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IMPROVEMENT OF FAST AND EFFECTIVE NUMERICAL METHODS FOR EVALUATION OF SCINTILLATION GAMMA-RAY SPECTRA

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AUTHOR'S REVIEW

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Scientific problem formulation

Gamma-ray detection is a considerably complicated, multi-step process. When gamma-rays enter the **scintillation crystal**, they interact primarily with the bound electrons from the iodine atoms in the crystal. The binding energy of an electron in the iodine is only 33keV and so the recoiling electron takes most of the energy of the incident γ-ray. This recoil electron passes through the NaI crystal and loses energy by ionisation and electronic and thermal excitations. This excitation energy is given off in various ways, a fixed fraction of the electron energy will be converted to visible photons (300-600nm), thus a single high energy gamma ray produces a flash of photons which then collide onto the photocathode of the **photomultiplier** tube. These photons will produce photoelectrons from the photocathode surface of the photomultiplier via the photoelectric effect. A cascade of electrons is produced along the multiplier to give an electrical pulse at the anode which is proportional to the energy of the incident gamma-ray. Pulses from the anode are fed through the **amplifier** and into the multi-channel analyser for analysis. In case of a NaI(Tl) scintillator, the number of channels are 256, 512 or 1024. A multi-channel analyzer sorts the pulses according to height and counts the number in each channel to give an energy distribution of electrons, which is called “pulse height spectrum”.

The relationship between incident and observed spectrum can be described by a linear equation system. The solution of this system (called deconvolution), is generally a complex problem, because the solution is unstable with respect to the measurement error. The equation system is extremely sensitive to errors in the measured data, because the matrix of the system is always singular. The existence of error and the singularity of the system-matrix affects the process of deconvolution, and can lead to difficulties in solving the equation system. This work first of all investigates mathematical background of this problem.

To describe the problem in details, let's divide the measuring energy range into n parts, let $\mathbf{x} \in \Re^n$ be the real spectrum, and $\mathbf{y} \in \Re^m$ is the measured spectrum where m is the number of channels of a multi-channel analyzer. The relationship between incident and observed spectrum can be described by a linear equation system $\mathbf{y} = \mathbf{R} \cdot \mathbf{x} + \boldsymbol{\varepsilon}$ where $\mathbf{R} \in \Re^{mxn}$ is the **response matrix,** $\varepsilon \in \Re^m$ is an error or more accurately the **uncertainty of the measurement**. The components of the response matrix are depends on the detector characteristics, the size of the scintillation crystal, the shielding of the detector, the gamma ray energy, etc. Each column of the response is a **probability distribution**, the component R_{ij} is a probability of the event that a gamma photon, belongs to the j-th energy range will be detected in the i-th channel. The problem is obviously to determine x, the incident spectrum. From mathematical point of view, it means that the **inverse problem** must be solved. The solution method of inverse problem is called **deconvolution**.

From numerical point of view the deconvolution is a very critical, so-called **ill-posed** problem. A mathematical problem is **well-posed**, if it satisfies the following conditions:

1. **Existence**: For all suitable data there exists a solution of the problem in an appropriate sense.
2. **Uniqueness**: For all suitable data, the solution is unique.
3. **Stability**: The solution depends continuously on the data.

The solution of the equation system, is generally a complex problem, because the solution is unstable with respect to the measurement error, the equation system is extremely sensitive to errors in the measured data. From mathematical point of view the main problem is the singularity of response matrix, the existence of very small eigenvalues. The existence of error and the singularity of the response matrix affects the process of deconvolution, and can lead to difficulties in solving the equation system. The principal purpose of this dissertation, to develop numerical methods, which are significantly less sensitive to errors in the data.

Research methods

I studied Hungarian and international literature, to find out which are unsolved problems according to this question. First of all I treated the described question as pure mathematical problem. I studied several chapters of mathematics, examining the possibility of solving the ill-posed problem, using iterative algorithms. I used MATLAB for calculations, because this software had been designed especially for solving linear algebraic problems. In the first part of the work I made artificial gamma spectrum, consisting of noisy Gaussian distribution functions and generated an artificial response matrix. To test the methods efficiency, new iterative algorithms were tested first of all in this ideal case, with pure Gaussian response.

