



An improved spectral reconstruction method based on non-negative matrix factorization and multiplicative update rule: Framework and preliminary application on TROPOMI BRDF in 400–2400 nm

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ARTICLE INFO

Keywords:

Non-negative matrix factorization (NMF)
Multiplicative update (MU)
Spectral reconstruction
TROPOMI/GRASP BRDF
MODIS Nadir BRDF-adjusted reflectance (NBAR)
EMIT

ABSTRACT

This study presents a physically interpretable hyperspectral reconstruction framework based on Non-negative Matrix Factorization (NMF) with multiplicative update (MU) optimization to reconstruct continuous hyperspectral surface reflectance from satellite bidirectional reflectance distribution function (BRDF) products with limited spectral bands. The Sentinel-5P/TROPOMI BRDF monthly product generated using the Generalized Retrieval of Atmosphere and Surface Properties (GRASP) algorithm is extended from seven discrete spectral bands to a continuous spectral range of 400–2400 nm. Five representative spectral basis vectors extracted from the USGS/ASTER spectral libraries are combined with MU-based mixing-coefficient optimization to ensure physically meaningful, non-negative reconstruction. Compared with the conventional least-squares solution, the proposed MU optimization yields more robust non-negative coefficient estimation and consistently improves hyperspectral reconstruction performance. The reconstructed hyperspectral BRDF parameters exhibit physically consistent spatial distributions and pronounced seasonal variations across North America. Validation against monthly mean MODIS MCD43C4 Nadir BRDF-Adjusted Reflectance (NBAR) demonstrates excellent agreement in the visible and near-infrared regions (470–859 nm), with monthly mean differences generally within ± 0.01 and standard deviations of 0.02–0.04. In the shortwave infrared, larger discrepancies are observed over vegetation-dominated regions, where the monthly mean differences range from approximately -0.06 to -0.04 at 1240 and 1610 nm. Independent comparisons with EMIT Level-2A hyperspectral surface reflectance further confirm that the reconstructed spectra successfully reproduce the dominant hyperspectral characteristics of representative natural surfaces across the continuous 400–2400 nm spectral range. Despite the remaining shortwave-infrared underestimation, likely reflecting the limited representation of vegetation spectral variability in the selected spectral dataset, both the MODIS and EMIT validations confirm the overall robustness of the proposed framework. The proposed MU-based NMF framework provides a transparent solution for reconstructing continuous hyperspectral reflectance from satellite products with limited spectral bands, establishing a scalable methodological foundation for future cross-sensor harmonization and multi-resolution surface reflectance reconstruction.

1. Introduction

Satellite-based multispectral remote sensing has become an indispensable tool for Earth surface monitoring, offering broad spatial coverage and high-frequency revisit cycles [1–3]. However, the limited

spectral resolution of multispectral instruments often restricts their capacity to detect fine spectral features [4,5]. Such features are critical for accurately characterizing surface properties, especially in spectral regions where gas absorption or atmospheric correction introduces significant uncertainties [6–8]. While hyperspectral sensors provide far

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<https://doi.org/10.1016/j.jqsrt.2026.110140>

Received 26 December 2025; Received in revised form 31 July 2026; Accepted 14 September 2026

Available online 16 September 2026

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more detailed information, their operational use is often hampered by high deployment costs, relatively narrow swath widths, and limited temporal coverage [9–14].

To bridge the gap in spectral resolution, various reconstruction methods have been developed to estimate hyperspectral-like reflectance from a limited set of multispectral bands [15–18]. Previous research introduced a framework based on Non-negative Matrix Factorization (NMF) [19,20], utilizing Bidirectional Reflectance Distribution Function (BRDF) products generated from the Tropospheric Monitoring Instrument (TROPOMI) onboard Sentinel-5P satellite via the Generalized Retrieval of Atmosphere and Surface Properties (GRASP) algorithm [21–27]. This approach successfully demonstrated that visible-range reflectance (400 to 800 nm) could be efficiently reconstructed using a small number of isotropic coefficients [19]. Nevertheless, earlier implementations relied on unconstrained least-squares method (LSM), which can produce physically incompatible negative reflectance values and lack robustness when applied to heterogeneous surfaces.

Simultaneously, advances in deep learning have introduced neural networks, such as hyperspectral convolutional neural networks (HSCNN), hybrid convolutional neural network (CNN)-transformer model, high-resolution network (HRNet), and CNN-transformer combined block model (CTBNet), that excel at recovering dense spectral signatures from multispectral inputs [28–31]. While these and other optimization-based methods [32–34], like adaptive Wiener filtering, have improved spectral fidelity, they typically require vast amounts of labeled training data, are computationally expensive, and lack the physical transparency necessary for many practical applications. Alternatively, methods based on Principal Component Analysis (PCA) have proven effective for reconstructing visible to near-infrared (VIS-NIR) spectra, yet they suffer from orthogonality constraints and sign ambiguity, which limit the physical interpretability of the results [35–38].

The multiplicative-update (MU) rule was originally introduced by Lee and Seung as an efficient optimization algorithm for NMF, where both the basis matrix and the corresponding coefficient matrix are constrained to remain non-negative throughout the factorization process [20,39]. Owing to its simplicity, guaranteed non-negativity, and computational efficiency, the MU algorithm has been widely adopted in applications such as matrix decomposition and hyperspectral unmixing. However, despite its extensive use for NMF decomposition, its application as a non-negative least-squares (NNLS) solver for continuous spectral reconstruction from sparse multispectral observations has received little attention. In particular, when the spectral basis vectors are assumed to be known *a priori*, the reconstruction problem becomes a constrained coefficient estimation problem rather than an NMF decomposition problem. This distinction forms the methodological foundation of the present study.

Building upon the previously derived spectral basis vectors, this study proposes an enhanced spectral reconstruction framework by formulating the estimation of non-negative weighting coefficients as a series of NNLS subproblems. Instead of conventional least-squares fitting, the coefficient estimation is performed using a fully vectorized MU algorithm, which guarantees non-negative solutions while improving numerical stability and computational efficiency for large-scale remote sensing applications involving millions of pixels. The proposed framework preserves the physical interpretability of the reconstruction process, where the NMF-derived basis vectors represent characteristic spectral components, and the retrieved coefficients describe their relative contributions to the reconstructed continuous spectra.

The primary objectives of this work are to:

- (1) Develop an efficient NNLS reconstruction framework: Introduce a fully vectorized MU algorithm for solving the mixing coefficient estimation problem in continuous spectral reconstruction.

- (2) Expand the reconstruction capability: Demonstrate the feasibility of reconstructing continuous surface reflectance across the VIS and shortwave infrared (SWIR) spectral regions (400–2400 nm).
- (3) Demonstrate large-scale applicability and validation: Apply the proposed framework to monthly TROPOMI/GRASP BRDF products and evaluate the reconstructed spectra using complementary MODIS Nadir BRDF-Adjusted Reflectance (NBAR) and EMIT hyperspectral surface reflectance.

By developing an interpretable and efficient spectral enhancement framework, this work aims to advance surface reflectance retrieval and provide robust support for applications such as vegetation monitoring, atmospheric correction, and remote sensing product fusion.

2. Spectral reconstruction methodology via NMF

2.1. Principles of reflectance reconstruction using NMF

For a non-negative matrix $\mathbf{V} \in \mathbb{R}_{\geq 0}^{n \times m}$ representing a hyperspectral-like surface reflectance dataset, NMF aims to decompose $\mathbf{V}$ into two non-negative matrices $\mathbf{W} \in \mathbb{R}_{\geq 0}^{n \times r}$ and $\mathbf{H} \in \mathbb{R}_{\geq 0}^{r \times m}$, such that [20]:

$$\mathbf{V} \approx \mathbf{W}\mathbf{H}, \quad (1)$$

$$\begin{bmatrix} v_{1,1} & \cdots & v_{1,m} \\ \vdots & \ddots & \vdots \\ v_{n,1} & \cdots & v_{n,m} \end{bmatrix} \approx \begin{bmatrix} w_{1,1} & \cdots & w_{1,r} \\ \vdots & \ddots & \vdots \\ w_{n,1} & \cdots & w_{n,r} \end{bmatrix} \begin{bmatrix} h_{1,1} & \cdots & h_{1,m} \\ \vdots & \ddots & \vdots \\ h_{r,1} & \cdots & h_{r,m} \end{bmatrix}. \quad (2)$$

and with the matrix form:

Here, n represents the number of hyperspectral bands, m is the number of pixels (spectra), and r is the desired rank. $\mathbf{W}$ denotes the spectral basis matrix composed of statistical spectral components, while $\mathbf{H}$ denotes the corresponding mixing-coefficient matrix. For simplicity, let $\mathbf{v}_i$ and $\mathbf{h}_i$ denote the i -th columns of $\mathbf{V}$ and $\mathbf{H}$, respectively, where $i = 1, \dots, m$. Eq. (1) can then be expressed in the vector form as:

$$\mathbf{v} \approx \mathbf{W}\mathbf{h}. \quad (3)$$

Let $\Psi \in \mathbb{R}^{d \times n}$ denote the linear band-mapping operator, which projects the continuous hyperspectral reflectance onto the multispectral observation space according to the sensor's spectral response functions (SRFs). The multispectral reflectance vector and the corresponding basis matrix can then be expressed as

$$\begin{cases} \tilde{\mathbf{v}} = \Psi\mathbf{v} \\ \tilde{\mathbf{W}} = \Psi\mathbf{W} \end{cases} \quad (4)$$

where each row of Ψ represents the normalized SRF of one multispectral band. Consequently, the hyperspectral reconstruction model can be mapped into the multispectral observation space as

$$\tilde{\mathbf{v}} \approx \tilde{\mathbf{W}}\mathbf{h}, \quad (5)$$

which establishes the relationship between the observed multispectral reflectance and the continuous hyperspectral reflectance through the same non-negative coefficient vector $\mathbf{h}$. Therefore, the reconstruction problem is reformulated as estimating the coefficient vector from sparse multispectral observations, while the continuous hyperspectral reflectance can subsequently be recovered using the previously derived spectral basis vectors. Using the least-squares method (LSM), the mixing coefficients can be estimated as [19]:

$$\mathbf{h} \approx \tilde{\mathbf{W}}^+ \tilde{\mathbf{v}}, \quad (6)$$

where $\tilde{\mathbf{W}}^+$ denotes the pseudoinverse of $\tilde{\mathbf{W}}$. However, Eq. (6) does not guarantee that $\mathbf{h}$ will be non-negative. The resulting negative values may lead to physically impossible negative reflectance values in the reconstructed bands. Consequently, the reconstruction method must be

refined to include non-negative constraints.

2.2. Numerical solution for non-negative least-squares (NNLS)

Assuming that the subset matrices $\tilde{\mathbf{V}}$ and $\tilde{\mathbf{W}}$ are known and consist of pre-determined non-negative values, the objective is to solve for the unknown $\mathbf{H}$:

$$\min_{\mathbf{H} \geq 0} f(\mathbf{H}) = \|\tilde{\mathbf{V}} - \tilde{\mathbf{W}}\mathbf{H}\|_F^2, \quad (7)$$

where $\|\cdot\|_F^2$ denotes the squared Frobenius norm. Given that the subset basis-vector matrix $\tilde{\mathbf{W}}$ is fixed, Eq. (7) constitutes a standard non-negative least-squares (NNLS) problem [39].

2.2.1. Column-wise decoupling optimization

First, we express $\tilde{\mathbf{V}}$ and $\mathbf{H}$ in terms of their columns: $\tilde{\mathbf{V}} = [\tilde{\mathbf{v}}_1, \dots, \tilde{\mathbf{v}}_m]$ and $\mathbf{H} = [\mathbf{h}_1, \dots, \mathbf{h}_m]$, where $\tilde{\mathbf{v}}_j \in \mathbb{R}^n$ and $\mathbf{h}_j \in \mathbb{R}^k$. Substituting these into Eq. (7) yields:

$$f(\mathbf{H}) = \sum_{j=1}^m \|\tilde{\mathbf{v}}_j - \tilde{\mathbf{W}}\mathbf{h}_j\|_2^2. \quad (8)$$

In this formulation, each column can be treated as an independent NNLS sub-problem. Consequently, Eq. (8) can be decomposed into m independent optimization tasks:

$$\min_{\mathbf{h}_j \geq 0} \|\tilde{\mathbf{v}}_j - \tilde{\mathbf{W}}\mathbf{h}_j\|_2^2, (j = 1, \dots, m). \quad (9)$$

By solving Eq. (9) for each column, the results can be assembled to form $\mathbf{H}$. Various algorithms are available to solve this NNLS problem, including the active-set NNLS [40–42], projected gradient methods [43], and multiplicative update rules [39].

For a single-column problem in Eq. (9), the Karush-Kuhn-Tucker (KKT) optimality conditions are defined as:

$$\tilde{\mathbf{W}}^T(\tilde{\mathbf{W}}\mathbf{h}^* - \tilde{\mathbf{v}}) + \boldsymbol{\alpha}^* = \mathbf{0}, \mathbf{h}^* \geq 0, \boldsymbol{\alpha}^* \geq 0, \boldsymbol{\alpha}^* \odot \mathbf{h}^* = \mathbf{0}, \quad (10)$$

where the superscript “T” and “*” denote the transpose and optimal solution, respectively. Here, $\boldsymbol{\alpha}$ represents the vector of Lagrange multipliers, and $\odot$ denotes the Hadamard product. Here, the Hadamard product is the element-wise multiplication of two matrices of the same size, producing a new matrix whose entries are the products of corresponding elements. The active-set method enforces these conditions through iterative refinement.

2.2.2. Vectorized multiplicative update (MU) strategy

While column-wise loops are straightforward, a loop-free, fully vectorized NNLS solver is often more efficient for large-scale applications (e.g., $m \approx 10^6$ spectral pixels). In such cases, evaluating each column individually becomes computationally prohibitive. For the objective function in Eq. (8), the full-matrix gradient is expressed as:

$$\nabla f(\mathbf{H}) = \tilde{\mathbf{W}}^T(\tilde{\mathbf{W}}\mathbf{H} - \tilde{\mathbf{V}}) \in \mathbb{R}^{k \times m}, \quad (11)$$

and the corresponding KKT optimality conditions are:

$$\nabla f(\mathbf{H}^*) + \boldsymbol{\Lambda}^* = \mathbf{0}, \mathbf{H}^* \geq 0, \boldsymbol{\Lambda}^* \geq 0, \boldsymbol{\Lambda}^* \odot \mathbf{H}^* = \mathbf{0}, \quad (12)$$

where $\boldsymbol{\Lambda}$ represents the matrix of Lagrange multipliers and $\mathbf{H}^*$ denotes the optimal results. To satisfy these conditions, we employ the Lee-Seung multiplicative update rule [20,39], which operates on the entire matrix $\mathbf{H}$ simultaneously:

$$\mathbf{H} \leftarrow \mathbf{H} \odot \frac{\tilde{\mathbf{W}}^T \tilde{\mathbf{V}}}{\tilde{\mathbf{W}}^T \tilde{\mathbf{W}} \mathbf{H}}. \quad (13)$$

In this expression, all operations (including division) are performed

elementwise. In practical implementations, a small positive constant ϵ is added to the denominator of Eq. (13) to avoid division by zero and improve numerical stability. Starting with a strictly positive initialization $\mathbf{H}^{(0)}$, this rule automatically maintains the non-negativity constraint throughout the iteration process. This fully vectorized approach avoids an explicit loop over the m pixels, ensuring that $f(\mathbf{H}^{(i+1)}) \leq f(\mathbf{H}^{(i)})$ until convergence.

