Optical Wavefront Reconstruction: Numerical Theory

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Abstract

This work details the theory of projection techniques for numerical optical wavefront reconstruction. Computational wavefront reconstruction algorithms have been successfully applied for many years, however most of the fundamental mathematical questions about the behavior and properties of these algorithms remain open, in particular questions regarding existence, uniqueness and convergence. The theoretical results often cited for these algorithms do not apply to the problem of phase retrieval since the required hypotheses are not satisfied.

We briefly review an analysis of the central theoretical difficulties of the phase retrieval problem. We then propose techniques for avoiding numerical instabilities resulting from theoretical pathologies. In addition, we introduce a novel method for accelerating convergence with a technique we call *extended least squares*. Our results are compared to the performance of similar projection algorithms.

Optical wavefront reconstruction algorithms have been employed in crystallography, microscopy and optical design for three decades. Among the first of such algorithms is the celebrated Gerchberg-Saxton algorithm [8]. Since the introduction of the Gerchberg-Saxton algorithm numerous variations have been studied [1,6,7,12,13,16–19,21,22]. Projection algorithms in convex settings have been well understood since the early 1960's [4,9,10,20,23,24]. The phase retrieval problem, however, involves *nonconvex* sets. For this reason, the convergence properties of the Gerchberg-Saxton algorithm and its variants are not completely understood. In 1981 Hayes [11] showed that the solution to the two dimensional phase retrieval problem *for a single band-limited image*, if it exists, is almost surely unique up to rotations and linear shifts. While this result is of fundamental importance, it does not apply to many of the algorithms used for phase retrieval. For example, a projection technique proposed in 1973 by Misell [17] applies projections onto several images in a cyclic manner in order to find the wavefront aberration common to all the images. It is shown in [15] that in many practical situations, in particular in the presence of noise, the underlying problem that this and similar algorithms [6] attempt to solve has no solution. Thus, while the uniqueness result of Hayes remains valid for bandlimited signals, it says nothing about the uniqueness of *approximate* solutions in the event that a true solution does not exist, that is when the feasible set is empty. In the convex setting, when the constraint sets onto which the projections are computed do not intersect, convergence of projection algorithms is an open question [5]. Much less is known about the nonconvex setting.

The similarity between projection algorithms and line search methods applied to a particular error metric has been known for some time [3, 6, 8]. A precise analysis of this correspondence, however, has proven elusive. In 1985 Barakat and Newsam [2, 3] developed an approach modeled on the projection theory for convex sets. A well known fact from convex analysis is that the gradient of the squared distance to a convex set is *equivalent* to the direction toward the projection onto the set. To extend this property to the nonconvex sets, Barakat and Newsam require the projection operators to be single-valued, however there is no known example of a nonconvex set for which the projection operator is single-valued. Indeed, we show that the projections in the case of phase retrieval are multi-valued and that the squared set distance is not differentiable in the classical sense. The source of the difficulty is the nonconvexity of the underlying sets and the nonsmoothness of the error metric. The precise relationship between the projections onto image constraints and *subdifferentials* of the corresponding nonsmooth distance metric are detailed in [14]. The numerical phenomenon of stagnation that is commonly observed with projection-type algorithms can be associated with the multi-valuedness of the projection. Extensions to projection algorithms have been proposed to overcome stagnation [6]. These methods seem to be very robust and efficient in practice [21]. Their success warrants precise mathematical analysis which has yet to be done.

In our approach the subtleties of subdifferentials are avoided with the use of a smooth perturbation of the error metric. We compare the numerical performance of projection algorithms to standard line search algorithms applied to a perturbed least squares error metric. In addition, we investigate a novel approach which we call *extended least squares*, together with limited memory and trust region techniques for stabilizing and accelerating first-order analytic algorithms. The objective associated with the extended least squares

technique includes a regularization term and allows us to adaptively correct for the relative variability in image data. The extended least squares approach has great potential for future research. In our implementations we chose the simplest possible regularizing functional in the objective, *i.e.* a constant. Even this simple choice had a dramatic effect on the performance of the algorithms. This opens the door to a search for optimal regularization. There are two different ways to interpret the extended least squares regularization term, the first and perhaps most natural is statistical, the second is purely algorithmic. Under the statistical interpretation, the regularization term is viewed as the variance or spatial correlation of the data sets. The method is very general and applies to a wide variety of observations and statistical models. Under the algorithmic interpretation, the regularizing term is simply a merit function and can be used to tackle the problem of algorithm stagnation in the middle iterations. The adaptive weighting strategy allows one to include several different metrics in the same objective, one that is more effective for the middle regions and one that is more effective near a local solution.

