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Generalized Proximal Smoothing for Phase Retrieval

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Phase retrieval has been fundamental to several disciplines, ranging from imaging, microscopy, crystallography and optics to astronomy. It aims to recover an object only from its Fourier magnitudes. Without the Fourier phases, the recovery can be achieved via iterative algorithms when the Fourier magnitudes are sampled at a frequency sufficiently finer than the Nyquist interval. In 1972, Gerchberg and Saxton developed an iterative algorithm for phase retrieval, utilizing the magnitude of an image and the Fourier magnitudes as constraints [1]. In 1982, Fienup generalized the Gerchberg-Saxton algorithm by developing two iterative algorithms: error reduction (ER) and hybrid input-output (HIO), which use a support and non-negativity as constraints in real space and the Fourier magnitudes in reciprocal space [2]. In 1998, Miao, Sayre and Chapman proposed, when the number of independently measured Fourier magnitudes is larger than the number of unknown variables associated with a sample, the phases are in principle encoded in the Fourier magnitudes and can be retrieved by iterative algorithms [3]. These developments finally led to the first experimental demonstration of coherent diffractive imaging (CDI) by Miao and collaborators in 1999 [4], which has stimulated wide spread research activities in phase retrieval, CDI/ptychography, and their applications in the physical and biological sciences [5].

The phase retrieval algorithms iterate between real and reciprocal space using zero-density region and the Fourier magnitudes as dual-space constraints. A support is typically defined to separate the zero-density region from the object. In the presence of experimental noise and missing data, phase retrieval becomes much more challenging, and the ER and HIO algorithms may only converge to sub-optimal solutions. Simply combining ER and HIO still suffers from stagnation and the iterations can get trapped at local minima [2]. To alleviate these problems, more advanced phase retrieval algorithms have been developed such as the shrink-wrap algorithm and guided HIO (gHIO) [6,7]. Recently, Rodriguez et al. proposed to impose the smoothness constraint on the no-density region outside the support by applying Gaussian filters [8]. The resulting oversampling smoothness (OSS) algorithm successfully reduces oscillations in the reconstructed image, and is more robust to noisy data than the existing algorithms. Here, we present an optimization-based phase retrieval method, termed generalized proximal smoothing (GPS), which effectively addresses the noise in both real and Fourier spaces [9]. Motivated by the success of OSS, GPS incorporates the idea of Moreau-Yosida regularization with heat kernel smoothing to relax the support constraint into a continuous penalty term [10]. We further relax the magnitude constraint into a least squares fidelity term, for de-noising in Fourier space. To minimize the resulting primal-dual formulation, GPS iterates back and forth between efficient proximal mappings of the two relaxed functions, respectively.

To demonstrate the applicability of GPS to biological samples, we did phase retrieval on a diffraction pattern taken of a *S. Pombe* yeast spore taken at beamline BL29 at SPring-8 [11]. We did 500 independent, randomly seeded reconstructions with each algorithm and recorded the R factor in reciprocal space (R_F), excluding the missing center. The sequence of low-pass filters was chosen to be the same as in OSS. The top row of Fig. 1 is the mean of the best 5 reconstructions obtained by the respective algorithm. The second row shows the variance of the same 5 reconstructions. HIO achieved R_F = 15.70 +/- 0.53%, while OSS achieved R_F = 9.78 +/- 0.20% and GPS achieved R_F = 8.67 +/- 0.03%.

In conclusion, we have developed a fast and robust phase retrieval algorithm (GPS) for the reconstruction of images from noisy diffraction intensities [9]. GPS shows more reliable and consistent results than OSS and HIO for the reconstruction of weakly scattering objects such as biological specimens. Looking forward, we aim to explore the role of dual variables in non-convex optimization. Smoothing the dual variable, which is equivalent to smoothing the gradient of convex conjugate, represents a new and effective technique that can in principle be applied to other non-smooth, non-convex problems.

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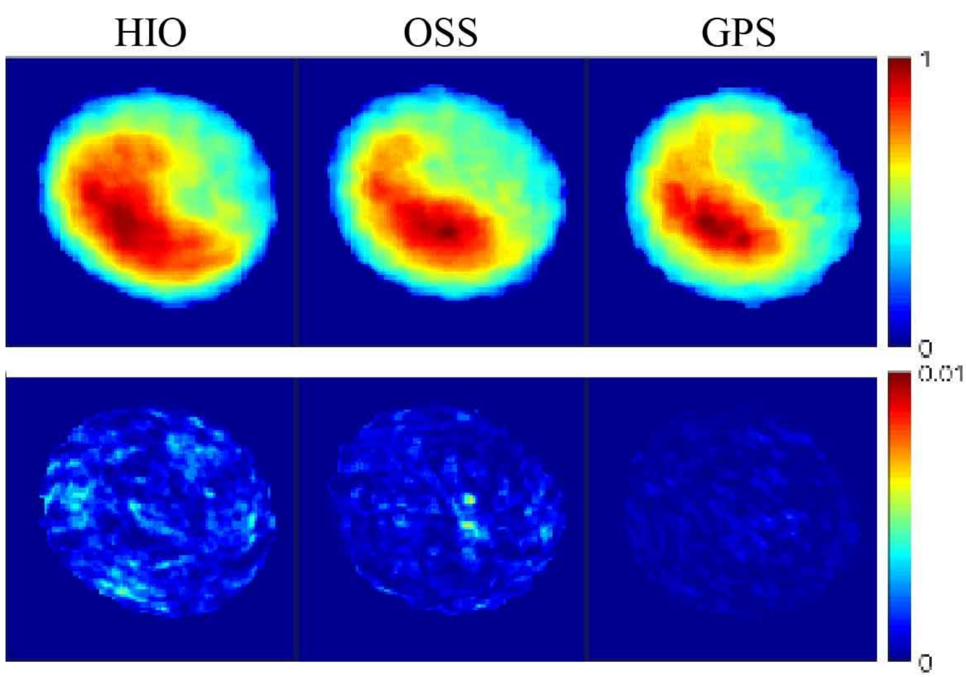

Figure 1. *S. pombe* yeast spore reconstructions. Means (first row) and variance (second row) were computed from the best 5 of 500 independent reconstructions.