After this research I examined experimentally detected spectra. I managed to make real spectra using three different gamma-ray detectors. There were available nine different isotopes for experiments, I made nearly fifty gamma-ray spectra. I used these spectra to test effectiveness of worked out algorithms.

Since the objective of many radiation measurements has been to deduce energy distribution of incident radiation, it is essential to understand the detector response for incoming radiation. The response matrix of the scintillation detector were obtained using the Monte Carlo method applying simple, analytical approximations of the full energy peak and the Compton continuum. The production of the response is essentially based on the peak to total ratio, the detector resolution, and other calibrations, which functions were determined experimentally. The obtained response matrix were compared with experimental values and a good agreement was found.

A brief presentation of the research, conducted chapter by chapter

In the **first chapter** I showed the topicality of the subject on the basis of the literature research. This chapter also includes research objectives and a presentation of the methods leading to realize them. I described classical methods and showed their insufficiency.

The **second chapter** is the main chapter of the dissertation. In this chapter I studied classical deconvolution methods, and the possibilities to improve them and I developed some new faster and more effective algorithms. I showed, that classical iterative methods also can be successfully applied to solve the problem.

But classical methods for solving equation systems are not efficient enough, therefore, in order to find stable solution the method of regularization must be applied. This means, that the original problem is replaced by an approximate one, the solutions of which are significantly less sensitive to errors in the data. This dissertation presents some effective regularisation techniques. But I showed, that the traditional regularisation not efficient enough.

Maximum entropy method is a probabilistic method, which can be successfully applied to deconvolution of gamma-ray spectra. The maximum entropy model has several advantages over conventional methods. It provides a better resolution than linear regularisation methods, the solution is positively constrained, and it also allows one to include the additional χ^2 statistic to compensate for the fluctuations in real spectra. But I showed, that this algorithm is very slow, and the resolution is not satisfactory. I proved, that the speed of the algorithm can be improved if rare matrices are applied.

Maximum likelihood estimation is a very effective statistical method used to calculate the best way of fitting a mathematical model to some data. Modelling real data by estimating maximum likelihood offers a way of tuning the free parameters of the model to provide an optimum fit. The expectation maximization algorithm is used in statistics for finding maximum likelihood estimates of parameters in probabilistic models, where the model depends on unobserved variables. This method is also very important if one have to determine the activity of the isotope. This question I studied in the third chapter.

I developed some new, very effective numerical algorithms, which are faster than traditional methods, and I proved, that the resolution of these new methods are much better. I modified classical regularization methods, I introduced the "weighted regularization", and proved that this method much less sensitive to the regularization parameter. This is an effective method which satisfies the following two conditions. The method **provides hidden photo peaks** also, in the form of Dirac-delta function, and **separate overlapping Gaussians**.

I also considered the described linear algebraic equation system as a quadratic programming optimization problem. For solution I employed two efficient mathematical programming methods. First of all, the conjugate gradient method, and after that the active set method. The **conjugate gradient method** is an efficient algorithm for the numerical solution of linear equation systems, whose matrix is symmetric and positive definite. This iterative method can be successfully applied also in numerical solution of optimization problems, such as the described quadratic programming problem. The **active set method** operates as an outer or controlling algorithm. Applying this method, the solution is always positive definite.

Cardinal question, in the connection of each algorithm, the **inversion method** of the response matrix. The traditional inversion is absolutely unsuitable. Much more effective the generalised inverse, but to calculate this inverse matrix needs very much operation. For this reason I examined other possibilities to provide inverse matrix. I proved that the Cholesky-deconvolution and the QR deconvolution also can be successfully applied to calculate inverse of the response matrix. I described two independent algorithms, in which these two inversion method is applied, and proved that these methods much faster than providing singular value decomposition.

