Artificial neural network as a tool for preliminary analysis of time resolved fluorescence data

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The time resolved fluorescence spectroscopy is a very important experimental tool for study the complex biomolecular objects and systems, including lipids, membranes, proteins, DNA, etc. These methods provide detailed information about structure and dynamic of these systems [1]. The analysis of spectroscopic data may be complex because of several reasons: there could be a number of unknown parameters in an experimental system; almost all dependencies between them and the processes taking place are non-linear; and experimental data are distorted by noises and inaccuracies of a registration system. These facts impel to analyze experimental data *via* the multi-parametric optimization approach (fitting). General scheme of the proposed method is the following: the model that describes studied processes is selected from all possible models, initial estimations for the model parameters are made, and the optimization algorithm is starting to modify these parameters trying to achieve a coincidence between experimental and calculated data [2]. For the successful application of the fitting procedure, the selected model must be an adequate and the initial estimation for its parameters should be sufficiently good. Consequently, the tasks of model recognition and initial estimations arise. The first task can be accomplished using *a priori* knowledge about the system. Unfortunately, it is not always possible, because this information may be the object of the research itself. To perform the second task, specific algorithms of data analysis can be implemented. However, these algorithms are strictly specialized, and cannot be applied in the general case. For example, the Laplace transform allows analyzing multi-exponential fluorescence decay model but it cannot be used for stretched exponential model.

Therefore, in this paper we propose to use artificial neural networks [3] to solve the tasks of model selection and initial parameter estimation. Neural networks are widely used in a variety of disciplines, including the application of such techniques to the data acquisition and triggering of high energy physics detectors. Their robustness provides successful data analysis in the presence of statistical fluctuations and noise.

The proposed approach was tested on the simulated fluorescence decays. It showed rather good results in prediction of the model for fluorescence data. For the case of multi-exponential fluorescence decay analysis, the mean probability to obtain the correct lifetime values within the error range of ±10% was approximately 80%. It should be noted that the method is applicable in the case of non-exponential decays. The method works with convoluted data. The absence of the deconvolution procedure gives a significant increase to the noise stability of the method.

1. J. R. Lakowicz, *Principles of fluorescence spectroscopy*, New York, 1999.
2. Yatskou, M.M.; et. al. *J. Phys. Chem. A* **2001**, *105*, 9498–9508.
3. M. Bishop *Neural Networks for Pattern Recognition*, Oxford: Clarendon Press, 1997.