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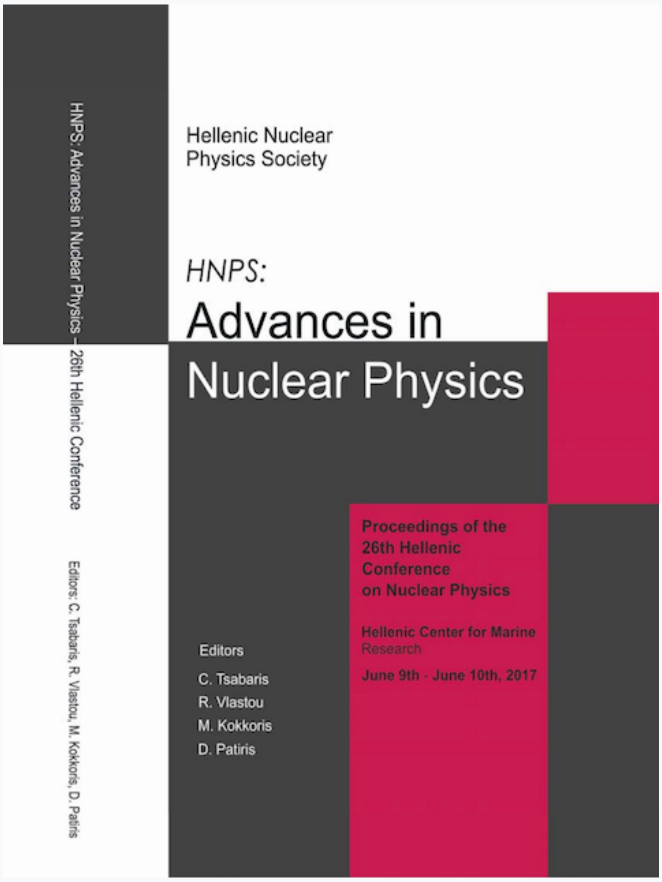

A comparative study of curve-fitting algorithms used for radiation detector efficiencies

M. Lykiardopoulou, A. Khaliel, T. J. Mertzimekis

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A comparative study of curve-fitting algorithms used for radiation detection efficiencies

Eleni-Marina Lykiardopoulou[1,*], Ahmed Khaliel[1], Theo J. Mertzimekis[1]

[1] *Department of Physics, Zografou Campus, GR-15784, University of Athens*

Abstract Non-linear-curve fitting is an essential tool for unfolding physical properties behind experimental data. In the present work, a part of experimental nuclear data from two proton-capture reactions were used to deduce the absolute efficiencies of HPGe detectors. The efficiency data were fitted with a fifth-order Debertin polynomial function using five different software packages. The aim of this work was to compare the calculated fitting parameters, as well as the relative errors of the resulting fitting parameters. The data were treated using gnuplot v5.0, ROOT v5.34.36 (open source), Origin v8.0, Mathematica v10, and MATLAB R2011a (commercial) and their default algorithms (Levenberg-Marquardt, Davidon-Fletcher-Powell and Trust Region Algorithm). In all cases, the data points were assigned with their instrumental weights, i.e. the reciprocal of their squared error values. Although all algorithms seem to produce the same results for the fitting parameters, a remarkable difference in the respective standard deviations was noticed between software packages that use the Levenberg-Marquardt (gnuplot, Origin, Mathematica) or the Trust region (MATLAB) algorithm and the one that uses the Davidon-Fletcher-Powell algorithm (ROOT). The latter produced significantly lower standard deviation values, indicating a better “handling” of the minimization process.

Keywords detector efficiency, curve-fitting algorithms

INTRODUCTION

Non linear curve fitting is an essential tool for studying the behavior of various experimental results. In this work, absolute efficiency data for a HPGe detector are fitted by various different software programs using their default algorithms and a particular test function. Main focus of the test was to investigate any variations in the resulting values of the fitting parameters, as well as their respective statistical errors.

