberrations, but they could not be removed by calibration. A picture of the experimental system for DSH curvature sensor is given in Figure 6.4.

It is essentially important to align the lenslet arrays of channel #0, 1, 2 with the center of the pupil image of the testing mirror. Then we can move the lenslet array in channel #1 and
channel#2 a differential distance independently to achieve the 2-D slope differential measurements. In the experimental system we developed, the differential values are about 222.25 μm in the x-direction and 150 μm in the y-direction, which are about 1/8 and 1/12 of the lenslet pitch size, separately.

The video cameras used in this setup were three Watec LCL-902 Monochrome CCD cameras, which have a resolution of 768×494 pixels² with the pixel size of 8.4×9.8 μm² (EIA,
RS-170). The size of the sensing area of the CCD camera was 6.4×4.8 mm², and the light sensitivity 0.01 Lux.

A NI-IMAQ PCI_1409 image acquisition board (National Instruments) was used as a frame grabber to acquire images from the CCD cameras. The board is compatible with double-speed 60 frames per second progressive scan cameras and delivers up to 60dB dynamic range, which corresponds to 10 bits or 1024 gray scales. It has 16 MB of onboard memory used to temporarily store the image being transferred to the PCI bus. The PCI_1409 board has up to four input ports, so we connected the three CCD cameras located in the three output channels to this

Figure 6.4 Picture of the experimental system for the DSH curvature sensor
board. The NI-IMAQ Vision development module was used to provide LabView related functions, which allowed us to perform various operations on the acquired images.

![Experimental System for Differential Shack-Hartmann Curvature Sensor](image)

Figure 6.5 GUI of the DSH sensor experimental setup

The Graphic User Interface (GUI) developed for the experimental setup with LabView graphic language is shown in Figure 6.5. Although in field applications it is required to sample all of the data simultaneously to reduce vibration sensitivity, for a first proof of concept demonstration, where we were limited by our hardware budget we sampled each of the grid
coordinates serially rather than in parallel. An indicator located on the up-left corner of the GUI shows the sampling process, and the individual images of the 52 Hartmann grid points were shown in an array on the right side of the GUI according to their original positions. A button immediately above the process indicator was used to switch between the calibration process and the measurement process. Once the data was obtained from measurement and calibration, wavefront estimations were computed with a zonal wavefront estimation algorithm described in Section 6.4.

### 6.4 Curvature-based zonal wavefront estimation

Given the wavefront curvature data obtained from the slope differential measurements and the boundary gradients obtained from slope measurements, the wavefront values may be estimated. On the basis of wavefront Laplacian curvature measurements inside the pupil and the slope measurement at the pupil boundary, Roddier and Roddier proposed a zonal iterative FT-based wavefront estimation algorithm. Chanan established a zonal least-squares wavefront estimation algorithm for curvature data obtained on a square domain. In this section, a zonal least-squares-based estimation algorithm for curvature data based on Taylor series is proposed.

The 8×8 S-H grid used for this experimental system is shown in Figure 6.6. For convenience, we index the square S-H grid array with the SNS mode (i= 1, 2…m (m=t×t)) as shown in Figure 5.2. The discretization of Poisson equation yields a normal equation set for the least-squares-based wavefront estimation (Zou & Rolland 2005).

For a curvature-based zonal wavefront estimation, the estimation algorithm becomes very simple because various mathematical frame works needed for estimating the Laplacian
curvatures from slope data at each given grid point are avoided. Instead, the Laplacian curvatures are directly obtained from measurements at each point where the wavefront value is evaluated, which forces the Southwell geometry, a geometry that yields the best error propagation in wavefront estimation as detailed in Chapter 5.

For any interior point within the sampling domain, the least-squares-based normal equations for wavefront estimation are always of the same form, which is

\[
\begin{align*}
& w_{i-j} + w_{i-t} - 4w_j + w_{i+1} + w_{i+1} = a^2(c_{x,i} + c_{y,i}).
\end{align*}
\]

Figure 6.6 A 52-point S-H Grid

For any interior point within the sampling domain, the least-squares-based normal equations for wavefront estimation are always of the same form, which is

\[
\begin{align*}
& w_{i-j} + w_{i-t} - 4w_j + w_{i+1} + w_{i+1} = a^2(c_{x,i} + c_{y,i}).
\end{align*}
\]

For a regular discretization mesh illustrated in Figure 6.6, all the boundary points can be categorized into two types: the line boundary points and the corner boundary points. As
illustrated in Figures 6.7 and 6.8, there are only eight boundary local geometries that are needed to be taken care of for a given sampling domain. In the following, we will derive the normal equations for wavefront estimation for each of the eight local geometries.

For the line boundary points illustrated in Figure 6.7(a), the curvature in the x-direction at this point can be approximated by

$$w_{i+1} - 2w_i + w_{i-1} = a^2 c_{x,j}. \tag{6.7}$$

![Figure 6.7 The edge points](image)

In order to couple Poisson equation with the boundary condition, we need to estimate the boundary slope that is normal to the boundary line. Given the Taylor expansion in the y-direction, we have

$$w_{i+1} = w_i - a s_{y,i} + \frac{a^2}{2!} c_{y,j} + \cdots, \tag{6.8}$$

where $s_{y,i}$ is the slope in the y-direction at point $i$. If we ignore the higher order terms and add Eqs. (6.7) and (6.8) together, we obtain the normal equation for the boundary points that shares a boundary geometry shown in Figure 6.7(a) as

$$w_{i+1} - 3w_i + w_{i-1} + w_{i+1} = a^2 \left( c_{x,j} + \frac{1}{2} c_{y,j} \right) - a s_{y,i}. \tag{6.9}$$
Performing similar operations for the other local boundary geometries illustrated in Figure 6.7(b)-(d) yields

\[ w_{i+1} - 3w_i + w_{i-1} = a^2 \left( c_{y,i} + \frac{1}{2} c_{x,i} \right) + as_{y,i}, \]  
\[ w_{i+1} - 3w_i + w_{i-1} = a^2 \left( c_{y,i} + \frac{1}{2} c_{x,i} \right) + as_{x,i}, \]  
\[ w_{i-1} - 3w_i + w_{i+1} = a^2 \left( c_{y,i} + \frac{1}{2} c_{x,i} \right) - as_{x,i}. \]  
(6.10)  
(6.11)  
(6.12)

