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A New Algorithm for Processing Beta-Gamma Coincidence Spectra Based on the Maximum Likelihood Estimation

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Poster No. P3.5-442

All-Russian Research Institute of Automatics (VNIIA)

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ABSTRACT

- A new algorithm for analysis of beta-gamma radioxenon spectra is presented.
- The algorithm allows simultaneous processing of the signal in all β-γ regions of interest (ROI) using the least-squares and maximum-likelihood estimations.
- All formulas, if they have a closed form, are given in vector and matrix forms.
- The XeMat program was developed for processing beta-gamma spectra using the new algorithm, and the activities and the air activity concentration of xenon were calculated using the data obtained by the Monitoring System of Xenon Isotopes (MIKS) in 2020.

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INTRODUCTION

The International Monitoring System for the Comprehensive Nuclear-Test-Ban Treaty includes measurements of radioxenon isotopes that are likely to be detectable at locations far from a suspected test site.

Some Detection systems like the Russian MIKS system, create 2D (256×256 channels) β-γ coincidence energy spectra using a plastic scintillator cell to detect conversion electrons and betas and a NaI(Tl) crystal to detect gamma- and X-rays. These β-γ spectra are used to estimate the activity of the radioxenon isotopes in the air.

The most important approaches to estimating the activity using beta-gamma spectra are:

- the Net Count Calculation (NCC) method, also called ROI method;
- the Standard Spectrum Method also called the SDAT method or the Spectral Unmixing method;
- Machine learning and Neural Networks.

If the counting rate is high, all methods are consistent and similar. Differences will be visible only for low statistics.

The activity estimation at low statistics is a difficult problem. Detector calibration drift distort spectra. Another important problem is the interference of spectra of relevant xenon and radon isotopes. For example, if the beta resolution for the ^{131m}Xe and ^{133m}Xe metastable isotopes is low, the task of determining their activities becomes an ill-posed problem.

In this case, we consider the Standard Spectrum Method and a derivative from it, also called the ROI simultaneous fitting method.

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METHODS

Standard spectrum method for radioactivity estimation

Linear spectral unmixing

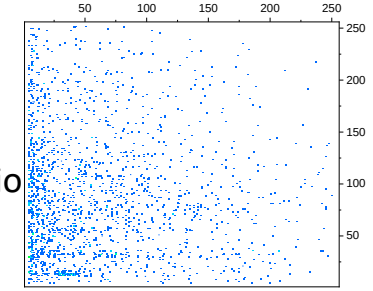
Column-vectors

$$\vec{c} - k_s \vec{b} = \sum_{i=1}^{5} \mu_i \vec{r}_i$$

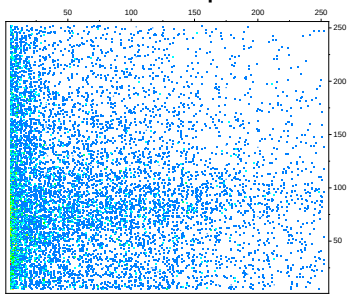
μ_i – amount (unknown) of the *i*th nuclide in the mixture;

$k_s = t_S / t_D$ – time acq. ratio

$\vec{c}$ = SAMPLE Spectrum

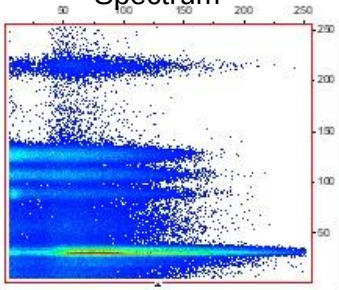


$\vec{b}$ = DETBK Spectrum

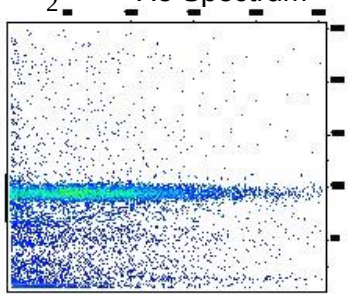


Reference β-γ spectra

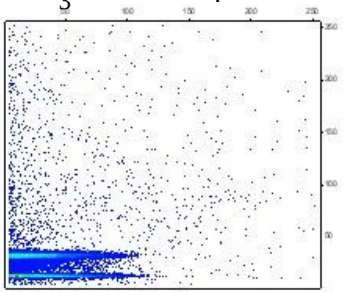
$\vec{r}_1$ = ^{222}Rn(daughters) Spectrum



