

Perspective

Paradigm shift in nuclear magnetic resonance relaxation spectra inversion: The relay and integration of regularization, machine learning, and quantum computing

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Abstract:

Nuclear magnetic resonance technology has been widely applied in deep geo-energy fields, including deep earth oil and gas exploration, geothermal resource exploration, carbon dioxide geological sequestration, and underground hydrogen storage. The reliability of these applications is directly affected by the accuracy of nuclear magnetic resonance relaxation spectra inversion. However, the inverse problem is inherently ill-posed and therefore the effective inversion strategy with appropriate constraints is required. The evolution of nuclear magnetic resonance relaxation spectra inversion has been marked by three major methodological milestones. The classical regularization method, exemplified by Tikhonov regularization, establishes the mathematical foundation; the machine-learning approach, particularly deep neural networks, is reshaping the computational paradigm; and the quantum computing offers a forward-looking avenue for fundamentally overcoming the computational-complexity bottleneck associated with inversion. This work emphasizes that the three paradigms are not characterized by simple linear replacement, but rather by the succession and integration. Each generation builds on its predecessor and extends the boundaries of nuclear magnetic resonance inversion. Specifically, regularization provides mathematical rigor, machine learning enables data-driven adaptability, and quantum computing may unlock fundamental computational speedups. This perspective systematically describes this evolutionary trajectory and discusses future directions for the integration of these paradigms.

1. Introduction

Nuclear magnetic resonance (NMR) relaxation analysis has become a core technique for characterizing porous media in the field of energy geoscience. Whether applied to high precision core analysis at the laboratory or NMR logging in the complex downhole environment, one of the key steps in the technical workflow remains essentially the same, i.e., NMR relaxation inversion. NMR relaxation spectra are recovered from the time domain echo data through mathematical inversion, from which the key reservoir physical and chemical properties,

including porosity, permeability, saturation, oil viscosity, and pore structure (Guo et al., 2026a; Guo et al., 2026b), are subsequently extracted. Mathematically, this problem can be rigorously formulated as a Fredholm integral equation of the first kind. It involves applying the inverse Laplace transformation to multiexponential decay signals and represents a typical linear inverse problem (Ahola et al., 2015).

However, the inversion process is inherently ill-posed: weak random noise in the measured data may cause the inverted NMR relaxation spectra to exhibit severe nonphysical

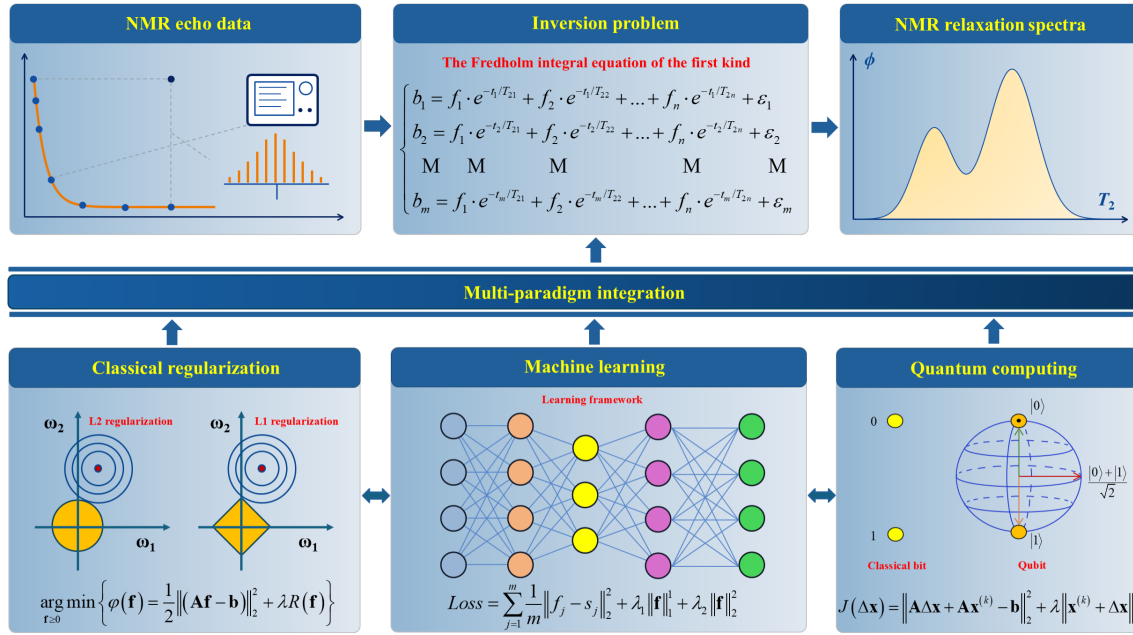


Fig. 1. NMR relaxation spectra inversion framework and the relationships among the classical regularization, machine learning, and quantum computing.

oscillations, multiple spurious peaks, or peak shifts. In the extreme cases, the inversion results may become entirely unsuitable for geological interpretation (Lamanna, 2005; Guo et al., 2026; Guo et al., 2018). Therefore, the performance of the inversion algorithm directly determines the reliability and accuracy with which NMR transforms raw data into reservoir information, making it a challenge in this field for decades.

