Metrology and Sensing

Lecture 12: Phase retrieval

2018-01-18

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## Preliminary Schedule

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<td>2</td>
<td>26.10</td>
<td>Wave optics</td>
<td>Basics, polarization, wave aberrations, PSF, OTF</td>
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<td>Moire principle, illumination coding, fringe projection, deflectometry</td>
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Content

- Introduction
- Algorithms
- Various practical aspects
- Accuracy
Wave front determines local direction of propagation
- Propagation over distance $z$: change of transverse intensity distribution
- Intensity propagation contains phase information
Wave Equation

- Maxwell equation for the field $E$, vectorial
  The spatial inhomogeneities couples the field components

- Homogeneous, without charges, non-conductive separation of vector components, scalar

- Time independence:
  Wave equation of Helmholtz
  In coordinate representation

- Wave number in medium refractive index $n$

- Fast $z$-oscillation separated
  Slowly varying envelope approximation

\[ \nabla^2 \vec{E} - \mu_0 \varepsilon_0 \varepsilon_r \frac{\partial^2 \vec{E}}{\partial t^2} + \nabla (\vec{E} \cdot \nabla \ln \varepsilon_r) = 0 \]

\[ \nabla^2 \tilde{E} = \mu \varepsilon \frac{\partial^2 \tilde{E}}{\partial t^2} \]

\[ \tilde{E}(\vec{r}, t) = \tilde{E}(\vec{r}) \cdot e^{i\omega t} \]

\[ \Delta \tilde{E} + k^2 \tilde{E} = 0 \]

\[ \frac{\partial^2 E}{\partial x^2} + \frac{\partial^2 E}{\partial y^2} + \frac{\partial^2 E}{\partial z^2} - \frac{n^2(x, y, z) \omega^2}{c^2} E = 0 \]

\[ k = \frac{\omega}{c} = \frac{2\pi n}{\lambda_o} = nk_o \]

\[ \tilde{E}(x, y, z) = \tilde{E}(x, y, z) \cdot e^{-ikz} \]

\[ - \frac{\partial^2 E}{\partial z^2} + 2ik \frac{\partial E}{\partial z} = \nabla_{\perp}^2 E + k^2 \left[ \frac{n^2(x, y)}{n_0^2} - n_o^2 \right] E \]
Fraunhofer Point Spread Function

- Rayleigh-Sommerfeld diffraction integral, Mathematical formulation of the Huygens-principle

\[
E_I(\vec{r}) = \frac{i}{\lambda} \iiint E(\vec{r}') \frac{e^{i \kappa|\vec{r} - \vec{r}'|}}{|\vec{r} - \vec{r}'|} \cos \theta \, dx' \, dy'
\]

- Fraunhofer approximation in the far field for large Fresnel number

\[
N_F = \frac{r_p^2}{\lambda \cdot z} \approx 1
\]

- Optical systems: numerical aperture NA in image space
  Pupil amplitude/transmission/illumination \( T(x_p, y_p) \)
  Wave aberration \( W(x_p, y_p) \)
  complex pupil function \( A(x_p, y_p) \)
  Transition from exit pupil to image plane

\[
E(x', y') = \iiint_{AP} T(x_p, y_p) \cdot e^{2\pi i W(x_p, y_p)} \cdot e^{\frac{2\pi i}{\lambda R_{AP}} (x_p x' + y_p y')} \, dx_p \, dy_p
\]

- Point spread function (PSF): Fourier transform of the complex pupil function

\[
A(x_p, y_p) = T(x_p, y_p) \cdot e^{2\pi i W(x_p, y_p)}
\]
Fresnel Diffraction

- Typical change of the intensity profile

- Normalized coordinates

\[ u = \frac{2\pi}{\lambda} \cdot \left( \frac{a}{f} \right)^2 \cdot z ; \quad v = \frac{2\pi}{\lambda} \cdot \left( \frac{a}{f} \right) \cdot r ; \quad \rho = \frac{r}{a} \]

- Diffraction integral

\[ E(u, v) = -\frac{2\pi ia^2 E_0}{\lambda f^2} \cdot e^{i(f/a)^2u} \cdot \int_0^1 J_0(\rho v) \cdot e^{-\frac{i}{2}u\rho^2} \rho \, d\rho \]
Propagation of Intensity

- Transport of intensity equation couples phase and intensity

\[ k \cdot \frac{\partial I(x, y, z)}{\partial z} = -\nabla[I(x, y, z) \cdot \nabla W(x, y)] \]

- Solution with z-variation of the intensity delivers start phase at \( z = 0 \)