Mathematical Essentials

- *Electromagnetic field:*

$$\boldsymbol{u} = (u_{re},\ u_{im}) \ \in L^2[\mathbb{R}^2, \mathbb{R}] \times L^2[\mathbb{R}^2, \mathbb{R}]$$

- *Object:*

$$\varphi \in L^2[\mathbb{R}^2, \mathbb{R}_+]$$

- *Data*:
  Field intensities for $m = 0, 1, 2, \ldots, M$:

$$\psi_m \in L^1[\mathbb{R}^2, \mathbb{R}_+] \cap L^2[\mathbb{R}^2, \mathbb{R}_+] \cap L^\infty[\mathbb{R}^2, \mathbb{R}_+]$$

- *Goal:*
  Find a field $\boldsymbol{u}$ and object φ satisfying

$$|\mathcal{F}_m[\boldsymbol{u}]| * \varphi = \psi_m \quad \forall m = 0, 1, 2, \ldots, M$$

  where $\mathcal{F}_m \ : \ L^2[\mathbb{R}^2, \mathbb{R}^2] \ \rightarrow \ L^2[\mathbb{R}^2, \mathbb{R}^2]$ is a unitary linear operator

An Optimization Approach

$$\begin{array}{ll} \text{minimize} & \displaystyle\sum_{m=0}^{M} \rho_m \left[\psi_m, |\mathcal{F}_m[\boldsymbol{u}]| * \varphi\ \right] \\ \text{over} & \boldsymbol{u} \in L^2[\mathbb{R}^2, \mathbb{R}^2] \times L^2[\mathbb{R}^2, \mathbb{R}^2] \\ & \varphi \in L^2[\mathbb{R}^2, \mathbb{R}_+] \end{array}$$

where ρ_m, $m = 0, 1, 2, \ldots$ are given measures of performance.

Wavefront reconstruction (aka Phase retrieval)