The implementation of the MU algorithm follows these steps:

Step 1: Pre-computation. Calculate the constant matrices $\tilde{\mathbf{W}}^T \tilde{\mathbf{V}} \in \mathbb{R}^{k \times m}$ and $\tilde{\mathbf{W}}^T \tilde{\mathbf{W}} \in \mathbb{R}^{k \times k}$ to optimize performance.

Step 2: Initialization. Initialize the mixing-coefficient matrix $\mathbf{H}^{(0)}$ with random positive values, such as $\mathbf{H}^{(0)} = \text{rand}(k, m)$.

Step3: Iteration. Update $\mathbf{H}$ using Eq. (13) for $i = 0, \dots, N - 1$ until the following convergence criterion is met:

$$\frac{\|\mathbf{H}^{(i+1)} - \mathbf{H}^{(i)}\|_F}{\|\mathbf{H}^{(i)}\|_F} \leq \epsilon, \quad (14)$$

where, ϵ is a convergence threshold and N is the maximum number of iterations.

Step 4: Output. Return the final mixing-coefficient matrix $\mathbf{H}^* = \mathbf{H}^{(N)}$.

Each iteration has a computational complexity of $O(k^2m)$. In practice, $N \in [150, 200]$ iterations are typically sufficient to reduce the relative reconstruction error below $\epsilon = 0.1\%$.

3. Reconstruction datasets and validation methods

Table 1 summarizes the spectral characteristics and temporal information of the USGS/ASTER spectral dataset, TROPOMI/GRASP BRDF, MODIS MCD43C4 NBAR, and EMIT L2A surface reflectance products used in this study.

3.1. USGS/ASTER spectral dataset

The U.S. Geological Survey Spectral Library Version 06 (USGS splib06) and the Advanced Spaceborne Thermal Emission and Reflection Radiometer (ASTER) spectral libraries are widely utilized reference datasets containing high-quality reflectance spectra of diverse natural and anthropogenic surface materials [44–46]. In this study, the combined dataset serves as the foundation for extracting continuous spectral basis vectors using NMF and is hereafter referred to as the USGS/ASTER spectral dataset.

Fig. 1 illustrates the USGS/ASTER spectral dataset used in this reconstruction study. The dataset consists of 297 reflectance spectra

Table 1

Spectral characteristics and acquisition dates of the USGS/ASTER spectral dataset, TROPOMI/GRASP BRDF, MODIS MCD43C4 NBAR, and EMIT L2A surface reflectance products used in this study.

Sensor/ Source	Product	Acquisition date	Spectral coverage used	Spectral sampling
USGS/ ASTER	Combined spectral dataset	N/A	400–2400 nm	Continuous hyperspectral (1 nm interval)
TROPOMI	GRASP monthly BRDF	Monthly mean (Dec 2019–Nov 2020)	416, 440, 494, 670, 747, 772, 2313 nm	7 discrete bands
MODIS	MCD43C4 monthly mean NBAR	Monthly mean (Dec 2019–Nov 2020)	470, 555, 645, 859, 1240, 1640, 2130 nm	7 broad bands
EMIT	L2A Surface Reflectance	Selected scenes (8 Aug. 2023 and 27 Jul. 2025)	400–2400 nm (from original 381–2493 nm)	Continuous hyperspectral (~7.5 nm interval), 285 (244 valid bands)

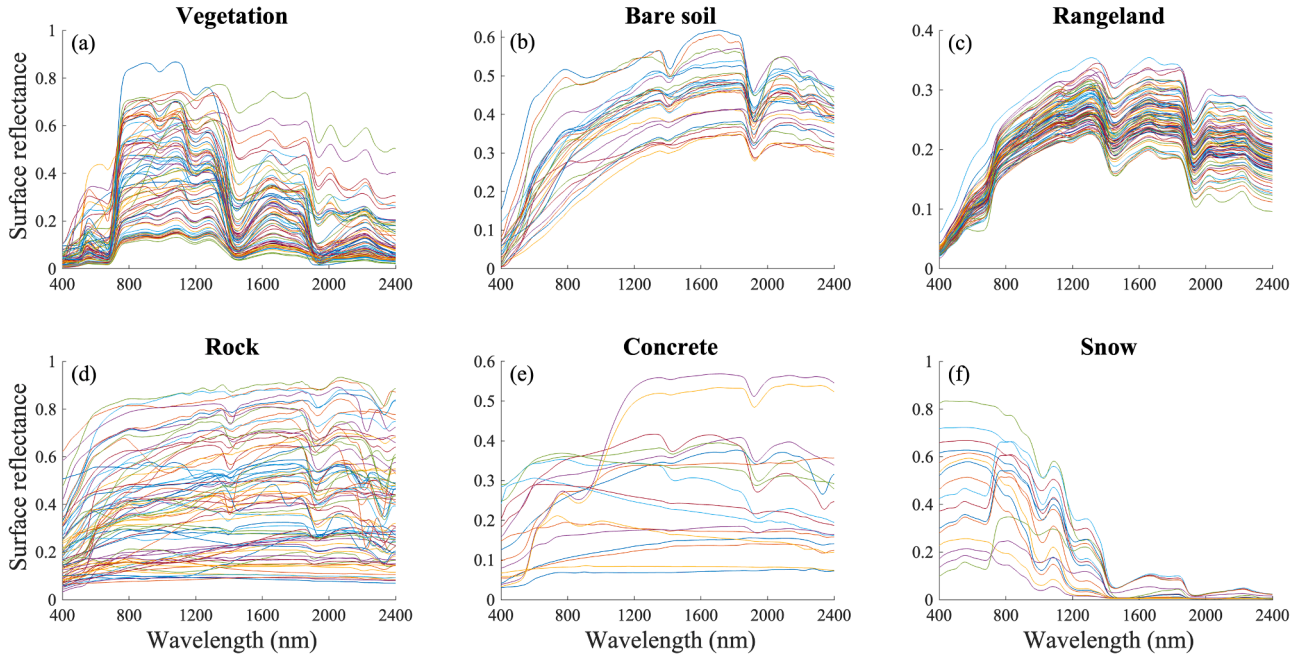


Fig. 1. Representative hyperspectral reflectance dataset consisting of 297 natural and man-made surface spectra selected from the USGS splib06 and ASTER spectral libraries. The USGS/ASTER spectral dataset covers six representative surface categories, namely vegetation, bare soil, rangeland, rock, concrete, and snow, over the wavelength range of 400 to 2400 nm.

selected for subsequent analysis. The six subplots present spectra of vegetation, bare soil, rangeland, rock, concrete, and snow over 400–2400 nm wavelength range. The diversity of these spectral signatures provides a representative dataset for evaluating spectral decomposition and reconstruction performance.

3.2. GRASP TROPOMI BRDF product characteristics

The GRASP TROPOMI v1.0 BRDF dataset is synthesized from observations acquired by the Sentinel-5P TROPOMI sensor [47], processed via the GRASP algorithm [24,25]. This publicly available product provides surface reflectance information across an extensive spectral range, spanning from UV to SWIR at ten discrete wavelengths. To ensure spatial consistency, TROPOMI radiance inputs are resampled onto a global 0.09° grid using an equidistant cylindrical projection referenced to the WGS84 ellipsoid. The retrieval accuracy is further bolstered by integrating auxiliary datasets, including ECMWF wind fields data and S5P NPP-VIIRS cloud masks. The final output is archived in NetCDF-4 format, featuring a nominal spatial resolution of approximately 10 km [24,25,48].

In this product, the directional dependence of surface reflectance is characterized using the Ross–Li semi-empirical kernel-driven model. For a surface characterized by the BRDF at wavelength λ , the corresponding spectral bidirectional reflectance factor (BRF) is mathematically defined as [49]:

$$\rho_s(\theta_0, \theta_v, \phi, \lambda) = k_{\text{iso}}(\lambda) \left[1 + k_{\text{geom}} f_{\text{geom}}(\theta_0, \theta_v, \phi) + k_{\text{vol}} f_{\text{vol}}(\theta_0, \theta_v, \phi) \right], \quad (15)$$

where the parameters θ_0 , θ_v , and ϕ represent the solar zenith, viewing zenith, and relative azimuth angles, respectively. The functions f_{geom} and f_{vol} are the geometric-optical and volumetric-scattering kernels, respectively. With this framework, $k_{\text{iso}}(\lambda)$ captures the isotropic reflectance component, while k_{geom} and k_{vol} are the wavelength-independent kernel-coefficients for geometric and volumetric scattering. This robust parameterization facilitates the modeling of multi-angular reflectance, providing the necessary data for the spectral reconstruction objectives of

this study. Once the coefficient vector $\mathbf{h}$ is determined, the reconstructed isotropic spectral coefficients $\mathbf{k}_{\text{iso}}^{\text{rec}} = [k_{\text{iso}}^{\text{rec}}(\lambda_1), \dots, k_{\text{iso}}^{\text{rec}}(\lambda_n)]^T$, are calculated as:

$$\mathbf{k}_{\text{iso}}^{\text{rec}} \approx \mathbf{W}\mathbf{h}, \quad (16)$$

where “rec” signifies the estimated values. Using the reconstructed coefficients, the BRF at an arbitrary target wavelength λ_i is then reconstructed as:

$$\rho_s^{\text{rec}}(\theta_0, \theta_v, \phi, \lambda_i) = k_{\text{iso}}^{\text{rec}}(\lambda_i) \left[1 + k_{\text{geom}} f_{\text{geom}}(\theta_0, \theta_v, \phi) + k_{\text{vol}} f_{\text{vol}}(\theta_0, \theta_v, \phi) \right], \quad (i = 1, \dots, n) \quad (17)$$

3.3. MODIS NBAR validation dataset

To validate the reconstructed results, this study utilizes the MODIS MCD43C4 (Collection 6.1) daily product, which provides Nadir BRDF-Adjusted Reflectance (NBAR). This dataset is generated by normalizing global surface reflectance to a standard viewing geometry (nadir view at local solar noon) using a sophisticated kernel-driven BRDF model inversion [50,51]. The algorithm aggregates multi-angle observations from the Terra and Aqua satellites over a 16-day period, applying a temporal weighting scheme to estimate isotropic, volumetric, and geometric kernels for each 0.05° Climate Modeling Grid (CMG) cell [52,53].

This MCD43C4 product is distributed on a 0.05-degree sinusoidal grid (approximately 5 km) and includes pixel-level quality flags and ancillary layers, such as local solar noon geometry, to support rigorous uncertainty filtering [54]. Compared to previous iterations, Version 6.1 offers superior calibration and cloud-screening, ensuring better temporal consistency between the Terra and Aqua records and enhancing the stability of long-term land surface monitoring applications. To match the temporal resolution of the monthly TROPOMI/GRASP BRDF product, the daily MODIS MCD43C4 NBAR observations and the associated local-noon solar zenith angles were averaged within each calendar month to generate monthly mean fields for the subsequent validation.

3.4. EMIT L2A surface reflectance dataset

To provide an independent hyperspectral evaluation of the proposed spectral reconstruction framework, the Earth Surface Mineral Dust Source Investigation (EMIT) Level-2A (L2A) surface reflectance product was used as an external validation dataset [55,56]. EMIT is a NASA Earth Ventures Instrument (EVI-4) imaging spectroscopy mission that provides hyperspectral surface reflectance observations over approximately 381–2493 nm with a spectral sampling interval of about 7.5 nm [57,58].

Because the TROPOMI/GRASP BRDF climatology used in this study was generated from monthly mean observations during December 2019–November 2020, whereas the EMIT mission became operational afterward, temporally coincident observations are unavailable. Therefore, representative cloud-free EMIT scenes over stable land-cover types were selected for hyperspectral validation. The original EMIT L2A surface data were spatially aggregated and resampled to the TROPOMI/GRASP BRDF grid by averaging all valid EMIT pixels within each TROPOMI grid cell.

3.5. Spectral reconstruction validation methods

The proposed reconstruction framework was evaluated using two

complementary validation strategies, and the overall validation workflow is illustrated in Fig. 2. First, continuous spectral basis vectors (400–2400 nm) were extracted from the USGS/ASTER spectral datasets using NMF. The derived basis vectors were subsequently used to reconstruct continuous isotropic reflectance spectra from the seven-band monthly TROPOMI/GRASP BRDF observations using both the least-squares method (LSM) and the multiplicative update (MU) algorithm. The reconstructed spectra were then evaluated through two independent validation pathways. The first employed the MODIS MCD43C4 monthly BRDF-adjusted reflectance (NBAR) product to assess the accuracy of the reconstructed multispectral reflectance after spectral convolution. The second utilized the EMIT L2A hyperspectral surface reflectance product to evaluate the capability of the proposed method to reconstruct continuous spectra over the wavelength range of 400–2400 nm.

3.5.1. Validation using MODIS NBAR

The MODIS-based validation was performed to evaluate the accuracy of the reconstructed monthly TROPOMI/GRASP spectra against the MODIS MCD43C4 monthly NBAR product. The LSM and MU algorithms were evaluated using an identical validation procedure to enable a direct comparison of their reconstruction performance. The reconstructed spectra obtained using the two algorithms were converted to

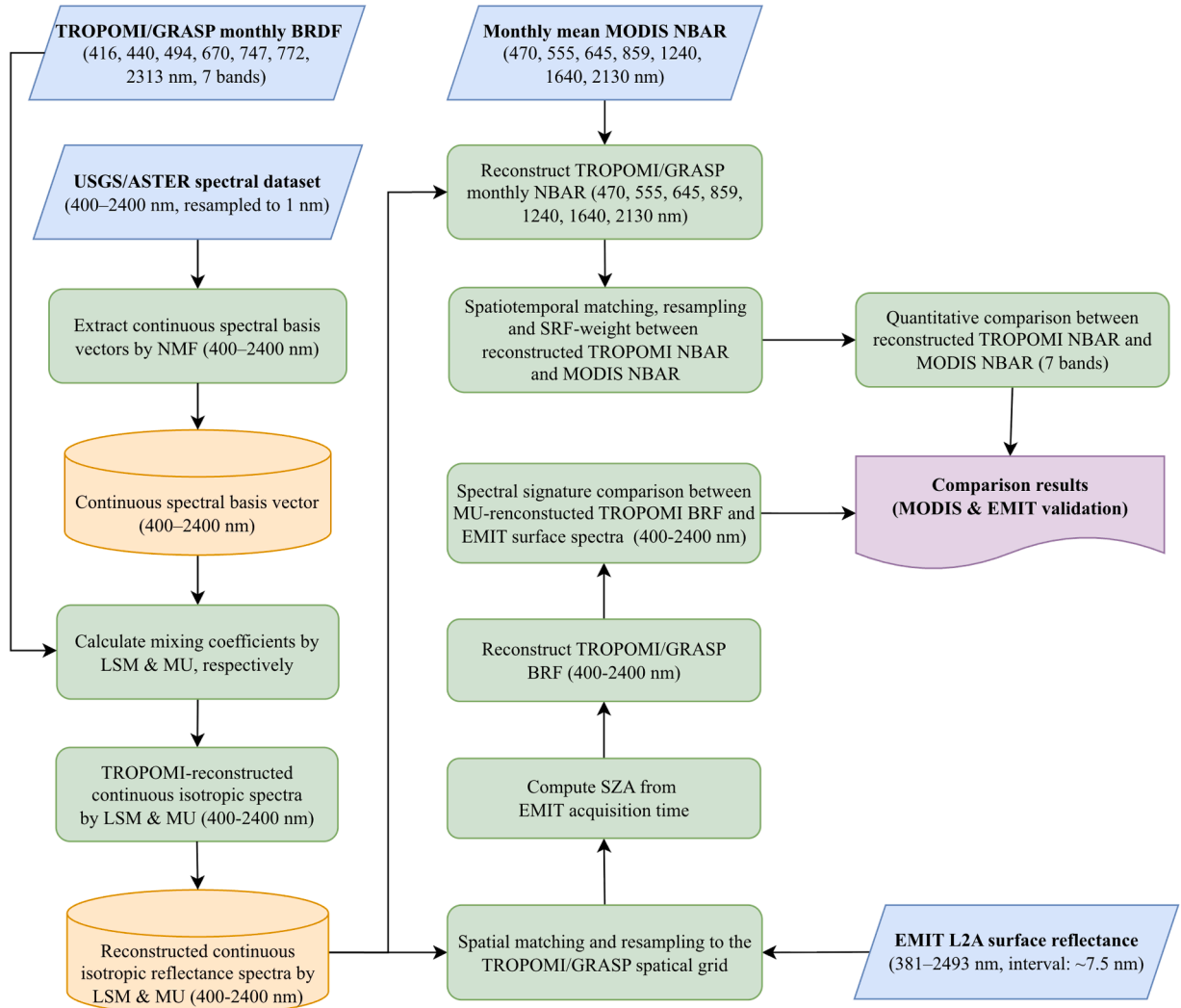


Fig. 2. Flowchart of the proposed NMF-based spectral reconstruction and validation framework, including the MODIS NBAR and EMIT hyperspectral validation pathways. Blue parallelograms represent the input datasets, green rounded rectangles denote the major processing and validation steps, orange cylinders indicate intermediate data products generated during the reconstruction process, and the purple document-shaped block summarizes the final validation results.