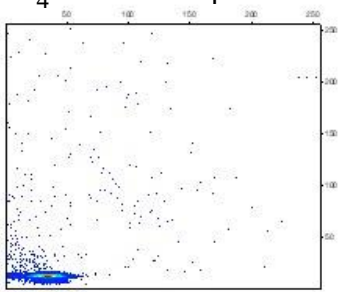
$\vec{r}_2$ = ^{135}Xe Spectrum



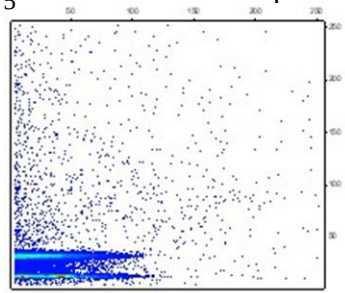
$\vec{r}_3$ = ^{133}Xe Spectrum



$\vec{r}_4$ = ^{131m}Xe Spectrum



$\vec{r}_5$ = ^{133m}Xe + ^{133}Xe Spectrum



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METHODS

Estimation as an inverse problem for linear regression

$$\vec{c} - k_s \vec{b} = \sum_{i=1}^{5} \mu_i \vec{r}_i \Leftrightarrow \vec{c}_b = \mathbf{R}\vec{\mu}$$

$$\vec{\mu} = \begin{bmatrix} \mu_1 \\ \vdots \\ \mu_5 \end{bmatrix} = ?$$

Calibration matrix

$$\mathbf{R} = \begin{bmatrix} \vec{r}_1 & \cdots & \vec{r}_5 \end{bmatrix} = \begin{bmatrix} R_{11} & R_{12} & \cdots & R_{15} \\ \vdots & \vdots & \ddots & \vdots \\ R_{k1} & R_{k2} & \cdots & R_{k5} \end{bmatrix}$$

- **R** is called the **calibration matrix** and represents the set of reference spectra generated by calibration, which will be used in an analysis;
- **R** is the **design matrix** for linear regression;
- **R** must be well-known;

If the Full spectrum is used, **R** is (k×5) matrix, where k = 256 × 256 = 65536.

If the ROI simultaneous method is used, **R** is (k×5) matrix, where k = number of ROIs.

About DETBK (really important for very low levels of activity)

In general, the background DETBK $\vec{b}$ can be processed in two ways: it can be viewed as a component (column-spectrum) in the matrix **R**, or subtracted from the observed distribution. In this case, we use only the second approach.

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METHODS

Four Estimators of the parameter vector for $\mathbf{R}\vec{\mu} = \vec{c}_b$

Method	Weighed Least Squares		Maximum Likelihood (Poisson)	
Function	$S(\vec{\mu}) = \left\| \mathbf{W}_c^{1/2} \left(\vec{c}_b - \mathbf{R}\vec{\mu} \right) \right\|^2 ; \mathbf{W}_c = \mathrm{diag}(\vec{c} + k_s^2 \vec{b})^{-1};$		$l(\vec{\mu}) = \sum_{i=1}^{n} c_i \ln([\mathbf{R}\vec{\mu}]_i + k_s b_i) - [\mathbf{R}\vec{\mu}]_i - k_s b_i; \; k_s \ll 1;$	
A priori	Without constraint	With constraint - non-negative	Without constraint	With constraint – non-negative
Estimator	$\vec{\mu}^*_{LS} = \arg\min_{\vec{\mu}} S(\vec{\mu})$	$\vec{\mu}^*_{NNLS} = \arg\min_{\vec{\mu}>\mathbf{0}} S(\vec{\mu})$	$\vec{\mu}^*_{ML} = \arg\max_{\vec{\mu}} l(\vec{\mu})$	$\vec{\mu}^*_{NNML} = \arg\max_{\vec{\mu}>0} l(\vec{\mu})$
Solution	$\vec{\mu}^*_{LS} = \left(\mathbf{R}^{\mathrm{T}} \mathbf{W}_c \mathbf{R} \right)^{-1} \mathbf{R}^{\mathrm{T}} \mathbf{W}_c \vec{c}_b$	Numerical, Quadratic programming	Numerical, Convex optimization	Numerical, Convex optimization
Characteristics	best linear unbiased estimator	biased estimator	best unbiased estimator for Poisson	biased estimator

