

An artificially intelligent look on the uranium enrichment determination problem using X- and gamma-ray spectroscopy: introducing a new isotopic code CAMILA for CZT and LaBr₃(Ce) detectors

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In the past decades, there has been a vast progress and development in the domain of artificial intelligence (AI) technologies and their practical application to various fields of science. Indeed, advanced statistical tools such as principal component analysis, distance and discrimination metric tools, as well as layered neural networks open a large array of data analysis and processing options. Among their potential advantages are the possibility to mitigate challenges of data sets analysis that are subject to noise and handling of large amounts of data. The former allows to extract the qualitative and quantitative information in cases when traditional statistical tools experience deficiencies either due to poor statistical quality of data and/or bias of different origin. The latter allows for an online processing of a large stream of data.

However, the domain of applied sciences where AI-based technologies are finding their rapidly developing application is a multidisciplinary domain that besides its instrumentation part requires also the methodological part in view of the algorithms used to effectively extract qualitative and quantitative information from the data sets. The latter implies a particular architecture of the sub-routines sequence implemented in the algorithm design, which in its turn requires clear designation of the specific tasks it is applied for.

Among such application domains is radiation detection, where room temperature semiconductor and scintillation devices such as CZT and LaBr₃(Ce) are proposed as promising candidates for uranium enrichment determination tasks, which set certain performance criteria for the algorithms. From a methodological point of view, the algorithms used to extract and analyze the spectral information consist of the two major parts – a model that is used to describe the physical interactions and a statistical tool used to analyze/infer the data for the corresponding qualitative and quantitative analysis of the sample attribute characteristics. One of the most commonly used concepts for such algorithms is based on the fundamental counting premise, usually referred to as the net peak area based methodology. The advantage of such a concept is that it implies constrained physical models for the physical interactions. However, a crucial disadvantage is that should the X- and gamma-ray signature photopeaks of radioisotopes be of worsened statistical quality, the resulting performance of the algorithm is degraded due to the conceptual inappropriateness of the model used to describe such noisy data and type of the statistical tool used to analyze it. The former is limited by the conceptual design of physical models used in classical spectra analysis algorithms, the latter is a direct consequence of a large degree of bias introduced by noise effects of different origin. In that respect, with introduction of room temperature medium resolution detector

designs, a large scientific gap has occurred. Thus, spectra analysis algorithms developed for traditional radiation detection systems based on cooled HPGe detectors require their specific spectroscopic performance, physical parameters and cannot be directly used with room temperature designs. Spectroscopic performance of room temperature medium resolution detectors is different in many ways to that of traditional ones. When used with traditional spectra analysis algorithms may yield erroneous data analysis results and low robustness, requiring adaptation of the mathematical formalism in their unfolding routines, models and statistical tools.

To overcome the conceptual deficiencies of the traditional net peak area based algorithms other methods for qualitative and quantitative information extraction can be used. Such methods imply a different conceptual design of the coupling physical model-statistical tool when extracting the information on the X-and gamma-ray signatures. The underlying idea of such methods is simply to avoid potential sources of bias due to degraded statistical quality, overlapping or bad signal-to-noise ratio and treat spectrum using higher dimensionalities with respect to its features. The conceptual basis for such novel methods is that spectrum is viewed as a layout of patterns corresponding to particular features of the sample assayed. In this respect, the traditional metrics of qualitative and quantitative information extraction can be avoided and replaced by analysis of the feature space and its functional behavior with respect to the attribute characteristics of the sample. Such novel concepts require advanced statistical tools (principal component analysis, distance metrics tools) and artificial intelligence (neural networks) to prepare the data sets, process, cluster and extract information from them.

However, there has yet been no comprehensive assessment of possible conceptual design of AI-based algorithms with respect to their architecture and underlying unfolding routines design applied to qualitative and quantitative X-and gamma-ray spectra analysis tasks and their performance evaluation with different strategies and case-scenarios. Conceptually, AI-based algorithms can be realized via different combinations of advanced statistical tools (such as principal component analysis, discrimination analysis and distance metrics tools) and neural networks. In that sense there are different strategies how the data sets can be prepared and processed from a methodological point of view.

The presented research aims not only to fulfil the mentioned scientific gap, but also proposes the conceptual design of such AI-based algorithms featuring neural networks and principal component analysis for uranium enrichment determination tasks and investigates their performance possibilities and limits in different experimental conditions. It is also a step towards the future research in the domain of artificial intelligence technologies applied for quantitative and qualitative X-and gamma-ray spectra analysis. Implemented routines are described in detail and results are presented.