HIR-Diff: Unsupervised Hyperspectral Image Restoration Via Improved Diffusion Models

Supplementary Material

1. Band Index Selection Using RRQR

1.1. Notation

The QR factorization of matrix $\mathbf{X} \in \mathbb{R}^{m \times n}$ is defined as

$$\mathbf{X} = \mathbf{Q}\mathbf{R} \equiv \mathbf{Q} \begin{bmatrix} \mathbf{R}_{11} \ \mathbf{R}_{12} \\ \mathbf{0} \ \mathbf{R}_{22} \end{bmatrix},$$
(25)

where $\mathbf{Q} \in \mathbb{R}^{m \times m}$ is an orthogonal matrix and $\mathbf{R} \in \mathbb{R}^{m \times n}$ is an upper triangular matrix. Then $\mathcal{R}_k(\mathbf{X})$ is defined as

$$\mathcal{R}_k(\mathbf{X}) = \begin{bmatrix} \mathbf{R}_{11} & \mathbf{R}_{12} \\ \mathbf{0} & \mathbf{R}_{22} \end{bmatrix}.$$
 (26)

For \mathbf{R}_{11} , $1/\omega_i(\mathbf{R}_{11})$ denotes the 2-norm of the *i*th row of \mathbf{R}_{11}^{-1} . For \mathbf{R}_{22} , $1/\gamma_i(\mathbf{R}_{22})$ denotes the 2-norm of the *j*th column of \mathbf{R}_{22} . Then $\rho(\mathbf{R}, k)$ is defined as

$$\rho(\mathbf{R},k) = \max_{\substack{1 \le i \le k\\1 \le j \le n-k}} \sqrt{\left(\mathbf{R}_{11}^{-1} \mathbf{R}_{12}\right)_{i,j}^2 + \left(\gamma_j(\mathbf{R}_{22})/\omega_i(\mathbf{R}_{11})\right)^2}.$$
(27)

 $\Pi_{i,j}$ denotes the permutation that interchanges the *i*th and *j*th columns of a matrix.

1.2. RRQR

In this section, we provide a more detailed description of the RRQR algorithm process [12] employed in our work. As introduced in Sect. 3.3, the RRQR is used to determine the band index $(i_1, i_2, ..., i_K)$ so that $|\det(\mathbf{V}_s)|$ is prevented from being zero and each band in the reduced image \mathcal{A} is able to encode different image information. Given a matrix $\mathbf{M} \in \mathbb{R}^{m \times n}$ with $m \ge n$, the QR factorization of \mathbf{M} with its columns permuted can be formulated as

$$\mathbf{M}\mathbf{\Pi} = \mathbf{Q}\mathbf{R} \equiv \mathbf{Q} \begin{bmatrix} \mathbf{R}_{11} & \mathbf{R}_{12} \\ \mathbf{0} & \mathbf{R}_{22} \end{bmatrix},$$
(28)

where $\mathbf{Q} \in \mathbb{R}^{m \times m}$ is an orthogonal matrix, $\mathbf{R} \in \mathbb{R}^{m \times n}$ is an upper triangular matrix and $\boldsymbol{\Pi}$ is a permutation matrix.

The RRQR aims to choose Π such that $\sigma_{\min}(\mathbf{R_{11}})$ is sufficiently large and $\sigma_{\max}(\mathbf{R_{22}})$ is sufficiently small, where $\sigma(\cdot)$ denotes the singular values. The RRQR factorization algorithm works by interchanging any pair of columns that sufficiently increases $|\det(\mathbf{R_{11}})|$, resulting in a large $|\det(\mathbf{R_{11}})|$. The details of the RRQR process are illustrated in Algorithm 2, where k and $f \ge 1$ are hyperparameters. It can be proven that $|\det(\mathbf{R_{11}})|$ increases strictly with every interchange and the algorithm is completed within a finite number of permutations. Readers