The development of NMR relaxation spectra inversion reveals a clear evolution across three technique paradigms: the classical regularization, machine learning, and the emerging quantum computing. Fig. 1 shows that a framework of principles for NMR relaxation spectra inversion and illustrates the relationships among the three categories of inversion algorithms. It should be noted that these paradigms are not characterized by simple linear replacement, but rather by the succession and integration (Arridge et al., 2019). The path of integration is expected not only to drive transformative advances in geophysical exploration but also to enable new breakthroughs in the NMR logging evaluation of complex reservoirs, including deep earth oil and gas reservoirs, geothermal reservoirs, and gas hydrate deposits.

2. Classical regularization method: The mathematical foundation for solving ill-posed problems

The regularization provides the most mature theoretical framework for addressing ill-posed inverse problems. The core strategy is to incorporate prior constraints, such as smoothness, nonnegativity, and spectral sparsity, into the objective function, thereby suppressing the strong sensitivity of the solution to noise. With an appropriate selection of the regularization parameter, the regularization method achieves a balance between

data fitting accuracy and solution stability. To date, it remains the most widely adopted and extensively validated inversion technique in industrial applications and engineering practice.

A representative classical method for NMR relaxation spectra inversion is the Tikhonov regularization. It employs an L_2 norm penalty term in the residual minimization objective to impose a smoothness constraint on the solution. The degree of smoothing is controlled by the regularization parameter (Butler et al., 1981). The commonly used regularization parameter selection strategy includes the S-curve method, the L-curve method, and generalized cross-validation (GCV) etc. It is noted that the regularization parameter affects the inversion results. Specifically, an excessively low regularization parameter increases the sensitivity of the solution to noise and compromises the stability, whereas an excessively large parameter causes over-smoothing and a consequent loss of the spectral resolution.

To address these limitations, various improved regularization strategies have been developed. For example, L_1 regularization imposes an L_1 -norm constraint to promote the spectra sparsity. Another strategy incorporates the maximum entropy criterion, leading to maximum entropy regularization that is well suited to data with a low signal to noise ratio (SNR). Furthermore, two different norms have been combined to construct a double regularization model, thereby achieving a better balance between sparsity and smoothness (Guo et al., 2018).

In a word, the regularization method is supported by a well-established theoretical framework and a clear mathematical and physical basis, while offering strong physical interpretability and relatively high computational efficiency. Nevertheless, their inherent limitations should not be overlooked. The selec-

tion of the regularization parameter may involve a degree of subjectivity, and the inversion results may become unstable when the SNR is low. In addition, predefined smoothness constraints may oversimplify the complex structure of the actual NMR relaxation spectra, obscuring minor spectra peaks or boundary features and consequently reducing the fine level in geological interpretation.

3. Machine learning method: A new data-driven paradigm

In recent years, machine learning, particularly deep learning, has driven a significant paradigm shift in NMR relaxation spectra inversion. In contrast to the conventional regularization strategy that relies on the designed mathematical constraints, the machine learning method learns the mapping between echo signal and relaxation spectra directly from a large dataset, without being restricted by predefined assumptions of smoothness or sparsity.

This transformation has been driven by three main factors. First, the large volumes of data accumulated from NMR logging and core experiments provide a substantial training basis for supervised learning. Second, the powerful nonlinear approximation capability of deep learning enables complex implicit relationships between echo trains and relaxation spectra to be effectively captured. Finally, the computational efficiency of neural networks during the inference stage is substantially higher than that of traditional iterative inversion, thereby providing feasible support for real-time well-logging interpretation.

Machine learning has recently achieved several notable milestones in this field. The research group of Professor Zhong Chen at Xiamen University proposed an uncertainty-aware deep learning method for Laplace NMR spectra reconstruction (Chen et al., 2025). The method employs a dual-branch network architecture and, for the first time, integrates uncertainty estimation into the reconstruction process while producing high-quality spectra. Consequently, the inversion results can not only be interpreted but also be accompanied by quantitative estimates of their reliability. This development marks a transition in deep learning for NMR inversion from black-box prediction to trustworthy reconstruction. Luo et al. (2025) proposed a lightweight multiscale neural network specifically designed for NMR relaxation data in porous media. It substantially reduces computational cost while maintaining inversion accuracy, demonstrating considerable potential for practical applications.

