Phase Retrieval and Support Estimation in X-Ray Diffraction

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Outline

• Phase retrieval applications

• Phase retrieval algorithms
  o Iterative Transform Algorithm
    – Hybrid input-output algorithm
  o Gradient search algorithms

• Support Constraint
  o Importance
  o Reconstructing object support from autocorrelation support
  o Tightening the support constraint
  o Several examples
Phase Retrieval Application: Imaging through Atmospheric Turbulence

- Problem: atmospheric turbulence causes phase errors, limits resolution

- Labeyrie’s stellar speckle interferometry yields Fourier magnitude
  - Incoherent (real, nonnegative) image

- Lensless imaging with laser illumination
  - Measure far-field speckle intensity
  - Complex-valued image

- Both mathematically similar to x-ray diffraction
PROCLAIM 3-D Imaging Concept
Phase Retrieval with Opacity Constraint LAser IMaging

- Tunable laser
- Direct-detection array
- Initial estimate from locator set
- Phase retrieval algorithm
- 3-D FFT
- Reconstructed object

\[ v_1, v_2, \ldots, v_n \]

Collected data set

Coherence 2005, JRF, 6/05-4
Determine Hubble Space Telescope Aberrations from PSF

Measurements & Constraints:
- Pupil plane: known aperture shape
  phase error fairly smooth function
- Focal plane: measured PSF intensity

Wavefronts in pupil plane and focal plane are related by a Fourier Transform
Next Generation Space Telescope
James Webb Space Telescope

- See red-shifted light from early universe
  - 0.6 to 28 µm
  - L2 orbit for passive cooling, avoiding light from sun and earth
  - 6 m diameter primary mirror
    - Deployable, segmented optics
    - Phase retrieval to align segments

http://ngst.gsfc.nasa.gov/
Optical Testing Using Phase Retrieval

Optical wave fronts (phase) can be measured by many forms of interferometry.

Novel wave front sensor: a bare CCD detector array, detects reflected intensity.

Wave front reconstructed in the computer by phase retrieval algorithm.

Approach:

Simulation Results:

- PSF1: Actual wrapped phase
- PSF2: Reconstructed wrapped phase
- True Phase
- Retrieved Phase

Part under test

Display of measured wavefront

CCD Array measures intensity of reflected wavefront

Illumination Wavefront

Computer
Image Reconstruction from X-Ray Diffraction Intensity

Coherent X-ray beam

Target

Collection of gold balls (has complex index of refraction)

Far-field diffraction pattern (Fourier intensity)

Detector array (CCD)
Phase Retrieval Basics

Fourier transform: \( F(u,v) = \int \int_{-\infty}^{\infty} f(x,y) e^{-i2\pi(ux + vy)} dx dy \)

\[ = |F(u,v)| e^{i\psi(u,v)} = \mathcal{F}[f(x,y)] \]

Inverse transform: \( f(x,y) = \int \int_{-\infty}^{\infty} F(u,v) e^{i2\pi(ux + vy)} dudv = \mathcal{F}^{-1}[F(u,v)] \)

Phase retrieval problem:

Given \( |F(u,v)| \) and some constraints on \( f(x,y) \),
Reconstruct \( f(x,y) \), or equivalently retrieve \( \psi(u,v) \)

\[ |F(u,v)| = |\mathcal{F}[f(x,y)]| = |\mathcal{F}[e^{ic} f(x - x_o, y - y_o)]| = |\mathcal{F}[e^{ic} f^* (-x - x_o, -y - y_o)]| \]
(Inherent ambiguities: phase constant, images shifts, twin image all result in same data)

Autocorrelation:

\[ r_f(x,y) = \int \int_{-\infty}^{\infty} f(x',y') f^* (x' - x, y' - y) dx' dy' = \mathcal{F}^{-1}[|F(u,v)|^2] \]

- Patterson function in crystallography is an aliased version of the autocorrelation
- Simply need Nyquist sampling of the Fourier intensity to avoid aliasing
Autocorrelation Function:

\[ r_f (x, y) = \int \int_{-\infty}^{\infty} f(x', y')f(\text{'}x - x, y' - y)dx'dy' = \mathcal{F}^{-1}[|F(u, v)|^2] \]

has all vector separations in object

If in repeated array, Object embedded in zeros by factor of 2

In repeated array, Object NOT embedded in zeros by factor of 2

\[ \Delta u \leq \frac{\lambda z}{(2D_u)} \]

Autocorrelation Function = Patterson function

Fourier intensities undersampled -- forced by crystallographic periodicity

Get Aliasing \[ \Delta u = \frac{\lambda z}{D_u} > \frac{\lambda z}{(2D_u)} \]

Autocorrelation Function

Fourier intensities adequately (Nyquist) sampled or oversampled

NO Aliasing
Constraints in Phase Retrieval

- **Nonnegativity constraint:** \( f(x, y) \geq 0 \)
  - True for ordinary incoherent imaging, crystallography, MRI, etc.
  - Not true for wavefront sensing or coherent imaging (sometimes x-ray)