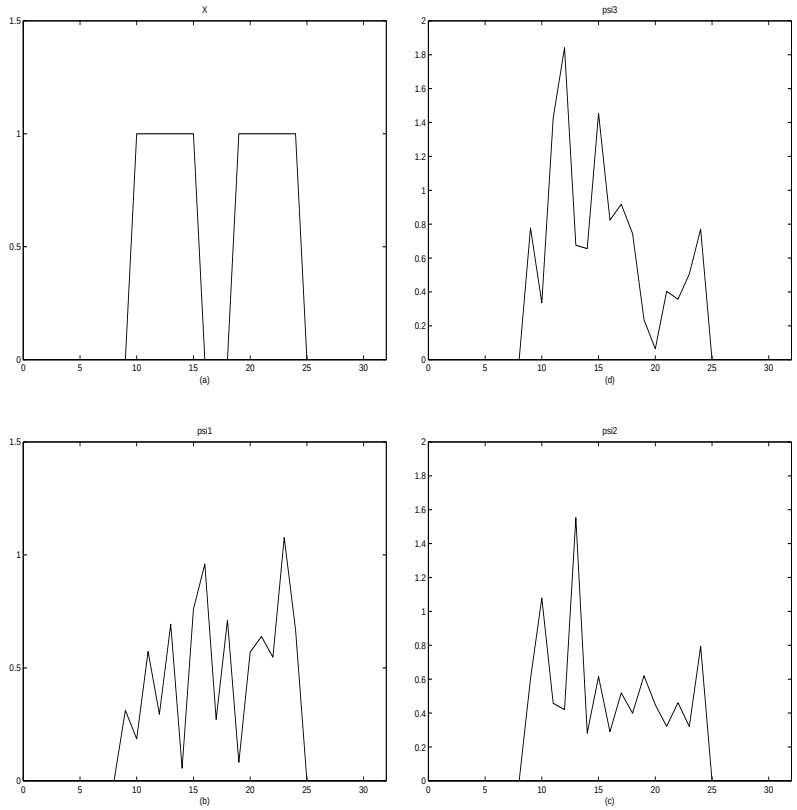
$$\varphi = \delta$$

Wavefront reconstruction/deconvolution

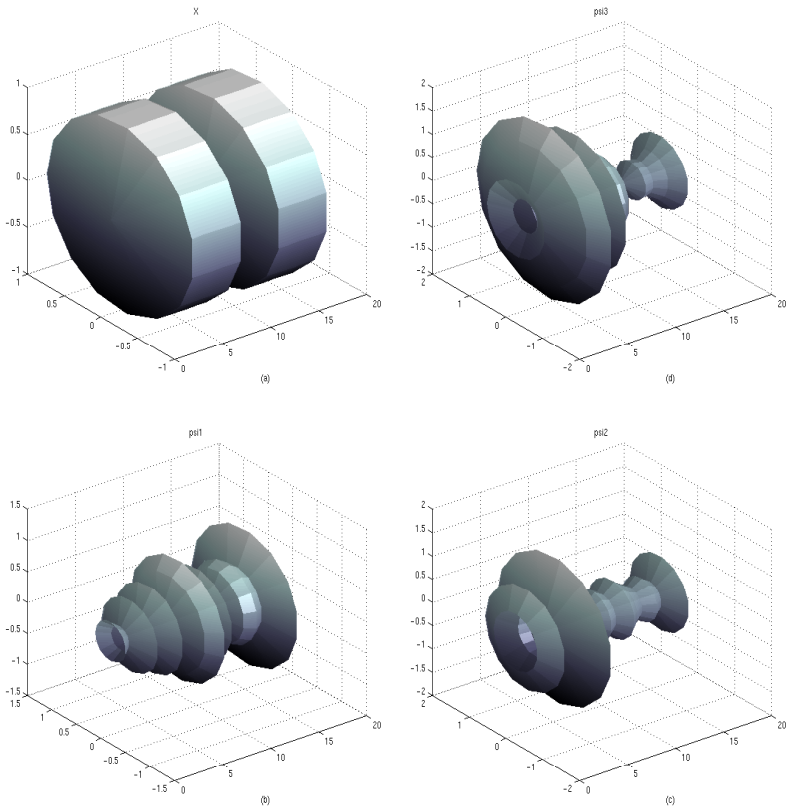
$$\varphi \text{ unknown}$$

Geometric Approaches

[Brégman, 65], [Gubin&Polyack, 67], [Gerchberg&Saxton, 72], [Misell, 73], [Fienup, 82], [Levi&Stark, 84] [Combettes, 90], [Bauschke&Borwein,96]



Geometric Approaches



Tube constraints. The vertical axis and the axis coming out of the page correspond to the real and imaginary components of the tubes. The horizontal axes correspond to the horizontal axes of the previous slide. Frame (a) represents the constraint set corresponding to frame (a) of the previous slide. Frames (b)-(d) represent the constraint sets corresponding to frame (b)-(d) of the previous slide.

Geometric Analysis

Given $\psi_m \not\equiv 0$, define

$$\mathbb{Q}_m \equiv \left\{ \boldsymbol{u} \in L^2[\mathbb{R}^2, \mathbb{R}^2] \ \mid |\mathcal{F}_m[\boldsymbol{u}]| = \psi_m \ a.e. \right\}$$

Property: The sets $\mathbb{Q}_m$ are neither weakly closed nor convex in $L^2[\mathbb{R}^2, \mathbb{R}^2]$ whenever ψ_m is not identically zero.

Geometric Analysis

- *Distance Function:*

$$\operatorname{dist}(x; \mathbb{Q}) = \inf_{u \in \mathbb{Q}} \|x - u\|$$

where $\mathbb{Q}$ is a subset of some normed space $\mathbb{X}$.

- *Projection Operator:*

$$\begin{aligned} \Pi_{\mathbb{Q}}[v] &= \arg\min_{u \in \mathbb{Q}} \|v - u\| \\ &= \{\bar{u} \in \mathbb{Q} : \|v - \bar{u}\| = \inf_{u \in \mathbb{Q}} \|v - u\|\} \end{aligned}$$

- *Tubes:*

Given $b \in L^2[\mathbb{R}^2, \mathbb{R}_+]$ with $b \not\equiv 0$.

$$\mathbb{Q}[b] \equiv \left\{ \boldsymbol{u} \in L^2[\mathbb{R}^2, \mathbb{R}^2] \mid |\boldsymbol{u}| = b \quad a.e. \right\}$$

Geometric Analysis

Define

$$\Pi[\boldsymbol{u}; b] = \{\pi[\boldsymbol{u}; b, \theta] \mid \theta \text{ measurable}\}$$

where

$$\pi[\boldsymbol{u}; b, \theta](\boldsymbol{x}) = \begin{cases} b(\boldsymbol{x})\frac{\boldsymbol{u}(\boldsymbol{x})}{|\boldsymbol{u}(\boldsymbol{x})|}, & \text{for } \boldsymbol{u}(\boldsymbol{x}) \neq 0 \\ \\ b(\boldsymbol{x}) \begin{pmatrix} \cos\theta(\boldsymbol{x}) \\ \sin\theta(\boldsymbol{x}) \end{pmatrix}, & \text{for } \boldsymbol{u}(\boldsymbol{x}) = 0 \end{cases}$$

Projection Theorem

For $b \in L^2[\mathbb{R}^2, \mathbb{R}_+]$ and $\boldsymbol{u} \in L^2[\mathbb{R}^2, \mathbb{R}^2]$,

- $\boldsymbol{v} \in \Pi[\boldsymbol{u}; b] \iff$

$$|\boldsymbol{v}(\boldsymbol{x}) - \boldsymbol{u}(\boldsymbol{x})| = \text{dist}\,(\boldsymbol{u}(\boldsymbol{x}); b(\boldsymbol{x})\mathbb{S}) \; a.e.$$

- $\Pi_{\mathbb{Q}[b]}[\boldsymbol{u}] = \Pi[\boldsymbol{u}; b]$, and

- $\text{dist}\,(\boldsymbol{u}; \mathbb{Q}[b]) = \|\,|\boldsymbol{u}| - b\|$.