- Determine phase from intensity distribution.
  - Inverse propagation problem: ill posed
  - Boundary condition: measured z-stack \( I(x,y,z) \)

- Algorithm for numerical solution
  - IFTA / Gerchberg Saxton (error reduction)
  - Acceleration (conjugate gradients, Fienup, ...)
  - Modal non least square methods
  - Extended Zernike method

- Applications:
  - Calculation of diffractive components for given illumination distribution
  - Wave front reconstruction
  - Phase microscopy
Principal Approach

- Given object $I_{\text{object}}(x)$
- Known illumination, usually incoherent
- Known measured image intensities $I_{\text{image}}(x',z)$ for several $z$-values
- To be calculated: transfer function of the system / pupil function
- Relationship: convolution

\[
I_{\text{object}}(x) \quad I_{\text{pupil}}(x_p) = A_{\text{pupil}}(x_p) \exp \left[ 2\pi i W(x_p) \right] \quad I_{\text{image}}(x',z)
\]
Retrieval: Intensity z-stack

- Stack of transverse intensity distributions \( I(x,y,z=\text{const}) \)
- Criteria for \( z \)-selection:
  - no truncation for outer \( z \)-planes
  - good resolution for focal point (>6 pixel per Airy diameter)
  - enough redundant data for noise, discretization and quantization
  - enough \( z \)-planes for far field and near field:
    at least \(-2R_u...+2R_u\)
Phase Retrieval

- Principle of phase retrieval for metrology of optical systems
- Measurement of intensity caustic z-stack
- Reconstruction of the phase in the exit pupil
Phase Space: 90° - Rotation

- Transition pupil-image plane: 90° rotation in phase space
- Planes Fourier inverse
- Marginal ray: space coordinate $x$ --- angle $\theta'$
- Chief ray: angle $\theta$ --- space coordinate $x'$
Phase Space Interpretation

- Known measurement of intensity in defocussed planes:
  - Several rotated planes in phase space
  - Information in and near the spatial domain
- Calculation of distribution in the Fourier plane
- Wave equation is valid
- Principle: Tomography
Phase Retrieval Illumination Setups

- **Pinhole object**
  - Deconvolution may be necessary
  - Illumination incoherent
  - Problems with pinhole

- **Epi-illumination**
  - Double pass with plane mirror
  - Only symmetrical aberrations
  - No field coma seen

- **Trans-illumination with objective**
  - Laser source, coherent
  - Calibration necessary
  - Speckle problem
Necessary known basic parameter for reconstruction:
1. wavelength $\lambda$
2. aperture in image space $\sin(u)$
3. pixel size of detector
4. pinhole size in object space
5. magnification $m$
6. z-values of z-stack

Critical data:
1. pixel size
2. size of pinhole (coherence, throughput)
3. deconvolution parameter of algorithm
4. background of intensity
5. selection of z-planes
Mathematical Formulation

- Mathematical description for Image formation, Integral equation, inverse problem

- Approximation with isoplanatic range: Psf shift invariant, convolution computed with Fourier methods

- Discretization: pixelized image delivers a linear system

- Solution via optimization due to noise and constraints

\[
I_{\text{image}}(x) = \int I_{\text{psf}}(x, x') \cdot I_{\text{object}}(x, x') \, dx' + I_{\text{noise}}(x)
\]

\[
I_{\text{image}}(x) = I_{\text{psf}}(x) \ast I_{\text{object}}(x) + I_{\text{noise}}
\]

\[
I_{\text{image}}(v) = I_{\text{psf}}(v) \cdot I_{\text{object}}(v) + I_{\text{noise}}
\]

\[
I_{jk}^{(ima)} = \sum_{j'} \sum_{k'} I_{j'-j,k'-k}^{(psf)} \cdot I_{j',k'}^{(obj)} + I_{jk}^{(noi)}
\]

\[
\bar{g} = A \cdot \bar{x} + \bar{n}
\]

\[
|A \cdot \bar{x} - \bar{b}|^2 = \min
\]

\[
\Phi = |A \cdot \bar{x} - \bar{b}|^2 + \mu \cdot |\bar{x}|^2 = \min
\]
Gerchberg-Saxton-Algorithm

- Iterative reconstruction of the pupil phase with back-and-forth calculation between image and pupil:
  IFTA / Gerchberg-Saxton

- Substitution of known intensity

- Problems with convergence:
  Twin-image degeneration

- Modified algorithms:
  1. Fienup-acceleration
  2. Non-least-square
  3. Use of pupil intensity
Possible numerical algorithms:

1. Fourier algorithm
2. NLSQ-algorithm with Zernike coefficients (modal)
3. Input-Output-algorithm according to Fienup
4. Yang-Gu-algorithm
5. Ping-Pong-algorithm
6. Gerchberg-Saxton-algorithm (error reduction)
7. Ferwerda-algorithm
8. Gradient methods
Check of Caustik

- Paraxial approximation:
  - quadratic curve of second moment of spot size
  - check of wrong data possible
  - deviations for larger aberrations
Example Phase Retrieval

- Evaluation of real data psf-stack
- Phase retrieval method
- Image z-stack

- Correlation of image
- Phase in pupil
Finite Size of Pinhole

- Image with finite size of the pinhole: convolution
- Characteristic diffraction structures hidden with growing size $D_{ph}$
- Deconvolution necessary for $D_{ph} > 0.3...0.4 \ D_{airy}$
- Pinholes larger than $4 \ D_{airy}$ are not feasible
Incoherent Image of a Pinhole

- Logarithm of intensity
- Diffraction ripples disappear with growing diameter $d$
Coherent Illuminated Pinhole

- Pinhole with coherent illumination: pupil apodization with Airy profile
- First zero at boundary of pupil for

\[
D_{PH} = \frac{1.22 \cdot \lambda}{\sin u} = D_{airy}
\]

\[
E(r_p) = 2J_1 \left( \frac{1.22 \cdot \pi \times \frac{D_{PH}}{D_{airy}} r_p}{1.22 \cdot \pi \times \frac{D_{PH}}{D_{airy}} r_p} \right)
\]
- Quas point source for the
  
  \[ 2a < 0.4 \cdot \mathcal{D}_{\text{Airy}} \]

- Criterion:
  intensity threshold of Airy function at 10% / 50%
Comparison of pinhole image with Airy-Psf:

Rms value of deviation

Coherent case: better approximation

Typical limits:
- Incoherent: \( D/D_{\text{airy}} < 0.4 \)
- Coherent: \( D/D_{\text{airy}} < 0.7 \)

<table>
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<th>Rms-limit</th>
<th>coherent</th>
<th>incoherent</th>
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<tr>
<td>0.01</td>
<td>( d = 0.670 )</td>
<td>( d = 0.338 )</td>
</tr>
<tr>
<td>0.02</td>
<td>( d = 0.867 )</td>
<td>( d = 0.458 )</td>
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Deconvolution - Algorithms

- Incoherent imaging with noise

\[ I_{\text{image}}(x) = I_{psf}(x) * I_{object}(x) + I_{noise} \]

- Wiener deconvolution with fixed Tikhonov regularization

\[ I_{object}(v) = \frac{I_{psf}^*(v) \cdot I_{image}(v)}{\|I_{psf}(v)\|^2 + \mu} \]

- Wiener deconvolution with variable Tikhonov regularization

\[ I_{object}(v) = \frac{I_{psf}^*(v) \cdot I_{image}(v)}{\|I_{psf}(v)\|^2 + \frac{P_{noise}}{P_{object}}} \]

- Lucy-Richardson deconvolution

\[ I_{obj}^{(k+1)}(x, y) = I_{obj}^{(k)}(x, y) \cdot \left[ I_{psf}(-x, -y)^* \cdot \frac{I_{image}(x, y)}{I_{psf}(x, y)^* \cdot I_{obj}^{(k)}(x, y)} \right] \]

- Wavelet-Deconvolution
Error in Phase Retrieval without Deconvolution

- Error of results, if no deconvolution is performed
- Error increases with pinhole size
- Deconvolution seems to be necessary for pinholes larger than 0.4 $D_{\text{airy}}$
Criteria for pinhole deconvolution:

1. minimal rms of stack sensitive for noise

2. Maximum correlation of the stacks robust, but less significant

3. Minimum entropy best results

\[ I_{\text{rms}} = \sqrt{\frac{\sum_{j} [I_{j}^{(\text{mod ell})} - I_{j}^{(\text{ist})}]^2}{n_x \cdot n_y \cdot n_z}} \]

\[ K = \frac{\iiint I_{\text{model}} \cdot I_{\text{ist}} \, dx \, dy \, dz}{\sqrt{\iiint I_{\text{model}}^2 \, dx \, dy \, dz \cdot \iiint I_{\text{ist}}^2 \, dx \, dy \, dz}} \]

\[ S = -\sum_{m,n} I_{mn} \cdot \ln I_{mn} \]
Iteration Phase Retrieval for finite sizes of Pinhole