For the corner points illustrated in Figure 6.8(a), the Taylor expansions can be given in the x- and y-directions as:

\[ w_{i+1} = w_i + as_{x,i} + \frac{a^2}{2!} c_{x,i} + \cdots, \]  
\[ w_{i+1} = w_i - as_{y,i} + \frac{a^2}{2!} c_{y,i} + \cdots. \]  
(6.13)  
(6.14)

![Figure 6.8 The corner points](image)

Adding the above two equations together and ignoring the higher order terms, we obtain the normal equation for the corner boundary points that share the local boundary geometry shown in Figure 6.8(a) as
Performing similar operations for the other local boundary geometries illustrated in Figure 6.8 (b)-(d) yields

$$w_{i+l} + w_{i+l} - 2w_i = a(s_{x,i} - s_{y,i}) + \frac{a^2}{2}(c_{x,i} + c_{y,i})$$

(6.15)

Writing the normal equations derived from the interior points and the boundary points in a proper order, we obtain the normal equation set, which may be expressed in matrix form as

$$AW = a^2F - aB$$

(6.19)

where $A$ is the normal matrix for zonal wavefront estimation, $W$ is the wavefront vector, $a$ is the pitch size of the S-H grid, $F$ is the vector of the weighted Laplacian curvature measurements, and $B$ is a vector of the boundary slopes that are normal to the edge. Compare with the algorithm obtained by Chanan, they both share the same matrix form. However, their boundary condition treatments are different, and therefore they are two different algorithms. The validation of this proposed algorithm is shown in Chapter 7.

Usually the optical surfaces have large errors near the edges. Variations in the boundary slopes may dramatically change the wavefront estimation results. Such a condition makes the wavefront estimation in optical testing challenging, because the boundary conditions are usually affected by large edge-slope defects. However, we can not discard the boundary conditions in wavefront estimation, because it contributes to the wavefront shape besides the wavefront...
orientation and defocus. As detailed in Chapter 3, the orientation of the wavefront is determined by the boundary slopes only, but the wavefront shape is determined by both the wavefront Laplacian and the boundary slopes.

6.5 Principal curvature computations

The normal curvature is the change of the surface normal in an osculating plane, and the principal curvatures at a non-umbilical point are the maximum and minimum values of the normal curvatures, say $\kappa_1$ and $\kappa_2$, in two perpendicular directions. Regarding a local patch on a surface, the principal curvatures are invariants, which are insensitive to the surface orientations.

In order to evaluate the principal curvatures, we assume that the neighborhood of a Hartmann grid point can be represented by a “Monge patch” of the form:

$$X = xe_1 + ye_2 + W(x,y)e_3$$

(6.20)

where $(e_1, e_2, e_3)$ is an orthogonal frame in Euclidean 3-D space. For a wavefront traveling in the $z$-direction ($e_3$), $W(x,y)$ is the “height” as a function of $x$ and $y$ in the pupil plane. Then the second fundamental form has a matrix form to describe the local surface shape as

$$\mathbf{II} = \begin{pmatrix} \omega_{ij}^{13} & \omega_{ij}^{14} \\ \omega_{ij}^{31} & \omega_{ij}^{32} \end{pmatrix},$$

(6.21)

where $\omega_{ij}^{kl}(i=1,2; j=1,2)$ defines the component in $e_i$ of the turning rate of the normal as you move the frame across the given point along $e_j$. Then at each “Monge patch”, the matrix $\mathbf{II}$ becomes
\[
\mathbf{II} = \begin{pmatrix}
c_x(i) & c_{x'\gamma}(i) \\
c_{y\gamma}(i) & c_y(i)
\end{pmatrix}, i = 1, 2, \ldots, m,
\] (6.22)

where the diagonal terms \(c_x(i)\) and \(c_y(i)\) are the wavefront normal curvatures in the x-direction and in the y-direction, i.e. \(c_x(i) = \frac{\partial^2 W}{\partial x^2}(i)\) and \(c_y(i) = \frac{\partial^2 W}{\partial y^2}(i)\); the off-diagonal terms \(c_{x'\gamma}(i)\) and \(c_{y\gamma}(i)\) are the corresponding twist curvature terms, i.e. \(c_{x'\gamma}(i) = \frac{\partial^2 W}{\partial x \partial \gamma}(i)\) and \(c_{y\gamma}(i) = \frac{\partial^2 W}{\partial y \partial \gamma}(i)\).

The determinant of matrix \(\mathbf{II}\), denoted as \(K\), is known as the Gaussian curvature, which measures the total spread of normal directions per unit surface area.\(^{46}\) The trace of the matrix \(\mathbf{II}\) is denoted as \(2H\), where \(H\) is known as the mean curvature, which is the average normal curvature taken over all tangent directions. Both Gaussian curvature and mean curvature are algebraic invariants,\(^{46}\) which means they do not change with rotation of the orthogonal frame \((\bar{e}_1, \bar{e}_2, \bar{e}_3)\) about the normal.

