METHOD OF MEASUREMENTS WITH RANDOM PERTURBATION

DMITRY FEDIN

Department of Mathematics and Mechanics, St. Petersburg State University, St. Petersburg 198904, Russia
fedind@gmail.com

YURY DEDKOV and SERGUEI MOLODTSOV

Institut für Festkörperphysik, TU Dresden, 011062 Dresden, Germany

Here we report on an application of simultaneous perturbation for stochastic approximation (SPSA) algorithm for filtering systematic noise (SN) in photoelectron spectra of solid state. In our analysis of the experimental data by means of SPSA algorithm we have used 50 photoelectron spectra where SN was introduced. We have found that the resulted SPSA-spectrum is in good agreement with the spectrum measured without SN.

1. Introduction

In many experiments physicists have to deal with the observation noise of unknown nature. Traditionally, the observed noise is assumed to be a mutual independent and zero-mean. These assumptions are often hard to justify in practice and without them, the validity of many algorithms is questionable in physics applications. For example, it is known that the standard "least-squares method" or the "maximum likelihood method" [1] give wrong estimates if the observed noise has an "unknown-but-bounded" deterministic nature or it is a probabilistic "dependent" sequence. As an example let us consider photoemission (PE) experiment where systematic noise (SN) of unknown nature appears at some particular kinetic energies. Such noise can introduce additional spectral features that can not be expected from theoretical consideration of electronic structure of solid. Since this noise is not zero-mean it can not be eliminated by simple increasing of the number of scans in PE experiment. One of the effective ways to deal with such noise is using of so-called simultaneous perturbation stochastic approximation (SPSA) algorithm. Generally, we use simultaneous perturbation of control input in order to enrich output information channel (PE intensity).

In the present work we demonstrate for a first time application of SPSA algorithm to analysis of photoemission spectra which include an arbitrary noise. PE spectra of the W(110) surface were collected with two independent photon sources, one of which was used as a probe and second one as a source of the noise. It was shown that the resulted spectrum after application of SPSA algorithm is in good agreement with the one measured without SN. On the basis of these results we conclude that application of SPSA algorithm can be useful for analysis of different experimental data (for example, photoelectron spectra). We can expect a wide application of this method for filtering out of systematic noises that can appear in different kind of measurement/experiments.

The manuscript is organized as following: Chapter 2 is devoted to description of the general aspects of SPSA algorithm, Chapter 3 – description of experimental details and measurement procedure, in Chapter 4 the application of SPSA algorithm for analysis of PE spectra is presented. Chapter 5 summarizes obtained results.

2. SPSA algorithm

Suppose that the observation (registered by some device) signal follows the model:

$$y = \phi\theta + v .$$

If the system is considered being steady-state (this mean that θ is a constant value) in order to define the unknown value of the parameter θ the standard method is used when series of experiments are repeated and the measurements data are averaged as usual. However, this method is applicable only supposing the independence and centering of the observation noise series. When it is impossible to repeat measurements many times the value y resulted in experiment under high level observation noise practically gives no information respectively the real value of the parameter θ. Otherwise, a simple averaging of the observation data is not valid at presence of the SN of the observation model. It may seem strange, but one of the effective ways to remove the systematic noise effect is using of the randomized algorithms for active measurements proposed in [2-5]. Then for the observations $\left\{ y_n \right\}$ relationships follow

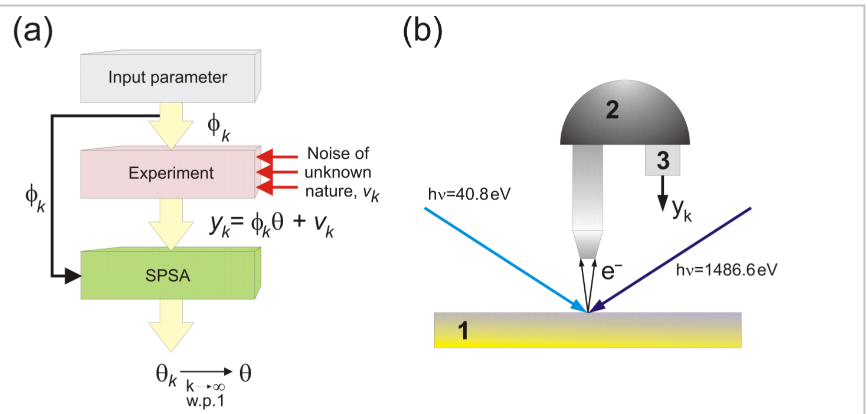

Fig. 1. (a) Principal scheme of the experiment with using SPSA algorithm for eliminating noises of unknown nature; (b) Scheme of the photoemission experiment where sample (1) is illuminated by two light sources, He IIα and Al Kα, electrons are analysed by photoelectron spectrometer (2) and detector (3) register signal y_k.

