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Stochastic projection methods and applications to some nonlinear inverse problems of phase retrieving

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Abstract

In this short paper we present a stochastic projection based Monte Carlo algorithm for solving a nonlinear ill-posed inverse problem of recovering the phase of a complex-valued function provided its absolute value is known, under some additional information. The method is developed here for retrieving the step structure of the epitaxial films from the X-ray diffraction analysis. We suggest to extract some additional information from the measurements which makes the problem well-posed, and with this information, the method suggested works well even for noisy measurements. Results of simulations for a layer structure recovering problem with 26 sublayers are presented.

Keywords: Stochastic projections; Inverse problem; X-ray diffraction; Epitaxial layers; Phase retrieving

1. Introduction

Stochastic models and Monte Carlo algorithms for solving inverse problems were intensively developed since the 1990s, as a result of a rapid progress in computer technology (e.g., see [8]). Monte Carlo methods are becoming increasingly important for the solution of linear and nonlinear inverse problems in situations, where the inverse problem is formulated as a search for generalized solutions fitting the data within a certain tolerance, defined by data uncertainties. In a deterministic formulation this implies that we search for solutions with calculated data whose distance from the observed is less than a fixed, positive number. Note that in statistical inference, the tolerance is not so strong: a large number of samples of statistically almost independent models from posterior probability distributions are sought. Such solutions are consistent with data and prior information, since they fit the data with a given statistical error [8]. As to some applications, we mention here the paper [1] where the authors used the Monte Carlo method to analyze the seismic waveform inversion problem in a Bayesian formulation, see also [6]. Closely

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related is the expectation–maximization (EM) algorithm for solving ill-posed equations. There is a large body of literature concerning the expectation–maximization (EM) algorithm, see, for instance, [5,9].

Another class of rather heuristic stochastic methods include Genetic algorithms (GA) which were originally devised as a model of adaptation in an artificial system, [4], see also [20]. Genetic algorithms belong in a sense to the class of Monte Carlo techniques, they use random numbers to control the sampling of a parameter space. In contrast to simulated annealing which uses an analogy with a physical optimization process, genetic algorithms are based on analogy with biological evolution and can be considered as a family of heuristic combinatorial search techniques that come from the concepts of natural genetics and the Darwinian theory of survival of the fittest.

It is well known that the phase retrieval arises in many practical problems, for instance, in X-ray crystallography, diffraction imaging and microscopy (e.g., see [2,16,3,7]) where the phase of the optical wave cannot be measured directly, instead, the detector measures only its magnitudes. We deal in this paper with recovering the height profile of the epitaxial layers from X-ray diffraction measurements.

From the original continuous formulation we turn to a discrete approximation, and transform the problem to a system of quadratic equations of high dimension. There are many different stochastic methods for solving large systems of linear and quadratic equations (e.g., see overviews given in [8,14]; see also [10,13,11]). In this paper we further develop a stochastic projection method which can be considered as a generalization of the randomization method first suggested in [15] and an approach first described in [19].

The deconvolution of X-ray diffraction profiles is a basic step in order to obtain reliable results on the microstructure of crystalline powder (crystallite size, lattice microstrain, etc.). The magnitude of the Fourier transform of some function is measurable, but not the phase. The "phase problem" in crystallography arises because the number of discrete measurements (Bragg peak intensities) is only half the number of unknowns (electron density points in space, see [21]).

We use in this paper the randomized version of the projection methods belonging to the class of row-action methods which work well both for systems with quadratic nonsingular matrices and for under- and overdetermined systems, as presented in our paper [11]. These methods belong to a type known as *Projection on Convex Sets* methods. This approach is beyond the conventional Markov chain based Neumann–Ulam scheme. The main idea is in a random choice of rows, or blocks of rows in the projection method so that in average, the convergence is improved compared to the conventional cyclic choice of the rows. This method was first suggested in [15], and become quite popular in many applied fields. In [11] we suggested an acceleration of the row projection method by using the Johnson–Lindenstrauss theorem to find, among the randomly chosen rows, in a sense an optimal row. We extend this randomized method for solving linear systems coupled with systems of linear inequalities. Applied to finite-difference approximations of boundary value problems, the method appears to be an extremely efficient Random Walk algorithm with a mean exponential convergence, and moreover, the cost does not depend on the dimension of the matrix but only on the number of nonzero entries in the rows. In addition, in contrast to the conventional Monte Carlo algorithm, the method calculates the solution in all grid points, and can be implemented easily on parallel computers.

2. Stochastic projection method for linear systems with constraints

In this paper we deal with a non-linear problem, with additional constraints. To make a smooth introduction to the randomized projection method, we explain the main idea for the case of a linear system of equations with constraints. But we should stress that when solving the ill-posed problem of retrieving by the projection method, we do not deal with any linear equation. Moreover, we will see that the relevant system of quadratic equations may have different number of rows and columns.

Assume we solve the following linear system

$$A\mathbf{y} = \mathbf{b},$$

where the measurement vector $\mathbf{b}$ has k_s components, the matrix A has k_s rows and m columns. Additionally, the following constraints should be satisfied: the solution components should be non-negative: $y_i \geq 0$, and they should satisfy the upper limit conditions $y_i \leq maxval_i$ for all $i = 1, \dots, m$.

The stochastic projection method for calculation of this linear constraints problem can be described as follows.