Geometric Analysis

Recall

$$\mathbb{Q}_m \equiv \left\{ \boldsymbol{u} \in L^2[\mathbb{R}^2, \mathbb{R}^2] \ \mid |\mathcal{F}_m[\boldsymbol{u}]| = \psi_m \ a.e. \right\}$$

Rewrite as

$$\mathbb{Q}_m = \mathcal{F}_m^* \mathbb{Q}[\psi_m]$$

Corollary

$$\Pi_{\mathbb{Q}_m}[\boldsymbol{u}] = \mathcal{F}_m^* \left[\Pi_{\mathbb{Q}[\psi_m]}[\mathcal{F}_m[\boldsymbol{u}]] \right]$$

and

$$\operatorname{dist}(\boldsymbol{u}; \mathbb{Q}_m) = \| \, |\mathcal{F}_m[\boldsymbol{u}]| - \psi_m \|$$

for all $\boldsymbol{u} \in L^2[\mathbb{R}^2, \mathbb{R}^2]$.

Projection Algorithms

- *General Projection algorithms:*

$$\boldsymbol{u}^{(\nu+1)} \in \left(\sum_{m=0}^{M} \gamma_m^{(\nu)} \left[(1-\alpha_m^{(\nu)})\mathcal{I} + \alpha_m^{(\nu)} \Pi_{\mathbb{Q}_m} \right] \right) [\boldsymbol{u}^{(\nu)}]$$

where

$$\alpha_m^{(\nu)} > 0, \ m = 0, 1, 2, \ldots \quad (\text{usually } \alpha_m^{(\nu)} \in [0, 2])$$

and

$$\gamma_m^{(\nu)} > 0, \ m = 0, 1, 2, \ldots \quad \text{with} \quad \sum_{m=0}^{M} \gamma_m^{(\nu)} = 1$$

- *Iterative transform algorithms*:

$$\boldsymbol{u}^{(\nu+1)} \in \left(\prod_{m=0}^{M} \left[(1-\alpha_m^{(\nu)})\mathcal{I} + \alpha_m^{(\nu)} \Pi_{\mathbb{Q}_m} \right] \right) [\boldsymbol{u}^{(\nu)}].$$

Gerchberg-Saxton: $M = 1, \ \alpha_0^{(\nu)} = \alpha_1^{(\nu)} = 1.$

Projection Algorithms

Change of variables

$$\lambda^{(\nu)}\beta_m^{(\nu)} \equiv \gamma_m^{(\nu)}\alpha_m^{(\nu)}$$

yields

$$\boldsymbol{u}^{(\nu+1)} \in \left(\mathcal{I} - \lambda^{(\nu)}\mathcal{G}^{(\nu)}\right)[\boldsymbol{u}^{(\nu)}].$$

where

$$\mathcal{G}^{(\nu)} \equiv \sum_{m=0}^{M} \mathcal{G}_m^{(\nu)} \quad \forall \nu$$

with

$$\mathcal{G}_m^{(\nu)} \equiv \beta_m^{(\nu)}\left(\mathcal{I} - \Pi_{\mathbb{Q}_m}\right)$$

(Note that $\sum_{m=0}^{M} \beta_m^{(\nu)} \neq 1$ in general and $\lambda^{(\nu)}$ is a *step length*)

Analytic Methods: the squared distance function

- *Squared set distance error*

$$E[\boldsymbol{u}] = \sum_{m=0}^{M} \frac{\beta_m}{2} \mathrm{dist}^{\,2}(\boldsymbol{u}; \mathbb{Q}_m)$$

where

$$\beta_m \geq 0 \quad m = 0, \ldots, M$$

and

$$\mathrm{dist}^{\,2}(\boldsymbol{u}; \mathbb{Q}_m) \equiv \| |\mathcal{F}_m[\boldsymbol{u}]| - \psi_m \|^2$$

- *Nonsmooth least squares minimization:*

$$\begin{array}{ll} \text{minimize} & E[\boldsymbol{u}] \\ \text{over} & \boldsymbol{u} \in L^2[\mathbb{R}^2, \mathbb{R}^2] \times L^2[\mathbb{R}^2, \mathbb{R}^2]. \end{array}$$

Analytic Methods: subdifferentials and projections

- *First-order variational principle:*

$$0 \in \partial E[\boldsymbol{u}_*].$$

where ∂ denotes a *subgradient* operator

- *Relation to projections:*

$$\partial \left(\mathrm{dist}^{\,2}(\boldsymbol{u}; \mathbb{Q}_m) \right) = 2\mathrm{cl}^{\,*} \left(\mathcal{I} - \Pi_{\mathbb{Q}_m} \right) [\boldsymbol{u}]$$

- *Subdifferential Calculus:*

$$\partial E[\boldsymbol{u}] \subset \sum_{m=0}^{M} \beta_m^{(\nu)} \mathrm{cl}^{\,*} \left(\mathcal{I} - \Pi_{\mathbb{Q}_m} \right) [\boldsymbol{u}].$$