MODIS-equivalent NBAR, and the validation procedure consisted of the following steps.

Monthly averaging and spatial matching. Daily MODIS MCD43C4 NBAR observations were averaged within each month to generate monthly mean NBAR fields. The corresponding daily solar zenith angles provided in the MCD43C4 product were averaged in the same manner to obtain the monthly mean local-noon solar zenith angle for each grid cell. The resulting monthly mean NBAR and solar zenith angle fields were then spatially resampled onto the 0.09° TROPOMI/GRASP grid.

Geometric standardization. For each month, the reconstructed TROPOMI/GRASP BRDF was evaluated using the monthly mean local-noon solar zenith angle derived from the MODIS MCD43C4 product, while the viewing zenith angle and relative azimuth angle were fixed at 0°. This procedure produced monthly mean TROPOMI/GRASP NBAR that is geometrically consistent with the MODIS NBAR observations.

Generation of MODIS-equivalent NBAR. The geometrically standardized continuous spectra were convolved with the MODIS spectral response functions (SRFs) to generate seven MODIS-equivalent reflectance bands centered at 470, 555, 645, 859, 1240, 1640, and 2130 nm [59].

Quantitative comparison. The reconstructed monthly TROPOMI/GRASP NBAR was compared directly with the corresponding monthly mean MODIS NBAR after spatial matching. The agreement between the two datasets was evaluated using statistical metrics including the correlation coefficient, RMSE, MAE, and spectral bias.

3.5.2. Validation using EMIT hyperspectral observations

Unlike the MODIS validation, which evaluates reconstructed broadband reflectance, the EMIT validation focuses on the accuracy of the reconstructed continuous hyperspectral spectra. Based on the superior performance of the MU algorithm in the MODIS validation, only

the MU-reconstructed spectra were considered in the subsequent analysis.

For each selected EMIT scene, the reconstructed TROPOMI spectra were converted from BRDF parameters to spectral BRF using the Ross–Li BRDF model. The solar zenith angle (θ_0) was calculated from the EMIT acquisition time and pixel geolocation, while the viewing zenith angle and relative azimuth angle were assumed to be $\theta_v = 0^\circ$ and $\phi = 0^\circ$, respectively, because the complete observation geometry is unavailable in the EMIT L2A product. Under this simplified geometry, the reconstructed BRF spectra were calculated according to Eq. (15).

Finally, the reconstructed BRF spectra were interpolated to the EMIT good wavelengths over the common spectral range of 400–2400 nm and directly compared with the EMIT L2A surface reflectance. The evaluation focused on representative hyperspectral signatures together with wavelength-dependent mean differences and corresponding standard deviations.

4. MU-optimized reconstruction results and analysis

4.1. Basis vector characterization and reconstruction fidelity

Fig. 3 compares the spectral basis vectors extracted by NMF using two representative desired ranks, $r = 5$ and $r = 6$. To improve readability, each basis vector is displayed individually rather than overlaying all components within a single panel, allowing a more direct comparison between the two decompositions. The extracted basis vectors should be regarded as statistical spectral components rather than strict physical endmembers. NMF identifies a nonnegative low-rank representation of the spectral library, and each basis vector therefore represents dominant spectral characteristics shared by multiple surface materials rather than a unique land-cover type.

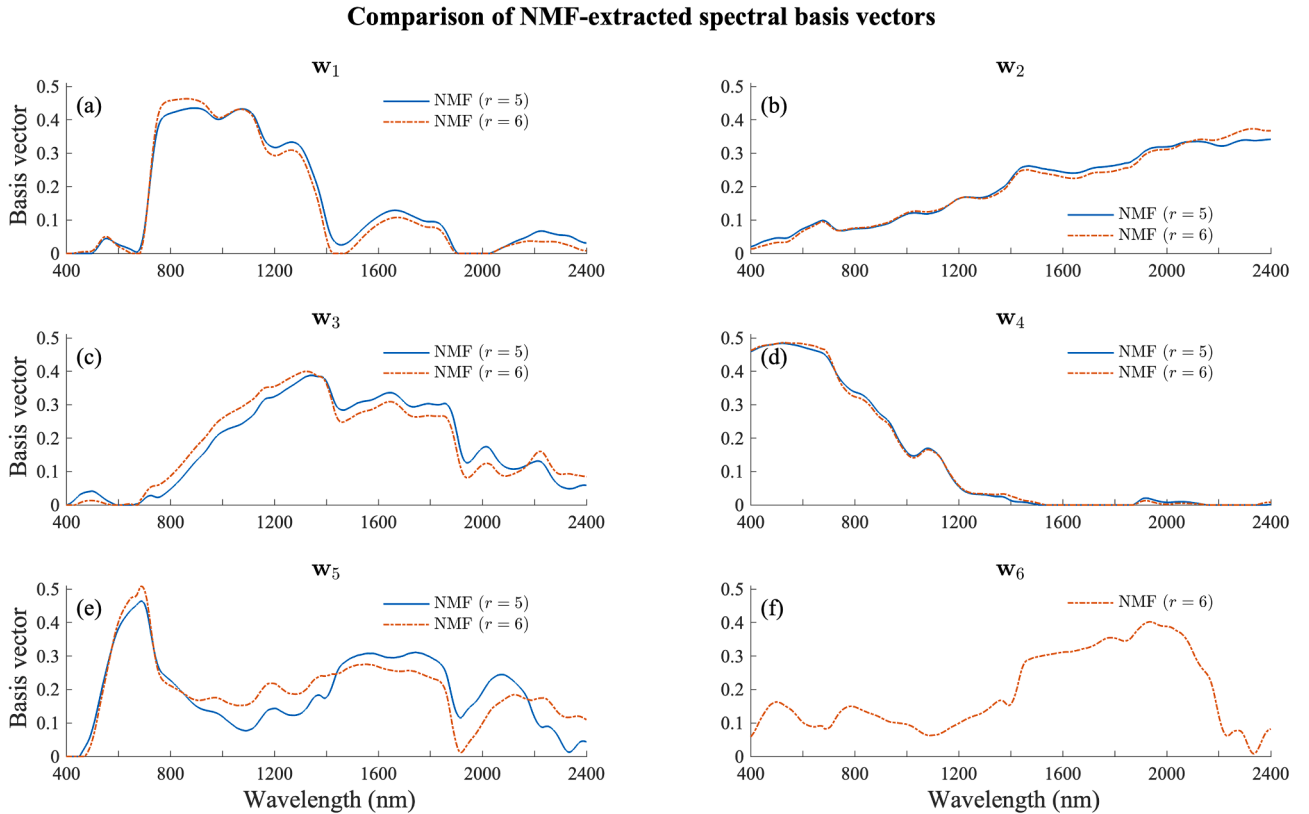


Fig. 3. Comparison of NMF-extracted spectral basis vectors obtained using desired ranks of $r = 5$ and $r = 6$ from the USGS/ASTER spectral dataset. Panels (a)–(f) correspond to basis vectors w_1 – w_6 , respectively. For each basis vector, the solutions obtained with $r = 5$ (solid blue) and $r = 6$ (dashed orange) are compared within the same panel. Each basis vector is displayed individually to improve readability. The first five basis vectors remain highly consistent between the two decompositions, whereas the additional basis vector w_6 , is introduced only in the $r = 6$ decomposition and primarily captures residual statistical spectral variability.

For the solution with $r = 5$, the five basis vectors exhibit distinct spectral characteristics. $\mathbf{w}_1$ resembles a vegetation-like spectral component, characterized by a pronounced red-edge transition near 700 nm, high reflectance throughout the NIR region, and distinct water-absorption features in the shortwave infrared SWIR. $\mathbf{w}_2$ corresponds to a bare-surface spectral component, resembling a smooth and gradually increasing reflectance from the visible to the SWIR region, a characteristic spectral behavior of many soil and exposed terrestrial surfaces. $\mathbf{w}_3$ captures transition-type spectral characteristics with broad SWIR absorption features associated with mixtures of mineral-rich and sparsely vegetated surfaces. $\mathbf{w}_4$ exhibits snow-like spectral behavior, with high visible reflectance followed by a rapid decrease in the SWIR due to strong ice absorption. $\mathbf{w}_5$ reflects the remaining dominant spectral variability associated with spectrally heterogeneous bright terrestrial surfaces.

Compared with the $r = 5$ solution, the first five basis vectors obtained with $r = 6$ remain highly consistent, indicating that the dominant low-dimensional spectral structure is stable. The additional component $\mathbf{w}_6$, primarily captures residual statistical variability rather than an independent spectral characteristic.

The selection of the desired rank is a critical step because it determines the balance between reconstruction fidelity, model complexity, and coefficient stability. If the desired rank is too small, distinct spectral characteristics may be merged into the same statistical component. Conversely, increasing the rank introduces additional components that must be estimated from the same limited multispectral observations, providing progressively smaller improvements in reconstruction accuracy while reducing component interpretability.

Fig. 4 summarizes the mean absolute error (MAE) and root mean squared error (RMSE), together with their corresponding standard deviations, obtained from NMF-based spectral reconstruction of the 297 reflectance spectra (400–2400 nm) shown in Fig. 1, for desired ranks from $r = 2$ to $r = 7$. Both reconstruction metrics decrease monotonically as the desired rank increases, although the improvement becomes noticeably smaller beyond $r = 5$, indicating diminishing returns with increasing model complexity.

The subsequent reconstruction is performed using only the seven monthly TROPOMI/GRASP BRDF bands (416, 440, 494, 670, 747, 772, and 2313 nm). Consequently, the desired rank is naturally constrained to $r \leq 7$, since the number of unknown NMF coefficients cannot exceed

the number of available multispectral observations if a unique coefficient solution is to be obtained.

The subsequent reconstruction is performed using only the seven monthly TROPOMI/GRASP BRDF bands (416, 440, 494, 670, 747, 772, and 2313 nm). Consequently, the desired rank is naturally constrained to $r \leq 7$, since the number of unknown NMF coefficients cannot exceed the number of available multispectral observations if a unique coefficient solution is to be obtained.

Considering both the statistical interpretability of the extracted basis vectors (Fig. 3) and the reconstruction performance (Fig. 4), $r = 5$ is adopted throughout this study. This configuration captures the dominant spectral variability while maintaining low reconstruction errors and a well-constrained coefficient estimation problem. Although slightly lower reconstruction errors are obtained for $r = 6$ and $r = 7$, the additional basis vectors mainly represent residual statistical variability and provide only marginal performance gains. Therefore, $r = 5$ offers a practical compromise between reconstruction accuracy, model simplicity, coefficient stability, and spectral interpretability.

4.2. Spatiotemporal dynamics and physical interpretability of mixing coefficients

The following reconstruction results in this section are obtained using the MU algorithm for coefficient optimization unless otherwise specified. Fig. 5 illustrates the monthly average spatial distribution of the MU-optimized mixing coefficients associated with the vegetation-like spectral component (denoted as $\mathbf{H}_1$) across North America. Due to strict quality control applied to the GRASP BRDF dataset, pixels contaminated by snow, ice, or clouds were excluded, resulting in varying data gaps that are particularly evident in high-latitude regions during winter. Panels (a)–(l) demonstrate a clear seasonal cycle: from January to March, vegetation coefficients remain generally low, with many northern regions showing sparse pixel availability. As spring shifts into summer (April–August), a marked increase in coefficients is observed throughout the central, eastern, and northern regions, reflecting vigorous canopy development and biomass accumulation. Following the autumn transition, these values steadily decline, aligning with the predictable patterns of seasonal vegetation senescence.

In contrast to the dynamic seasonal variations exhibited by the vegetation-like spectral component, Fig. 6 shows that the MU-optimized

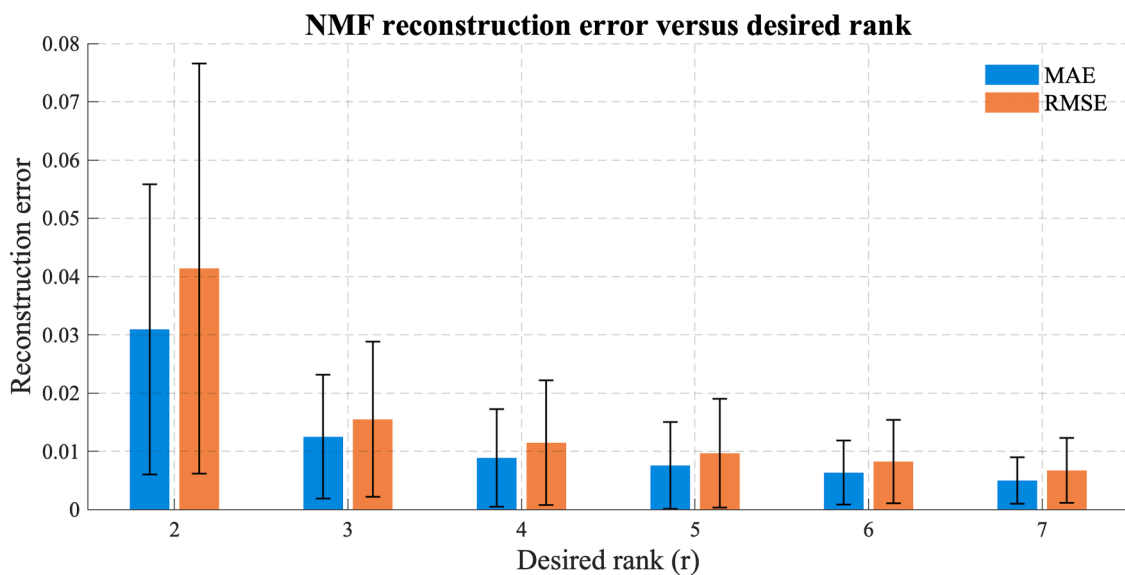


Fig. 4. Mean absolute error (MAE) and root mean squared error (RMSE), together with their corresponding standard deviations, as a function of the desired rank (r). The statistics were obtained from NMF reconstruction of the 297 USGS/ASTER reflectance spectra (400–2400 nm) using desired ranks from $r = 2$ to $r = 7$. Both metrics decrease with increasing rank, whereas the improvement becomes marginal beyond $r = 5$, supporting the selection of $r = 5$ for the subsequent spectral reconstruction.