By diagonalizing the matrix \(\mathbf{II}\) to rotate the orthogonal frame about \(\bar{e}_3\), the off-diagonal terms disappear. Then we obtain a new matrix \(\mathbf{II}'\) by

\[
\mathbf{II}' = \mathbf{P}^T \mathbf{II} \mathbf{P},
\] (6.23)

where \(\mathbf{P}\) is an orthogonal matrix defined by

\[
\mathbf{P} = \begin{bmatrix}
cos\theta & -\sin\theta \\
\sin\theta & \cos\theta
\end{bmatrix},
\] (6.24)

where the angle \(\theta\) is defined as the frame rotation angle. The new matrix \(\mathbf{II}'\) is therefore a diagonal matrix as

\[
\mathbf{II}' = \begin{pmatrix}
\kappa_x(i) & 0 \\
0 & \kappa_y(i)
\end{pmatrix},
\] (6.25)
where $\kappa_1(i) > \kappa_2(i)$ ($i=1, 2, ..., m$, where $m$ is the total number of the S-H grid points). $\kappa_1(i)$ and $\kappa_2(i)$ are the eigenvalues of the matrix $\mathbf{II}$, which are also known as the first and second principal curvatures that define the greatest and smallest normal curvatures at a given patch. Applying Eqs. (6.22), (6.24) and (6.25) in Eq. (6.23), we obtain a formula for the principal curvatures $\kappa_1$ and $\kappa_2$ as

$$\kappa_{1,2}(i) = \frac{c_x(i) + c_y(i) \pm \sqrt{(c_x(i) - c_y(i))^2 + 4c_{xy}(i)^2}}{2},$$

and a formula for the rotation angle (i.e. $\theta$ is the angle between the first principal curvature and the x-direction) as

$$\theta(i) = \frac{1}{2} \tan^{-1} \left( \frac{2c_{xy}(i)}{c_x(i) - c_y(i)} \right).$$

The principal curvatures can also be computed by evaluating the eigenvalues of matrix $\mathbf{II}$ with its characteristic equation as

$$\det(\kappa \mathbf{I} - \mathbf{II}) = 0,$$

which yields the same result. Additionally, the rotation angle $\theta$ can also be computed with the Euler's formula (1760) given by

$$\cos[2\theta(i)] = \frac{2c_x(i) - 2H(i)}{\kappa_1(i) - \kappa_2(i)},$$

where $H$ is the mean curvature

$$H(i) = \frac{(c_x(i) + c_y(i))}{2}.$$
Applying Eq.(6.26) in Eq.(6.31), we have

\[
\theta(i) = \frac{1}{2} \cos^{-1}\left( \frac{c_x(i) - c_y(i)}{\sqrt{(c_y(i) - c_x(i))^2 + 4c_{xy}(i)^2}} \right),
\]

(6.32)

which is equivalent to Eq.(6.27).

The principal curvatures and their directions are two important parameters of local surface shape. We showed how these parameters are estimated directly from the wavefront Laplacian curvatures and the twist curvature terms with matrix diagonalization method.

### 6.6 Summary

The DSH curvature sensor is derived from the S-H sensor, so it shares some important features of the S-H sensor. It is a real-time wavefront sensing, and the measurements are inherently two-dimensional and parallel. It yields good photon efficiency for all wavelength bands. The DSH curvature sensor shares some important features of Roddier’s curvature sensor. Theoretically it is independent of all types of vibrations and drifts, tip/tilts and whole body movements. Similar to Roddier’s curvature sensor, it is scale tunable by changing the differential values. After calibration, no external references are needed for all tests.

The DSH curvature sensor has its unique features. (1) Compare with the CGS sensor and the curvature profiling technique, the DSH curvature sensor provides a more convenient way to measure the twist curvature terms, while Roddier’s curvature sensor only yields the Laplacian curvature measurements. The twist curvature terms are important parameters for computing the principal curvatures and directions, because they provide more information about the exact shape of the wavefront. (2) The DSH curvature measurements are performed at the pupil of the optical
system under test, so the difficulties associated with the operations close to the caustic zone in Roddier’s curvature sensor are avoided. As pointed out by its inventor, Roddier’s curvature sensor is valid only for the defocused images taken outside of the caustic zone, inside which the rays coming from different sample pupil points intersect together. Unfortunately the size of the caustic zone is related with the aberrations of the system under test and the atmospheric turbulence-induced seeing blur, so there is no general rule to apply. (3) The DSH curvature sensor does not have a $2\pi$-ambiguity problem, while most of the irradiance-based phase retrieval methods do. This feature makes the DSH curvature sensor work well with large aberrations, while Roddier’s curvature sensor is good in accuracy only for small aberrations. (4) The DSH curvature sensor provides a means to remove the need to scan as the profiling curvature sensing does, and avoids the scan errors and nonlinearity problems. As the DSH curvature sensor measures the curvatures by simultaneously acquiring 2-D slope differentials via three channels, it is totally insensitive to all types of vibrations and drifts, both in surface height and in surface slope, so the vibration-induced accuracy degradation is avoided during curvature measurements.

Koenderink pointed out that “it would be better, of course, to sample even higher order properties of the surface (such as curvature) directly instead of having to infer them from point or facet samples”. From the normal curvature measurements, we showed how to compute the principal curvatures and their directions. The principal curvatures contain more shape information of wavefront than Laplacian curvature, and further more than slope data. Future work will include review of the mathematical literature for estimating wavefront shape directly from the principal curvatures and their directions and potentially the development of new algorithms as well for optical testing instead of the existing Laplacian curvature-based algorithms.
CHAPTER SEVEN: SIMULATION AND ERROR ANALYSIS

In this chapter, we first numerically validate the curvature-based zonal wavefront estimation algorithm with a test wavefront given by a Zernike polynomial. Then an error analysis of the DSH sensor is provided.

