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

Petr V. Nazarov, Maryna V. Repich, Vladimir V. Apanasovich
Department of System Analysis, Faculty of Radio Physics, Belarusian State University,
Skaryna Ave 4, 220050, Minsk, Belarus. E-mail: nazarov@tut.by

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.