Analytic Methods: perturbed least squares

Perturbed squared set distance error:

$$E_\epsilon[\boldsymbol{u}] = \sum_{m=0}^{M} \frac{\beta_m}{2} \left\| \frac{|\mathcal{F}_m[\boldsymbol{u}]|^2}{\left(|\mathcal{F}_m[\boldsymbol{u}]|^2 + \ \epsilon^2\right)^{1/2}} - \psi_m \right\|^2$$

Define $r : \mathbb{R}^2 \times \mathbb{R}_+ \to \mathbb{R}$

$$r(\boldsymbol{u}; b, \epsilon) = \frac{|\boldsymbol{u}|^2}{\left(|\boldsymbol{u}|^2 + \epsilon^2\right)^{1/2}} - b \quad (\approx |\boldsymbol{u}| - b)$$

and $J : L^2[\mathbb{R}^2, \mathbb{R}^2] \to \overline{\mathbb{R}}$

$$J[\boldsymbol{u}; b, \epsilon] = \int_{\mathbb{R}^2} r^2(\boldsymbol{u}(\boldsymbol{x}); b(\boldsymbol{x}), \epsilon) d\boldsymbol{x}.$$

Then

$$E_\epsilon[\boldsymbol{u}] \equiv \sum_{m=0}^{M} \frac{\beta_m}{2} \left(J[\cdot; \psi_m, \epsilon] \circ \mathcal{F}_m\right)[\boldsymbol{u}].$$

Analytic Methods: properties of the perturbed squared set distance error

Theorem

For all $\epsilon \neq 0$ and $b \in L^1 \cap L^2 \cap L^\infty$ nonnegative

- $J[\,\cdot\,; b, \epsilon]$ is finite-valued,
- $J[\,\cdot\,; b, \epsilon]$ is Fréchet differentiable,
- $\nabla J[\,\cdot\,; b, \epsilon]$ is globally Lipschitz continuous.

Corollary

E_ϵ is finite-valued, and Fréchet differentiable with globally Lipschitz continuous derivative

Analytic Methods: properties of perturbed squared set distance error

Gradients:

$$\nabla E_\epsilon[\boldsymbol{u}] =$$

$$\sum_{m=0}^{M} \beta_m \mathcal{F}_m^* \left[r[\mathcal{F}_m[\boldsymbol{u}]; \psi_m, \epsilon] r'[\mathcal{F}_m[\boldsymbol{u}]; \psi_m, \epsilon] \mathcal{F}_m[\boldsymbol{u}] \right]$$

where

$$r'[\mathcal{F}_m[\boldsymbol{u}]; \psi_m, \epsilon] = \frac{|\mathcal{F}_m[\boldsymbol{u}]|^2 + 2\epsilon^2}{\left(|\mathcal{F}_m[\boldsymbol{u}]|^2 + \epsilon^2\right)^{3/2}}$$

Analytic Methods: the perturbed squared set distance error and projections

Theorem

If $E[\boldsymbol{u}] < \delta$, there exists an $\epsilon > 0$ such that

$$\|\nabla E_\epsilon[\boldsymbol{u}] \; - \; \boldsymbol{v}\| \; < \; C\delta^{1/2}$$

for all $\boldsymbol{v} \in \; \mathcal{G}[\boldsymbol{u}]$ where

$$\mathcal{G} = \sum_{m=0}^{M} \beta_m \left(\mathcal{I} - \Pi_{\mathbb{Q}_m}\right)$$

and

$$C = \sqrt{2} \sum_{m=0}^{M} \beta_m^{1/2} \left(1 + \sqrt{2}\beta_m^{1/2}\right)$$

Analytic Methods: extended least squares [Bell et al, 96]

- *Extended least squares objective:*

$$L_\epsilon[\boldsymbol{u}, \boldsymbol{\beta}] =$$

$$\sum_{m=0}^{M} -ln(2\pi\beta_m) + \beta_m \left(J[\mathcal{F}_m[\boldsymbol{u}]; \psi_m, \epsilon] + G_m[\boldsymbol{u}] \right).$$

- *Optimization problem:*

$$\begin{array}{rl} \text{minimize} & L_\epsilon[\boldsymbol{u}, \boldsymbol{\beta}] \\ \text{over} & \boldsymbol{u} \in L^2[\mathbb{R}^2, \mathbb{R}^2],\ 0 < \boldsymbol{\beta} \end{array}$$

Analytic Methods: extended least squares

Lemma

Set

$$G_m[\boldsymbol{u}] = c_m \quad m = 0, 1, 2, \ldots, M$$

and

$$\boldsymbol{\beta}_*[\boldsymbol{u}] \equiv (\beta_{0*}[\boldsymbol{u}], \ldots, \beta_{M*}[\boldsymbol{u}])$$

where

$$\beta_{m*}[\boldsymbol{u}] = \left(J[\mathcal{F}_m[\boldsymbol{u}]; \psi_m, \epsilon] + c_m\right)^{-1}, \; m = 0, \ldots, M$$