7.1 Numerical validation of the proposed algorithm

In order to validate the wavefront estimation algorithm proposed in Chapter 6, the following procedures were adopted. First, a wavefront function was generated as the original wavefront by using a known Zernike polynomial. Then the first and the second derivatives of this given wavefront were computed at each grid point. Based on the generated curvature data, the wavefront was estimated with the proposed algorithm. For evaluating the proposed wavefront estimation algorithm, the wavefront was also estimated from the generated slope data with a common iterative wavefront estimation algorithm. This iterative algorithm was used as the ground truth for evaluating a Gerchberg-Saxton iterative wavefront estimation algorithm in our previous work presented in Chapter 4. Comparisons were made between the original and the estimated wavefronts. The differences between them were used as metrics for evaluating the proposed curvature-based algorithm.

The original wavefront function in this simulation was defined by a Zernike polynomial as

$$W(\rho, \theta) = W_0 Z_{\rho}^0 (\rho, \theta), \quad (7.1)$$
where $Z^6_1(\rho, \theta) = \sqrt{5}(6\rho^4 - 6\rho^2 + 1)$ is the term for primary spherical aberration in Zernike polynomials with $0 < \rho \leq 1$, $0 \leq \theta < 2\pi$, and $W_0 = \frac{7}{3}\lambda$. As defined by the Zernike polynomial, the RMS value of the introduced wavefront is $W_0(-2.33\lambda)$. If the radius of the wavefront test pupil is $R$, then we can write the original wavefront in the Cartesian coordinate form as

$$W(x, y) = W_0\sqrt{5} \left( \frac{6(x^2 + y^2)^2}{R^4} - 6\frac{x^2 + y^2}{R^2} + 1 \right).$$  \hfill (7.2)

Accordingly, the first derivatives (slopes) of the given wavefront can be derived as

$$\frac{\partial W}{\partial x}(x, y) = \frac{12\sqrt{5}W_0}{R^2}\left( \frac{2(x^2 + y^2)}{R^2} - 1 \right)x,$$  \hfill (7.3)

$$\frac{\partial W}{\partial y}(x, y) = \frac{12\sqrt{5}W_0}{R^2}\left( \frac{2(x^2 + y^2)}{R^2} - 1 \right)y,$$  \hfill (7.4)

and the second derivatives (curvatures) of the given wavefront can be derived as

$$\frac{\partial^2 W}{\partial x^2}(x, y) = \frac{12\sqrt{5}W_0}{R^2}\left( \frac{2(x^2 + y^2)}{R^2} - 1 \right)x,$$  \hfill (7.5)

$$\frac{\partial^2 W}{\partial y^2}(x, y) = \frac{12\sqrt{5}W_0}{R^2}\left( \frac{2(x^2 + y^2)}{R^2} - 1 \right)y.$$  \hfill (7.6)

Given the wavefront slope and curvature data on a 8×8 grid (shown in Figure 6.6) by Eqs.(7.3)-(7.6), we can estimated the wavefront with the zonal curvature-based wavefront estimation algorithm proposed in Chapter 6. The contour plot of the estimated wavefront from curvature data is shown in Figure 7.1(a), and the wavefront estimated from slope data is shown in Figure 7.1(b) for comparison. Both wavefronts were estimated by zonal least-squares algorithms with the Southwell geometry. Figure 7.1(c) shows the original wavefront with the
8×8 discretization grid. In Figures 7.1 and 7.2, the “Ave” stands for the mean value of the wavefront, and the “Var” stands for the RMS value of the wavefront.

Figure 7.1 Wavefront estimation with an 8×8 grid array

(a) Estimated wavefront from curvature data. (b) Estimated wavefront from slope data. (c) Original wavefront on an 8×8 grid. (d) Deviation error map of the estimated wavefront from curvature data. (e) Deviation error map of the estimated wavefront from slope data.

The difference between the estimated wavefront and the original wavefront is referred to
as the wavefront deviation error of the proposed wavefront estimation. The wavefront RMS deviation error is defined as the root-mean-square value of the difference between the two wavefronts at each grid point. The RMS value of the curvature-based wavefront is $2.47\lambda$ ($\lambda=632.8\text{nm}$ for this chapter), the RMS value of the slope-based wavefront is $2.21\lambda$, and the RMS value of the original wavefront is $2.51\lambda$. The wavefront deviation error maps generated by the curvature-based and slope-based wavefront estimations are shown in Figures 7.1(d) and (e), which are shown to have RMS deviation errors of $1.144\lambda$ and $0.572\lambda$, respectively.

It can be observed that the coarse grid sampling is the main cause of the large deviation RMS errors. To get insight into the impact of the grid sampling size on the deviation error when the exit pupil is fixed, we provide another simulation example of wavefront estimation with a $30\times30$ grid array in Figure 7.2. The estimated wavefronts from curvature and slope data are shown in Figure 7.2(a)-(b), and the original wavefront with the $30\times30$ grid array is shown in Figure 7.2(c). The RMS value of the curvature-based wavefront is $2.387\lambda$, the RMS value of the slope-based wavefront is $2.392\lambda$, and the RMS value of the original wavefront is $2.390\lambda$. The corresponding wavefront deviation error maps of the curvature and slope-based wavefront estimations are shown in Figure 7.2(d)-(e), in which the RMS deviation errors are $0.081\lambda$ and $0.041\lambda$, respectively.