MU-optimized mixing coefficients for the vegetation-like spectral component

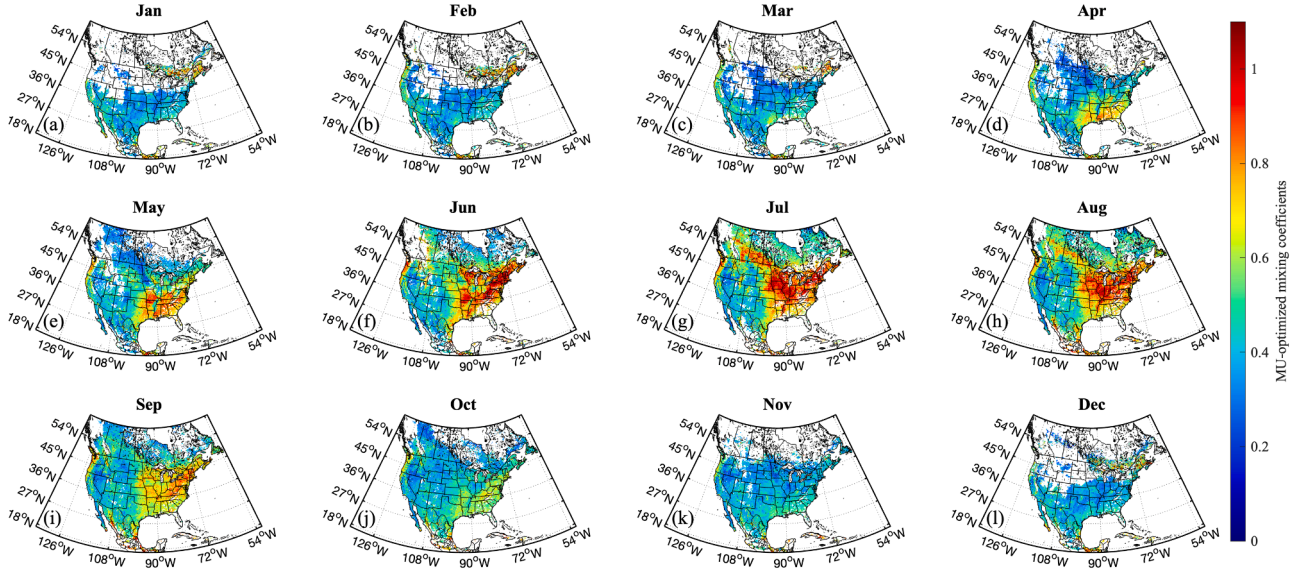


Fig. 5. Spatiotemporal distribution of the mixing coefficients for the vegetation-like spectral component across North America. Panels (a–l) show the monthly mean distributions of the mixing coefficients optimized using the MU algorithm. Maps for January through November are generated from the corresponding monthly mean GRASP BRDF products in 2020, whereas the December map is generated from the December 2019 monthly mean product because of the corresponding 2020 data are unavailable. Unless otherwise noted, all subsequent figures follow the same data selection convention. Spatial gaps indicate regions excluded due to rigorous quality control protocols applied to the GRASP BRDF dataset.

MU-optimized mixing coefficients for the bare-surface spectral component

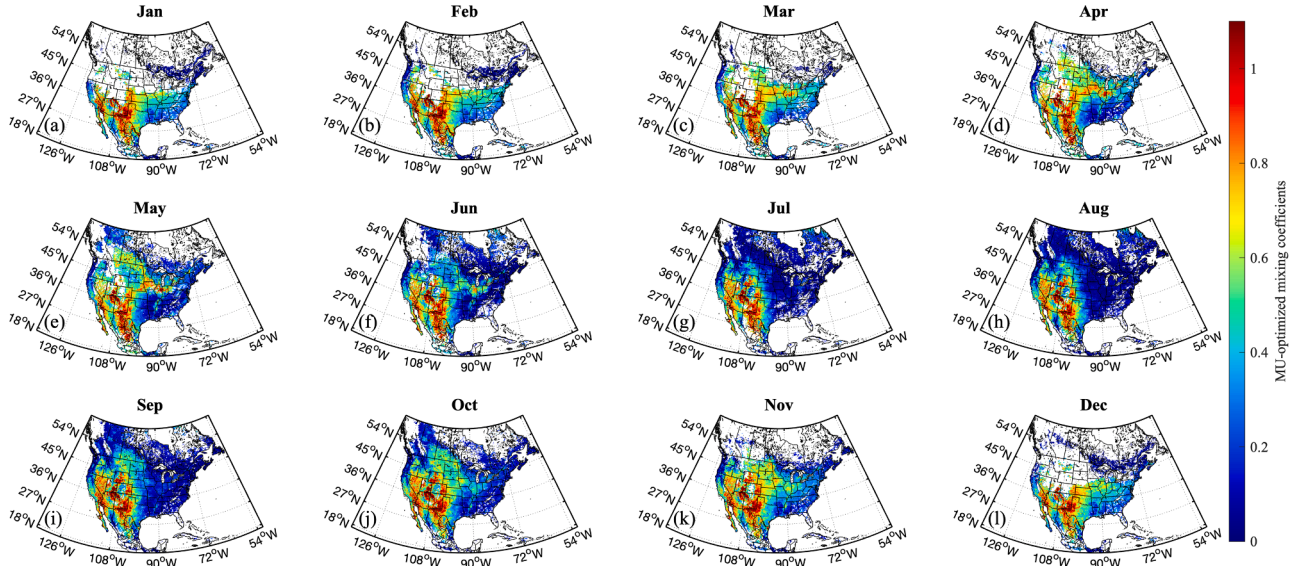


Fig. 6. Spatiotemporal distribution of mixing coefficients for the bare-surface spectral component across North America. Panels (a–l) show the monthly mean distributions of the MU-optimized mixing coefficients. High coefficient values primarily occur over arid and semi-arid zones.

mixing coefficients for the bare-surface spectral component (denoted as H_2) maintain relatively stable regional spatial patterns throughout the year. The highest soil coefficients are persistently concentrated in the arid and semi-arid zones of the southwestern United States, northern Mexico, and central-western North America, where sparse vegetative cover allows surface reflectance to closely mirror typical soil spectral signatures. While these coefficients slightly decrease during the peak growing season as vegetation thrives, they tend to rise during autumn and winter in agricultural zones. This rise is driven by the combined influence of crop harvesting, vegetation senescence, and the resulting exposure of bare surfaces.

The spatiotemporal distributions of these coefficients exhibit clear, physically meaningful, and complementary patterns. The vegetation endmember rises significantly during the growing season, while the bare soil-like endmember maintains high values in arid regions or increases when vegetation declines. A distinct inverse relationship is observed in agricultural and mid-latitude regions: during spring and summer, the rapid growth of vegetation drives its mixing coefficient upward while the bare soil contribution diminishes accordingly. Conversely, in autumn and winter, this trend reverses as surface exposure increases. This complementary behavior validates the independence and representativeness of the extracted NMF endmembers, confirming that the $r =$

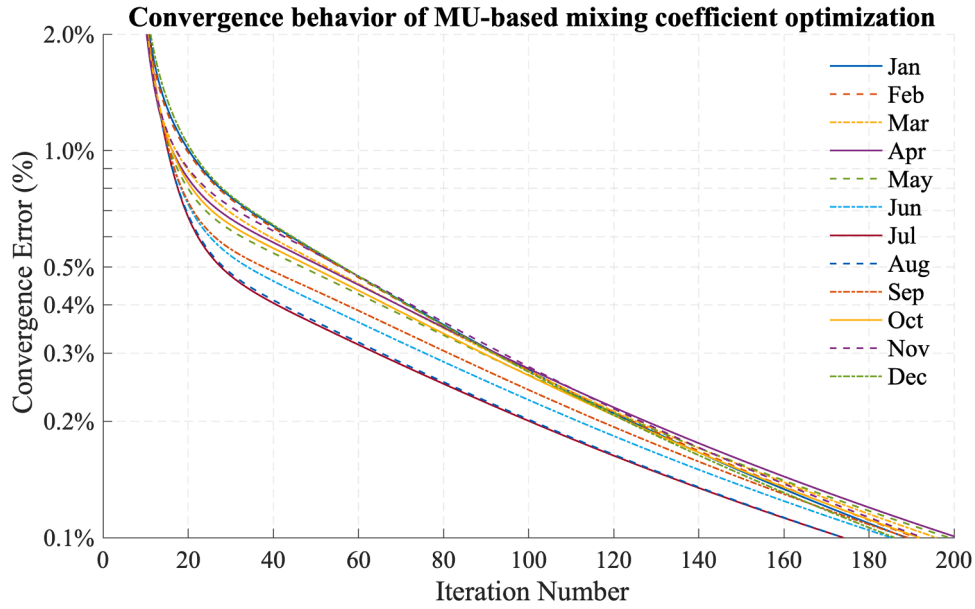


Fig. 7. Iterative convergence profiles of the MU algorithm for mixing coefficient optimization. The plot illustrates the monotonic decrease in convergence error with increasing iteration count across different months. Individual colors and line styles differentiate the results for January to December.

5 configuration accurately distinguishes and quantifies the spectral contributions of primary land cover types.

Furthermore, Fig. 7 characterizes the convergence behavior of the MU algorithm for mixing coefficient optimization across different monthly data scenarios. The convergence error consistently and monotonically decreases as iterations proceed, demonstrating the inherent stability of the NMF approach. While initial error levels and early descent rates vary by month, likely due to seasonal variations in surface spectral complexity, the curves for all months follow a similar convergence trajectory. After approximately 170–200 iterations, the relative convergence errors fall below the predefined stopping criterion of 0.1% and stabilize thereafter, indicating satisfactory convergence of the MU optimization. This suggests that seasonal variations have limited influence on the algorithm's ultimate stability, underscoring the robustness of the MU solver for processing the seasonally varying GRASP TROPOMI BRDF dataset.

4.3. Spatial fidelity and spectral continuity of the reconstructed BRDF

Fig. 8 provides a three-dimensional visualization of the spectral reconstruction, illustrating the transformation from seven discrete TROPOMI/GRASP spectral bands to continuous hyperspectral reflectance over North America. The left panels show the original multi-spectral isotropic reflectance at seven wavelengths (416, 440, 494, 670, 747, 772, and 2313 nm), whereas the right panels present the corresponding continuous hyperspectral results spanning 400–2400 nm. The reconstructed hyperspectral cubes preserve the overall spatial distribution and reflectance gradients of the original multispectral observations while providing smooth, continuous spectral variations across the measured wavelengths. July and October are shown as representative examples to illustrate the reconstruction under different seasonal surface conditions. The purpose of this visualization is to demonstrate the concept and qualitative performance of the proposed spectral reconstruction rather than to interpret seasonal surface characteristics.

To further evaluate the physical consistency of the proposed framework, Figs. 9 and 10 present the monthly spectral evolution of the reconstructed isotropic reflectance at eight representative terrestrial sites, with the odd and even months displayed separately for improved visualization. These sites were selected along two latitudinal transects (33.23°N and 39.53°N) to capture diverse longitudinal surface

conditions. The continuous curves represent the MU-optimized NMF-reconstructed hyperspectral reflectance, while the open circles denote the original TROPOMI/GRASP BRDF isotropic parameter values at the anchor wavelengths. For visual clarity, only five of the seven anchor wavelengths are shown. Overall, the reconstructed spectra accurately capture the overall spectral trends of the discrete observations while exhibiting smooth and physically realistic behavior across the VIS, NIR, and SWIR regions.

It should be noted that the reconstructed curves are not expected to pass exactly through every anchor point. Rather than fitting each wavelength independently, the MU algorithm optimizes the mixing coefficients by jointly considering information from all seven anchor wavelengths. Since the TROPOMI/GRASP BRDF isotropic parameters may contain retrieval uncertainties and individual anchor wavelengths may occasionally deviate from the spectral characteristics represented by the extracted NMF basis vectors, slight adjustments are introduced to achieve a more globally consistent hyperspectral reconstruction. As the transects extend eastward across the continent, variations in surface composition are reflected in distinct differences in reflectance magnitude and seasonal variability. Nevertheless, the reconstructed spectra consistently preserve smooth and physically consistent spectral behavior across diverse geographic regions and seasons.

4.4. Correlation analysis between NMF mixing coefficients and vegetation indices

Fig. 11 illustrates the density scatterplots correlating the MU-optimized mixing coefficients with classic vegetation indices, with H_1 corresponding to the vegetation-like spectral component and H_2 corresponds to the bare-surface spectral component, providing a quantitative validation of their physical significance. The Enhanced Vegetation Index (EVI), Normalized Difference Vegetation Index (NDVI), and Normalized Difference Water Index (NDWI) are calculated using the reconstructed isotropic coefficients at specific wavelengths.

Here, the EVI is calculated by [60,61]:

$$EVI = G \frac{k_{iso}^{NIR} - k_{iso}^{red}}{k_{iso}^{NIR} + C_1 k_{iso}^{red} - C_2 k_{iso}^{blue} + L}, \quad (18)$$

where k_{iso} represents the reconstructed isotropic coefficient, the blue, red, and NIR bands correspond to 470, 670, and 870 nm, respectively,