Only the LS has a closed-form and covariance matrix

$\vec{\mu}^*_{LS} = \left(\mathbf{R}^{\mathrm{T}} \mathbf{W}_c \mathbf{R} \right)^{-1} \mathbf{R}^{\mathrm{T}} \mathbf{W}_c \vec{c}_b, \quad \mathbf{K}_{\vec{\mu}} = \left(\mathbf{R}^{\mathrm{T}} \mathbf{W}_c \mathbf{R} \right)^{-1}$ Goodness of fit $\chi^2_{k-n} = \vec{\varepsilon}^{\mathrm{T}} \mathbf{W}_c \vec{\varepsilon}$, $\vec{\varepsilon}$ is the residual

- Non-negative a priori constraint lead to a bias in estimators, which is a characteristic of regularization.
- According to the Mean Squared Error (MSE), biased estimators NNLS and NNML are better than unbiased LS and ML.
- The ML approach has the advantage over LS when the counting rate is very low and background is well known

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METHODS

The ROI simultaneous fitting method

Standard spectrum method (full-spectrum analysis)

Creating ROI and Grouping spectral data

loss of information and reducing the degree of orthogonality

Increase Robustness

ROI simultaneous fitting (ROI analysis)

How to optimally create the set of Regions Of Interest?

- ROIs should not overlap;
- ROIs should contain only the useful signal and give orthogonal spectra vectors;
- the number and shape of the ROIs in a β-γ spectrum should be correlated with the stability of the calibration.

Tradeoff: Efficiency vs. Robustness

The region-of-interest approach provides a robust estimator

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RESULTS

Matrix form of activity calculation including gas background and correction factors

Activity at acquisition start

$$\vec{\mathrm{A}} = \mathbf{H}\left(\vec{\mu}^{*} - \mathbf{F}\vec{\eta}^{*}\right).$$

Activity concentration (average)

$$\vec{\mathrm{A}}_c = V_0^{-1}\mathbf{G}_p\mathbf{G}_s\mathbf{\Gamma}\vec{\mathrm{A}}.$$

$\left\{\vec{\mu}^{*}, \vec{\eta}^{*}\right\}$ - unmixing solutions for SAMPLE and GASBK spectra.

Standard correction factors in matrix form

factor chain ^{133m}Xe-->^{133}Xe

$$\mathbf{\Gamma} = \begin{bmatrix} 1 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & -\gamma \\ 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 1 \end{bmatrix}$$

GASBK factors Matrix

$$\mathbf{F} = \begin{bmatrix} F_{11} & 0 & 0 & 0 & 0 \\ 0 & F_{22} & 0 & 0 & 0 \\ 0 & 0 & F_{33} & 0 & f \\ 0 & 0 & 0 & F_{44} & 0 \\ 0 & 0 & 0 & 0 & F_{55} \end{bmatrix};$$

$\vec{\lambda} = \left[\lambda_1 \quad \cdots \quad \lambda_5\right]^{\mathrm{T}}$ $\left\{^{222}\mathrm{Rn}, ^{135}\mathrm{Xe}, ^{133}\mathrm{Xe}, ^{131m}\mathrm{Xe}, ^{133m}\mathrm{Xe}\right\}$

$\mathbf{H} = \mathrm{diag}(G_{\lambda_i t_{sr}} / (t_{sl} \cdot I_i)), i = \overline{1,5}$ - activity factors;

$G_{\lambda t} = \lambda t / \left(1 - e^{-\lambda t}\right)$ - decay-corr. *acquisition*;

$\mathbf{G}_p = \mathrm{diag}(e^{\lambda_i t_p}), i = \overline{1,5}$ - decay-corr. *processing*;

$\mathbf{G}_s = \mathrm{diag}\left(\lambda_i t_a / \left(1 - e^{-\lambda_i t_a}\right)\right), i = \overline{1,5}$ - decay-corr. *sampling*;

$$F_{jj} = \frac{G_{\lambda_j t_{gr}}}{G_{\lambda_j t_{sr}}} \frac{t_{sl}}{t_{gl}} e^{-\lambda_j \tau}; \; f = \frac{G_{\lambda_5 t_{gr}}}{G_{\lambda_3 t_{sr}}} \frac{t_{sl}}{t_{gl}} \frac{I_3}{I_5} \frac{\lambda_3}{\lambda_5 - \lambda_3} \left(\mathrm{e}^{-\lambda_3 \tau} - \mathrm{e}^{-\lambda_5 \tau}\right);$$