For both examples if we decompose the estimated wavefronts into the Zernike polynomials (for $t>5$), a spherical aberration of $2.33\lambda(\sim7/3\lambda)$ can be retrieved, which is the original aberration value that was introduced by Eq. (7.2). This provides a validation of the curvature-based zonal wavefront estimation algorithm proposed in this dissertation.
Further study shows that the deviation error of the slope-based wavefront is only half that of the curvature-based wavefront, as shown in Figure 7.3, and both of them decrease exponentially with an increase in the sampling grid size. After removal of the piston error and the tip/tilt error in the estimated wavefront, we found that the deviation error in the estimated
wavefront is mainly the defocus value (>98%). In Figure 7.3, curves 1 and 2 are the plots of the deviation errors of the curvature-based and slope-based wavefront estimations versus the grid size, and the curves 3 and 4 are the plots of the corresponding defocus values. It is interesting to notice that the defocus value in the curvature-based estimation is twice that of the slope-based estimation but of different sign. As shown in Figure 7.3, the curvature-based defocus value is negative, while the slope-based defocus value is positive.

The RMS value of the discretized original wavefront is the RMS value of the true wavefront values computed on the whole grid. Although the RMS wavefront deviation error is defined as the RMS difference between the estimated wavefront value and the original wavefront value at each grid point, the RMS value of the discretized original wavefront differs from the RMS value of the continuous true wavefront (which is $7\lambda/3$ in this example) as a result of wavefront discretization. The difference between the two RMS wavefront values is defined as
the wavefront discretization error. As shown in Figure 7.4, the discrete sampling becomes denser as the grid size increases, and the wavefront discretization error tends to zero.

In the above numerical simulations, the pupil size is about 15mm in diameter, which corresponds to an 8×8 grid array with a pitch size of 1.79mm. When the grid size is increased, the pitch size of the S-H grid decreases for a fixed pupil. For the case of a 40×40 grid size (the maximum grid size in simulation), the pitch size of the S-H grid is 0.36mm.

![Wavefront discretization error versus discretization grid size](image)

Figure 7.4 Wavefront discretization error versus discretization grid size

### 7.2 Error analysis of wavefront measurement

Because the DSH curvature sensor is based on the S-H sensor, its measurement capability is limited by the dynamic range of the S-H sensor in each channel, while its measurement accuracy is limited by the sensitivity of the S-H sensor in each channel. We shall provide an analysis of dynamic range and sensitivity, and exemplify this analysis using spherical aberration.
as the departure aberration from an ideal shape. The dynamic range and sensitivity will be computed in both slope values and number of waves of wavefront departure utilizing the experimental setup parameters given in Chapter 6.

For a wavefront with third-order spherical aberration of $W_{040}$, we have

$$W(x,y) = W_{040} \rho^4 = \frac{W_{040}}{R^4} (x^2 + y^2)^2.$$  \hspace{1cm} (7.7)

where $R$ is the pupil radius at the optics under test (e.g. a mirror), and $0 \leq \rho \leq 1$ is the normalized pupil radius, and $x$ and $y$ in Eq. (7.7) are physical dimensions within the pupil. Differentiating Eq. (7.7) yields wavefront slopes in the $x$-and $y$-direction as

$$S_x = \frac{\partial W}{\partial x}(x,y) = \frac{4W_{040}}{R^4} (x^2 + y^2)x,$$  \hspace{1cm} (7.8)

$$S_y = \frac{\partial W}{\partial y}(x,y) = \frac{4W_{040}}{R^4} (x^2 + y^2)y.$$  \hspace{1cm} (7.9)

### 7.2.1 Dynamic range

The dynamic range is defined as the largest wavefront slope that can be measured. Given that the pitch size of the lenslet array is $1.79\text{mm}$, and the focal length of the lenslet array is $90\text{mm}$, the maximum slope that the lenslet array can sense can be determined by

$$\tan \theta_{\text{max}} = 1.79 / (2 \times 90) \approx 0.00994 \text{ radian},$$  \hspace{1cm} (7.10)

so the dynamic range of the S-H sensor is $\theta_{\text{max}} = \pm 0.57^\circ$, which corresponds to a local wavefront slope error of $\theta_{\text{max}} d / D = \pm 3'.35$ arc minutes at the mirror surface, where $d=15\text{mm}$ is the exit pupil size at the lenslet and the $D=152.4\text{mm}$ is the mirror size.
In expressing this slope error in terms of the wave number of wavefront error, we shall note that spherical aberration displays its largest amount of slope value at the edge of the pupil, and the aberration is rotationally symmetric. Thus considering the edge of the mirror pupil in the x-direction (i.e. \( x=R=76.2\,\text{mm}, \ y=0 \)), we establish that

\[
W_{040} = \frac{S_x R^4}{4 x^2} = \frac{\theta_{\text{max}} \ d \ R}{4D} = \frac{0.00994 \times 15 \times 76.2}{4 \times 152.4} = 0.0186 \text{mm} \approx 29.5 \lambda , \quad (7.11)
\]

where the \( \lambda \) equals 0.6328nm. Thus the dynamic range at the mirror is quantified to be in slope measurements \( \pm 3'.35 \) arc minutes or in wavefront amplitudes about \( \pm 30 \) waves.

7.2.2 Sensitivity

The sensitivity of a S-H sensor is defined as the smallest slope data that can be measured. Assuming that a S-H spot centroid position can be acquired with an accuracy of one tenth of a pixel size when a high quality camera is used, the smallest measurable slope value is

\[
\theta_{\text{min}} = \frac{\sigma_{\text{CCD}}}{\beta f} \quad (7.12)
\]

where \( \beta = 1/2.3 \) is the magnifying power from the lenslet array image plane to the CCD camera, and \( f = 90\,\text{mm} \) is the focal length of the lenslet array. Assuming a CCD camera with 8.4 \( \mu \text{m} \) pixel size, then

\[
\theta_{\text{min}} = 0.84 \times 10^{-3} \,\text{mm} \times 2.3 / 90\,\text{mm} = 2.147 \times 10^{-5} \text{radian} = 4.4 \text{arc sec} , \quad (7.13)
\]

which corresponds to a wavefront slope error at mirror surface of \( \theta_M = \theta_{\text{min}} d / D = 0.43 \text{arc sec} \).
To estimate the smallest value of $W_{040}$ that can be measured, we consider the edge of the mirror pupil in the x-direction (i.e. $x=R=76.2\,\text{mm}$, $y=0$), where the wavefront have its maximum slope

$$S_{\text{max}} = \frac{4W_{040}}{R}, \quad (7.14)$$

To make the wavefront sensible for the S-H sensor, the maximum wavefront slope $S_{\text{max}}$ should be at least as big as the smallest measurable slope value $\theta_{\text{min}}$, and then we establish that

$$W_{040} = \frac{\theta_{\text{min}} Rd}{4D} = \frac{2.147 \times 10^{-5} \times 76.2\,\text{mm} \times 15\,\text{mm}}{4 \times 152.4\,\text{mm}} = 0.04\,\mu\text{m} \approx 0.0636\lambda. \quad (7.15)$$

where $\lambda$ equals 0.6328nm. The above analysis shows that given a RMS CCD centroiding error of $\frac{1}{10}$ pixel, $\lambda/15$ is the smallest third-order spherical aberration (P-V) that our experimental system can sense, and 0.43 arc sec is the smallest wavefront slope value sensible at the mirror surface. It is to be noted that the accuracy of the CCD camera, along with the quantity of the S-H spots, drives the magnitude of the slope measurement error. Therefore, based on the special requirement for testing applications, a high performance CCD is desirable.

### 7.2.3 Accuracy

In the following, we will show how much wavefront measurement accuracy that an S-H sensor of the DSH experimental system can achieve, when the error propagation in wavefront estimation is considered. For the Laplacian curvature-based wavefront estimation, either the Fried geometry or the Southwell geometry can be applied. Because of its convenience for wavefront estimation and its low error propagation behavior, the Southwell geometry was
adopted in our work. For the slope-based wavefront estimation in each channel, the error propagation coefficient was given in Chapter 5 by

$$\eta_s = \frac{\sigma_w^2}{\sigma_s^2} = K_s \eta_S$$  \hspace{1cm} (7.16)

where $K_s = A_0 (m-t)/m = 0.875 A_0$ for the Southwell geometry. $A_0$ is the pitch area of the sampling grid, and $\eta_S$ is the WFD-based error propagation coefficient defined by Eq.(5.36) and estimated by Eq.(5.39). For a $8 \times 8$ sampling grid,

$$\eta_S = 0.2861 + 0.41 \ln(t) = 1.1387 ,$$  \hspace{1cm} (7.17)

thus $\eta_S = 0.875 A_0 \times 1.1387 = 0.9963 A_0$. Therefore, the mean variance of the wavefront estimation error is given as

$$\sigma_w^2 = \eta_S \sigma_s^2 = 0.9963 A_0 \sigma_s^2 .$$  \hspace{1cm} (7.18)

Since the equally spaced sampling grid is square, and its pitch area is $A_0 = a^2$, then Eq. (7.18) yields

$$\sigma_w = \sigma_s \sqrt{\eta_S} = \sqrt{0.9963 \frac{a \sigma_{\text{CCD}}}{\beta f}} .$$  \hspace{1cm} (7.19)

Therefore, the RMS wavefront estimation error with an $8 \times 8$ sampling grid can be estimated by

$$\sigma_w = \sqrt{0.9963 \times \frac{1.79 \text{mm} \times 0.84 \mu\text{m} \times 2.3}{90 \text{mm}}} = 0.0384 \mu\text{m} = 0.061 \lambda ,$$  \hspace{1cm} (7.20)

where $\lambda$ equal to 632.8nm.

The analysis shows that if the RMS wavefront slope measurement error of an S-H sensor is $1/10$ pixel, the RMS wavefront estimation error will be $\lambda/16$. Since the wavefront estimation
error is driven by both the pitch size of the sampling grid and the CCD centroiding accuracy, a smaller wavefront estimation error may be obtained if a smaller grid size is adapted.

7.3 Summary

In this chapter, we validate the accuracy of the zonal curvature-based wavefront estimation algorithm presented in Chapter 6. We provide an analysis of the dynamic range, the instrument sensitivity, and the wavefront estimation accuracy of the DSH curvature experimental system under development. As part of the lessons learned, the camera we considered for methodology development was found to have dead space in one direction which resulted in data missing during measurements, thereby a low CCD centroiding accuracy. A high performance CCD camera will be necessary for the application of optical testing where wavefront estimation at level of $\lambda/4$–$\lambda/100$ may be required.
CHAPTER EIGHT: SUMMARY OF CONTRIBUTIONS AND CONCLUSION

With developments in active and adaptive optics, ophthalmology, and optical shop testing wavefront sensing has become increasingly prevalent. Wavefront sensing can involve either direct or indirect OPD measurements. This dissertation focused on indirect OPD sensing, specifically the parameter-based wavefront sensing. Three major contributions were made for optimizing wavefront sensing techniques. First, an iterative zonal wavefront estimation algorithm for any irregular pupil shape was presented; secondly, a theoretical study of error propagation for zonal wavefront estimations was performed; thirdly, a differential Shack-Hartmann curvature sensor was proposed and implemented.