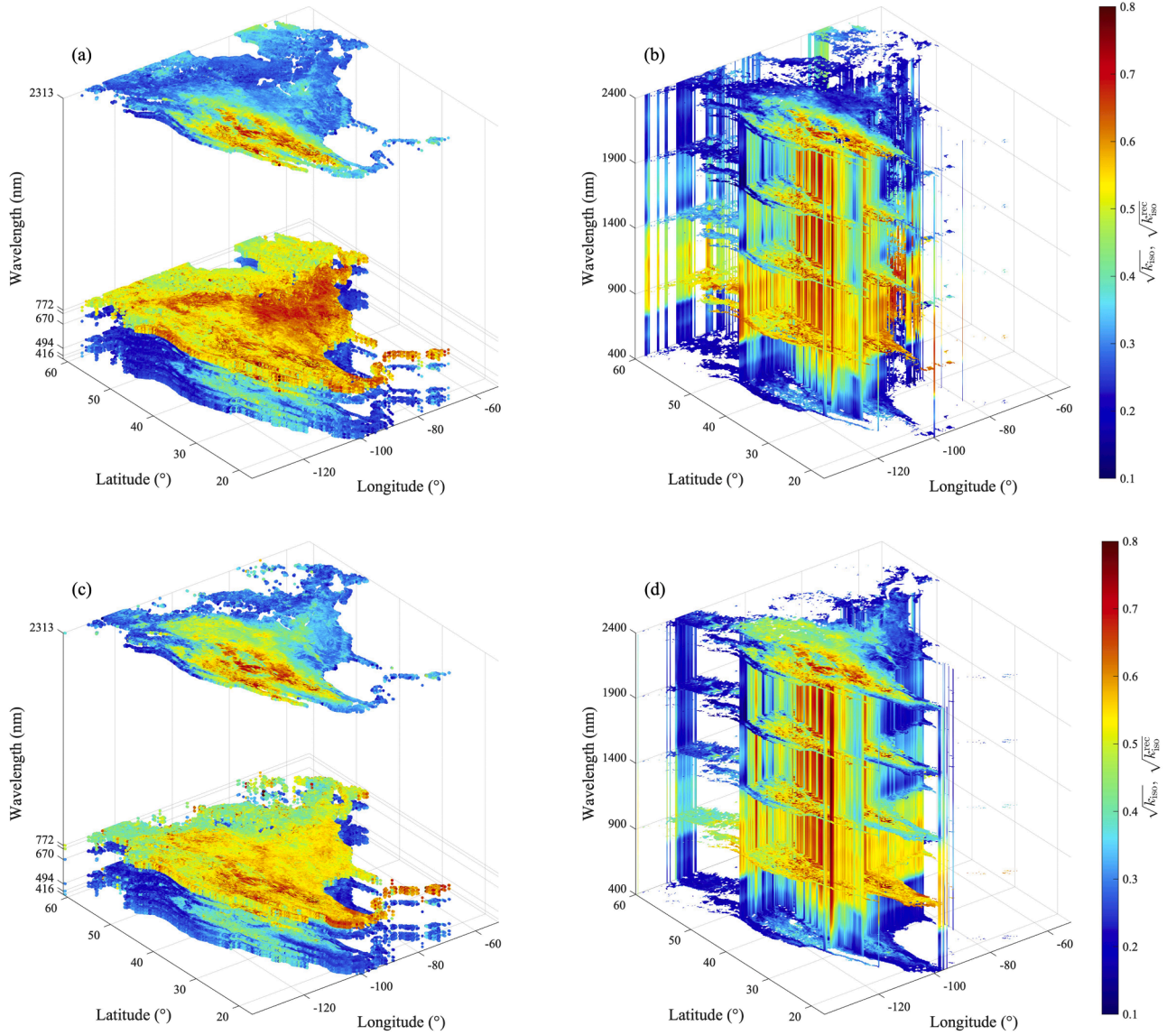


Fig. 8. Three-dimensional visualization of the spectral reconstruction from seven discrete bands to continuous hyperspectral reflectance. The left panels illustrate the original multispectral isotropic coefficients at TROPOMI/GRASP wavelengths (416, 440, 494, 670, 747, 772, and 2313 nm), while the right panels present the corresponding reconstructed hyperspectral results spanning 400–2400 nm. Panels (a) and (b) correspond to July, and panels (c) and (d) correspond to October. To enhance visual contrast, a square-root scaling is applied to the color bar.

with the parameter values of $L = 1$, $C_1 = 6$, $C_2 = 7.5$, and $G = 2.5$. Meanwhile, the NDVI is derived by [62]:

$$\text{NDVI} = \frac{k_{\text{iso}}^{\text{NIR}} - k_{\text{iso}}^{\text{red}}}{k_{\text{iso}}^{\text{NIR}} + k_{\text{iso}}^{\text{red}}} \quad (19)$$

where the red and NIR bands align with EVI. Additionally, the NDWI is typically calculated using [63,64]:

$$\text{NDWI} = \frac{k_{\text{iso}}^{\text{NIR}} - k_{\text{iso}}^{\text{SWIR}}}{k_{\text{iso}}^{\text{NIR}} + k_{\text{iso}}^{\text{SWIR}}} \quad (20)$$

where NIR and SWIR denote the reconstructed 870 and 2130 nm bands.

The vegetation-like MU-optimized mixing coefficient (H_1) exhibits a strong positive relationship with EVI, with the highest correspondence observed during the peak growing season (July). Although the correlation becomes slightly weaker in October, the overall seasonal evolution of H_1 remains consistent with the transition from vigorous vegetation growth to autumn senescence. Conversely, the bare-surface MU-optimized mixing coefficient (H_2) shows a pronounced negative relationship

with both NDVI and NDWI throughout the two representative seasons, reflecting the increasing contribution of exposed soil and sparsely vegetated surfaces. Rather than emphasizing the correlation coefficients themselves, these results demonstrate that the extracted MU-optimized mixing coefficients exhibit physically interpretable seasonal behavior and spatial consistency with major land-cover characteristics and phenological transitions, supporting the physical plausibility of the reconstructed hyperspectral reflectance.

5. Validation of spectral reconstruction using MODIS NBAR and EMIT products

To compare the spectral reconstruction performance of the LSM and MU-optimized NMF methods using the GRASP TROPOMI BRDF monthly product, monthly mean MODIS MCD43C4 NBAR data and the corresponding monthly mean local-solar-noon solar zenith angles were generated by averaging the daily products for each month over the period from December 2019 to November 2020. The reconstructed GRASP TROPOMI NBAR results were calculated using Eq. (17),

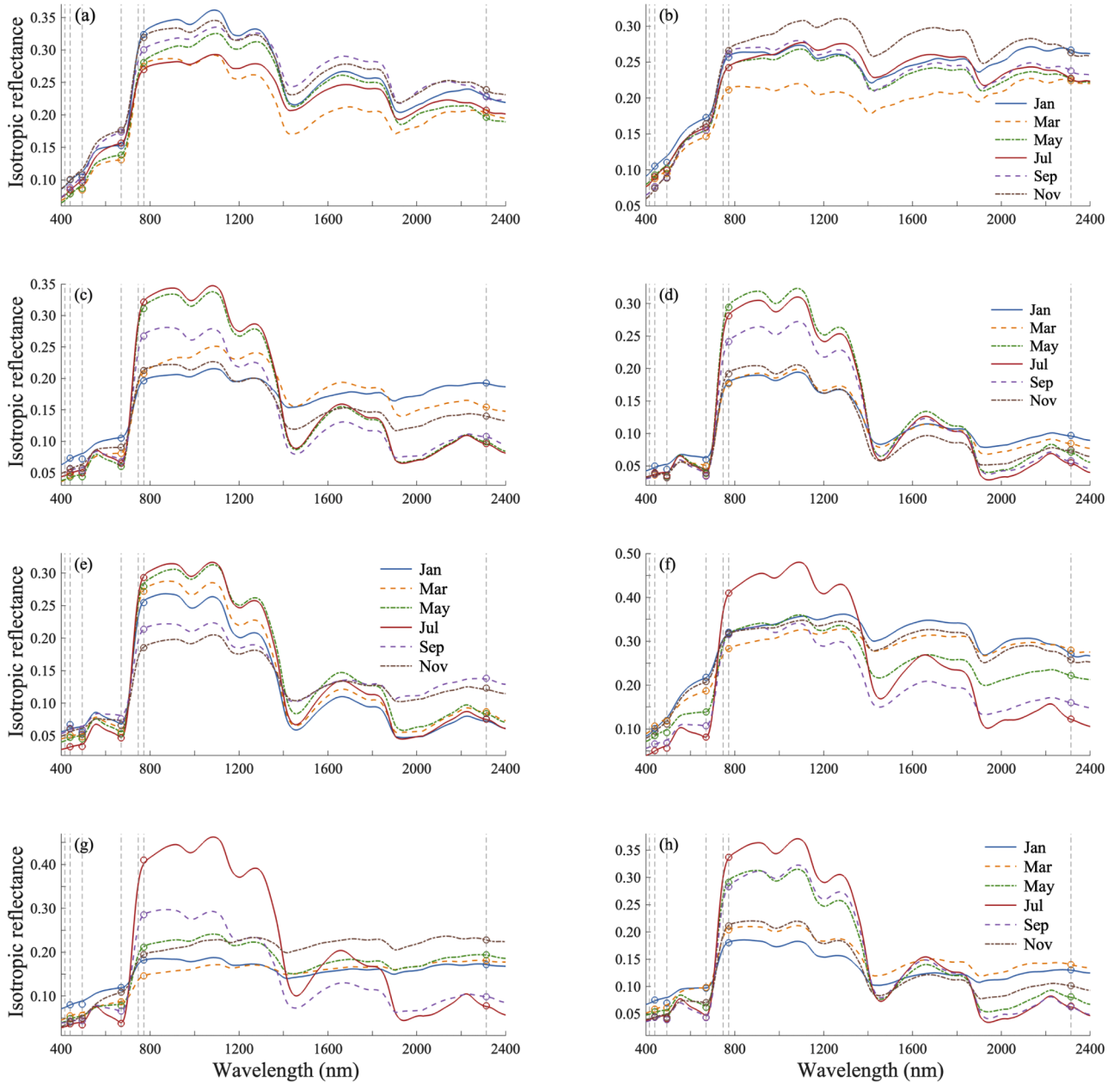


Fig. 9. Monthly spectral evolution of reconstructed isotropic reflectance at eight selected terrestrial sites for the odd months (January, March, May, July, September, and November). The continuous curves (solid and dashed lines) represent the MU-optimized NMF-reconstructed hyperspectral output from 400 to 2400 nm. The vertical gray dashed lines mark the seven TROPOMI/GRASP anchor wavelengths (416, 440, 494, 670, 747, 772, and 2313 nm). Open circles, shown in the corresponding monthly colors, denote the original TROPOMI/GRASP BRDF isotropic parameter values at the anchor wavelengths used for spectral reconstruction. For visual clarity, the markers at 416 and 747 nm are omitted because they would overlap with those at the adjacent wavelengths. Panels (a–d) correspond to sites located at 33.23°N (116.51°W, 106.61°W, 97.98°W, and 88.27°W), while panels (e–h) correspond to sites located at 39.53°N (122.89°W, 98.25°W, 89.26°W, and 75.86°W).

combining the NMF-reconstructed spectral isotropic term with the original wavelength-independent volumetric and geometric BRDF coefficients. For comparison with MODIS, both datasets were evaluated under a common NBAR geometry, with the solar zenith angle specified as the corresponding monthly mean local-solar-noon value, the viewing zenith angle fixed at 0°, and the relative azimuth angle set to 0° to represent the standard nadir-viewing geometry. Details of the supplementary validation method using EMIT hyperspectral observations are provided in Section 3.5 and are not repeated here; only representative validation results are presented in this section.

5.1. SRF-weighted spectral harmonization for MODIS NBAR comparison

To facilitate a rigorous comparison between the reconstructed TROPOMI spectra at 1-nm resolution and the MODIS NBAR product, a spectral harmonization procedure based on the MODIS spectral response function (SRF) was implemented. The USGS/ASTER spectral dataset was convolved with the SRFs of the first seven MODIS bands (Terra and Aqua), to generate SRF-weighted reflectance that is spectrally consistent with the MODIS observations. Fig. 12 illustrates the resulting relationships, where a linear regression model $y = ax + b$, was established between the original spectral dataset reflectance (x) and the corresponding SRF-weighted reflectance (y). The resulting linear coefficients, a and b ,

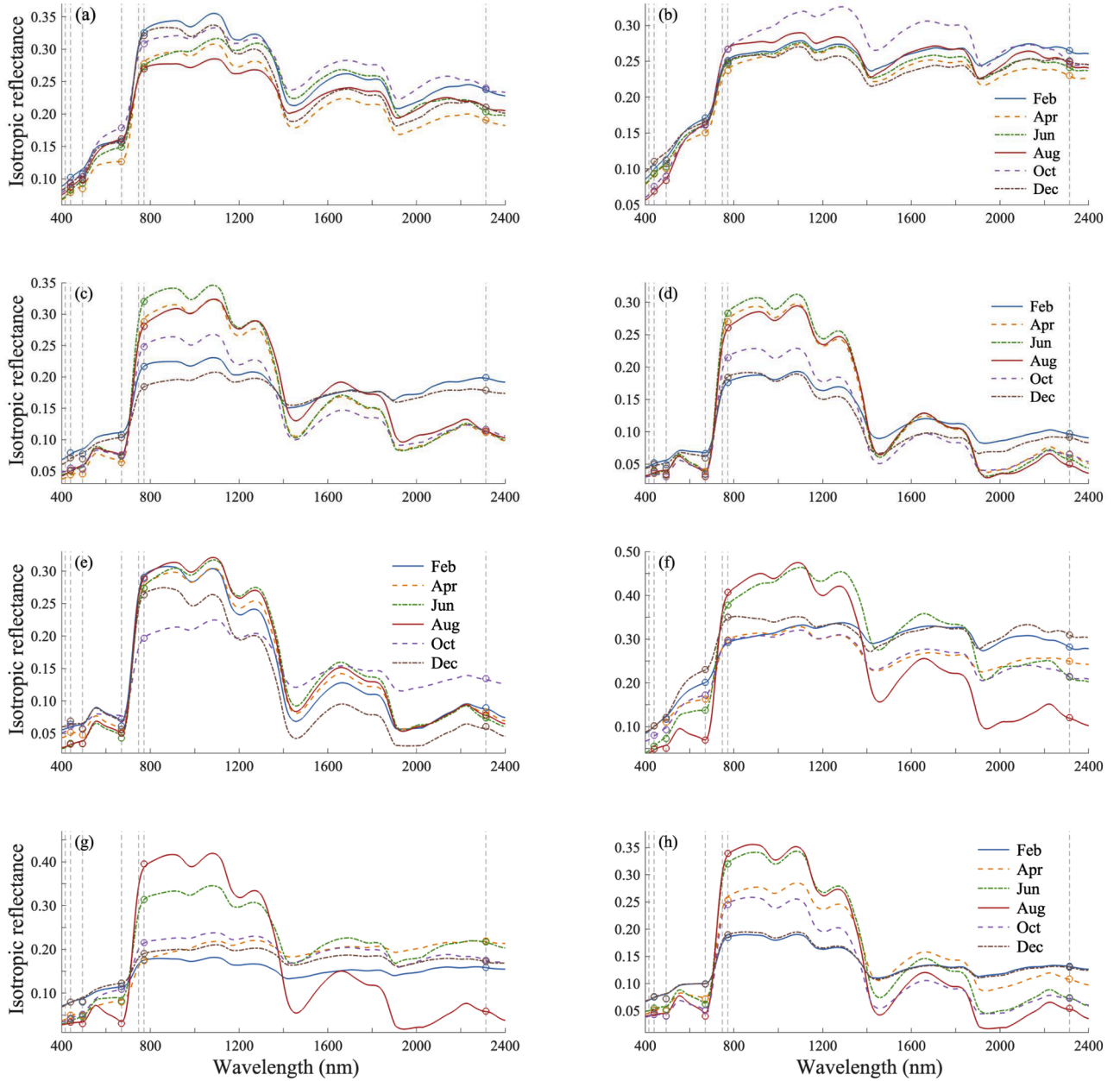


Fig. 10. Same as Fig. 9, but for the even months (February, April, June, August, October, and December).

for the seven MODIS bands are summarized in Table 2. The strong agreement observed across all seven bands demonstrates the robustness of the linear transformation, providing a consistent basis for evaluating the reconstructed TROPOMI NBAR against the MODIS NBAR product under MODIS-equivalent spectral conditions.

5.2. Spatial comparison with MODIS NBAR

Figs. 13 and 14 present cross-sensor spatial comparisons between the MODIS NBAR product and the MU-optimized reconstructed (MU-reconstructed) MODIS-equivalent TROPOMI NBAR for July and October 2020, respectively. Across the VIS and NIR bands (470 to 859 nm), the two datasets demonstrate excellent agreement in reproducing major surface features and spatial gradients across North America. This agreement confirms that the proposed NMF framework effectively preserves the spatial structure of the original BRDF during hyperspectral reconstruction. However, differences become more apparent in the

SWIR bands in both July and October. At 1240 and 1610 nm, the MU-reconstructed MODIS-equivalent TROPOMI NBAR generally exhibits slightly lower reflectance than the MODIS NBAR product over much of the eastern United States, whereas the spatial agreement remains comparatively good at 2130 nm. These spatial differences are further quantified in Section 5.3 and are independently evaluated using EMIT hyperspectral observations in Section 5.4.