$V_0[\mathrm{m}^3] = \dfrac{V_{Xe}\,[\mathrm{cm}^3]}{0.086\,[\mathrm{cm}^3/\mathrm{m}^3]}$ - Air volume;

We used different estimators and select the NNLS for the ROI simultaneous fitting and NNML for the full spectrum approach. These estimators are the biased and regularized estimators. However, it is more convenient to use the LS approach for error handling, since it gives a covariance matrix. For example, if the correction factor matrices are non-random, $\mathbf{K}_A = \mathbf{H}\left(\mathbf{K}_{\boldsymbol{\mu}} + \mathbf{F}\mathbf{K}_{\boldsymbol{\eta}}\mathbf{F}^{\mathrm{T}}\right)\mathbf{H}^{\mathrm{T}}$, *where* $\mathbf{K}_{\vec{\mu}} = \left(\mathbf{R}^{\mathrm{T}}\mathbf{W}_c\mathbf{R}\right)^{-1}, \mathbf{K}_{\eta} = \left(\mathbf{R}^{\mathrm{T}}\mathbf{W}_d\mathbf{R}\right)^{-1}$.

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RESULTS

Matrix form of MDA and MDC calculations

$\mathbf{R} = [\vec{r}_1 \ \cdots \ \vec{r}_5]$ – calibration matrix full spectrum or **ROI**

$\vec{c}$ - *Sample;*

$\vec{b}$ - *DetBk;*

$\vec{n} = \theta(\vec{\mu}^* - \mathbf{F}\vec{\eta}^*), \quad \theta(\cdot)$ – Heaviside;

$$\tilde{\mathbf{\Omega}}_j = \mathrm{diag}\left(\vec{c} + k_s^2\vec{b} - n_j\vec{r}_j\right),\ j = 1..5 \setminus \{3\};$$

^{133m}Xe -->^{133}Xe

$$\tilde{\mathbf{\Omega}}_3 = \mathrm{diag}\left(\vec{c} + k_s^2\vec{b} - (n_3 - \chi n_5)\vec{r}_3\right);$$

Tensor $\mathbf{K}^j = \left(\mathbf{R}^{\mathrm{T}}\tilde{\mathbf{\Omega}}_j^{-1}\mathbf{R}\right)^{-1} \Rightarrow \sigma_{0j} = \sqrt{K_{jj}^j};$

$L_d{}^j = k^2 + 2k\sigma_{0j} = k^2 + 2k\sqrt{K_{jj}^j}$ – Currie limit, $k=z_{1-\alpha}$

$\vec{L}_d = [L_d^1 \cdots L_d^5]^{\mathrm{T}}, \ \overrightarrow{\mathrm{MDC}} = [\mathrm{MDC}^1 \cdots \mathrm{MDC}^5]^{\mathrm{T}};$

$\overrightarrow{\mathrm{MDA}} = \mathbf{H}\vec{L}_d;$

$\overrightarrow{\mathrm{MDC}} = V_0^{-1}\mathbf{G}_p\mathbf{G}_s \cdot \overrightarrow{\mathrm{MDA}};$

$\{\vec{\mu}^*, \vec{\eta}^*\}$ – unmixing solutions for SAMPLE and GASBK spectra.

How many nuclide spectra should a priori be in R?

MDA depends on a priori knowledge of the presence of nuclides in a sample.

- If too few spectra are included in **R**, the estimates will be biased, with the bias depending on the concentration of the neglected nuclides, and on the relationship between the spectra of the neglected nuclides and the spectra of the accounted nuclides.
- On the other hand, including too many spectra in R leads to a loss of precision, i.e., to an increase in the standard errors of the estimates. The estimates, however, remain unbiased.
- A more accurate calculation is possible in a non-negative case, but the Monte Carlo method is necessary.