In the **third chapter** I examined the possibilities to determine activity of isotopes in the case of overlapping photo peaks, and when several isotopes radiates at the same time. I deduced two independent algorithms which can be successfully applied in the above mentioned case. The first method is based on the Gaussian normal equation, and leads to the simple linear iteration. This method separates overlapping Gaussian functions. The second method, which can be applied in the most general case, is deduced applying the maximum likelihood principle. Employing this algorithm the response matrix must be known. The procedure of making the response, I examined in the fifth chapter.

In the **fourth chapter** I examined the role of noise in the deconvolution methods. Applying the discrete Fourier-transform I proved, that the smoothing convolution procedure damages the properties of the solution. The resolution is much worse and false photo peaks appear in the solution. But it came to light, that if the spectrum contains extremely strong noise, the deconvolution methods also give the correct solution. By the way, applying the Fourier transform, I described how to provide the second derivative of the spectrum, and examined the properties of this classical method.

In the **fifth chapter** I studied the way of producing the response matrix. I described the method, how to calibrate a scintillation detector. I examined in details the way of generating a photopeak and the Compton continuum. I improved the approximation of the photo peak and the Compton continuum, using some easy manageable analytical functions. I worked out a Monte Carlo method, to generate response matrix. I validated the method using theoretical and measured spectra. I proved, that the described Monte Carlo method can be successfully applied to generate response matrix. At last, using experimental gamma-ray spectra, I proved, that deconvolution methods and generated response matrix together is fast and efficient procedure to identify unknown isotopes.

New scientific results

THESIS I. Applying methods of linear algebra and mathematical programming I worked out new iterative algorithms, which can be successfully applied to deconvolution of scintillation gamma-ray spectra.

1. I applied successfully the conjugate gradient method and the active set method.
2. I worked out an efficient algorithm, applying the singular value decomposition of singular matrices.
3. Introducing the method of “weighted regularization” I considerably improved the efficiency of regularization techniques.

THESIS 2. Applying the results of deconvolution techniques, I deduced iterative algorithms, which are applicable to determine the activity of isotopes in the case of overlapping spectra.

1. Applying the Gaussian normal equation I deduced an iterative technique to resolve overlapping gamma lines analytically.
2. Applying the maximum likelihood estimation I worked out a nonlinear equation, which can be successfully applied to estimate activity in case of overlapping gamma-ray spectra.

THESIS 3. I described a procedure to calibrate a scintillation gamma detector, and I calibrated all of three detectors, what I used to produce experimental spectra.

THESIS 4. I constructed a Monte Carlo algorithm for generating a response matrix for a scintillation detector. I validated the method and gave the response matrices of three detectors.

1. I improved the analytical approximation of the Gaussian photo peak, and described a Monte Carlo procedure to generate it.
2. I improved the analytical approximation of the Compton continuum in the case when $E < 1$ MeV and when $E > 1$ MeV, and described a Monte Carlo procedure to generate it.

THESIS 5. I assembled a MATLAB-implemented software system, which can be applied, in the case of an arbitrary scintillation detector, to carry out the next procedure:

1. Calibrating operation.
2. Generation of the response matrix.
3. Using deconvolution algorithms, isotopes can be identified.
4. Can be calculated the activity.

Possibilities for using results; recommendations

There are a lot of scientific problems, especially in natural and technical sciences, but economy and logistics can be mentioned too, which lead to ill conditioned or ill posed linear algebraic problems. New iterative algorithms, which were developed in this dissertation can be successfully applied for solution of these problems.

1. Military application: Identify radiating isotopes in the field.
2. Disaster defence application: Dirty bomb or nuclear events.
3. Gamma astronomy: To examine gamma ray bursts.
4. Measuring technical application: In some parameter fitting problem.
5. In economy: Portfolio analysis.
6. In technical examinations: Multi variable, ill conditioned optimization problems.
7. In logistics: Solving the transporting problem.