Algorithm 2. KKOK Algorithm	Algorithm	2:	RROR	Algorithn
-----------------------------	-----------	----	------	-----------

Input: \mathbf{M}, k, f Output: Permutation matrix $\mathbf{\Pi}$ Compute $\mathbf{R} := \mathcal{R}_k(M)$ and $\mathbf{\Pi} = \mathbf{I}$ while True do step 1: Compute $\rho(\mathbf{R}, k)$ step 2: if $\rho(\mathbf{R}, k) \leq f$ then Break; step 3: Find *i* and *j* such that $\rho(\mathbf{R}, k) > f$ step 4: Compute $\mathbf{R} := \mathcal{R}_k(\mathbf{R}\mathbf{\Pi}_{i,j+k})$ and $\mathbf{\Pi} := \mathbf{\Pi}\mathbf{\Pi}_{i,j+k}$ end return $\mathbf{\Pi}$

could refer to [12] for more detailed proof. We replace M in Eq.(28) with V^{T} and we have

$$\mathbf{V}^{\mathrm{T}} \mathbf{\Pi}_{\mathbf{v}} = \begin{bmatrix} \mathbf{Q}_{v} \mathbf{R}_{v1} \ \mathbf{Q}_{v} \mathbf{R}_{v2} \end{bmatrix}$$
(29)

We define $\mathbf{V}_s^{\mathrm{T}}$ as $\mathbf{Q}_v \mathbf{R}_{v1}$ and then we could readily obtain $|\det(\mathbf{V}_s)| = |\det(\mathbf{R}_{v1})|$. Therefore, by solving the RRQR factorization problem of \mathbf{V}^{T} utilizing the algorithm proposed in [12], the permutation matrix $\mathbf{\Pi}_v$ is obtained and $|\det(\mathbf{V}_s)|$ is maximized. The indices corresponding to the first K columns of the permuted \mathbf{V}^{T} are defined as the band selection index.

2. Diffusion Model

In HIR-Diff, we employ a pre-trained diffusion model proposed in [10] to generate the reduced image A. The diffusion model is a U-Net proposed in [40] and is trained on an amount of 3-channel remote sensing images without human supervision. Since the network requires the input image to be 3-channel, the rank value K in our work is set as 3 so that the reduced image A with 3 channels can be denoised with the pre-trained network. Although the rank value is small, we found that it is sufficient to restore the image details and helps to keep noise out of the estimated coefficient matrix E and the restored image, since the matrix V obtained from the SVD of the observed image as introduced in Sec. 3.3 is cleaner and the low-rank property enables noise reduction of the restored image.

3. Coefficient Matrix Estimation

In our work, we employ SVD and RRQR to estimate the coefficient matrix \mathbf{E} as introduced in Sec. 3.3. The visualization results of the estimated \mathbf{E} for the WDC dataset



Figure 5. The visualization results of the estimated **E**. Least Square and Ground Truth (LS) denote the coefficient matrix **E** estimated by employing the least square method with the observed image and the clean image, respectively. Ours and Ground Truth (SVD) denote the coefficient matrix **E** estimated using SVD and RRQR proposed in our work with the observed image and the clean image, respectively.

are demonstrated in Fig. 5. The results of the matrix **E** estimated using the least square method proposed in [38] is also provided for comparison. Specifically, the least-squares method directly selects several bands from the observed image \mathcal{Y} as the reduced image \mathcal{A} , and then estimates the coefficient matrix E by solving the least-squares problem.

$$\arg\min_{\mathbf{E}} ||\mathcal{Y} - \mathcal{A} \times_3 E||_F^2 \,. \tag{30}$$

Since there is a lot of noise in the reduced image A as the observed image suffers from various degradation, the estimated **E** is unreliable, resulting in undesirable HSI restoration performance. On the contrary, our estimated coefficient matrix **E** is robust to noise and exhibits a high degree of similarity to ground truth, verifying the effectiveness of our estimation method.