$$y_n = \phi_n\theta + v_n, n = 1, 2, \dots ,$$

where $v_1, v_2, \dots$ are the observation noises. Denote $\Delta_n = \phi_n - M_\phi, n = 1, 2, \dots$ as centralized outputs. Keeping in mind a statistical nature of the control actions $\{\phi_n\}$ suppose they are a sequence of independent bounded random values with known nonzero mean value $M_\phi \neq 0$, positive bounded dispersion $\sigma_\phi^2 > 0$ and bounded forth moment M_4^4 [1]. The idea of the least mean squared method dated still from Gauss and Legendre, is based on averaging of n successive observation data multiplied by the corresponding values of the control actions. According to the strong large numbers law the sequence of estimates in scope of the usual mean squared method at presence of random independent observation noise with bounded statistical moments,

$$\theta = \frac{\sum_{i=1}^{n} \phi_i y_i}{\sum_{i=1}^{n} \phi_i^2}$$

converges at $n \to \infty$ with the probability 1 to the value θ + $\frac{M_\phi M_v}{\sigma_\phi^2}$, where M_ϕ is a mean value of the control actions. Consequently, at rather large number of observations and the known value M_v the problem on the determination of the value θ is solved. If the value M_v is unknown or the sequence of the observation noises is unknown and probably not random the classical algorithm is not valid. Multiplying by centralized outputs Δ_n both parts of the relationship determining the observations, after some simple manipulation one can get

$$\Delta_n y_n = \theta\Delta_n^2 + \theta\Delta_n M_\phi + \Delta_n v_n$$

Summarizing and averaging the first N observations results

$$\frac{1}{N}\Delta_n y_n = \theta\frac{1}{N}\Delta_n^2 + \frac{1}{N}(\theta\Delta_n M_\phi + \Delta_n v_n)$$

The fist and the second terms in the right-hand part under the adopted suppositions according to the strong large number law, at $n \to \infty$ with probability 1 tend to $\theta\sigma_\phi^2$ and zero, correspondingly. It can be shown in the same way that the last member at $n \to \infty$ tends to zero. From there it follows that at $\phi_1 \neq M_\phi$ the sequence of estimations $\{\hat{\theta}_n\}$, formed by the rule

$$\theta = \frac{\sum_{i=1}^{n}(\phi_i - M_\phi)y_i}{\sum_{i=1}^{n}(\phi_i - M_\phi)^2},$$

converges at $n \to \infty$ with probability 1 to θ.

Now let us consider the linear regression model

$$y_n = \phi_n^T\theta^n + v_n,\ \theta^n = \theta + w^n,\ n = 1,2,\ldots \qquad (1)$$

with outputs (observations) $y_n \in \mathbb{R}$ and inputs $\phi_n \in \mathbb{R}$ and noises $v_n \in \mathbb{R}^r$, $w^n \in \mathbb{R}$ (linearly dependent noise). Therefore we want to estimate θ using the observations $y_n, \phi_n, n = 1, 2, \ldots$.

Note that this conditions are different from those in standard assumption in the task of estimating the parameters of linear regression model with arbitrary input signal (i.e. [6, 7]). For example we do not need the condition $E\{v_n\} = 0$ and the assumption $\{v_n\}_{n\geq 1}$ is a sequence of independent variables with the same probability distribution.

