MS.62.3

Relaxed averaged alternating reflections for diffraction imaging

Russell Luke
University of Delaware, Mathematical Sciences, 501 Ewing Hall, Newark, Delaware, 19716, USA, E-mail：rluke@math.udel.edu

We report on progress in algorithms for iterative phase retrieval. The theory of convex optimisation is used to develop and to gain insight into counterparts for the nonconvex problem of phase retrieval. We propose a relaxation of averaged alternating reflectors and determine the fixed point set of the related operator in the convex case. A numerical study supports our theoretical observations and demonstrates the effectiveness of the algorithm compared to the current state of the art.

Keywords: phase retrieval, projection, inconsistent feasibility

MS.62.4

Reduced-rank extension of BLUE and deep lipschitzian gradient projector for inverse problems

Isao Yamada, Tomasz Piotrowski, Masao Yamagishi
Tokyo Institute of Technology, Department of Communications and Integrated Systems, Meguro-ku Ookayama 2-12-1-S3-60, Tokyo, 152-8550, Japan, E-mail：isao@comm.ss.titech.ac.jp

This talk is divided into 2 parts as follows. In the 1st part of this talk, we introduce one of the central ideas of the MV-PURE (Minimum-Variance Pseudo-Unbiased Reduced-Rank Estimator), by Yamada and Elbadraoui (2006) and Piotrowski and Yamada (2008), which is a novel estimator for ill-conditioned inverse problems. The MV-PURE is a reduced-rank extension of the Gauss-Markov estimator (BLUE: Best Linear Unbiased Estimator) and defined as a closed form solution of a hierarchical nonconvex constrained optimization problem. The MV-PURE achieves the minimum variance among all solutions of the first stage optimization problem for minimizing, under a rank constraint, simultaneously all unitarily invariant norms of an operator applied to the unknown parameter vector in view of suppressing bias of the estimator. The MV-PURE offers a unified view for many estimators including the well-known estimators: the Gauss-Markov (BLUE) estimator, the generalized Marquardt's reduced-rank estimator and the minimum-variance conditionally unbiased affine estimator subject to linear restrictions. In the 2nd part of this talk, we introduce an idea of the deep lipschitzian gradient projector which is defined by Yamagishi and Yamada (2008) as the metric projection onto the level set of the best lower bound of a convex function which is assumed to be (i) bounded below, and (ii) differentiable and its derivative is lipschitzian. The deep lipschitzian gradient projector is computationally efficient and can approximate the level set of the convex function better than the subgradient projector, hence it can improve many computational methodologies employing the subgradient projector as one of their key players.

Keywords: inverse problem, MV-PURE, lipschitzian gradient projector

MS.62.5

Solution to the phase problem for surface X-ray diffraction

Paul F Lyman, Valentin L. Shneerson, Russel Fung, Ross J. Harder, Somendra S. Parihar, H. T. Johnson-Steigelman, Dilano K. Saldin
University of Wisconsin-Milwaukee, Physics, 1900 E Kenwood Blvd., Milwaukee, WI, 53211, USA, E-mail：plyman@uwm.edu

Directly inverting x-ray data requires determining the unmeasured phases (the "phase problem"). We propose a general solution to the phase problem for surface x-ray diffraction (SXRD) termed the *phase and amplitude recovery and diffraction image generation method* (PARADIGM); atomic structures from a single surface domain or from multiple, symmetry-related domains on a known bulk structure may be recovered. Diffraction *rods* in reciprocal space may be *oversampled* relative to the Nyquist frequency of the height of the selvedge. An iterative algorithm alternately satisfies known constraints of the oversampled data in real and reciprocal space, and progressively determines the amplitudes and phases of the surface structure factors. A Fourier transform then constructs an "image" of the selvedge. Using this method, the atomic positions on a Au(110)-(2x1) surface have been visualized directly from the data. (See figure.) This breakthrough allows an automated, model-independent way to determine unknown surface structures. We have applied this method to several heretofore unknown surface phases: Sb/Au(110)-c(2x2) and even the multi-domain Sb/Au(110)-($\sqrt{3}$x$\sqrt{3}$) R54.7° structure.
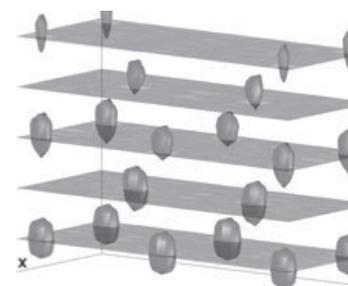
Keywords: phase determination methods, real-space refinement methods, surface reconstruction

MS.63.1

Photoreduction of metalloprotein active sites by synchrotron radiation

Britt Hedman[1], Mary C Corbett[2], Matthew J Latimer[1], Thomas L Poulos[3,4], Irina F Sevrioukova[3], Keith O Hodgson[1,2]
[1]Stanford University, SSRL, 2575 Sand Hill Road MS 69, Menlo Park, CA, California, 94025, USA, [2]Department of Chemistry, Stanford University, Stanford, CA 94305, USA, [3]Departments of Molecular Biology & Biochemistry, University of California, Irvine, CA 92697, USA, [4]Departments of Physiology & Biophysics, and Chemistry, University of California, Irvine, CA 92697 USA, E-mail：hedman@ssrl.slac.stanford.edu

X-ray damage to protein crystals is assessed on the basis of the degradation of diffraction intensity, yet this measure is not sensitive to the rapid changes that occur at photosensitive groups, such as the active sites of metalloproteins. X-ray absorption spectroscopy (XAS) has been used to study the x-ray dose-dependent photoreduction of crystals of the [Fe(2)S(2)]-containing metalloprotein, putidaredoxin. A dramatic decrease in the rate of photoreduction, followed through changes in the XAS edge structure, is observed in crystals cryocooled with liquid helium at 40 K as compared to those cooled with liquid nitrogen at 110 K, showing structural changes consistent with active site cluster reduction at 110 K, but not at 40 K, even after an eight-