If $c_m > 0$ then

$$L_\epsilon[\boldsymbol{u}, \boldsymbol{\beta}_*[\boldsymbol{u}]] \leq L_\epsilon[\boldsymbol{u}, \boldsymbol{\beta}] \qquad \forall \boldsymbol{\beta} > 0$$

Analytic Methods: reduced extended least squares objective

Substitute $\boldsymbol{\beta}_*[\boldsymbol{u}]$ for $\boldsymbol{\beta}$ to obtain the reduced objective

$$R_\epsilon[\boldsymbol{u}] = \sum_{m=0}^{M} ln(J[\mathcal{F}_m[\boldsymbol{u}]; \psi_m, \epsilon] + c_m)$$

where

$$R'_\epsilon[\boldsymbol{u}][\boldsymbol{w}] =$$

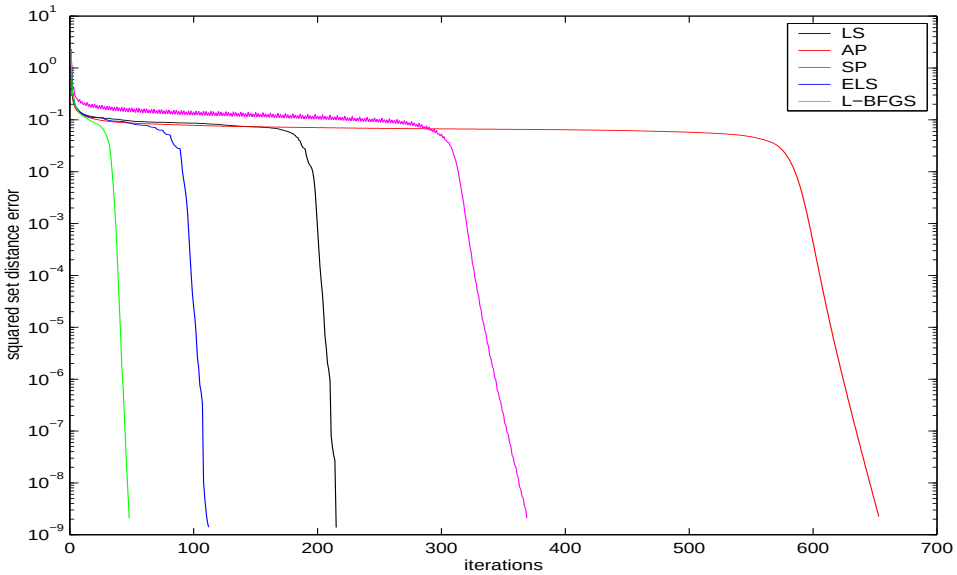
$$\sum_{m=0}^{M} \left(J[\mathcal{F}_m[\boldsymbol{u}]; \psi_m, \epsilon] + c_m\right)^{-1} \left(J[\cdot; \psi_m, \epsilon] \circ \mathcal{F}_m\right)' [\boldsymbol{u}][\boldsymbol{w}]$$

