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# Review of Nuclear Quadrupole Resonance Signal Processing and Analysis Methods

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**ABSTRACT** This article presents a structured and comprehensive review of signal processing and analysis methods used in nuclear quadrupole resonance (NQR), with a focus on their performance under real-world operating conditions, where signals are typically weak, noisy, and highly sensitive to environmental influences. Classical approaches, including Fourier analysis, wavelet transforms, adaptive and matched filtering, as well as high-resolution spectral estimation techniques, are considered with respect to their ability to enhance signal detectability and frequency resolution. Particular attention is devoted to modern machine learning-based methods, including deep neural networks and hybrid architectures, which enable automatic feature extraction and demonstrate high robustness in low signal-to-noise ratio conditions. Each group of methods is systematically analyzed according to a set of practical criteria, including noise immunity, computational complexity, adaptability to nonstationary environments, sensitivity to parameter variations, and suitability for implementation in portable or resource-constrained NQR systems. The review highlights key challenges in current research, such as the lack of standardized and representative training datasets, limited interpretability of learning-based models, and difficulties associated with deploying computationally intensive algorithms in compact instrumentation. It is shown that no single signal processing approach provides a universally optimal solution across all operating scenarios. Instead, the most promising direction lies in the development of hybrid signal processing frameworks that combine classical preprocessing techniques with data-driven machine learning models. The presented analysis provides a methodological basis for the informed selection and design of robust, adaptive NQR systems intended for practical applications in security screening, material characterization, and chemical substance identification under diverse and challenging conditions.

**KEYWORDS** nuclear quadrupole resonance, data analysis, artificial intelligence, artificial neural networks, intelligent system.

## I. INTRODUCTION

The method of nuclear quadrupole resonance (NQR) is based on the absorption of radiofrequency energy due to changes in the orientation of the nuclear quadrupole moments in a non-uniform electric field created by external charges relative to the nucleus. Quadrupolar energy levels in a solid arise from the interaction of nuclear quadrupole moments with the electric field gradient at the resonating nucleus location; therefore, the NQR spectrum reflects the distribution of electron density near a specific atom. This is what makes the NQR method unique in the study of subtle structural features of chemical compounds.

Unlike nuclear magnetic resonance, NQR does not require the application of an external magnetic field, enabling the development of more compact instruments suitable for field measurements. This feature expands the applicability of the method in environments where magnetic fields are impractical or technically challenging, such as in security systems for detecting explosives and narcotic substances in non-metallic containers [1].

Pulsed NQR techniques, particularly Fourier spectroscopy, allow the analysis of small-mass samples from fractions of a gram which makes them attractive for applied analysis. Modern NQR signal processing methods aim to increase detection sensitivity and improve the accuracy of spectral analysis [1]. However, low signal-to-noise ratio (SNR) and the high sensitivity of NQR signals to external factors such as temperature, mechanical

vibrations, and crystal lattice defects significantly complicate their reliable detection under field conditions [1, 2]. This creates additional challenges for stable measurements and especially hinders the construction of compact, energy-efficient spectrometers, where the stability and sensitivity of hardware components must be maintained regardless of environmental variations.

Over the past few decades, a wide range of NQR signal processing methods have been developed. Among them, traditional algorithms – fast Fourier transform (FFT), wavelet transform, adaptive filtering – play a key role in the preprocessing stage and spectral analysis [3, 4]. At the same time, the growth in computational capabilities has increased interest in applying Machine Learning (ML) methods, particularly deep neural networks – Convolutional Neural Networks (CNNs), Recurrent Neural Networks (RNNs), autoencoders, and transfer learning technologies [5].

The aim of this review is to systematize both traditional and modern approaches to NQR signal processing, analyze their advantages and limitations, and substantiate the potential for combining methods to improve the efficiency of spectroscopic analysis.

## II. OVERVIEW OF NQR SIGNAL PROCESSING METHODS

**A. Traditional approaches to NQR signal processing.** Traditional methods for processing NQR signals form the foundation for the primary analysis of experimental data and laid the groundwork for modern automated systems.

Their main objective is to improve the SNR, identify frequency components, suppress interference, and restore the informative part of the signal. Since free induction decay (FID) signals are typically short and nonstationary, the effectiveness of algorithms largely depends on their ability to capture both temporal and spectral features simultaneously.

One of the most common techniques is the FFT, which enables conversion from the time to frequency domain for spectral analysis. FFT offers high computational efficiency and real-time data processing capability. However, its limitations become apparent when dealing with short or noisy signals, where time-localized spectral analysis is required [3].

To overcome these limitations, wavelet transform methods have been introduced, allowing for multilevel signal analysis with simultaneous localization in both time and frequency domains. Wavelet-based techniques have proven particularly effective in processing weak or distorted NQR echoes by enabling clear detection of spectral variations over short time intervals [4]. Among the effective modern modifications, the WICAML algorithm stands out as an interference-resistant method based on Gabor-Morlet wavelet analysis. It enables the estimation of the time-frequency structure of disturbances and suppresses components with varying amplitude and phase without distorting the resonance response [6]. A comparative evaluation of WICAML with other preprocessing techniques is shown in Fig. 1.

Another important category includes adaptive filtering methods that suppress noise components while preserving the informative content of the signal. For example, the Wiener filter minimizes the mean square error between the observed and estimated signals. The multistage Wiener filter avoids computationally intensive matrix inversion while maintaining effective interference suppression. The Kalman filter performs well under dynamic conditions or limited a priori knowledge of the signal model. Fig. 2 presents the results of Kalman filtering evaluated under two scenarios: direct estimation of the NQR signal and indirect estimation through noise modeling. The results demonstrate high adaptability, although the accuracy strongly depends on the quality of the training data and covariance matrices [7].

One critical external factor influencing NQR signal parameters is ambient temperature. Temperature fluctuations cause resonance frequency drift, which may shift the spectrum beyond detection range. To address this, [8] proposed a frequency scanning method within a  $\pm 2$  kHz range around the excitation frequency, effectively compensating for temperature variations up to  $\pm 16$  K. This approach ensures stable signal detection without complex thermal control, which is crucial for portable NQR systems.

Traditional approaches offer a high degree of interpretability, algorithmic stability, and simplicity of hardware implementation, making them suitable for systems with limited computational resources. However, their primary limitations include poor robustness under complex interference conditions, limited generalizability to atypical signals, and the need for manual parameter

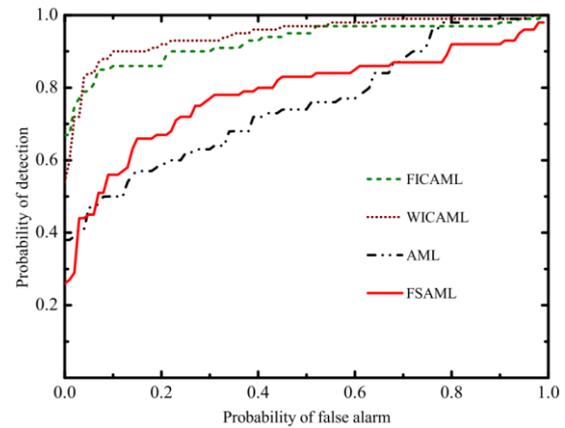


FIG. 1. ROC curve for the WICAML interference suppression method compared to other preprocessing techniques [6].

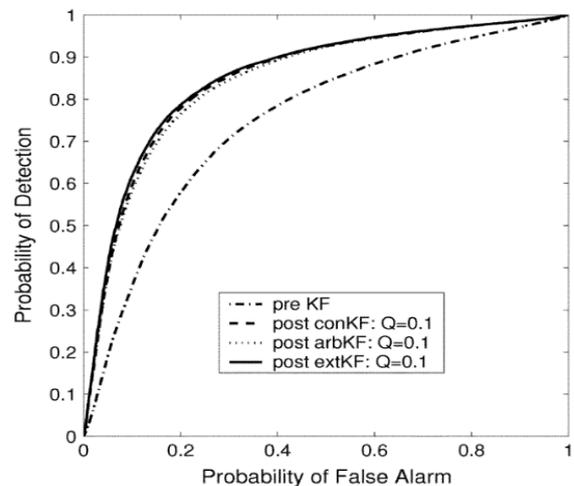


FIG. 2. ROC curves comparing Kalman filter configurations: no filter, standard, correlated-noise-adapted, and autoregressive-model-based filters [7].

tuning for each specific task [2]. These shortcomings have driven growing interest in more adaptive machine learning-based signal processing methods that can automatically extract meaningful features even under high noise levels.

**B. Statistical and spectral methods.** One of the key objectives in NQR signal analysis is accurate localization of spectral components, which is especially challenging under low SNR conditions, frequency component overlap, or limited FID signal duration. In such cases, traditional Fourier-based methods often exhibit insufficient spectral resolution, necessitating the use of high-precision spectral estimation techniques.

Among the most effective approaches is the Approximate Maximum Likelihood (AML) algorithm, which optimizes the estimation of sinusoidal signal parameters by maximizing a likelihood criterion under practical constraints. Advanced versions of this method that account for noise correlation and structural signal properties can significantly improve estimation accuracy in high-noise environments [4]. In particular, [9] demonstrated that modeling exponential spin echo decay improves signal detectability under severe noise. Fig. 3 presents experimental comparisons of enhanced AML algorithm variants.

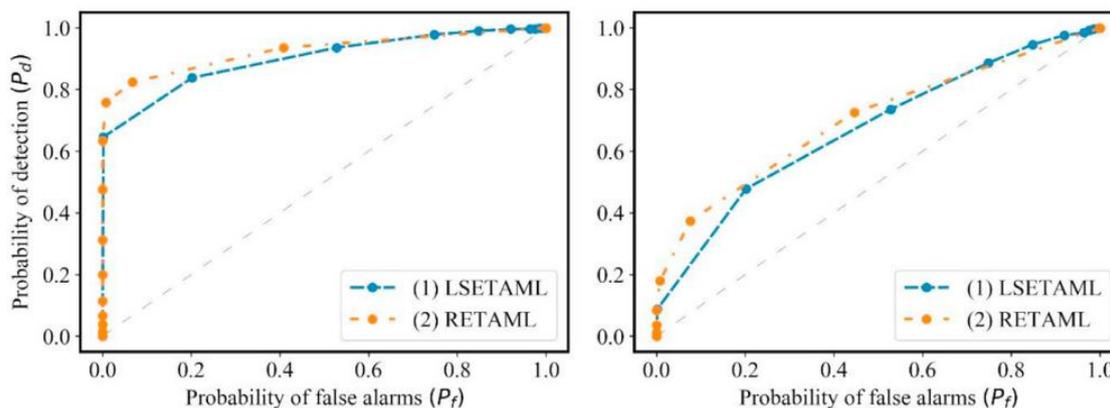


FIG. 3. ROC curves for enhanced AML algorithms: (1) LSETAML; (2) RETAML, tested on noisy data with SNR = -30 dB (left) and -35 dB (right) [4].

When the shape of the target signal is known a priori, matched filtering can be used to amplify components corresponding to a reference template while suppressing noise. This approach is widely employed in detection systems for explosives and narcotics, where high sensitivity is required even under strong noise [3]. In [7], a two-stage adaptive filtering scheme based on the Kalman filter is proposed for both direct and indirect estimation configurations. In indirect mode, the background noise is modeled as the system state, while the NQR echo is treated as an observed noisy output. This enables adaptive signal separation even under significant thermal drift and low SNR, thereby opening the door to combining statistical techniques with preliminary filtering in spectral analysis tasks.

A notable contribution to improved spectral resolution comes from subspace methods, particularly Multiple Signal Classification (MUSIC) and Estimation of Signal Parameters via Rotational Invariance Techniques (ESPRIT). These approaches rely on separating the signal and noise subspaces using eigenvalue decomposition of the covariance matrix, allowing precise frequency estimation even in the presence of overlapping components [4]. The MUSIC method provides high frequency resolution but requires prior knowledge of the number of spectral components, while ESPRIT is more noise-resilient and computationally efficient.

To enhance spectral analysis stability under fluctuating noise and complex signal structure, nonparametric techniques such as Capon-APES Average (CAPA) and its improved version Echo Train Capon-APES Average (ETCAPA) are also applied. ETCAPA allows estimating the structure of echo trains in NQR signals using stepwise adaptive smoothing of amplitude-time characteristics, making it an effective method for processing multicomponent responses in complex experimental conditions [4].

Despite their strengths, high-resolution spectral estimation methods have several limitations. They demand significant computational resources, are sensitive to noise modeling errors, and require thorough signal preprocessing to ensure stable performance. In portable or resource-constrained NQR systems, these limitations hinder widespread adoption due to the high computational cost and the need for precise hardware calibration [2].

**C. Machine learning-based methods for NQR signal processing.** The development of ML techniques, particularly deep learning, has opened new opportunities for analyzing complex and noisy NQR signals. Unlike traditional algorithms, ML methods are capable of automatically extracting informative features, adapting to data-specific characteristics, and providing high generalization performance without manual parameter tuning.

One of the most widely used approaches is the application of CNNs architectures, which have demonstrated strong capabilities in identifying essential features even in high-noise conditions. These networks effectively handle short and unstable FID signals – typical of NQR – and adapt flexibly to different types of input data without requiring complex preprocessing. Architectures such as AlexNet, LeNet-5, and hybrid CNN-LSTM models have shown strong performance in NQR signal classification tasks, achieving substance detection accuracy above 98 % [5]. Fig. 4 illustrates the ROC curve for one of the convolutional network architectures.

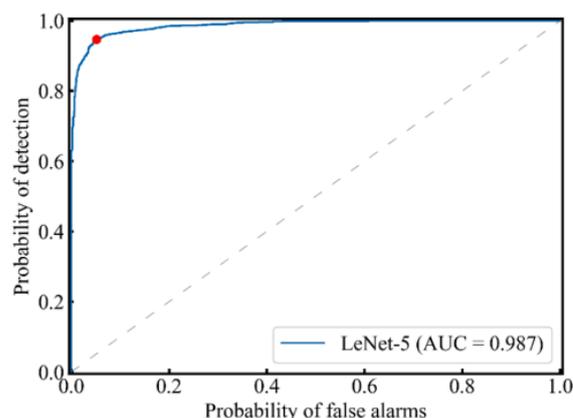


FIG. 4. ROC curve for a neural network based on the LeNet-5 architecture, evaluated on a prepared dataset of 20,000 NQR signals [5].

A convolutional neural network was used for NQR signal classification under challenging conditions. The authors reported an accuracy of 95 % for substance detection at a SNR of -15 dB on a training dataset of 4,000 NQR signals. However, the accuracy declined rapidly at SNR = -20 dB, though it still outperformed other considered approaches. This trend is shown in Fig. 5.

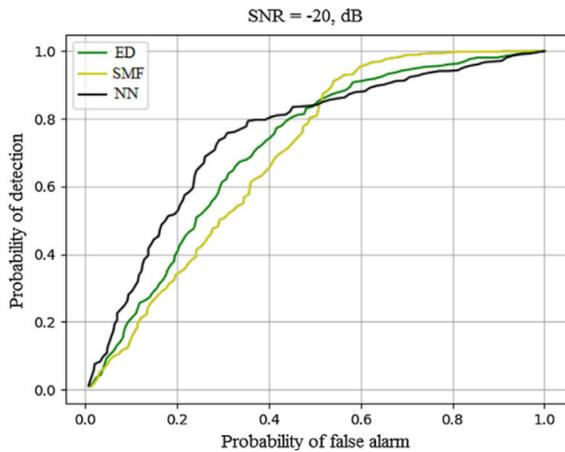


FIG. 5. ROC curve for a neural network evaluated at an SNR of -20 dB.

In [4], four machine learning models were compared in the context of NQR signal classification under noisy conditions. Figures 6 and 7 show the ROC curves for the evaluated methods: k-nearest neighbors (k-NN), support vector machines (SVM), a fully connected neural network (NN), and an ensemble classifier (EC). The ensemble method achieved the highest detection accuracy in severely noisy environments, with SNR values down to -45 dB and temperature variation of 10 K.

Another promising approach involves autoencoders – neural networks trained to compress and reconstruct input data with minimal loss. Owing to their ability to preserve essential signal characteristics while suppressing noise, autoencoders have proven effective in processing images

and time-series data [10]. Adapting these techniques for NQR signals offers a promising path toward improving sensitivity in subsequent spectral analysis stages.

Transfer learning is another avenue that enables reusing models pre-trained on related tasks, followed by fine-tuning on NQR-specific data. This approach significantly reduces the amount of required training data without compromising accuracy [5].

For tasks requiring the modeling of temporal dependencies, RNNs, particularly Long Short-Term Memory (LSTM) architectures, are appropriate. When combined with CNNs, these models can capture both spatial and temporal dependencies in NQR signals, which significantly enhances reconstruction and classification performance [5].

Furthermore, combining neural network architectures with stochastic resonance mechanisms offers additional benefits. In [11], it was shown that employing stochastic resonance together with artificial neural networks enables the detection of ultra-weak NQR signals even under strong noise conditions. As shown in Fig. 8, neural-network-based methods outperform conventional approaches in high-noise experimental scenarios.

Despite these advantages, deep learning techniques face several challenges: high computational requirements, the need for large volumes of quality training data, and difficulties in result interpretation. As a response, explainable machine learning is gaining traction, aiming to enhance model transparency in critical applications such as security and medical diagnostics [5].

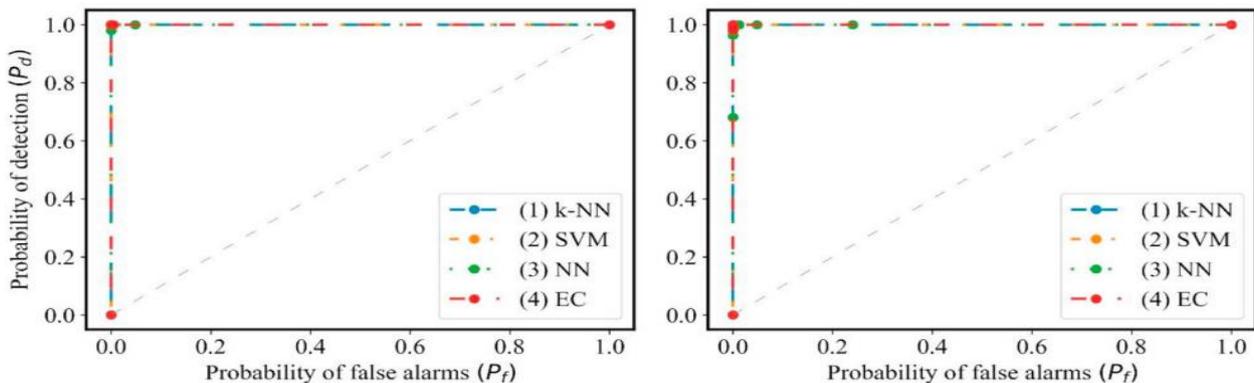


FIG. 6. ROC curves for classification algorithms at SNR = -30 dB (left) and -35 dB (right) [4].

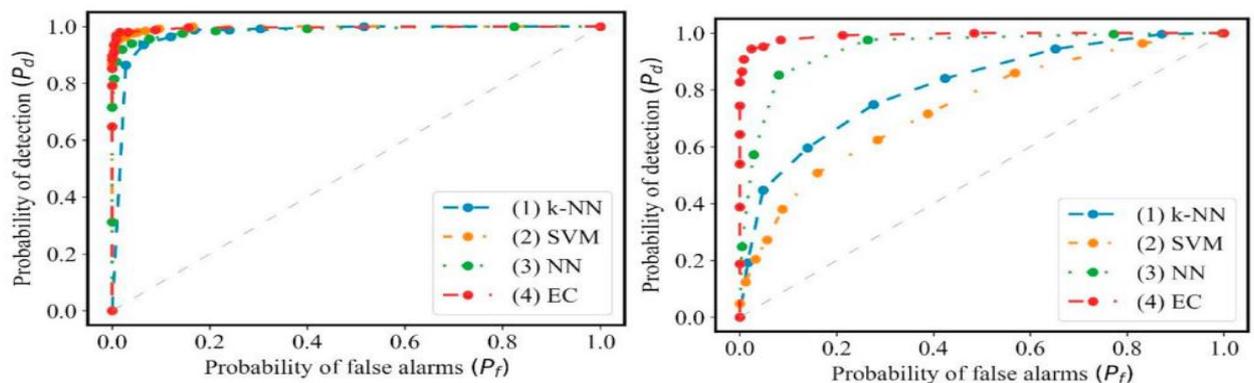


FIG. 7. ROC curves for classification algorithms at SNR = -45 dB (left) and at SNR = -45 dB with a temperature variation of 10 K (right) [4].

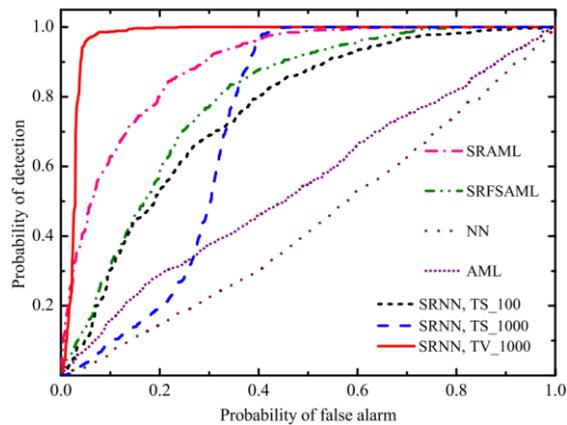


FIG. 8. ROC curves for stochastic resonance-based methods under experimental conditions with SNR = -38 dB [11].

### III. COMPARATIVE ANALYSIS OF EXISTING NQR SIGNAL PROCESSING METHODS AND THEIR LIMITATIONS

The comparison of NQR signal processing methods should be based on several key criteria: the ability to detect weak signals under low SNR conditions, robustness to interference, consideration of the signal's temporal structure, generalizability of results, and computational resource requirements.

Traditional methods, such as FFT and wavelet transform, are fast, easy to implement, and well-suited for preliminary data processing. They perform adequately under moderate noise levels but struggle with short or heavily corrupted signals, as they do not always allow accurate localization of frequency changes over time [3].

Adaptive methods, including Wiener and Kalman filters, offer better performance in non-stationary noise environments and help preserve the core signal content. As noted in [4], these filters are especially effective under unstable conditions; however, their performance depends heavily on the quality of initial estimates and they typically do not provide high spectral resolution in complex scenarios.

High-resolution spectral estimation methods such as MUSIC and ESPRIT are capable of identifying frequency components even in the presence of overlapping spectra and low SNR down to -20 dB [4]. These techniques are well-justified in applications requiring high precision, but they demand significant computational resources and careful calibration of the hardware setup.

ML approaches, particularly artificial neural networks, exhibit strong noise robustness and high detection accuracy for NQR signals. Although the training phase can be computationally intensive, once trained, these models operate rapidly and efficiently. Studies [5, 11] have shown that deep neural networks can reliably detect NQR signals in extremely noisy conditions, with SNR as low as -40 dB – well beyond the effective range of traditional techniques.

In summary, none of the analyzed approaches is universally optimal: traditional and adaptive methods offer speed and stability at moderate noise levels, while high-resolution spectral methods ensure precision under more demanding conditions but at the cost of higher

computational requirements. ML methods yield the best results in highly noisy environments, although their deployment is constrained by the need for large labeled datasets and challenges related to model interpretability. In this context, hybrid approaches that combine the strengths of different techniques and can adapt to varying operational conditions appear to be the most promising for robust and efficient NQR signal analysis.

### IV. FUTURE DIRECTIONS IN NQR SIGNAL PROCESSING METHODS

The processing of NQR signals remains a complex challenge due to the short duration of signals, high sensitivity to noise, and instability of signal parameters under changing environmental conditions. Despite the wide range of available methods – from classical spectral analysis to deep neural networks – none alone provides an optimal combination of accuracy, adaptability, and computational efficiency. This issue becomes even more critical when attempting to scale such solutions for portable or resource-constrained systems.

Most existing NQR systems are optimized for narrow laboratory tasks, such as detecting a single target substance under stable conditions [2]. These systems are generally ineffective in complex, multicomponent environments, where detection accuracy significantly deteriorates due to spectral overlap and fluctuating background noise. Moreover, in many cases, the results are difficult for users to interpret, which limits adoption in critical fields such as security screening and pharmaceutical quality control.

A promising direction involves the development of adaptive hybrid architectures that integrate classical preprocessing methods (e.g., wavelet analysis or matched filtering) with the powerful classification and signal reconstruction capabilities of neural networks. Combined models – particularly those incorporating CNNs and LSTM architectures – have already demonstrated strong potential in low-SNR scenarios [12].

Special attention should also be given to the creation of open and representative training datasets, which would help standardize ML model training and improve reproducibility across research studies. The current lack of sufficiently large and diverse NQR data corpora remains a significant bottleneck to the advancement of deep learning in this field [9].

Another important avenue is the integration of explainable machine learning, aimed at improving model transparency in high-stakes applications. In safety, medical, or quality control settings, it is crucial not only to obtain accurate predictions but also to understand the reasoning behind them. Explainable approaches can help visualize the key signal features that influence classification outcomes and enhance user trust in automated decisions.

In conclusion, the future of NQR signal processing lies in holistic solutions that combine algorithmic precision, interpretability, and computational efficiency – capable of adapting to the complex and unpredictable conditions of real-world applications.

## V. CONCLUSION

This paper presents a systematic review of signal processing methods for nuclear quadrupole resonance. We compared the capabilities of classical approaches – such as fast Fourier transform, wavelet analysis, and adaptive filtering – with state-of-the-art machine learning-based algorithms. Each group of methods was evaluated in terms of noise robustness, adaptability, computational complexity, and generalization capabilities.

Special attention was paid to the practical application of nuclear quadrupole resonance systems, particularly their performance under real-world conditions, where signals often exhibit low signal-to-noise ratios and unstable structural characteristics. It was shown that deep neural network-based methods can achieve high accuracy even in extremely noisy environments, significantly outperforming classical algorithms.

At the same time, it was emphasized that most existing solutions remain limited in scope, often tailored to detecting specific substances under laboratory conditions. This highlights the need for further development of adaptive systems capable of handling a broader range of signals across diverse environments.

Looking ahead, it is advisable to integrate classical preprocessing techniques with modern neural network architectures, improve model interpretability, and build open-access training datasets. These steps will significantly expand the practical applicability of nuclear quadrupole resonance technology.

## AUTHOR CONTRIBUTIONS

S.H., A.S. – conceptualization, methodology, investigation, writing (original draft preparation), writing (review and editing).

## COMPETING INTERESTS

The authors declare no conflict of interest.

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# Огляд методів оброблення та аналізу сигналів ядерного квадрупольного резонансу

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**АНОТАЦІЯ** У статті представлено структурований і комплексний огляд методів оброблення та аналізу сигналів ядерного квадрупольного резонансу (ЯКР) з акцентом на їхню ефективність в умовах реального середовища, де вимірювані сигнали, як правило, є слабкими, зашумленими та високочутливими до впливу зовнішніх чинників. Розглянуто класичні підходи, зокрема аналіз Фур'є, вейвлет-перетворення, адаптивну й узгоджену фільтрацію, а також методи спектрального оцінювання високої роздільної здатності, які застосовуються для підвищення завадостійкості та точності локалізації частотних компонентів. Окрему увагу приділено сучасним методам машинного навчання, включно з глибокими нейронними мережами та гібридними архітектурами, здатними автоматично виокремлювати інформативні ознаки сигналів і демонструвати високу ефективність за низьких відношень сигнал/шум. Кожну групу методів проаналізовано за сукупністю практично важливих критеріїв, зокрема шумостійкістю, обчислювальною складністю, адаптивністю до нестационарних умов, чутливістю до зміни параметрів сигналу та придатністю для реалізації у портативних або обмежених за ресурсами ЯКР-системах. У межах огляду також окреслено ключові проблеми сучасних досліджень у галузі ядерного квадрупольного резонансу, серед яких відсутність стандартизованих і репрезентативних навчальних наборів даних, обмежена інтерпретованість моделей машинного навчання, а також складність упровадження обчислювально затратних алгоритмів у компактні вимірювальні комплекси. Показано, що жоден із розглянутих підходів не забезпечує універсального рішення для всіх умов експлуатації та прикладних задач. Найперспективнішим напрямом розвитку є створення гібридних підходів, що поєднують класичні методи попередньої обробки сигналів із можливостями машинного навчання. Проведений аналіз формує методологічну основу для обґрунтованого вибору та проектування надійних і адаптивних ЯКР-систем, орієнтованих на практичне застосування у сфері безпеки, аналізу матеріалів та ідентифікації хімічних сполук у складних умовах.

**КЛЮЧОВІ СЛОВА** ядерний квадрупольний резонанс, аналіз даних, штучний інтелект, штучні нейронні мережі, інтелектуальна система.



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