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RESULTS

Software XeMat

The **XeMatrix** is a software tool developed by VNIIA. It utilizes the **Standard-spectrum and simultaneous-fitting methods** for the purpose of analyzing β-γ coincidence radioxenon spectra. Spectra are read in the International Monitoring System (IMS) pulse height data (PHD) format. The final result is the activity and activity concentration for ^{135}Xe, ^{133}Xe, ^{131m}Xe, and ^{133m}Xe.

All of the above formulas are implemented in the XeMat algorithm:

- the library of Reference β-γ spectra saved in **R** matrix, taking efficiency normalization into account;
- selection of a set of ROIs based on the Efficiency vs. Robustness tradeoff;
- unmixing calculation by the four estimators for the sample and the gas background spectra, which allows one to control the goodness of fit and blunders such as background variation (estimates should not be very different from each other);
- the closed form of the LS-approach and covariance matrix are used to calculate the errors;
- the ability to set a priori thresholds for detection of each nuclide: MDA and MDC depend on a priori knowledge of nuclide presence.

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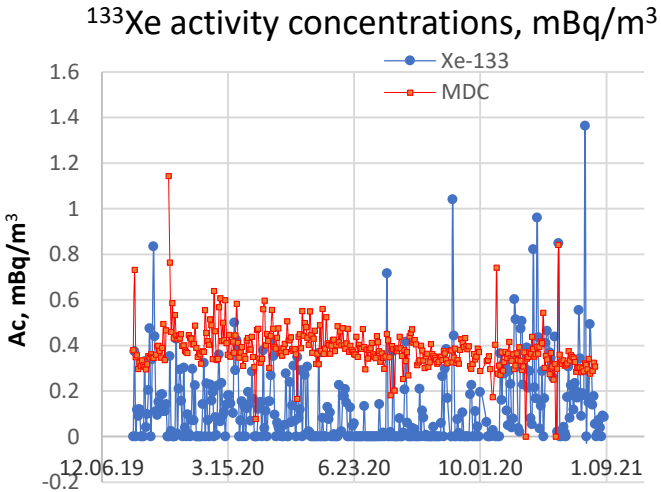
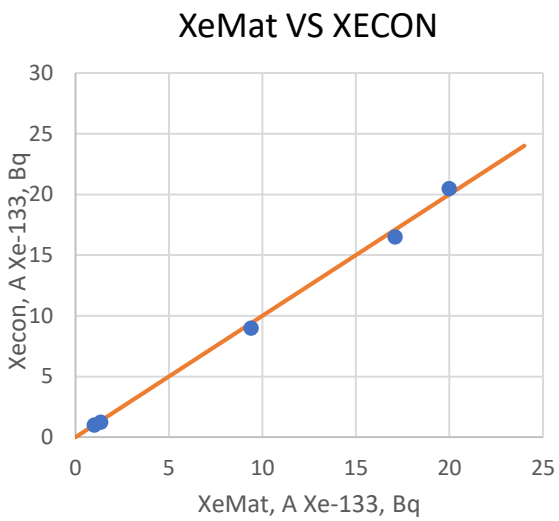
RESULTS

Activity concentration calculated using XeMat (MIKS data)





Some results are presented. In the future, we plan a more detailed study on the comparison of different approaches to processing of xenon spectra.

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CONCLUSIONS

Conclusion

- The simultaneous ROI fitting method is a derivation from the Standard Spectral Method. The simultaneous ROI fitting approach is based on the principle of maximum likelihood and is both intuitive and flexible.
- Four Estimators of the solution to the inverse problem (unmixing) were studied. The Maximum Likelihood (Poisson) approach will have the advantage over Least Squares when the counting rate is very low and the background is well known. Only the Least Squares has a closed-form and covariance matrix. According to the Mean Squared Error (MSE), the biased NNLS and NNML estimators are better than the unbiased LS and ML.
- The library of reference beta-gamma spectra must include relevant xenon spectra, and the background DETBK spectrum can be processed in two ways: it can be viewed as a component (column-spectrum) in the calibration matrix R, or subtracted from the observed distribution. If the background is stable over time, the second approach must be chosen.
- Regions of interest should be set based on the Efficiency vs. Robustness tradeoff. If the calibration is stable, one should work with the full spectrum without ROIs.
- The MDA is directly derived from the calibration matrix. A priori knowledge can be added in the non-Bayesian version in the form of thresholds for each nuclide.
- Comparison between XeMat and the XECON show good agreement.