For parameter-based wavefront sensing, either wavefront slope or wavefront curvature or a combination are measured within the pupil under test. One problem encountered in the slope-based wavefront estimation is how to handle wavefront estimation with irregular pupil shapes. In optical shop, optical elements can be round, square, or circular but with central obscuration, etc. A zonal wavefront estimation algorithm was proposed based on a least-squares linear equation system and Gerchberg-Saxton iterations. A domain extension technique was used to transform the irregular pupil into a square shape, and a serial numbering scheme was adopted for indexing the sampling grid inside the square domain to make the wavefront estimation matrix regular, symmetric and pre-defined. Gerchberg-Saxton iterations were employed to extrapolate the slope data outside the original pupil. The deviation error induced in the wavefront domain extension was then reduced to less than $\lambda/100$, and the convergence was showed to occur within a few iterations. It is believed to be the first implementation of the Gerchberg-Saxton algorithm.
with a least-squares linear system technique. The strength of the approach lies in the fact that the least-squares-based Gerchberg-Saxton algorithm does not suffer from the $2\pi$-phase ambiguity problem commonly encountered in Fourier-based approaches. As a result the least-squares-based Gerchberg-Saxton algorithm is superior for estimating large aberrations. A theoretical analysis shows that this algorithm is not only computationally efficient but also yields low error propagation.

Error propagation is an important parameter in evaluating slope-based wavefront estimation. Based on the serial numbering scheme, wavefront estimation matrices for the Hudgin, Southwell and Fried geometries were established. It was shown that the error propagation coefficient can be expressed as a function of the eigenvalues of the wavefront-estimation-based matrix, where the error propagation behavior differs with the different parity of the grid size. For wavefront estimation with a “zero point” chosen, odd-number grid sizes were shown to be preferable to even-number grid sizes. This formulation confirms Noll’s theoretical result if the Southwell geometry is adopted with the odd-number grid sizes.

From the wavefront difference-based wavefront estimation to the wavefront slope-based wavefront estimation, if the effect of the pitch size is not considered, the error propagator does not change much for the Hudgin and the Southwell geometries, but it becomes four times worse for the Fried geometry. In sum, the Southwell geometry is recommended as the best error propagator for both the difference-based and slope–based wavefront estimations.

For curvature-based wavefront estimation, a differential Shack-Hartmann (DSH) curvature sensor was proposed, which measures wavefront curvatures by measuring the differentials of the wavefront slopes at each Shack-Hartmann grid point in parallel. An
algorithm for zonal wavefront estimation from curvature measurements was proposed and demonstrated. For slope differential measurements at each S-H grid point, the Southwell geometry has been demonstrated to be the best choice. The curvature-based wavefront estimation algorithm was shown to be equivalent to the slope-based wavefront estimation algorithm for the Southwell geometry, but it is much simpler and more convenient to apply. Furthermore, curvature data acquired by the DSH sensor is expected not to suffer from vibration induced noise, a current limitation of most slope-based sensors and some curvature sensors.

The principal curvatures and their directions are two important parameters in characterizing the wavefront local shape, which are the maximum and minimum curvatures of any local patch on the surface in two orthogonal directions. It is known that the principal curvatures can be computed from the Laplacian curvatures and the twist curvature terms. We provide in this dissertation a means with the DSH sensor to measure such components for the first time. Previous curvature sensors essentially focused on measuring solely the Laplacian curvatures, which is not sufficient to compute the principal curvatures and directions of a local patch for describing the local wavefront shape.

The main merits of the DSH sensor are its immunity to vibrations, its ability to better measure the twist curvature terms, and its capability with high sampling to estimate the mid-spatial frequency error as well as the low-spatial frequency, which move the wavefront sensing technique to the next level of profilometry accuracy. Finally, with efficient two-dimensional curvature measurements in parallel, the problems associated with one-dimensional point-by-point-scan curvature profiling are avoided.

161
Future work will involve the comprehensive engineering investigation of the DSH sensor for various applications. The design of the instrument will differ based on the requirements for sensitivity and dynamic range. In developing any DSH instrument, care will need to be taken in easing the alignment of the three channels and minimizing spurious aberrations introduced by components that make up the system. It is also of interest to investigate algorithms for wavefront estimation directly from the principal curvatures and directions and yield insight into the ability of this parameterization to best represent overall local and global shape. Finally, any departure in estimated shape from a defined gold standard should be correlated to the impact of such errors on the performance metrics of various tasks linked to specific applications.
APPENDIX  DERIVATION OF EQS. (4.11), (4. 12), (4.26) AND (4. 27)
The $n^{th}$ derivative of the wavefront at point $i$ is denoted as \( \frac{\partial^n W}{\partial y^n} \), and the $n^{th}$ derivative of the wavefront at the midpoint between the points $i$ and $i+1$ as \( \frac{\partial^n W}{\partial y^n} \text{ at } \frac{i+i}{2} \). According to Taylor’s series, we can write

\[
w_i = w_{i+\frac{1}{2}} - \frac{a \frac{\partial W}{\partial y}}{2} \bigg|_{i+\frac{1}{2}} + \frac{a^2 \frac{\partial^2 W}{\partial y^2}}{4 \times 2!} \bigg|_{i+\frac{1}{2}} - \frac{a^3 \frac{\partial^3 W}{\partial y^3}}{8 \times 3!} \bigg|_{i+\frac{1}{2}} + \frac{a^4 \frac{\partial^4 W}{\partial y^4}}{16 \times 4!} \bigg|_{i+\frac{1}{2}} + O(a^5), \quad (A1)
\]

and

\[
w_{i+\frac{1}{2}} = w_i + \frac{a \frac{\partial W}{\partial y}}{2} \bigg|_{i+\frac{1}{2}} + \frac{a^2 \frac{\partial^2 W}{\partial y^2}}{4 \times 2!} \bigg|_{i+\frac{1}{2}} - \frac{a^3 \frac{\partial^3 W}{\partial y^3}}{8 \times 3!} \bigg|_{i+\frac{1}{2}} + \frac{a^4 \frac{\partial^4 W}{\partial y^4}}{16 \times 4!} \bigg|_{i+\frac{1}{2}} + O(a^5). \quad (A2)
\]