5.3. Statistical assessment of reconstruction performance

Figs. 15–17 summarize the monthly statistical evaluation of the reconstruction performance. Fig. 15 presents the signed differences between the MU-reconstructed MODIS-equivalent TROPOMI NBAR and the MODIS NBAR reference, while Figs. 16 and 17 provide a quantitative comparison of the LSM and MU reconstructions using MAE, RMSE, and Pearson correlation coefficients (R).

The signed differences indicate that the MU reconstruction exhibits

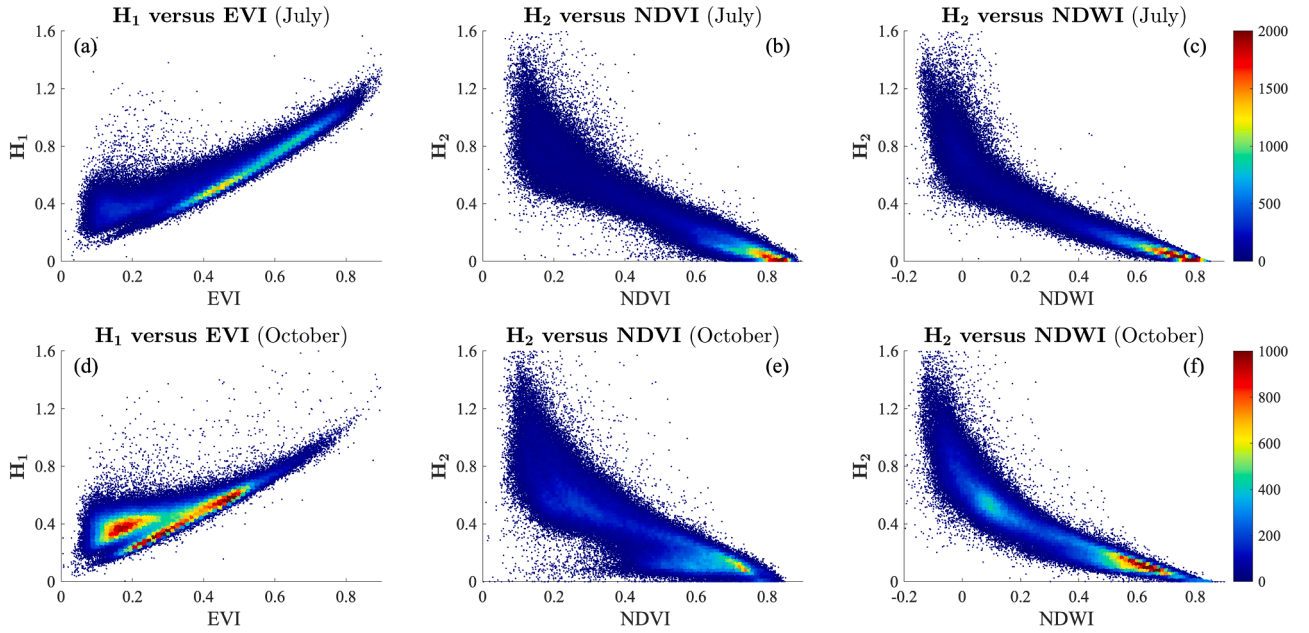


Fig. 11. Statistical relationships between MU-optimized mixing coefficients and spectral vegetation indices. Panels (a) to (c) represent July conditions (growing season), while panels (d) to (f) correspond to October (senescence season). The color gradient indicates the point density, with each row sharing a common scale. The strong positive correlation of H_1 with EVI and the pronounced negative correlation of H_2 with NDVI and NDWI highlight the clear physical interpretability of the extracted endmembers. Pearson correlation coefficients (R) for each scenario are provided as (a) 0.91, (b) -0.94 , (c) -0.94 , (d) 0.79, (e) -0.87 , and (f) -0.91 .

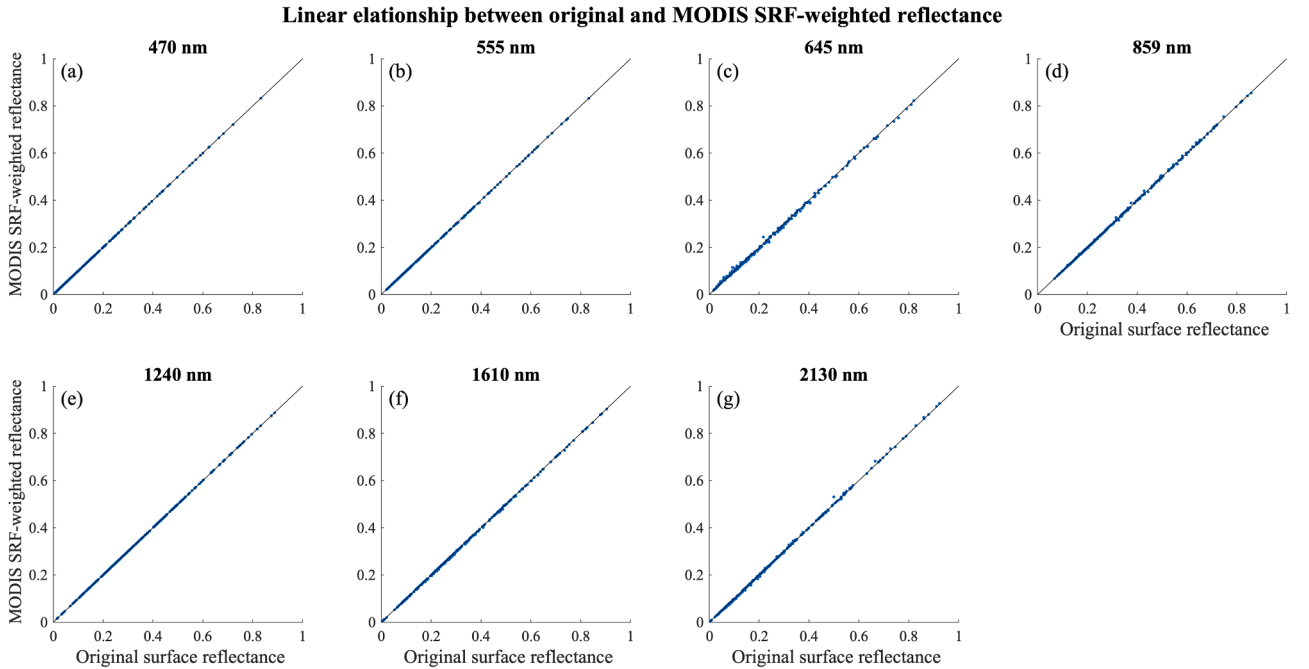


Fig. 12. Linear relationships between the original surface reflectance of the USGS/ASTER spectral dataset and the corresponding MODIS SRF-weighted reflectance for the seven MODIS bands.

only small systematic biases in the VIS and NIR bands (470, 555, 645, and 859 nm), with monthly mean differences generally remaining within ± 0.01 . Larger discrepancies are confined to the SWIR bands, where the 1240 nm and 1610 nm bands exhibit persistent negative biases of approximately -0.04 to -0.06 , while the 2130 nm band shows a moderate seasonal dependence with summer differences of about 0.02 – 0.03 .

The MAE and RMSE statistics further demonstrate the advantage of the MU optimization over the conventional LSM approach. In the VIS

and NIR bands, the MU reconstruction maintains MAE values below 0.03 and RMSE values below 0.05, compared with 0.03–0.05 and 0.05–0.08, respectively, for LSM. The improvement becomes substantially more pronounced in the SWIR region, where the MU reconstruction typically achieves MAE values of 0.02–0.06 and RMSE values of 0.04–0.08, substantially lower than the corresponding LSM ranges of 0.08–0.14 and 0.12–0.20. The largest improvement is observed at 2130 nm, where the MU reconstruction effectively suppresses the seasonal error increase present in the LSM solution.

Table 2

Linear calibration coefficients (a and b) for converting the original USGS/ASTER spectral reflectance to the corresponding MODIS SRF-weighted reflectance at seven MODIS bands, based on linear regression between the original and SRF-weighted reflectance.

Wavelength bands	a	b
470 nm	0.9999	$-1.744\text{e-}05$
555 nm	0.9988	$-4.997\text{e-}04$
640 nm	0.9912	$-2.887\text{e-}05$
859 nm	1.002	$-1.469\text{e-}03$
1240 nm	1.000	$1.906\text{e-}04$
1640 nm	0.9997	$-1.728\text{e-}03$
2130 nm	1.007	$-2.382\text{e-}03$

The superiority of the MU optimization is further confirmed by the Pearson correlation coefficients. Although both methods reproduce the seasonal variability of MODIS NBAR, the MU reconstruction consistently achieves higher correlations across all wavelengths and months. In the VIS and NIR bands, correlation coefficients generally exceed 0.90 during the summer growing season. More importantly, the MU reconstruction substantially improves the correlations in the SWIR bands while reducing the seasonal fluctuations observed for LSM.

Collectively, the simultaneous reduction in MAE and RMSE, together with the consistently higher correlation coefficients, demonstrates that the MU-reconstructed MODIS-equivalent TROPOMI NBAR achieves substantially better agreement with the MODIS NBAR product than the conventional LSM solution, confirming the effectiveness of the proposed multiplicative-update optimization framework.

5.4. Hyperspectral validation using EMIT observations

Fig. 18 presents the two representative EMIT-L2A surface reflectance scenes selected for hyperspectral validation together with their spatial aggregation onto the TROPOMI/GRASP BRDF grid. Considering the relatively narrow EMIT swath (approximately 80 km) and the limited

availability of cloud-free observations, two representative scenes were selected to provide complementary validation over contrasting land-cover types. The first scene (EMIT_L2A_RFL_001_20230808T174016_2322012_013) represents a desert-dominated surface in the arid southwestern United States and was compared with the spectra reconstructed from the August monthly TROPOMI/GRASP BRDF. The second scene (EMIT_L2A_RFL_001_20250727T194032_2520813_018) represents a cropland-dominated surface in the central United States and was compared with the spectra reconstructed from the July monthly TROPOMI/GRASP BRDF. Despite the reduced spatial resolution after aggregation, the dominant surface characteristics remain well represented, providing a consistent basis for hyperspectral comparison.

Fig. 19 presents the corresponding hyperspectral comparisons between the MU-reconstructed BRF spectra and the EMIT L2A surface reflectance. The comparison was performed using the EMIT *good-wavelengths*, which provide nearly continuous spectral coverage over approximately 400–1330 nm, 1450–1780 nm, and 1950–2400 nm after excluding channels strongly affected by atmospheric absorption. For both representative scenes, the reconstructed spectra reproduce the overall spectral characteristics observed by EMIT across the shared spectral range. Over the desert scene, the reconstructed spectra accurately capture the gradual increase in reflectance from the visible to the near-infrared region together with the major SWIR absorption features. Likewise, the cropland scene preserves the pronounced vegetation red-edge near 700 nm and the characteristic water absorption features in the SWIR region, indicating that the proposed framework effectively reconstructs both mineral and vegetation spectral signatures from the limited multispectral TROPOMI observations.

Fig. 19(e) and (f) further provide a quantitative evaluation through the wavelength-dependent mean differences and corresponding standard deviations. For the desert scene, the mean differences remain close to zero across most wavelengths, generally within approximately ± 0.03 . The cropland scene exhibits good agreement in the visible region, while a modest positive difference occurs across the vegetation red-edge

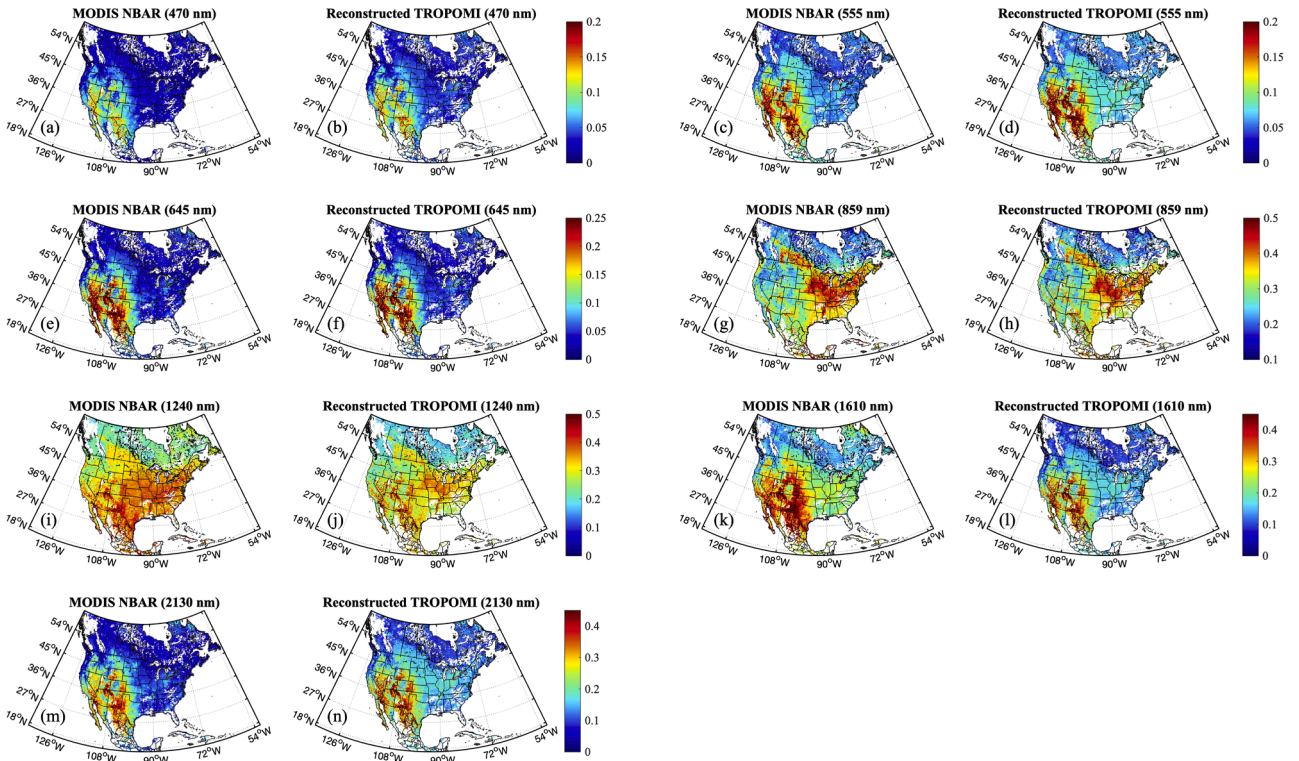


Fig. 13. Spatial comparison between the monthly mean MODIS NBAR product and the corresponding MU-optimized reconstructed MODIS-equivalent TROPOMI NBAR over North America at seven MODIS band center wavelengths (470, 555, 645, 859, 1240, 1610, and 2130 nm) for July 2020.