The fitting was performed for eleven (11) different sets of Efficiency vs. Energy data using a standard ^{152}Eu point source. The data were fitted with the function originally proposed by Debertin to model absolute efficiencies of radiation detectors.

$$f(x) = Aln(x) + Bln(x)/x + Cln^2(x)/x + Dln^4(x)/x + Eln^5(x)/x$$

In the study, the following software packages were tested:

- OriginPro 8.0 (commercial)
- Gnuplot 5.0 (open source)

* Corresponding author, email: marilena_lkl@hotmail.com

- Mathematica 10 (commercial)
- MATLAB R2011a (commercial)
- ROOT 5.34.36 (open source)

NON-LINEAR CURVE FITTING ALGORITHMS

A significant process in the non-linear curve fitting is calculating the Inverted Hessian Matrix:

$$H^{\mu\nu} = \left\| \frac{\partial^2 f}{\partial \mathrm{x}^{\mu}\, \partial x^{\nu}} \right\|^{-1}$$

The Inverted Hessian Matrix's diagonal elements give the mean square uncertainty for each of the variables, while the off-diagonal elements determine the correlations among them. Due to the complexity of calculating the Hessian matrix directly, all the aforementioned software packages use algorithms that calculate the latter iteratively. The difference in the final efficiency errors lies in the different iterative process that each algorithm uses to calculate the Hessian Matrix. OriginPro 8, Gnuplot 5.0 and Mathematica 10, as well as previous versions of these software packages, use the least-squared method along with the **Levenberg-Marquardt iteration algorithm** [1,2]. In this algorithm, the Hessian matrix is being approximated by the product of the Jacobian matrix (first derivatives matrix) and its transverse.

The default algorithm used by MINUIT, the minimization package included in ROOT, is **MIGRAD**. The latter is a stable variation of the Davidon-Fletcher-Powell variable-metric algorithm [3], which is based on a quasi-Newton method. In this algorithm, a matrix H is initially chosen and modified iteratively. The conditions that are being imposed to the approximate Hessian matrix are:

H has to be positive-definite and symmetric and,

$y_{\mathrm{r}} = \mathrm{H_k r_k}$, where $\mathrm{r_k} = \mathrm{x_{k+1}} - \mathrm{x_k}$ and $\mathrm{y_k} = \nabla f(x_{k+1}) - \nabla f(x_k)$

MATLAB's curve-fitting tool (cftool) uses the least squares method by default, along with the **Trust-region Algorithm**. In contrast to the previous methods, in this algorithm the iteration step size is decided before the direction of the process. This step size defines a "Trust Region" in which the approximate function (usually quadratic) is trusted to behave as the original one.

RESULTS AND COMPARISON

From the eleven sets of efficiency curves, here we present sets for two different HPGe detectors, which were used to calibrate the detectors during experimental investigations of (p,γ) reactions suffering low statistics. From the present validation analysis, we expect to find the best analysis algorithm for reducing the impact of the experimental uncertainties in the detector efficiencies on the final estimated experimental error.

Coef.	Origin 8.0	Gnuplot 5.0	Mathematica 10	MATLAB R2011a	ROOT 5.34.36
A σ(A)	-0.0009508 0.0006892	0.0009502 0.0005279	-0.0009502 0.0005279	-0.0014 0.001329	-0.001045 0.00001796
B σ(B)	-5.9942 3.0800	-5.9906 3.0800	-5.9906 3.0802	7.9890 7.2410	-5.9940 0.0037
C σ(C)	2.1368 1.0980	2.1355 1.0980	2.1355 1.0981	2.8570 2.5980	2.1587 0.0014
D σ(D)	-0.06840 0.03634	-0.06836 0.03635	-0.06836 0.03635	-0.09291 0.08719	-0.07058 0.00005
E σ(E)	0.006579 0.003514	0.006575 0.003515	0.006575 0.003515	0.008989 0.008506	0.006897 0.000007

Table 1. Coefficients for the detector #2 (90 deg)

Coef.	Origin 8.0	Gnuplot 5.0	Mathematica 10	MATLAB R2011a	ROOT 5.34.36
A σ(A)	-0.004900 0.000669	-0.004900 0.000669	-0.004904 0.000669	-0.005739 0.001611	-0.004892 0.000093
B σ(B)	-30.81 3.90	-30.81 3.90	-30.81 3.90	-35.46 8.35	-30.73 0.20
C σ(C)	10.896 1.390	10.896 1.390	10.896 1.390	12.56 3.00	10.087 0.053
D σ(D)	-0.35331 0.04594	-0.35331 0.04594	-0.35331 0.04594	-0.40910 0.10170	-0.35240 0.00136
E σ(E)	0.03395 0.00444	0.03395 0.00444	0.03395 0.00444	0.03939 0.00998	0.03387 0.00020

Table 2. Coefficients for the detector #1 (15 deg)

CONCLUSIONS

Efficiency curve fitting was performed in five different software environments. While the value of each parameter seems to be the same in almost all software packages, its corresponding estimated uncertainty varies significantly, an effect attributed to the different fitting algorithms employed. Fitting with ROOT produces the smallest uncertainties, while MATLAB R2011a provides the largest ones.