- The **support** of an object is the set of points over which it is nonzero
  - Meaningful for imaging objects on dark backgrounds
  - Wavefront sensing through a known aperture

- A good support constraint is essential for complex-valued objects
  - Coherent imaging or wave front sensing

- **Atomiticity** when have angstrom-level resolution
  - For crystals -- **not** applicable for coarser-resolution, single-particle

- **Object intensity constraint** (wish to reconstruct object phase)
  - E.g., measure wavefront intensity in two planes (Gerchberg-Saxton)
  - If available, supercedes support constraint
First Phase Retrieval Result

(a) Original object, (b) Fourier modulus data, (c) Initial estimate
(d) – (f) Reconstructed images — number of iterations: (d) 20, (e) 230, (f) 600

Iterative Transform Algorithm

START:
Initial Estimate

\[ g \]

\[ \mathcal{F} \{ \} \]

\[ G = |G| e^{i\phi} \]

Constraints:
Support, (Nonnegativity)

Form New Input
Using Image
Constraints

\[ g' \]

\[ \mathcal{F}^{-1} \{ \} \]

\[ G' = |G'| e^{i\phi} \]

Satisfy Fourier
Domain
Constraints

Measured Data:
Magnitude, IFI

\[ \sqrt{\text{Measured intensity}} \]

Hybrid Input-Output version

\[ g_{k+1}(x,y) = \begin{cases} 
  g'_k(x,y), & (x,y) \in \text{Support} \\
  g_k(x,y) - \beta g'_k(x,y), & (x,y) \notin \text{Support}
\end{cases} \]
Iterative Transform Algorithm Versions: Error-Reduction versus HIO

- **Error reduction algorithm**
  \[ g_{k+1}(x) = \begin{cases} 
  g_k'(x), & x \in S \text{ and } g'_k(x) \geq 0 \\
  0, & \text{otherwise} 
\end{cases} \]
  - Satisfy constraints in object domain
  - Equivalent to projection onto (nonconvex) sets algorithm
  - Equivalent to successive approximations
  - Similar to steepest-descent gradient search
  - Proof of convergence (weak sense)
  - In practice: slow, prone to stagnation, gets trapped in local minima

- **Hybrid-input-output algorithm**
  \[ g_{k+1}(x) = \begin{cases} 
  g_k'(x), & x \in S \text{ and } g'_k(x) \geq 0 \\
  g_k(x) - \beta g'_k(x), & \text{otherwise} 
\end{cases} \]
  - Uses negative feedback idea from control theory
    - \( \beta \) is feedback constant
  - No convergence proof (can increase errors temporarily)
  - In practice: much faster than ER
  - Can climb out of local minima at which ER stagnates
Image Reconstruction from Simulated Speckle Interferometry Data

Labeyrie’s stellar speckle interferometry gives this

Error Metric versus Iteration Number

RMS ERROR $E_0$

ITERATION $k$

Error Reduction

Hybrid Input-Output
Nonlinear Optimization Algorithms
Employing Gradients

Minimize Error Metric, e.g.:  
\[ E = \sum_u W(u)[|G(u)| - |F(u)|]^2 \]

Contour Plot of Error Metric

Repeat three steps:
1. Compute gradient:  
   \[ \frac{\partial E}{\partial p_1}, \frac{\partial E}{\partial p_2}, \ldots \]
2. Compute direction of search
3. Perform line search

Gradient methods:
- (Steepest Descent)
- Conjugate Gradient
- BFGS/Quasi-Newton
- …
Analytic Gradients with Phase Values as Parameters

\[
E = \sum_u W(u)[|G(u)| - |F(u)|]^2
\]

\[
G(u) = \mathcal{P}[g(x)]
\]

Optimizing over \( g(x) = g_R(x) + ig_I(x) = m_o(x)e^{i\theta(x)} \), \( \theta(x) = \sum_{j=1}^J a_j Z_j(x) \)

For point-by-point pixel (complex) value, \( g(x) \),
\[
\frac{\partial E}{\partial g(x)} = 2 \text{ Im}\left\{ g^*^{W*}(x) \right\}
\]

For point-by-point phase map, \( \theta(x) \),
\[
\frac{\partial E}{\partial \theta(x)} = 2 \text{ Im}\left\{ g(x) g^{W*}(x) \right\}
\]

For Zernike polynomial coefficients,
\[
\frac{\partial E}{\partial a_j} = 2 \text{ Im}\left\{ \sum_x g(x) g^{W*}(x) Z_j(x) \right\}
\]

where
\[
G^W(u) = W(u) \left[ |F(u)| \frac{G(u)}{|F(u)|} - G(u) \right], \quad \text{and} \quad g^W(x) = \mathcal{P}^\dagger \left[ G^W(u) \right]
\]

\( \mathcal{P}[\cdot] \) can be a single FFT or multiple-plane Fresnel transforms with phase factors and obscurations.

Analytic gradients very fast compared with calculation by finite differences.