The machine learning method possesses several advantages, including rapid inference once trained, no requirement for explicitly constructed regularization terms, and the ability to learn mapping relationships adaptively from the training data. However, their limitations are equally evident. Their generalization performance depends strongly on the coverage of the training data, while their limited interpretability may lead to unreliable predictions when they are applied beyond the training. The current research therefore focuses on integrating data-driven approaches with physical priors to achieve both computational efficiency and robustness, as exemplified by the

introduction of physics-informed neural networks (PINNs).

4. Quantum computing: A future breakthrough in inversion?

If the introduction of machine learning represents an order-of-magnitude advance in inversion algorithms, quantum computing may bring about a paradigm-level revolution. Although the direct application of quantum computing to NMR relaxation spectra inversion remains at a very early exploratory stage, the potential impact is worthy to evaluate.

Quantum computing and NMR techniques share a deep and intrinsic connection. NMR is one of the earliest physical platforms for quantum information processing, in which nuclear spins serve as qubits and are manipulated by radiofrequency pulses to implement quantum gate operations. This reciprocal relationship offers a unique perspective, namely that NMR can not only provide a physical platform for quantum computing but may also benefit from the powerful computational capabilities of quantum computing in signal processing. They both create a mutually reinforcing cycle.

From the perspective of inversion computation, quantum computing may offer fundamental breakthroughs in two respects. The first is exponential speedup (Harrow et al., 2009). NMR relaxation spectra inversion involves large-scale matrix operations and iterative optimization, whose computational cost on a classical computer increases rapidly with problem size, such as the number of sampling points and echoes. A low-rank matrix approximation based on quantum singular value decomposition has the potential to achieve exponential speedup for a few certain subproblems (Ilmavirta et al., 2025). The second is enhanced global optimization capability. The inversion is essentially a constrained nonlinear optimization problem and is therefore highly susceptible to local optima. By exploiting quantum tunneling to efficiently traverse the energy landscape, quantum annealing algorithms may significantly improve the ability to escape local traps and approach the global optimum.

There is some preliminary evidence of the practical quantum computing potential for solving the inverse problem. Maletín et al. (2025) solved the 1D acoustic approximation seismic inversion problem on a hybrid quantum-classical annealer, demonstrating its feasibility on larger-scale problems. Wang and Wen (2025) proposed an iterative quantum annealing inversion algorithm for seismic data processing. Compared with the classical method, this algorithm achieved a similar accuracy in both linear and nonlinear tomography experiments. It provides a strong support for the practical application of quantum computing in field of the geophysical inversion.

However, a substantial gap remains between theoretical feasibility and practical implementation. The number of fault-tolerant qubits and their coherence times remain fundamental bottlenecks. For NMR relaxation spectra inversion in energy geoscience, the application of quantum computing is still at an early exploratory stage. Nevertheless, given the inherent ill-posedness and computational complexity of the inversion problem, quantum computing undoubtedly represents a frontier research direction that warrants sustained attention.

5. Conclusion and prospect

From the Tikhonov regularization to deep neural networks and, more recently, to the emerging quantum computing approaches, the evolution of NMR relaxation spectra inversion reflects the broader trajectory of computational science. This progression extends from manually designed constraints in regularization, through constraints learned from data in machine learning, to quantum enabled breakthroughs beyond classical computational constraints. Each step marks a significant advance in how the ill-posedness of inversion is addressed.

However, the central argument of this perspective is that these three paradigms are not characterized by simple linear replacement, but rather by “succession and integration”. Regularization contributes mathematical rigor, enabling inherently ill-posed inversion problems to be solved stably within a classical framework. Machine learning introduces data-driven adaptability, and it moves inversion from “manual parameter tuning” toward “automatic learning”. Quantum computing, in turn, holds the potential to unlock computational speedups rooted in physical principles, thereby making problems with exponential computational complexity potentially tractable.

The future direction lies not in “trade-offs” among the three, but in their “synergy”. Physics-informed neural networks (PINNs) embed the physical priors embodied in regularization into deep learning architectures, thereby enhancing the interpretability of neural networks. Hybrid quantum-classical algorithms integrate quantum acceleration modules with a classical optimization procedure, gradually moving toward practical implementation. Learnable regularizers, meanwhile, incorporate data-driven principles into regularization theory, allowing constraints to evolve from fixed, predefined forms to adaptive, learned ones. These frontier explorations of cross-paradigm integration are no longer merely theoretical concepts but are beginning to define the practical landscape of the next generation of NMR relaxation spectra inversion.

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Conflicts of interest

The authors declare no competing interest.

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