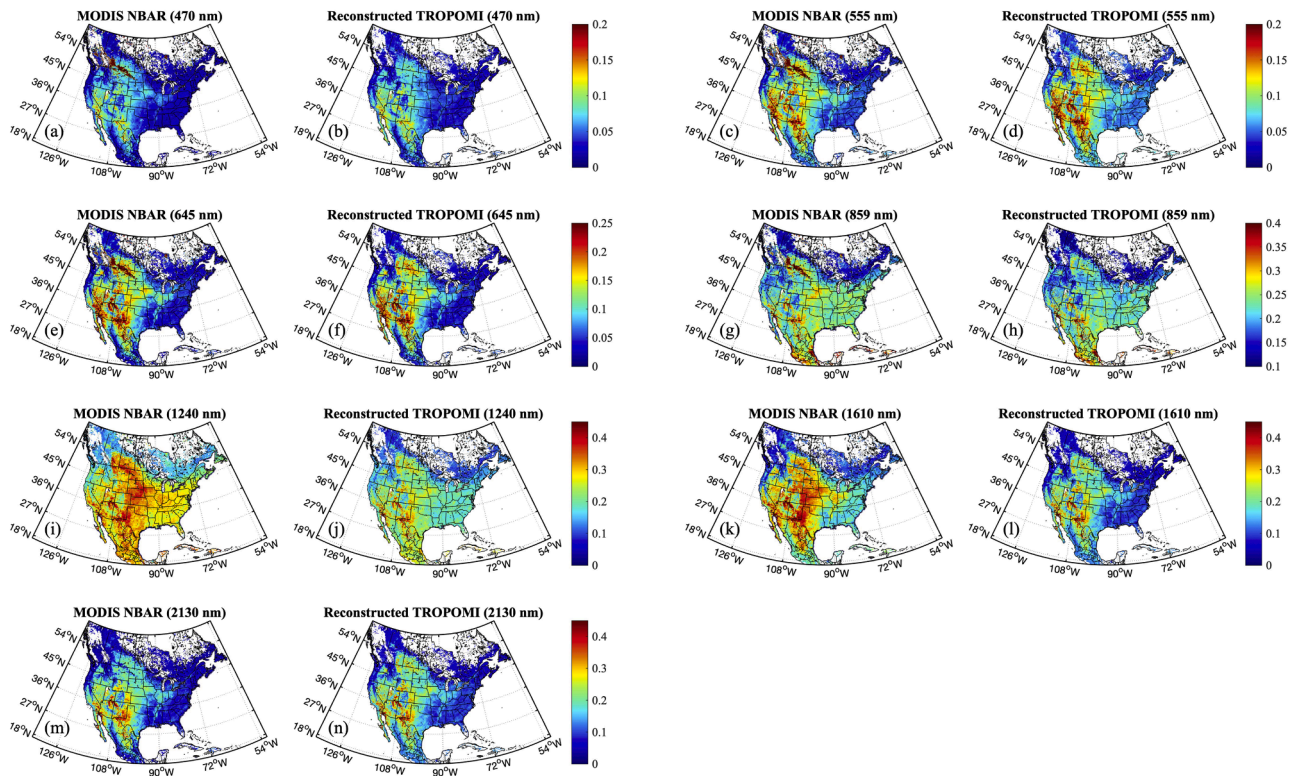


Fig. 14. Same as Fig. 13, but for October 2020.

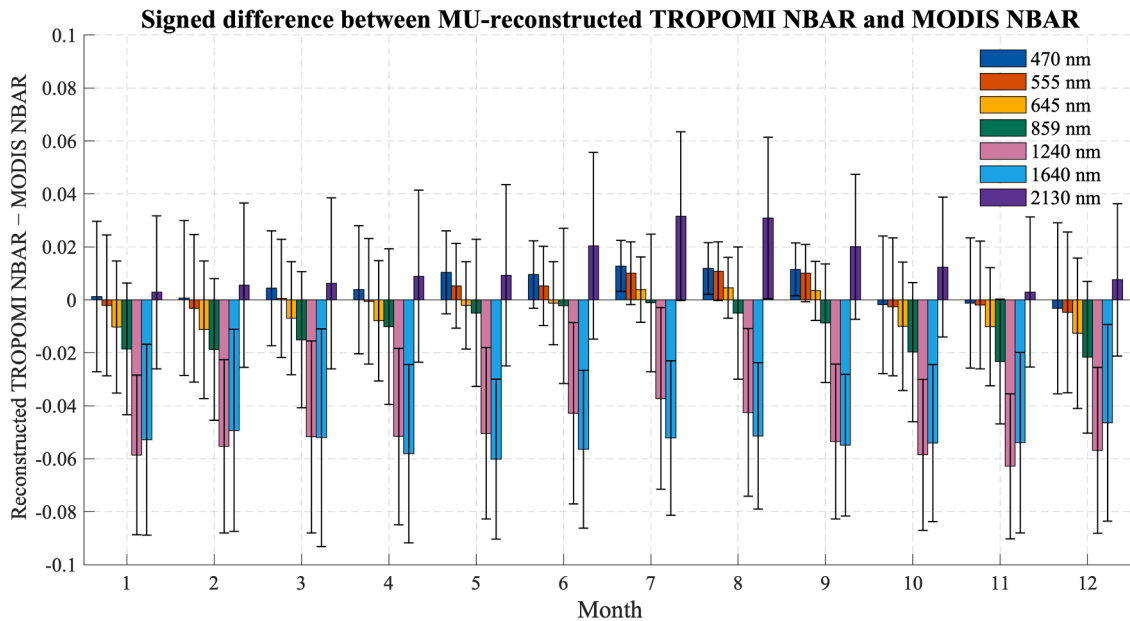


Fig. 15. Monthly mean signed differences (bars) and corresponding standard deviations (error bars) between the MU-optimized reconstructed (MU-reconstructed) MODIS-equivalent TROPOMI NBAR and the MODIS NBAR (TROPOMI – MODIS) at seven MODIS band center wavelengths (470, 555, 645, 859, 1240, 1610, and 2130 nm) from December 2019 to November 2020.

and early near-infrared region, reaching approximately +0.03 around 800 nm. The differences subsequently become negative beyond approximately 1100 nm and increase in magnitude across portions of the SWIR region, with the mean difference (MU-reconstructed BRF – EMIT) reaching approximately −0.06 to −0.08 between about 1300 and 1800 nm. This indicates that the reconstructed TROPOMI BRF is lower than the corresponding EMIT surface reflectance over much of this

spectral interval, consistent with the summer underestimation observed for the SWIR bands in the MODIS NBAR validation (Fig. 15). For both representative scenes, the wavelength-dependent mean differences are generally small relative to the corresponding within-scene spectral variability, indicating that the reconstructed spectra successfully capture the dominant hyperspectral characteristics observed by EMIT despite localized systematic differences.

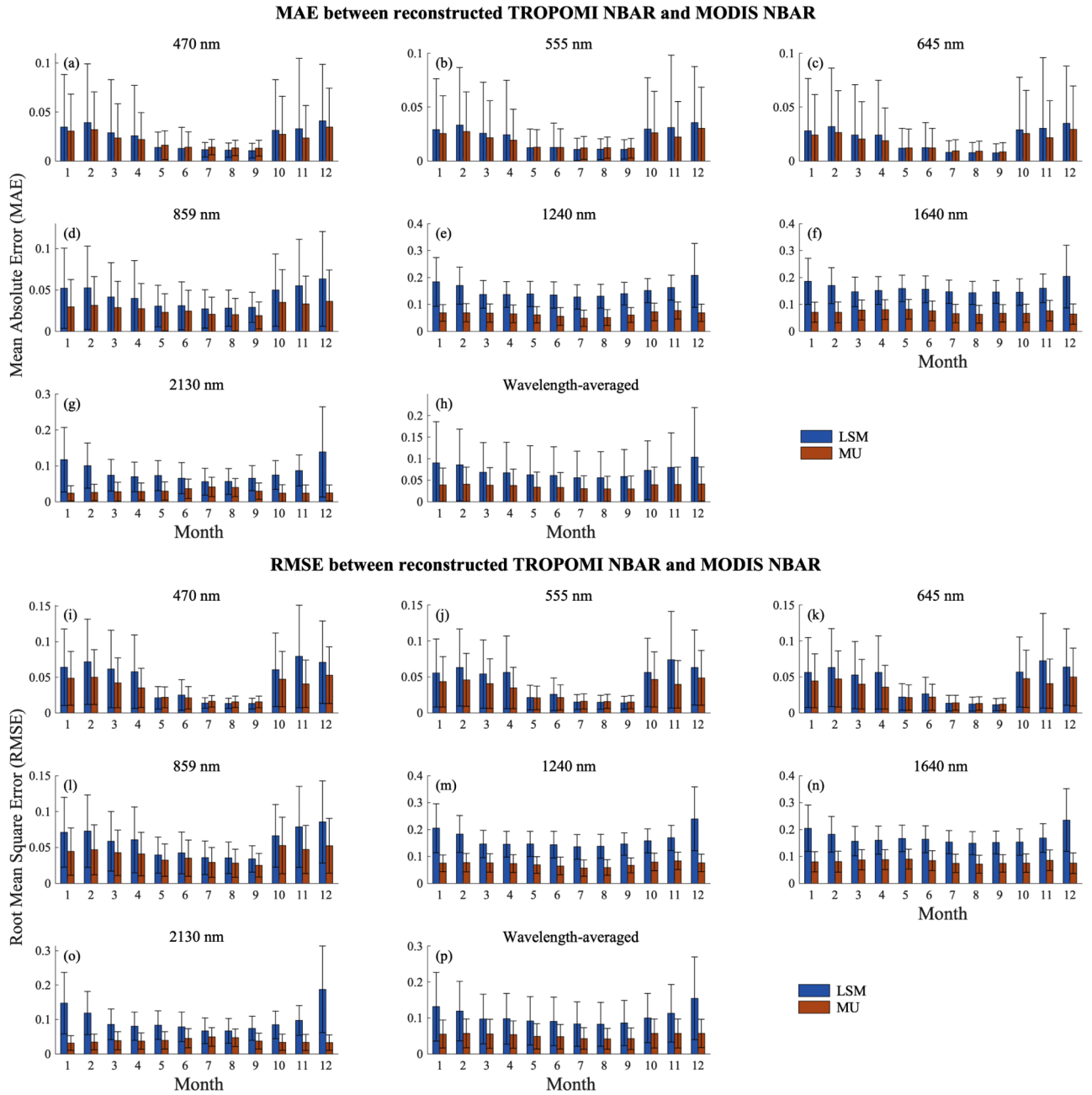


Fig. 16. Monthly mean MAE and RMSE, with corresponding standard deviations, between the reconstructed MODIS-equivalent TROPOMI NBAR and the MODIS NBAR product for the LSM and MU methods at the seven MODIS band center wavelengths and the wavelength-averaged result across the seven MODIS bands, from December 2019 to November 2020.

The EMIT validation complements the MODIS NBAR evaluation presented in Sections 5.2 and 5.3 by extending the assessment from multispectral consistency to continuous hyperspectral reconstruction. Together, these results support the capability of the proposed MU-based framework to accurately reconstruct continuous surface reflectance spectra over the 400–2400 nm wavelength range from the limited multispectral information provided by the TROPOMI/GRASP BRDF product.

6. Discussions

The MODIS NBAR and EMIT hyperspectral validations consistently demonstrate that the proposed MU-optimized NMF framework provides robust hyperspectral reconstruction from satellite BRDF products with

limited spectral bands. While excellent agreement is achieved across most visible and NIR wavelengths, systematic underestimation persists over vegetation-dominated regions, particularly around 1240 and 1610 nm in the SWIR region. The consistency of these differences across the MODIS spatial comparison, statistical evaluation, and independent EMIT hyperspectral validation suggests that they primarily reflect the reconstruction framework's current representational capability rather than the mixing-coefficient optimization strategy itself.

The observed SWIR underestimation underscores the importance of spectral library completeness in physics-based hyperspectral reconstruction. The present study uses 297 spectra from the USGS/ASTER spectral libraries, of which only 76 are vegetation spectra. Consequently, the vegetation-like basis vector extracted by NMF captures only the dominant statistical characteristics of the available vegetation

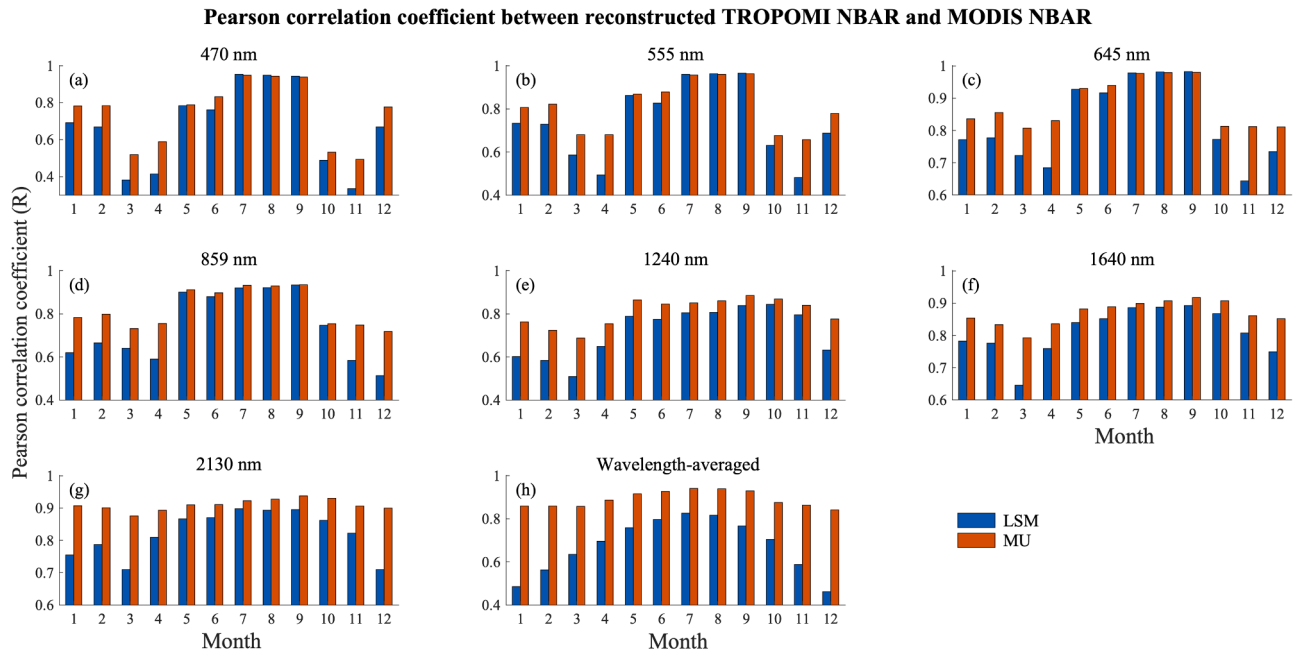


Fig. 17. Monthly mean Pearson correlation coefficients (R) between the reconstructed MODIS-equivalent TROPOMI NBAR and the MODIS NBAR product for the LSM and MU methods at the seven MODIS band center wavelengths and the wavelength-averaged result across the seven MODIS bands, from December 2019 to November 2020.