In the Chapter 2 of [2] is shown that under these assumptions we can effectively use the

SPSA algorithm or randomized least-square method. In our paper we will use SPSA algorithm which is following:

$$\theta^n = \theta^{n-1} - \alpha_n \Gamma \Delta_n \left(\phi_n^T \theta^{n-1} - y_n \right), n = 1, 2, ... \qquad (2)$$

where $\alpha_n \geq 0$ is nonrandom sequence which is defining the step of the algorithm, and Γ is some positively definite matrix. $\phi_1, \phi_2, ...$ are realization of sequence of bounded independent random variables with the same probabilistic distribution, known mathematical expectation. M_ϕ, with finite, positive dispersion $\sigma^2 > 0$, with 3rd moment about mean zero and finite 4th central moment M_4^4. Note that vectors $\phi_n, E\{\phi_n\}$ (and thus $\Delta_n = \phi_n - E\{\phi_n\}$ called sample perturbation) are assumed to be known. Figure 1(a) shows the principal scheme of the experiment where SPSA algorithm is applied. Experimentalist choose the parameter ϕ_n randomly. The noise of unknown nature, v_n, appears in the experiment and results of observations, y_n, has to be analysed. Following the consideration presented above in the chapter we have to come to the real estimated value, θ, at $n \to \infty$ with probability equal to one.

3. Photoemission experiment

PE spectra [8] were measured from W(110) single crystal kept at room temperature. Experiments were performed in the setup based on the hemispherical energy analyser (SPECS PHOIBOS 150) [9]. The overall-system energy resolution accounting for the thermal broadening was set to 150 meV and electrons were collected in angle-integrated mode around surface normal. The base pressure was in the range of 1×10^{-10} mbar. Prior to experiment, the W(110) crystal was carefully cleaned by repeated cycles of heating up to 1300^{o}C in oxygen ambient pressure of 5×10^{-8} mbar for 15 min each and subsequent flashing up to 2300^{o}C. After such procedure the crystal was kept in vacuum for 24 hours in order to passivate the surface of the crystal by residual gases in the experimental chamber. This step is necessary for the better stability of the crystal surface in the long-time experiment. Photoemission is a surface sensitive method and absorption of residual

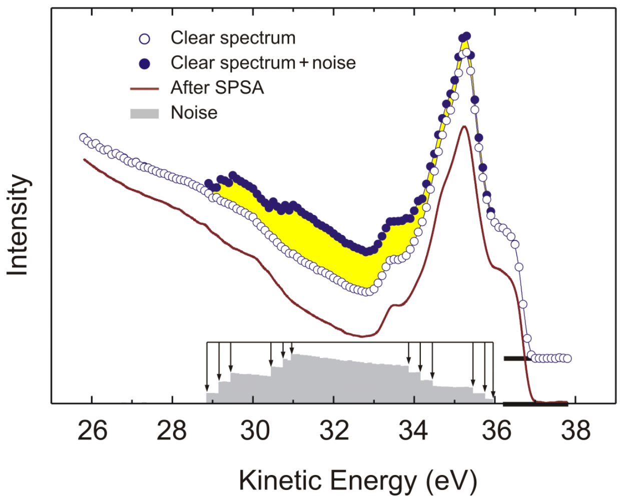

Fig. 2. Experimental photoelectron spectra of the valence band of W(110) obtained with He IIα radiation with (open circles) and without (closed circles) SN. Spectrum obtained after application of SPSA algorithm to the series of 50 experimental spectra is shown by straight line. The gray area in the low part of the plot is a SN. 12 black arrows show control points used for demonstration of the convergence dynamic of algorithm.

gases can drastically change the shape of photoemission spectra. As an excitation light sources in photoemission experiment we have used He IIα resonance line ($h\nu$ = 40.8 eV) and Al Kα emission line ($h\nu$ = 1486.6 eV) in order to produce "studied photoemission signal" and "noise", respectively. The scheme of the experiment is shown in Fig. 1(b). Photoemission spectra were collected in the range of 25.8 - 37.8 eV of kinetic energy of emitted photoelectrons. In this case the He IIα radiation of random intensity produce photoemission spectrum of the valence band of W(110) surface (Fig. 2, open circles). In the same time experimentalist knows the intensity of incoming He IIα radiation. The photocurrent produced in this process can be written

$$j(E_{kin}) = I \cdot DOS(E_{kin}) \cdot \frac{d\sigma(E_{kin})}{d\Omega},$$

where I is the intensity of the light source (He IIα), DOS is the density of states of W(110) surface $d\sigma / d\Omega$ is the cross-section of the photoemission process, $E_{kin}=h\nu$-W-E_B is the kinetic energy of the photoelectron (W-work function of the material, E_B-binding energy of the electron in the solid). Since $d\sigma / d\Omega$ is practically constant in the small energy range the total photocurrent can be written as

$$j(E_{kin}) = I \cdot const \cdot DOS(E_{kin}).$$

It is proportional to density of states and to intensity of incoming radiation.