COMPARATIVE PLOTS

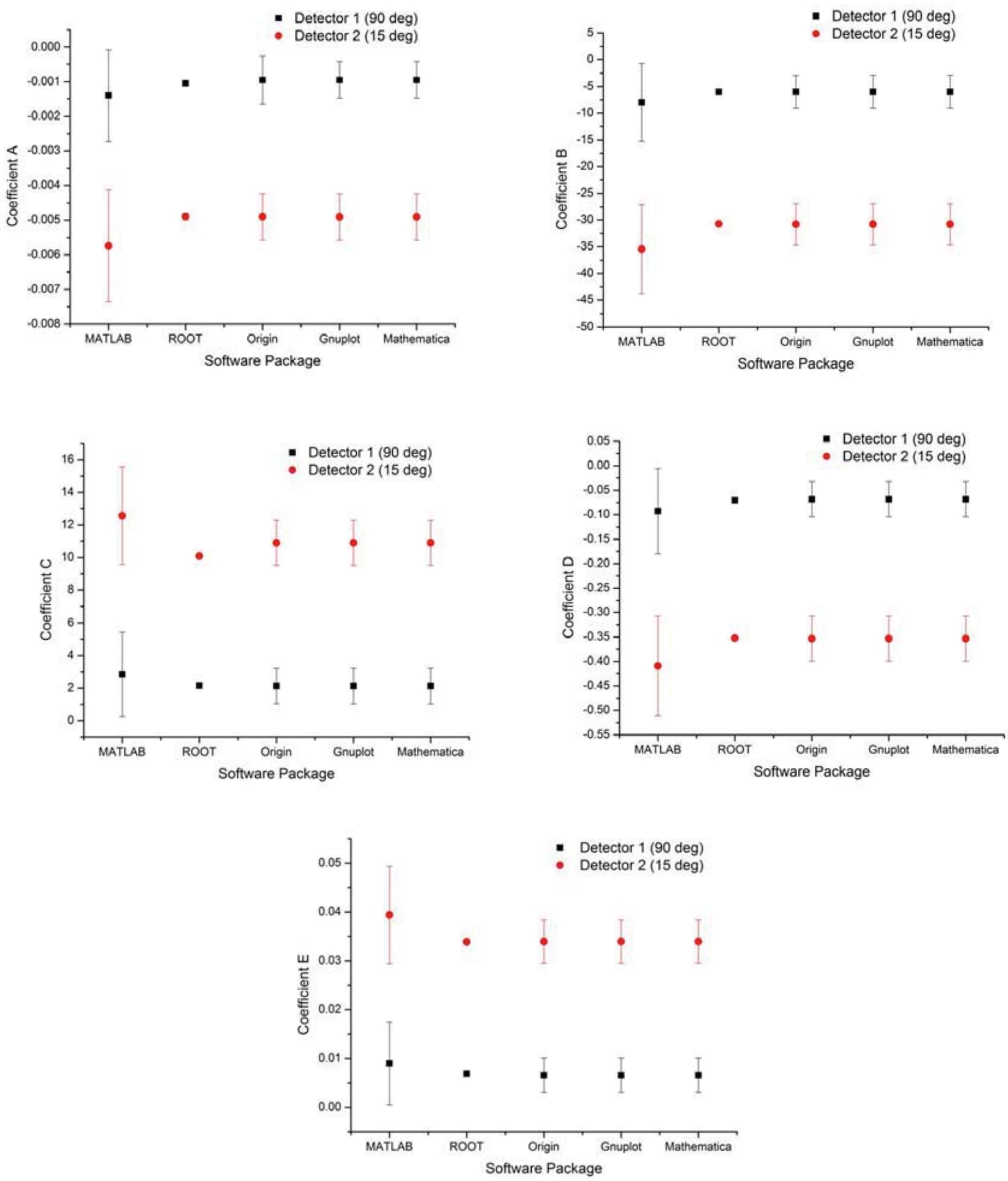

Fig. 1. Values of coefficients: a) A, b) B, c) C, d) D, e) E, according to equation (1), estimated by the software packages used in the present study.

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