is globally Lipschitz

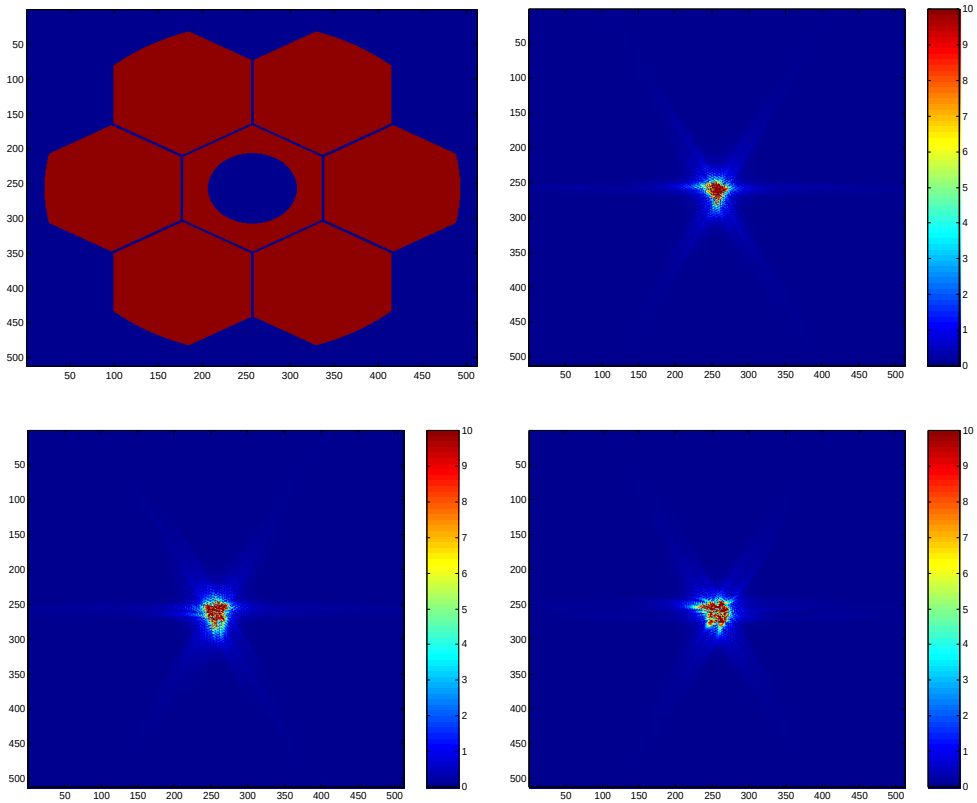
Results

Table 1: Relative cpu time of projection and analytic algorithms averaged over 30 random trials. The baseline is the LS algorithm. Outliers were not included in the totals for algorithms with an asterisk.

	No Noise			Noise					
	$E \leq 20e^{-9}$			$E \leq 0.05$			$E \leq 0.0138$		
	mean	low	high	mean	low	high	mean	low	high
LS	248	99	970	161	68	483	222	159	518
AP*	2.29	99	1680	2.7	126	1765	2.3	162	1808
SP*	.96	72	591	1.19	35	746	-	-	-
ELS	.66	74	365	.77	35	258	.84	76	304
L-BFGS	.29	41	196	.44	37	159	.47	72	182

