Quantum Spectral Unmixing: Emerging Directions in Hyperspectral Image Unmixing

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Abstract*—Spectral unmixing (SU) aims to decompose mixed hyperspectral pixels into constituent endmember signatures and their corresponding fractional abundances, enabling material identification at sub-pixel resolution. Conventional SU methodologies, comprising dimensionality reduction, endmember extraction, and abundance estimation, have achieved significant progress; however, their performance remains constrained by nonlinear mixing effects, spectral variability, and the increasing computational complexity associated with high-dimensional hyperspectral data. Recent advances in quantum computing offer promising computational paradigms for addressing these challenges through quantum principal component analysis (QPCA), quantum kernel methods, and variational quantum algorithms (VQAs), particularly within hybrid quantum–classical optimization frameworks designed for Noisy Intermediate-Scale Quantum (NISQ) devices. This review systematically examines the evolution of spectral unmixing from classical to emerging quantum paradigms by establishing a stage-wise correspondence between conventional SU operations and their quantum counterparts. Furthermore, it critically discusses the theoretical foundations, computational advantages, practical implementation challenges including quantum data encoding, Quantum Random Access Memory (QRAM) assumptions, hardware noise, and reproducibility and outlines future research directions toward scalable, transparent, and reproducible quantum spectral unmixing frameworks for next-generation hyperspectral remote sensing applications.

Keywords— hyperspectral imaging, spectral unmixing, endmember extraction, abundance estimation, quantum machine learning, variational quantum algorithms, hybrid optimization.

I. INTRODUCTION

Hyperspectral and multispectral imaging sensors often capture mixed pixels, where the recorded spectrum represents a combination of multiple surface materials within a single pixel. Spectral unmixing (SU) addresses this problem by decomposing the observed spectrum into the spectral signatures of the constituent materials, known as endmembers, and estimating their corresponding abundance fractions. This enables material identification at the sub-pixel level and has become an essential component of numerous remote sensing applications, including mineral exploration, precision agriculture, urban monitoring, environmental forensics, disaster assessment, and ecosystem monitoring [1], [2].

For many years, the Linear Mixing Model (LMM) has been the predominant framework for spectral unmixing. It assumes that each observed pixel can be represented as a weighted linear combination of endmember spectra while satisfying the abundance non-negativity and sum-to-one constraints [3]. Although this assumption simplifies the unmixing process and provides physically interpretable results, it is often insufficient for real-world scenarios. In practice, multiple scattering, intimate material mixtures, atmospheric effects, varying illumination conditions, sensor noise, and terrain-induced spectral variability introduce nonlinear interactions that cannot be adequately represented by a simple linear model. Consequently, a wide range of extended linear models, nonlinear mixing models, sparse representation techniques, and, more recently, deep learning-based approaches have been developed to improve unmixing performance under complex imaging conditions [4-8].

The progression of these methodologies, from conventional linear models to modern data-driven and quantum-inspired approaches, is summarized in Figure 1. Despite these methodological advances, spectral unmixing remains computationally intensive, particularly for contemporary hyperspectral datasets containing hundreds of spectral bands and millions of pixels. Core processing stages including dimensionality reduction, endmember extraction, abundance estimation, and optimization incur substantial computational costs as data volume increases, making large-scale and near real-time analysis a persistent challenge. These computational limitations have motivated the exploration of quantum computing as a potential alternative, where quantum

algorithms are investigated as counterparts to key stages of the classical spectral unmixing pipeline.

Rather than replacing the conventional spectral unmixing workflow, quantum computing seeks to accelerate or enhance specific computationally intensive stages through quantum algorithms and optimization techniques. Establishing a correspondence between classical processing stages and their emerging quantum counterparts provides a systematic framework for understanding current research trends and identifying potential computational advantages. A conceptual comparison of the conventional and quantum spectral unmixing workflows is presented in Figure 2, highlighting the relationship between corresponding processing stages and illustrating the motivation for quantum-enabled spectral unmixing.

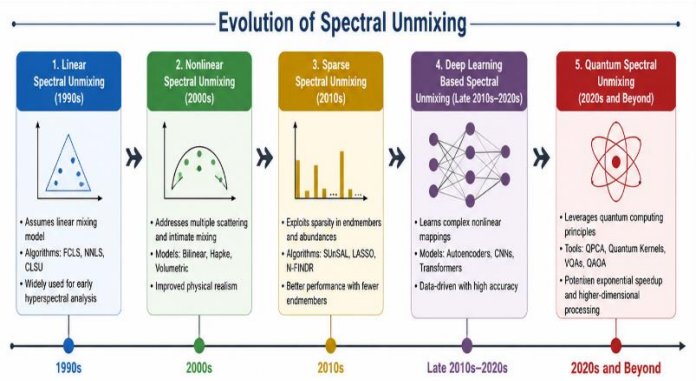


Figure 1 Evolution of spectral unmixing methodologies from conventional linear models to quantum-enabled computational approaches

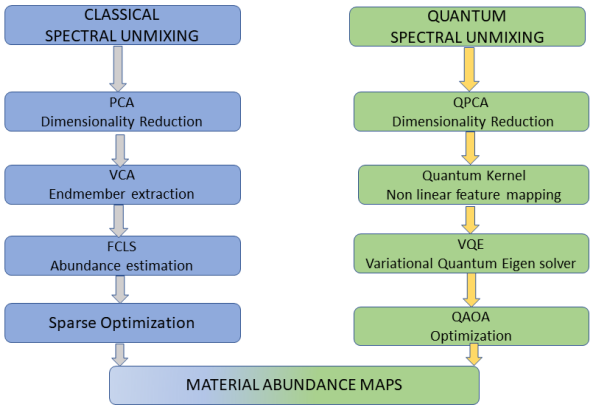


Figure 2 Classical Spectral Unmixing Vs Quantum Spectral Unmixing

In recent years, quantum computing has attracted considerable attention as a potential solution to computationally intensive problems in machine learning and data analysis. By exploiting quantum mechanical principles such as superposition, entanglement, and interference, quantum algorithms have the potential to accelerate several linear algebra operations that form the basis of many spectral unmixing techniques. Emerging approaches, including Quantum Principal Component Analysis (QPCA), quantum kernel methods, and Variational Quantum Algorithms (VQAs), have shown promise for dimensionality reduction, nonlinear feature representation, and optimization within hybrid quantum - classical frameworks designed for Noisy Intermediate-Scale Quantum (NISQ) devices [9-12]. Although these methods are still at an early stage of development, they provide an interesting direction for addressing some of the computational limitations of classical spectral unmixing.

While a number of review articles have discussed either hyperspectral spectral unmixing or quantum machine learning, relatively few have examined how quantum computing can be integrated across the complete spectral unmixing pipeline. Questions related to quantum data encoding, Quantum Random Access Memory (QRAM), hardware limitations, reproducibility, and benchmark datasets remain largely unexplored in the context of remote sensing, leaving several important research challenges open.

Motivated by these observations, this review brings together the foundations of classical spectral unmixing and the latest developments in quantum computing to provide a comprehensive overview of Quantum Spectral Unmixing (QSU). The review first revisits the principles of conventional spectral unmixing before discussing emerging quantum approaches for dimensionality reduction, endmember extraction, abundance estimation, and optimization. It further examines the practical challenges associated with implementing these methods on current quantum hardware, including data encoding, QRAM assumptions, device noise, and scalability. Finally, the paper identifies key research gaps and outlines future directions that may guide the development of efficient, scalable, and reproducible quantum spectral unmixing frameworks for next-generation hyperspectral remote sensing.

II. Classical Spectral Unmixing Pipeline

A typical SU pipeline is depicted through Figure 1. A typical spectral unmixing pipeline consists of three main stages:

1. **Dimensionality Reduction (DR)**: Techniques such as Principal Component Analysis (PCA), Minimum Noise Fraction (MNF), or autoencoders are applied to reduce redundancy, suppress noise, and project high-dimensional hyperspectral data into a more tractable subspace.
2. **Endmember Extraction (EE)**: Algorithms such as Vertex Component Analysis (VCA), N-FINDR, SISAL, and HySime-based subspace estimation are employed to identify candidate pure spectral signatures from the reduced data.
3. **Abundance Estimation (AE)**: Once endmembers are obtained, abundances are estimated by solving a constrained inverse problem subject to non-negativity and sum-to-one constraints. Approaches include Fully Constrained Least Squares (FCLS) and sparse regression-based techniques.

Although the LMM remains computationally efficient and physically interpretable, its simplifying assumptions often limit its applicability in complex natural environments where nonlinear interactions dominate Therefore to

address the limitations of the basic Linear Mixing Model (LMM), several extended models have been proposed to better account for spectral variability in real-world hyperspectral data. The Perturbed Linear Mixing Model (PLMM) incorporates additive perturbations to endmember spectra, providing pixel-specific flexibility to capture distortions caused by illumination changes, atmospheric effects, or sensor noise. However, this adaptability comes at the cost of increased computational complexity due to the large number of free parameters [1]. The Extended Linear Mixing Model (ELMM) introduces pixel-wise scaling factors applied to endmembers, offering a simpler representation of illumination and shadow variability. While computationally more efficient, its reliance on linear scaling makes it less capable of representing more complex distortions [2]. The Augmented Linear Mixing Model (ALMM) extends these ideas by decomposing each observation into a scaled endmember dictionary and a complementary variability spectral library, jointly learned under low-coherence constraints. This approach captures richer spectral distortions and improves robustness in challenging environments [3]. Collectively, these models bridge the gap between idealized linear assumptions and the complexities of natural scenes.

From a broader perspective, spectral unmixing techniques can be classified as linear or nonlinear. Linear methods including LMM and its extensions (PLMM, ELMM, ALMM) assume that each mixed pixel is a weighted linear combination of endmembers subject to abundance non-negativity and sum- to-one constraints. These methods are computationally efficient, interpretable, and widely applied in areas such as mineral mapping and urban monitoring. However, they often fail to adequately model nonlinear interactions. By contrast, nonlinear spectral unmixing (NL-SU) explicitly accounts for multiple scattering, topographic effects, and canopy interactions through nonlinear mixing functions. Common approaches include bilinear models, which introduce cross- terms between endmembers; the Polynomial Post-Nonlinear Mixing Model (PNMM), which applies polynomial functions to capture higher-order distortions; kernel-based unmixing methods, which project spectra into high-dimensional feature spaces for improved separability and neural network methods which learn complex nonlinear relationships directly from hyperspectral data [4], [5]. While nonlinear models provide a more realistic representation of natural mixing processes, they are computationally intensive, prone to overfitting, and less interpretable than linear approaches. The trade-off between model complexity, interpretability, and accuracy continues to drive interest in hybrid methods and emerging quantum- assisted unmixing frameworks. **Table 1. provides a comparative summary of linear and nonlinear spectral unmixing techniques in classical spectral unmixing.**

Table 1 Linear Spectral Unmixing *vs* Non- linear Spectral Unmixing

Sr. No	Linear Spectral Unmixing	Nonlinear Spectral Unmixing
1	Each pixel is a linear combination of endmembers weighted by abundances	Pixel spectrum is generated by nonlinear interactions (e.g., scattering, multiple reflections).
2	y=Ax+ n (linear system with ANC/ASC constraints).	y=f(A,x)+ n, where f is a nonlinear function (bilinear, polynomial, kernel).
3	FCLS, P L M M , E L M M , ALMM, sparse regression approaches.	Bilinear models, polynomial post-nonlinear mixing model (PNMM), k e r n e l -based S U , neural networks.
4	Simple, interpretable, computationally efficient; widely used in real applications.	Captures real-world phenomena (multiple scattering, c a n o p y e f f e c t s , atmospheric interactions).
5	Struggles with spectral variability, nonlinear mixing, noise sensitivity	Computationally intensive, risk of overfitting, limited interpretability.
6	Mineral mapping, urban monitoring, scenarios with limited variability.	Vegetation studies, aquatic environments, complex topography, strongly nonlinear scenes.

III. QUANTUM SPECTRAL UNMIXING:

EMERGING METHODS AND NECESSITY

A key distinction between classical and quantum spectral unmixing (QSU) lies in their computational scaling across the main stages of the unmixing pipeline. For dimensionality reduction, classical PCA has a time complexity of O(n^3) for an n×n covariance matrix, which becomes prohibitive for high-dimensional hyperspectral cubes. In contrast, Quantum PCA (QPCA), introduced by Lloyd et al. [9], can estimate principal components in polylogarithmic time O(log n) under favorable data-access assumptions, thereby offering exponential improvement in scalability. For endmember extraction, classical methods such as VCA or N-FINDR rely on geometric simplex assumptions that degrade under nonlinear mixing. Here, quantum kernels and feature maps embed spectra into high-dimensional Hilbert spaces, enabling linear separability of nonlinear mixtures without exponential cost [13], [14]. Finally, for abundance estimation, classical constrained least-squares regression typically requires O(n^2m) time for n pixels and m endmembers, while quantum linear solvers

such as those proposed by Gribling et al. [15] and Shaik et al. [17] solve similar systems in time polylogarithmic in, given efficient quantum state preparation. Variational quantum algorithms (VQAs) further provide a NISQ-compatible pathway for constrained optimization [14]. Collectively, these comparisons highlight where quantum approaches hold potential advantages: (i) QPCA for scalable dimensionality reduction, (ii) quantum kernels for nonlinear separability, and (iii) quantum solvers and VQAs for accelerated abundance estimation. We conceptualize a Quantum Spectral Unmixing (QSU) framework by extending the classical spectral unmixing pipeline Figure 3

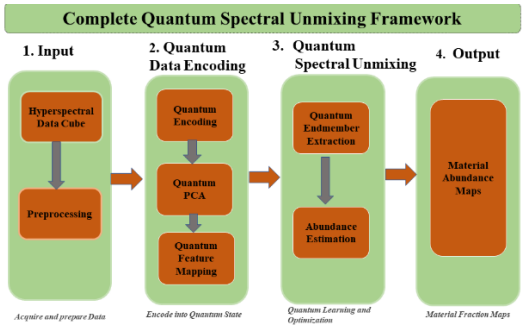


Figure 3 Quantum Spectral Unmixing

Classical approaches become computationally expensive as the dimensionality of hyperspectral datasets increases. For instance, Principal Component Analysis (PCA) is widely used for dimensionality reduction, but it scales polynomials with the number of pixels and spectral bands and may lose subtle spectral variability that is essential for endmember separability. Quantum computing introduces new computational primitives that can mitigate these bottlenecks, motivating the exploration of QSU.

One promising direction is Quantum Principal Component Analysis (QPCA), introduced by Lloyd, Mohseni, and Rebentrost [9], which can estimate principal components in logarithmic time with respect to the input dimension under certain data-access assumptions. In contrast, classical PCA requires polynomial time. In hyperspectral unmixing, this translates into the ability to process extremely high- dimensional cubes more efficiently while preserving geometric structure necessary for endmember identification. Thus, QPCA represents a paradigm shift for dimensionality reduction in SU. Moreover, quantum circuits can also be designed for abundance estimation via optimization, offering computational advantages for high-dimensional data.

Beyond dimensionality reduction, quantum kernels and feature maps have been explored as a means of embedding hyperspectral spectra into high-dimensional Hilbert spaces, where mixed pixels may become more linearly separable. Di Marcantonio et al. [12] and Li et al. [13] demonstrated that this property is crucial for endmember extraction, since many classical algorithms (e.g., VCA, N-FINDR) assume simplex geometry that is often violated by nonlinear mixing. Quantum feature embeddings expand the representational space without incurring an exponential increase in computational cost, thereby improving the detection of pure spectra.
For abundance estimation, which is typically formulated as a constrained least-squares regression problem, Variational Quantum Algorithms (VQAs) have been proposed as efficient solvers. Cimini et al. [14] showed how VQAs can be adapted for photonic multiphase sensing, while Gribling et al. [15] and Shaik et al [17] developed quantum linear system solvers and regression models tailored for abundance estimation under non-negativity and sum-to-one constraints. These approaches combine shallow parameterized circuits with classical optimization loops, making them suitable for deployment on Noisy Intermediate-Scale Quantum (NISQ) devices.

An early attempt at an end-to-end pipeline is the PRIME framework, proposed by Lin and Lin [16], which introduced a "virtual quantum prism" for blind multispectral unmixing. Their approach expands spectra into a quantum feature space to emulate additional virtual bands, applies convex-geometry unmixing, and then maps estimated endmembers back to the original space. While designed for multispectral data, PRIME provides a conceptual template for hyperspectral QSU, demonstrating how quantum-enhanced preprocessing can support more effective unmixing.

Finally, evidence from related hyperspectral classification tasks further supports feasibility. Shaik et al. [17] implemented quantum support vector machines (QSVMs) and quantum pseudo-labeling strategies on PRISMA satellite data, reporting competitive accuracy compared to classical baselines while also analyzing device noise and resource trade-offs. Although these works address classification rather than unmixing, they validate encoding schemes and quantum kernel methods that are directly transferable to SU pipelines.
In summary, the necessity of QSU stems from three key aspects

- **Scalability:** Algorithms like QPCA provide asymptotic speedups over classical PCA, enabling more efficient dimensionality reduction of large hyperspectral cubes.
- **Nonlinear Separability:** Quantum kernels offer richer feature spaces that enhance endmember extraction under nonlinear mixing conditions.
- **Optimization Efficiency:** VQAs and quantum linear solvers can accelerate abundance estimation, particularly under constraints.

Collectively, these developments suggest that QSU can alleviate the long-standing challenges of computational complexity, spectral variability, and nonlinear mixing in hyperspectral analysis

IV Discussion

While hyperspectral unmixing has been studied extensively using classical approaches, the application of quantum computing to spectral unmixing is still in its early stages. Rather than simply adapting existing quantum algorithms to remote sensing problems, Quantum Spectral Unmixing (QSU) opens up opportunities to develop new quantum methods specifically designed for the characteristics of hyperspectral data.

One of the first challenges is data encoding. Before any quantum algorithm can be applied, the high-dimensional spectral

information must be converted into quantum states. Common encoding methods, such as amplitude and angle encoding, can require complex state preparation and significant computational resources, particularly for large hyperspectral datasets. In addition, many theoretical studies assume the availability of efficient Quantum Random Access Memory (QRAM) to load data into quantum processors. At present, however, scalable and fault-tolerant QRAM has not yet been realized, making efficient data loading one of the major practical limitations for implementing QSU on real quantum hardware.

Another important aspect is the interpretation of computational complexity. Quantum algorithms such as Quantum Principal Component Analysis (QPCA), Variational Quantum Algorithms (VQAs), and quantum optimization methods have demonstrated promising theoretical advantages for certain linear algebra and optimization problems. However, these advantages generally rely on assumptions such as efficient state preparation, reliable quantum memory, and sufficiently capable quantum hardware. Consequently, while quantum methods may offer significant computational benefits in the future, their practical performance for hyperspectral unmixing on today's Noisy Intermediate-Scale Quantum (NISQ) devices remains an active area of research. Variational quantum algorithms, although attractive for abundance estimation, are also affected by hardware noise, decoherence, and optimization issues such as barren plateaus, highlighting the need for improved circuit designs and more effective error-mitigation techniques.

Another area that deserves attention is benchmarking. Classical spectral unmixing has benefited from widely used datasets such as Samson, Jasper Ridge, and Urban, which have enabled consistent comparison of different algorithms over many years. Similar benchmark datasets and evaluation protocols are still lacking for QSU. Developing quantum-ready benchmark datasets, simulation frameworks, and standardized evaluation procedures will be essential for assessing future quantum algorithms fairly and reproducibly.

In the near term, quantum-inspired algorithms provide a practical way to investigate many of these ideas using classical computing platforms while quantum hardware continues to evolve. At the same time, combining quantum computing with deep learning appears to be a particularly promising research direction. Hybrid quantum-classical models that integrate quantum kernels, variational circuits, and neural networks could provide more flexible solutions for nonlinear spectral unmixing and other challenging hyperspectral analysis tasks.

Overall, Quantum Spectral Unmixing should be viewed as a long-term research direction rather than a mature technology. Although current hardware limitations prevent immediate large-scale deployment, continued advances in quantum processors, data encoding strategies, benchmarking methodologies, and hybrid algorithms are likely to accelerate progress in this field. By bringing together developments from quantum computing and hyperspectral image analysis, QSU has the potential to become an important area of interdisciplinary research and may contribute to the next generation of computational methods for remote sensing.

V. Conclusion

Spectral unmixing remains a fundamental component of hyperspectral image analysis, enabling material identification at the sub-pixel level for applications such as environmental monitoring, precision agriculture, mineral exploration, and urban mapping. Although substantial progress has been achieved through linear, nonlinear, sparse representation, and deep learning-based approaches, challenges related to computational complexity, spectral variability, and nonlinear mixing continue to limit their performance, particularly for large-scale hyperspectral datasets.

This review has examined the evolution of spectral unmixing methods and explored how recent advances in quantum computing may contribute to addressing some of these challenges. By bringing together developments in quantum linear algebra, variational optimization, and quantum machine learning, the review provides a unified perspective on the emerging field of Quantum Spectral Unmixing (QSU). Rather than viewing quantum computing simply as a faster alternative to classical computation, the discussion highlights its potential to introduce new computational paradigms for selected stages of the spectral unmixing workflow.

One of the key contributions of this review is the synthesis of currently dispersed research into a coherent framework that connects classical spectral unmixing with emerging quantum approaches. The proposed taxonomy and conceptual workflow illustrate how techniques such as Quantum Principal Component Analysis (QPCA), quantum kernel methods, and variational quantum algorithms may be incorporated into dimensionality reduction, feature mapping, and abundance estimation. At the same time, the review emphasizes that many of these approaches remain at an early stage of development and that their practical advantages will depend on continued progress in quantum hardware, efficient quantum data encoding, scalable state preparation, and rigorous experimental validation.

Several important research challenges also remain unresolved. Efficient data loading, the absence of practical and scalable QRAM, hardware noise, limited qubit resources, and the lack of standardized quantum benchmarking datasets continue to restrict the practical deployment of QSU. Addressing these limitations will require close collaboration between the remote sensing and quantum computing communities, together with the development of reproducible benchmarks and hybrid quantum-classical algorithms that can be evaluated on realistic hyperspectral datasets.

Overall, Quantum Spectral Unmixing represents a promising and rapidly evolving research direction at the intersection of remote sensing and quantum computing. While practical large-scale implementation is still some distance away, ongoing advances in quantum hardware, algorithms, and software ecosystems are expected to expand the range of feasible applications. As these technologies mature, QSU has the potential to become an important computational framework for next-generation hyperspectral image analysis while simultaneously stimulating new research in quantum algorithms tailored to Earth observation problems.

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DECLARATIONS

ETHICS APPROVAL AND CONSENT TO PARTICIPATE: This study did not involve human participants, animals, or plant experiments. The research is based entirely on publicly available hyperspectral datasets and computational analyses. Therefore, ethics approval and consent to participate were not required

CONSENT FOR PUBLICATION: Not applicable.

AVAILABILITY OF DATA AND MATERIALS: No new datasets were generated or analyzed during this study. This review is based on published literature and publicly available resources cited in the manuscript.

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AUTHORS' CONTRIBUTIONS Rashmi Kumaria Nitwane conceived the study, performed the literature review, analyzed the published research, prepared the figures and tables, and drafted the manuscript. Vaishali D. Bhagile and Ratnadeep R. Deshmukh provided academic guidance, reviewed the manuscript critically, and approved the final version.

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