Subtracting Eq.(A1) from Eq.(A2) yields

\[
w_{i+\frac{1}{2}} - w_i = a \frac{\partial W}{\partial y} \bigg|_{i+\frac{1}{2}} + \frac{a^3 \frac{\partial^3 W}{\partial y^3}}{4 \times 3!} \bigg|_{i+\frac{1}{2}} + O(a^5). \quad (A3)
\]

Adding Eq.(A1) and Eq.(A2) yields

\[
w_{i+\frac{1}{2}} + w_i = 2w_{i+\frac{1}{2}} + \frac{a^2 \frac{\partial^2 W}{\partial y^2}}{4} \bigg|_{i+\frac{1}{2}} + \frac{a^4 \frac{\partial^4 W}{\partial y^4}}{8 \times 4!} \bigg|_{i+\frac{1}{2}} + O(a^5). \quad (A4)
\]

Replacing $w$ with $\frac{\partial W}{\partial y}$ in (A4) yields

\[
\frac{\partial W}{\partial y} \bigg|_{i+\frac{1}{2}} + \frac{\partial W}{\partial y} \bigg|_{i} = 2 \frac{\partial W}{\partial y} \bigg|_{i+\frac{1}{2}} + \frac{a^2 \frac{\partial^2 W}{\partial y^2}}{4} \bigg|_{i+\frac{1}{2}} + \frac{a^4 \frac{\partial^4 W}{\partial y^4}}{8 \times 4!} \bigg|_{i+\frac{1}{2}} + O(a^5). \quad (A5)
\]

Ignore the high order terms in (A5), we have

(164)
Applying Eq. (A6) in Eq.(A3) yields
\[
w_{i+l} - w_i = \frac{a}{2} \left( \frac{\partial W}{\partial y} \bigg|_{i+l} + \frac{\partial W}{\partial y} \bigg|_i \right) - \frac{a^3}{12} \frac{\partial^3 W}{\partial y^3} \bigg|_{i+\frac{l}{2}} + O(a^5).
\] (A7)

Again, replacing \( w \) with \( \frac{\partial W}{\partial y} \) in Eq.(A7) yields
\[
\frac{\partial W}{\partial y} \bigg|_{i+l} - \frac{\partial W}{\partial y} \bigg|_i = \frac{a}{2} \left( \frac{\partial^2 W}{\partial y^2} \bigg|_{i+l} + \frac{\partial^2 W}{\partial y^2} \bigg|_i \right) - \frac{a^3}{12} \frac{\partial^4 W}{\partial y^4} \bigg|_{i+\frac{l}{2}} + O(a^5).
\] (A8)

It was shown in literature that
\[
w_{i+l} - 2w_i + w_{i-l} = a^2 \frac{\partial^2 W}{\partial y^2} \bigg|_i + \frac{a^4}{12} \frac{\partial^4 W}{\partial y^4} \bigg|_i + O(a^6),
\] (A9)

From (A9), we have
\[
\frac{\partial^2 W}{\partial y^2} \bigg|_i = \frac{w_{i+l} - 2w_i + w_{i-l}}{a^2} - \frac{a^2}{12} \frac{\partial^4 W}{\partial y^4} \bigg|_i + O(a^4).
\] (A10)

Applying Eq. (A10) in Eq.(A8) yields
\[
\frac{\partial W}{\partial y} \bigg|_{i+l} - \frac{\partial W}{\partial y} \bigg|_i = \frac{a}{2} \left( \frac{w_{i+2} - 2w_{i+1} + w_i}{a^2} + \frac{w_{i-1} - 2w_i + w_{i+1}}{a^2} \right) - \frac{a^3}{24} \left( \frac{\partial^4 W}{\partial y^4} \bigg|_{i+\frac{l}{2}} + \frac{\partial^4 W}{\partial y^4} \bigg|_i \right) - \frac{a^3}{6} \frac{\partial^4 W}{\partial y^4} \bigg|_{i+\frac{l}{2}} + O(a^5),
\] (A11)

or
\[
\frac{\partial W}{\partial y} \bigg|_{i+l} - \frac{\partial W}{\partial y} \bigg|_i = \frac{1}{2a} \left( w_{i+2} - w_{i+1} - w_i + w_{i-1} \right) - \frac{a^3}{6} \frac{\partial^4 W}{\partial y^4} \bigg|_{i+\frac{l}{2}} + O(a^5).
\] (A12)
If we neglect the higher order small-value terms on the right side of Eq. (A12) and denote the first derivative of the wavefront in the y-direction as $s_y$, then Eq.(12) becomes

$$s_{y,i+2} - s_{y,i+1} = \frac{1}{2a} \left( w_{i+3} - w_{i+2} - w_{i+1} + w_i \right),$$  \hspace{2cm} (A13)

where $i=1,2,..., t-3$; $t+1,t+2,..., 2t-3$, $...$, $m-3$.

Similarly in the z-direction, we can write

$$s_{z,i+t} - s_{z,i+2t} = \frac{1}{2a} \left( w_i - w_{i+t} - w_{i+2t} + w_{i+3t} \right),$$  \hspace{2cm} (A14)

where $i=1,2,..., t$, $t+1,t+2,..., 2t$, $...$, $m-3t$. 

166
LIST OF REFERENCES