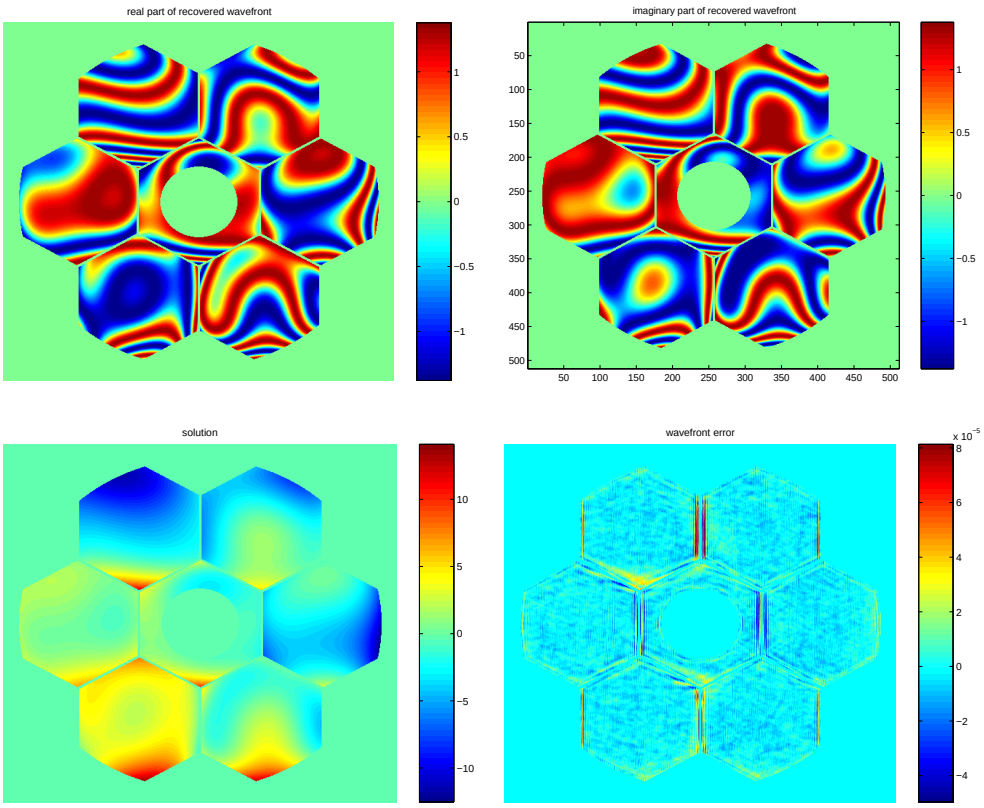


Analytic Methods: results



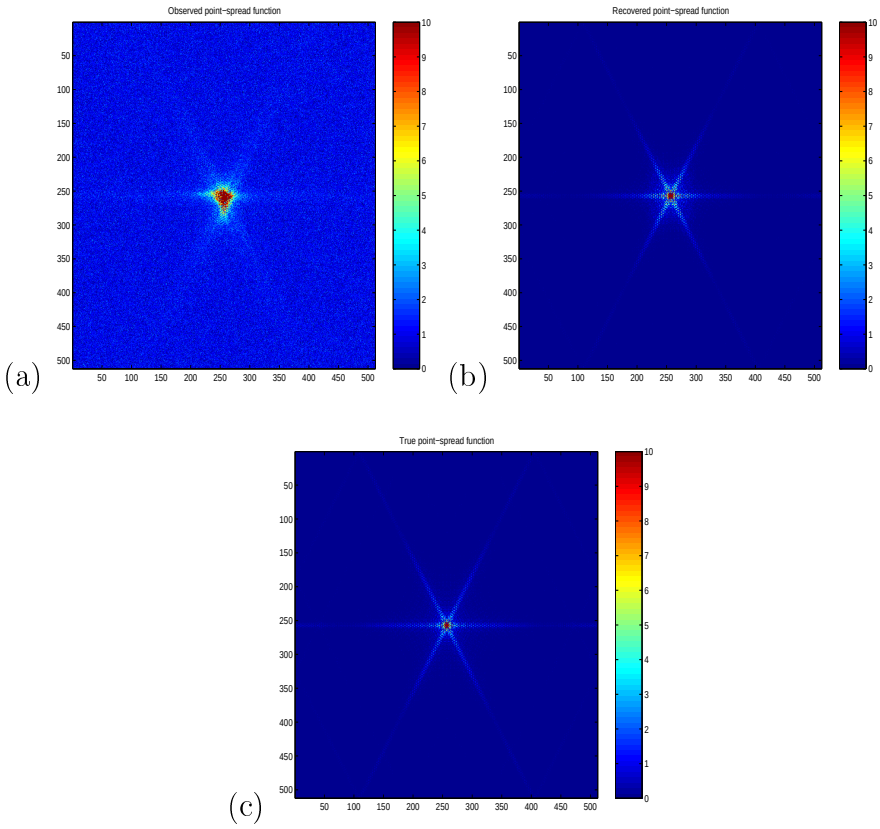
Aperture and noiseless image data for a segmented pupil on a 512 by 512 grid. The 3 diversity images are the optical system's response to a point source at focus, and plus/minus defocus respectively.

Analytic Methods: results



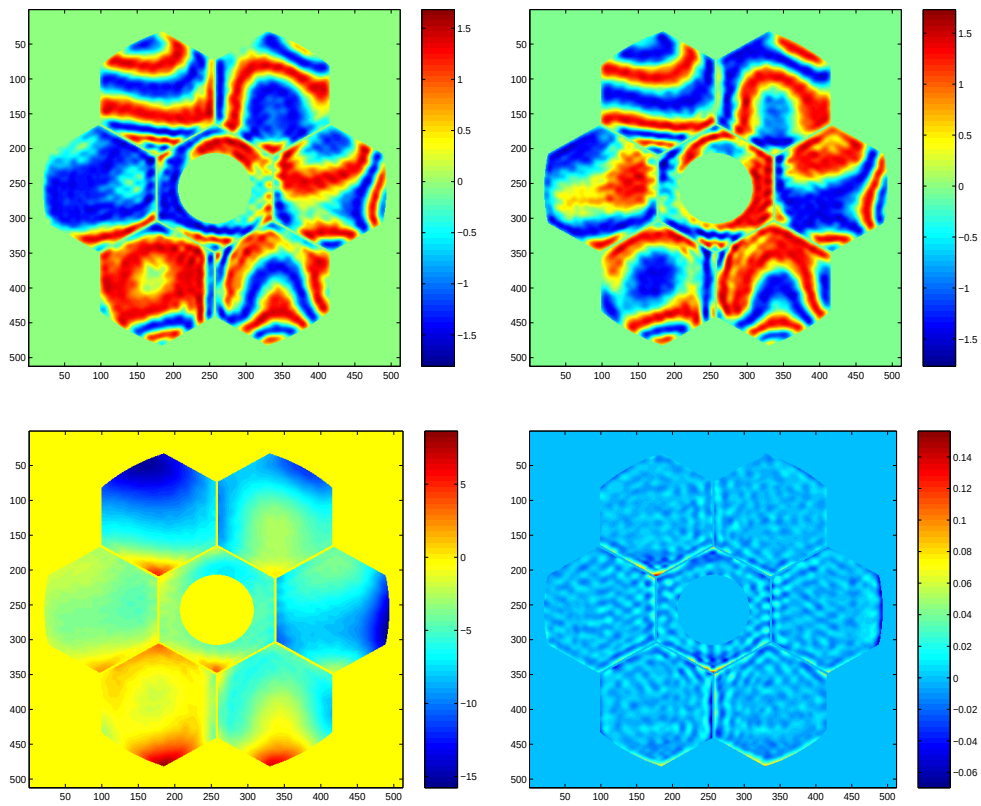
Aberrated wavefront for the segmented pupil recovered from 3 noiseless diversity point source images on a 512 by 512 grid. The wavefront phase is unwrapped and compared to the true phase. The wavefront error is in units of wavelength.

Analytic Methods: results



(a) Noisy point-spread function for a segmented pupil on a 512 by 512 grid. (b) Recovered point-spread function. (c) True point-spread function.

Analytic Methods: results



Aberrated wavefront for the segmented pupil recovered from 3 noisy diversity point source images on a 512 by 512 grid. The wavefront phase is unwrapped and compared to the true phase. The wavefront error is in units of wavelength. The ridges in the wavefront error is due to Gibbs phenomenon associated with the noise filter.

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