In every spectrum the "noise" [$N(E_{kin})$] was introduced by switching-on the x-ray source in the range of 28.8 - 35.9 eV of kinetic energy and resulted spectrum in this case is shown by closed circles in Fig. 2. In such way introduced noise represents secondary electrons in the x-ray spectrum of the W(110) surface. This source of electrons is independent on the first one produced by He IIα radiation.

From this consideration we can rewrite the total photocurrent in the following form:

$$j(E_{kin}) = I \cdot const \cdot DOS(E_{kin}) + N(E_{kin}) .$$

This expression is analogous to the general equation of linear regression model (1):

$$y_n = \phi_n^T \theta^n + v_n ,\ \theta^n = \theta + w^n ,\ n = 1,2,\ldots$$

where y_n=$j(E_{kin})$, ϕ_n=I, ϕ_n =const*$DOS(E_{kin})$, v_n=$N(E_{kin})$. And v_n is a systematic noise.

4. Experimental data proceeding

To proceed experimental data we used SPSA algorithm (2) with $\alpha_n \Gamma = 1/(\sigma_n^2 n)$. In our notation it will be:

$$\theta^n = \theta^{n-1} - \frac{\phi_n - M_\phi}{\sigma_\phi^2 n}(\phi_n \theta^{n-1} - y_n)$$

For the analysis we have used 50 scans of PE spectra where SN was introduced. Figure 2 shows us that spectrum obtained after application of SPSA algorithm is in a good agreement with clear spectrum without SN. Figure 3 shows us the evaluation of estimated value θ_k . Here we can see that around 20 step the estimation process almost stabilized. And from the step 46 we have the most precise estimation.

5. Conclusions

We showed that the application of SPSA algorithm is effective way to deal with SN in linear regression model. As an example we applied this algorithm to filtering of random noise in PE spectra. Here we have found that set of 50 spectra is already enough in order

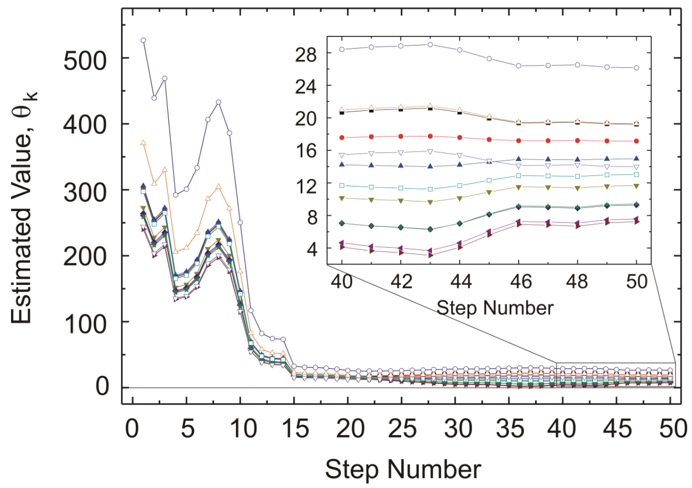

Fig. 3. Convergence of the SPSA algorithm: the estimated values $const \cdot DOS(E_{kin})$ of 12 control points marked by arrows in Fig. 2.

to eliminate systematic error. On the basis of these results we conclude that application of SPSA algorithm can be useful for analysis of different experimental data (for example, photoelectron spectra).

References

[1] S. Brandt, *Statistical and Computational Methods in Data Analysis*, 2nd ed. (Elsevier, New York, 1983).

[2] O. N. Granichin and B. T. Polyak, *Randomized Algorithms of Estimation and Optimization Under Almost Arbitrary Noise* (Nauka, Moscow, 2003).

[3] O. N. Granichin, Vestnik Leningr. Univ. Math. **21**, 92 (1988).

[4] A. V. Goldenshluger and B. T. Polyak, Mathematical Methods of Statistics **2**, 18 (1993).

[5] O. N. Granichin, Automat. and Remote Contr. **63**, 25 (2002).

[6] B. Polyak and Y. Tsypkin, Avtomatika i Telemekhanika **3**, 71 (1979).

[7] B. T. Polyak, Automat. Remote Control **51**, 937 (1990).

[8] S. Hüfner, *Photoelectron Spectroscopy*, 3rd. ed. (Springer, Berlin, 2003).

[9] http://www.specs.de

[10] O. N. Granichin, Vestnik Leningrad Univ. Math. **21**, 92 (1988).