- Possibilities with / without deconvolution
Measuring Setup with Magnification

- Transfer of coherent field

\[ I_{exact}(x) = \left| A_{psf1}(x) \otimes A_{psf2}(x) \right|^2 \]

- Frequency space

\[ I_{exact}(v) = \left[ A_1(v) \cdot A_2(v) \right] \otimes \left[ A_1^*(v) \cdot A_2^*(v) \right] \]

- Therefore the phase is added

\[ A(v) = T(v) \cdot e^{2\pi iW} \]

\[ I_{exact}(v) = \left[ T(v) \cdot e^{2\pi iW} \right] \otimes \left[ T(v) \cdot e^{-2\pi iW} \right] \]

\[ T(v) = T_1(v) \cdot T_2(v) \]

\[ W(v, z) = W_1(v) + W_2(v, z) \]
Measuring Setup with Magnification

Local energy flow directed
Phase Retrieval with Apodization

- Analysis taking apodization into account greatly improves the result
Phase Retrieval with Apodization

- If the pupil shows a significant illumination distribution: apodization must be taken into account
- Apodization can be fitted too
- Better: measured apodization used

![Graph showing the effect of apodization on rms intensity over iterations.](image)
Phase Retrieval with Apodization

- Retrieval without / with Apodization
- Correlation over z
- Scaling / Normalization:
  - Intensity
  - Energy
- Problem: SNR in strong defocussed planes

\[
\Delta z = -2R_E \\
\Delta z = -1R_E \\
\text{Focus} \\
\Delta z = +1R_E \\
\Delta z = +2R_E
\]

I_{max} = 5.1\%  
I_{max} = 9.8\%  
I_{max} = 42\%
- Determination background intensity preferred: corner, every z-plane individually
- Truncation of outer region without signal
- Subtraction of underground signal
- Noise depends on light level
- Defocussed z-planes more critical
- Modal fit with Zernikes is low pass filter
Centering - Line of Sight

Centering of z-stack images:
1. Line of sight
   (centroid moves exactly on a line))
2. Systematic errors due to mechanical inaccuracy (line tilt)
3. Statistical errors
Problems for truncation of the beam profiles: errors in centroid determination.
Object Space Defocussing

a) defocussing in image space

\[ \text{object plane} \rightarrow \text{lens} \rightarrow \text{pupil} \rightarrow \text{several detector planes} \]

Intensity caustic \( I(x,y,z) \)

b) defocussing in object space

\[ \text{several object planes} \rightarrow \text{lens} \rightarrow \text{pupil} \rightarrow \text{one fixed detector plane} \]

Intensity caustic \( I(x,y,Z_{\text{obj}}) \)
Object Space Defocussing

- Good Linearity of Zernike coefficients
- Small retrace non-linearity

\[ c_j(z) = c_{j_0} \cdot \left( 1 + \Delta c_{\text{lin}} \cdot \frac{\Delta z}{R_E} \right) \]
Phase Retrieval Accuracy

Evaluation of real measuring data

Comparison of Zernike coefficients with Hartmann test results: accuracy in the range $\lambda/100$
Circular symmetric contributions can be separated over defocussing range:
1. apodization: increase in diameter in focal region
2. finite pinhole size: uniform broadening vs defocus
3. spherical aberration: asymmetric around focal plane
Phase Retrieval Reproducability

- Reproducability of 3 measurements
- Very good agreement with uncertainties in the range of \( \lambda/100 \) for every Zernike coefficients for the first 36 terms
- No dependence on symmetry

![Graph showing the c_j(\lambda) values for different phase retrieval measurements.](image)
Example Residuum

- Comparison of intensity profile cross sections \( x / y \)
- Blue : Input
  Red : Model
Estimation of Accuracy

- Correlation matrix of NLSQ-fit can be used to estimate the accuracy
- Experience: largest error bars for circular symmetric aberrations
Problems and Suggestions

- Data not truncated
- Centering of stack images on common line
- Don’t use more than 36 Zernikes
- Pinhole not larger than $2 \times D_{\text{airy}}$
- Deconvolution for nearly incoherent illumination
- Preferred dynamic pinhole-match and forward convolution of finite size
- Proposed: $n > 7$ z-planes in the interval $-2 \text{Ru} \ldots +2 \text{Ru}$
- At least 6 detector pixels inside the Airy diameter in the focus plane
- Denoising of data
- Subtraction of background
- Low-pass filtering of Zernike modal functions in pupil
- If pupil apodization present: must be taken into account
- Normalization of intensity in every z-plane