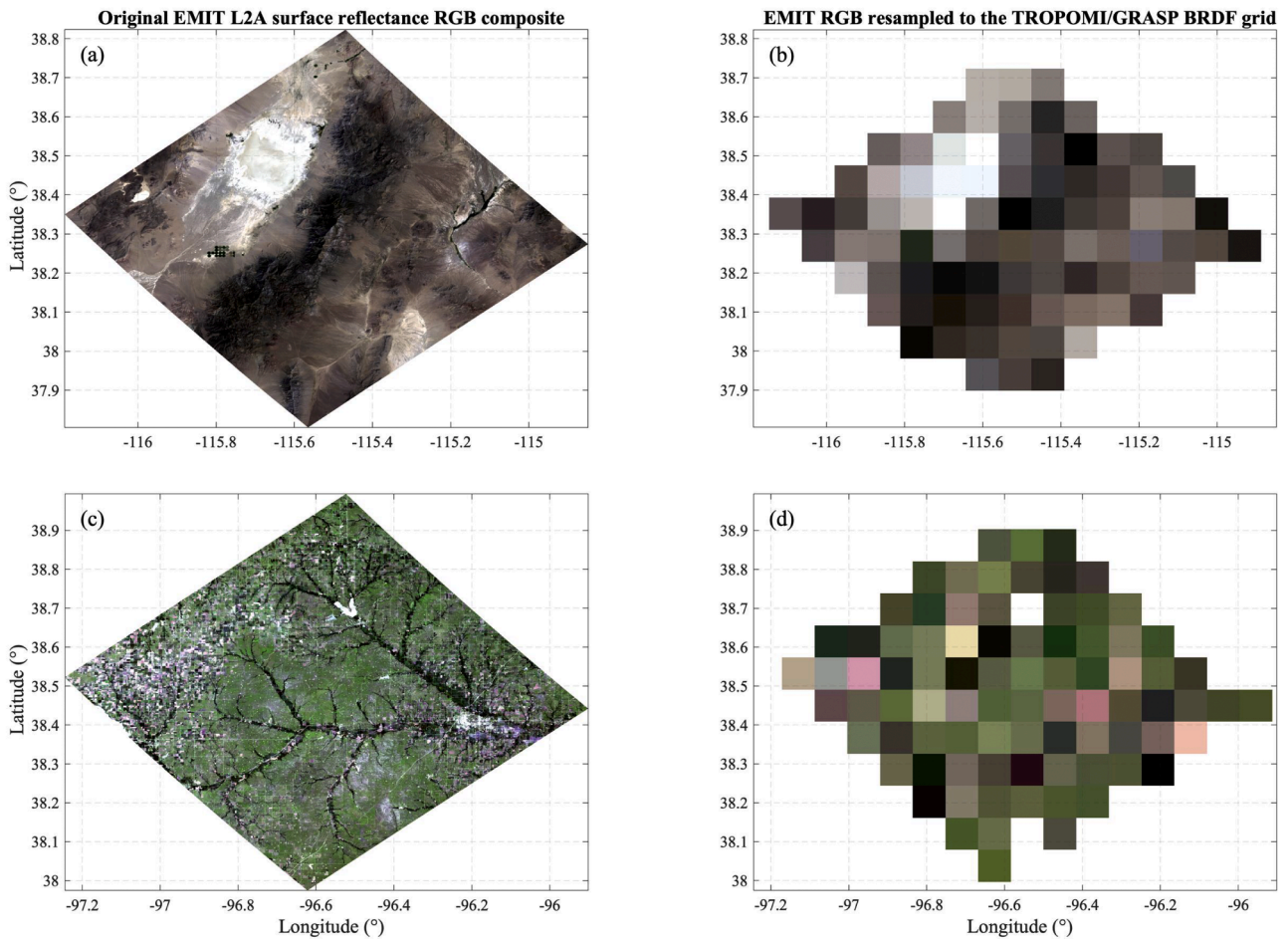


Fig. 18. Representative EMIT Level-2A (L2A) surface reflectance scenes selected for hyperspectral validation. The left column shows the original EMIT RGB composites, while the right column shows the corresponding observations after spatial aggregation and resampling onto the TROPOMI/GRASP BRDF grid. (a, b) Desert-dominated scene acquired on 8 August 2023. (c, d) Cropland-dominated scene acquired on 27 July 2025.

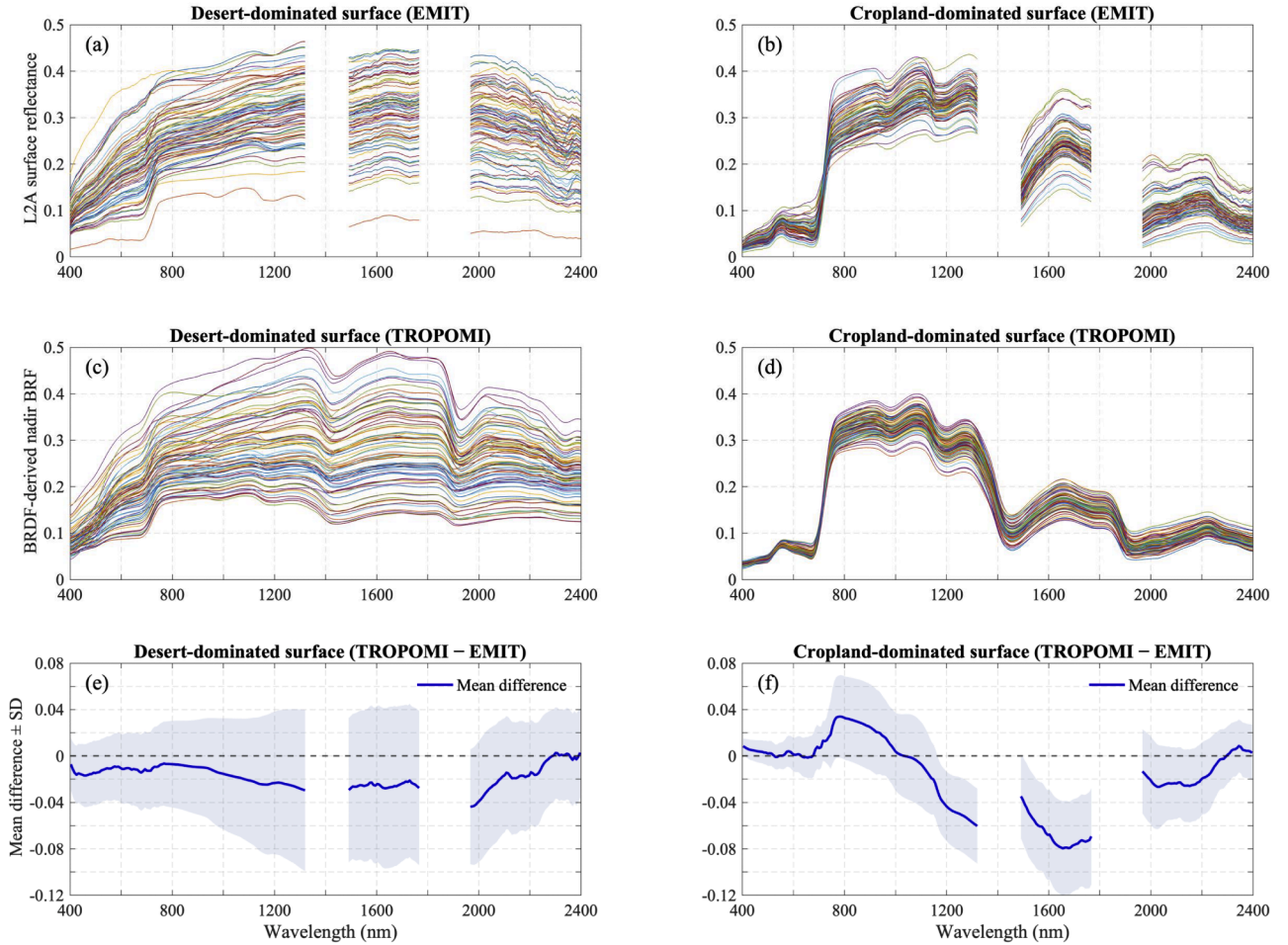


Fig. 19. Hyperspectral comparison between the MU-reconstructed BRF spectra and the EMIT L2A surface reflectance. (a, b) Representative EMIT L2A surface reflectance spectra for the desert and cropland scenes, respectively. (c, d) Corresponding MU-reconstructed BRF spectra for the two scenes. (e, f) Wavelength-dependent mean differences (MU-reconstructed – EMIT) with corresponding standard deviations for the desert and cropland scenes, respectively; solid lines denote the mean differences, and shaded regions represent one standard deviation.

samples, not the full diversity of vegetation spectral variability. This limitation is particularly evident in the SWIR region, where reflectance is strongly influenced by canopy structure, biochemical composition, and leaf water content. As a result, reconstructed spectra tend to underestimate reflectance over vegetation-dominated surfaces, especially at 1240 and 1610 nm. Future improvements are expected by incorporating more comprehensive spectral libraries, including the latest USGS Spectral Library Version 7 [44] together with the ECOSTRESS (Ecosystem Spaceborne Thermal Radiometer Experiment on Space Station) spectral library [46], which provides a more comprehensive statistical representation of vegetation and non-photosynthetic vegetation spectral variability. These expanded datasets should provide a more complete statistical representation of vegetation spectral variability and further improve reconstruction accuracy.

Another limitation arises from the use of a single global set of NMF basis vectors. Although this low-dimensional representation efficiently captures the dominant spectral characteristics of natural and man-made surfaces, a limited number of basis vectors ($r = 5$ in this study) cannot fully characterize the spectral diversity of heterogeneous land surfaces or spectrally mixed pixels. A natural extension of the proposed framework is therefore to introduce soft clustering prior to spectral reconstruction. Instead of representing all surfaces using a single global set of NMF basis vectors, the spectral dataset can first be partitioned into several statistical spectral classes. Each target pixel can then be assigned continuous membership weights across these classes, allowing class-specific basis vectors to reconstruct local spectral features. The final

hyperspectral reflectance would then be obtained through a weighted combination of the class-wise reconstructions, introducing additional statistical constraints while preserving the flexibility and physical interpretability of the MU optimization framework.

Residual differences are also influenced by differences between the TROPOMI/GRASP BRDF monthly product and the monthly-mean MODIS NBAR dataset generated in this study for validation. Although both datasets represent monthly mean surface reflectance, they are produced using different observation sampling, temporal compositing, quality-control filtering, and retrieval strategies, which inevitably introduce systematic discrepancies. In addition, the TROPOMI/GRASP BRDF monthly product provides no BRDF isotropic coefficients between 772 and 2313 nm. Consequently, surface reflectance within this broad spectral interval must be reconstructed statistically from the NMF basis vectors, making the results increasingly sensitive to both basis-vector representation and coefficient-estimation errors.

The proposed framework is also expected to exhibit different characteristics across satellite products with different spatial resolutions. Because moderate- and coarse-resolution observations generally contain a larger proportion of spectrally mixed pixels, the statistical representation provided by NMF may be particularly advantageous. Future work will therefore extend the proposed framework to multiple surface reflectance products spanning a broad range of spatial resolutions, including the MODIS MCD43C1 (0.05°) and MCD43A1 (500 m) BRDF products, the GOES-R Advanced Baseline Imager (ABI) Level-2 bidirectional reflectance factor (BRF) products (0.5–2 km), and Landsat

Collection 2 Level-2 (30 m) surface reflectance products, with independent validation provided by EMIT L2A hyperspectral observations. Such cross-sensor and multi-resolution evaluations will provide a more comprehensive assessment of the scalability and transferability of the proposed MU-based reconstruction framework across diverse Earth observation systems.

7. Conclusions

This study presented a training-free, physically interpretable hyperspectral reconstruction framework based on NMF to extend the monthly TROPOMI/GRASP BRDF product from seven multispectral bands to continuous surface reflectance spectra spanning 400–2400 nm. By combining physically interpretable NMF basis vectors with multiplicative-update (MU) mixing-coefficient optimization, the proposed framework reconstructs physically meaningful hyperspectral reflectance while naturally satisfying the non-negativity constraint. Comprehensive validation was performed using both the MODIS MCD43C4 NBAR product and independent EMIT L2A hyperspectral observations. The principal findings of this study are summarized as follows.

- (1) Robust hyperspectral reconstruction from limited multispectral observations. The proposed MU-optimized framework successfully reconstructs continuous hyperspectral surface reflectance from only seven TROPOMI/GRASP BRDF bands. The reconstructed hyperspectral isotropic parameters exhibit physically consistent spatial distributions and seasonal evolution across North America, while the extracted vegetation-like and bare-surface spectral components capture the dominant spectral characteristics of natural land surfaces.
- (2) Improved reconstruction performance through multiplicative-update optimization. Compared with the conventional least-squares solution, the MU optimization provides more robust coefficient estimation while preserving physically meaningful non-negative solutions. Validation against the MODIS MCD43C4 NBAR product demonstrates excellent agreement in the visible and near-infrared regions, and independent EMIT hyperspectral observations further confirm that the reconstructed spectra successfully reproduce the dominant hyperspectral characteristics of representative natural surfaces over the continuous 400–2400 nm spectral range.
- (3) Remaining limitations and future potential. Systematic underestimation is primarily observed over vegetation-dominated regions in portions of the SWIR region, highlighting opportunities for further improvement in spectral representation under limited multispectral constraints. Nevertheless, the overall consistency demonstrated by both the MODIS and EMIT validations indicates that the proposed framework provides a robust and reliable solution for continuous hyperspectral reconstruction from multispectral satellite observations.

The proposed MU-based NMF framework integrates physical interpretability, computational efficiency, and sensor independence into a unified reconstruction strategy. More broadly, this study demonstrates that physically interpretable spectral representations, when paired with multiplicative-update optimization, offer an effective and transparent alternative to purely data-driven hyperspectral reconstruction. This framework provides a scalable methodological foundation for future cross-sensor harmonization and multi-resolution surface reflectance reconstruction from satellite products with limited spectral bands, including BRDF, BRF, and surface reflectance products.

Declaration of generative AI and AI-assisted technologies in the manuscript preparation process

During the preparation of this work, the first author used Gemini to perform language polishing and structural refinement of the manuscript text. After using this tool, the first author reviewed and edited the content as needed to ensure scientific accuracy and takes full responsibility for the content of the published article.

CRediT authorship contribution statement

Weizhen Hou: Writing – review & editing, Writing – original draft, Visualization, Validation, Software, Methodology, Investigation, Formal analysis, Conceptualization. **Jun Wang:** Writing – review & editing, Supervision, Methodology, Funding acquisition, Formal analysis. **Xiong Liu:** Writing – review & editing, Supervision, Funding acquisition, Conceptualization. **Cheng Chen:** Writing – review & editing, Visualization, Validation, Data curation. **Xiaoguang Xu:** Writing – review & editing, Visualization, Validation.

Declaration of competing interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

Acknowledgments

This research was supported by the NASA TEMPO grant (NNL13AA09C) and Smithsonian Astrophysical Observatory's subaward S03939-01 to NASA grant (80NSSC22K1047). Besides, J. Wang's contribution is made possible by in-kind support through the Lichtenberger Family Chair Professor in Chemical Engineering at the University of Iowa. The authors express their sincere gratitude to Haesun Park from the School of Computational Science and Engineering at the Georgia Institute of Technology for providing the NMF_BPAS toolbox, which implements alternating non-negativity-constrained least squares and block principal pivoting/active set methods (<https://faculty.cc.gatech.edu/~hspark/nmfbpas.html>). We also acknowledge the use of the M_Map mapping package for MATLAB (University of British Columbia) in generating the geographic visualizations and cartographic projections presented in this study (<https://www-old.eoas.ubc.ca/~rich/map.html>). Meanwhile, we acknowledge the use of the MODIS MCD43C4 Collection 6.1 Nadir BRDF-Adjusted Reflectance (NBAR) product provided by the NASA Land Processes Distributed Active Archive Center (LP DAAC). We also gratefully acknowledge the U.S. Geological Survey (USGS) Spectral Library for providing valuable hyperspectral surface reflectance measurements used in this study. Furthermore, we acknowledge the use of the ASTER Spectral Library, which is now distributed as part of the ECOSTRESS Spectral Library maintained by the Jet Propulsion Laboratory (JPL) and NASA. Finally, we gratefully acknowledge NASA Earthdata for providing access to the EMIT Level-2A Estimated Surface Reflectance and Uncertainty and Masks (EMITL2ARFL, Version 001) dataset through the Earthdata Search portal.

Data availability

Data will be made available on request.

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