Support Constraints
Example of Algorithm for Deriving Bounds on Object Support

Object Support $S$

Forming Autocorrelation Support

$A = S - S \equiv \{x - y : x, y \in S\}$

Autocorrelation Support

$a_1, a_2 \ldots$ are “extreme points” they must all be contained in one translate of the object, $S$

$L = A \cap (A + a_1) \cap (A + a_2) \cap \ldots$

Triple Intersection Rule: [Crimmins, Fienup, & Thelen, JOSA A 7, 3 (1990)]
Triple Intersection for Triangle Object

- Family of solutions for object support from autocorrelation support
- Use upper bound for support constraint in phase retrieval
Fig. 7. Autocorrelation tri-intersection for sets consisting of a collection of distinct points. (a) Set $S$, (b) $A = S - S$, (c) and (d) locators of the form $L = A \cap (w + A)$. Intersecting (c) or (d) with (b) yields the unique solution (a).

Fig. 8. Autocorrelation intersection for redundant case. (a) Set $S$, (b) $A = S - S$, (c)–(e) locators of the form $L = A \cap (w + A)$, (f) intersection of (c) with (d), (g) another intersection of three translates of $A$. 
Arrangements of Points
Preventing Triple Intersection

Fig. 9. Redundancy types of relationships within $S$ that would violate Condition 1. (a) and (b) three vector separations add to zero, (c) one vector separation is twice another, (d) two vector separations are equal.
Reconstruction of Values of Collection of Points
Autocorrelation Support

Object Support

Forming the Autocorrelation Support

Autocorrelation Support
Locator Sets

Triple intersection rule
Includes all possible object supports that give rise to autocorrelation support
Combination of Locator Sets

- Must be able to restrict alignment horizontally and vertically, if half the autocorrelation width in each dimension and determine whether have twinned locator set.

- Then align and intersect locator sets to arrive at smaller (better) locator set.
Binary Object Example

Object

Autocorrelation (not binary)

Thresholded Autocorrelation
(Estimated Autocorrelation Support)
Finding Vertex Points on Autocorrelation Support

(Use Vertex Points for Triple Intersection)
3 Locator Sets and a Combination of Them
Gray-Level Object Example

Object

Autocorrelation

Autocorrelation (highly overexposed)

Thresholded Autocorrelation
Finding Vertex Points on Autocorrelation Support

Use Vertex Points for Triple Intersection
2 Locator Sets and a Combination

Object

Autocorrelation

Object

Autocorrelation (highly overexposed)
ST Object. The three concentric discs forming a pyramid can be seen as dark circles at their edges. The small piece on one of the two lower legs was removed before this photograph was taken.
PROCLAIM 3-D Imaging Concept
Phase Retrieval with Opacity Constraint Laser Imaging

- tunable laser
- direct-detection array

Collected data set $v_1, v_2, \ldots, v_n$

Initial estimate from locator set

Phase retrieval algorithm

3-D FFT

Reconstructed object
### 3-D Laser Fourier Intensity Laboratory Data

#### Data cube:

- 1024x1024 CCD pixels x 64 wavelengths

#### Shown at right:

- 128x128x64 sub-cube
  
  (128x128 CCD pixels at each of 64 wavelengths)
Imaging Correlography

- Get incoherent-image information from coherent speckle pattern
- Estimate 3-D Incoherent-object Fourier squared magnitude
  - Like Hanbury-Brown Twiss intensity interferometry
    \[ |F_1(u,v,w)|^2 \approx \langle [D_k(u,v,w) - I_o] \otimes [D_k(u,v,w) - I_o] \rangle_k \]
    (autocovariance of speckle pattern)
- Easier phase retrieval: have nonnegativity constraint on incoherent image
- Coarser resolution since correlography SNR lower

References:


Image Autocorrelation from Correlography
Thresholded Autocorrelation
Triple Intersection of Autocorrelation Support
Dilated Locator Set used as Support Constraint
Fourier Modulus Estimate from Correlography
Fourier Magnitude, DC Slice

Before Filtering  After Filtering
Incoherent Image
Reconstructed by ITA
Support Constraint from Thresholded Incoherent Image
Dilated Support Constraint from Thresholded Incoherent Image
Coherent Image Reconstructed by ITA from One 128x128x64 Sub-Cube
Example on Real X-Ray Data
(Data from M. Howells/LBNL and H. Chapman/LLNL)

(a) X-ray data
(b) Autocorrelation from (a)
(c) Initial Support constraint computed from (b)
(d) Electron micrograph of object
Status of Support Estimation

- “Shrink wrap” algorithm tries to find support dynamically during iterations, but all other phase retrieval algorithms need a support constraint.

- A low-resolution image of object by another sensor would help by providing a low-resolution support constraint, but phase retrieval works best with a fine-resolution support constraint.

- Have several methods for fine-resolution support from autocorrelation.

- Need to make support estimation from the autocorrelation more robust because of additional difficulties:
  - Missing data at low spatial frequencies because of the beam stop
  - Complex-valued objects
  - High levels of noise in single frames
  - 3-D support estimation has been done [1], but not as mature as 2-D

PROCLAIM:


Support Reconstruction and Locator Sets:


Imaging Correlography:


Iterative Transform Algorithm Phase Retrieval:


Sidelobe Removal: