Stochastic Enhancement of Graph and Rank Regularized Matrix Recovery (GRMR) for Spectral Image Recovery

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Abstract

The primary objective of this project was to enhance the methodology of a well-established paper, specifically focusing on the Graph and Rank Regularized Matrix Recovery (GRMR) for Snapshot Spectral Image Demosaicing. The innovation of Snapshot Spectral Imaging (SSI) lies in its ability to efficiently capture the spatio-spectral information of dynamic scenes on compact platforms. The inherent challenge in SSI is the balance between spatial and spectral resolution, as each pixel captures limited spectral data. To optimize this process, we introduced a stochastic component to the GRMR algorithm, effectively integrating variability into the rank determination during matrix recovery. This modification aims to leverage the stochastic nature of spectral data, accommodating variability and improving reconstruction fidelity. Our empirical tests, conducted on the same datasets utilized in the original paper, demonstrate that the stochastic-enhanced GRMR method yields improved results, indicating a promising direction for future advancements in spectral imaging technologies.

1 Introduction

Hyperspectral Imaging (HSI) is at the forefront of capturing the spectral signature at every spatial location within a scene, providing invaluable insights for diverse applications such as climate monitoring, medical diagnosis, precision agriculture, and food safety. The potential of HSI is vast, yet the acquisition of imagery with high spectral, spatial, and temporal resolution poses significant challenges. These challenges stem from the inherent trade-off between the dimensionality of the data and the physical constraints of detector arrays

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To address these challenges, Spectrally Resolved Detector Arrays (SRDA) have emerged, enabling the acquisition of a sub-sampled hyperspectral cube in a single exposure, ideal for dynamic scenes. This innovative approach associates each pixel with a specific spectral region, sacrificing spatial resolution to attain a high frame rate in spectral imaging. Figure 1 illustrates the concept of an SRDA-based SSI camera.

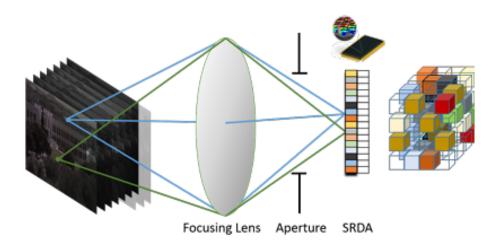


Figure 1: An SRDA-based SSI camera system where each detector element captures light from a specific spectral region.

Building on this paradigm, our work introduces an optimized Computational Spectral Imaging system that exploits spatial, spectral, and temporal correlations to estimate full-resolution HSI observations from a minimal number of snapshots. Leveraging spectral calibration and spatio-spectral correlations, we advance the original graph and rank regularized matrix recovery technique to new heights.

The mathematical framework of our optimization pivots on the minimization of the nuclear norm, formulated as:

minimize
$$||X||_* + \frac{1}{2}||A(X) - Y||_2^2 + \beta \operatorname{tr}(XLX^T),$$
 (1)

where the rank regularization is enhanced through a stochastic approach, thus addressing the limitations observed in previous implementations on complex datasets such as Sentinel-2 and others captured by actual SSI cameras.

This report unfolds the journey of this optimization, starting with a detailed analysis of the original approach, followed by a presentation of the enhanced stochastic optimization techniques, and culminating in experimental validations that solidify our contributions to the field of spectral imaging.

2 Theoretical Background

The Graph and Rank Regularized Matrix Recovery (GRMR) algorithm occupies a vital space in the domain of computational imaging, particularly within the context of Hyperspectral Imaging (HSI). GRMR is predicated on the principle of regularized optimization, where the objective is to recover high-fidelity images from undersampled data. This recovery is facilitated through the minimization of a cost function that balances the fidelity to the observed data and the imposition of a low-rank structure on the solution, leveraging the inherent spatial and spectral correlations.

Related optimization methods in this sphere often employ variations of matrix completion and recovery techniques, including methods like Principal Component Analysis (PCA) for dimensionality reduction and LASSO for sparse recovery. These methods share a common goal: to reconstruct or estimate the true signal from partial or noisy observations.

Stochastic methods in optimization introduce randomness into the algorithm to potentially escape local minima and explore the solution space more broadly. In our adaptation of GRMR, we interject stochasticity by incorporating a probabilistic decision into the rank selection process of the recovery algorithm. Specifically, we modify the rank determination step within the hard-thresholding operator traditionally used in GRMR. This operator typically retains the top r singular values of a matrix to approximate its lower-rank version. In our stochastic variant, named sGRMR, we introduce a coin toss mechanism to decide whether to use the predetermined rank r or a randomly chosen rank r' less than or equal to r for each iteration of the algorithm. This novel approach aims to enhance the robustness of the recovery process and is hypothesized to yield a more accurate reconstruction in scenarios where the spectral data is complex and the underlying model is not perfectly understood.

The integration of stochastic elements into optimization methods is not new; however, its application in the realm of HSI and SSI is innovative. It promises to mitigate some of the challenges posed by the high-dimensionality of HSI data and the undersampling inherent in SSI, ensuring that the reconstructed images maintain a balance between spatial and spectral resolution without being marred by the artifacts that deterministic methods might introduce.

3 Graph and Rank Regularized Matrix Recovery (GRMR)

The original Graph and Rank Regularized Matrix Recovery (GRMR) method is an advanced algorithm designed for the recovery of high-dimensional data matrices from undersampled observations. The methodology pivots on two main forms of regularization: rank and graph.

3.1 Rank Regularization

Rank regularization underpins the GRMR algorithm. It seeks to recover a data matrix X by minimizing the rank of X subject to the constraint that:

$$A(X) = A(M), (2)$$

where A is the acquisition operator, and M represents the subsampled measurements. In practice, direct rank minimization is NP-hard; therefore, the nuclear norm $||X||_*$, the sum of the singular values of X, is minimized as a convex surrogate for the rank function:

minimize_X
$$||X||_* + ||A(X) - A(M)||_F$$
. (3)

3.2 Graph Regularization

Graph regularization is utilized to encode the manifold structure of data, capturing spatial proximity. The graph Laplacian matrix L, an approximation to the Laplace-Beltrami operator, is employed in this context. The regularization term is formulated as:

$$||\nabla_g X||_F = \operatorname{tr}(XLX^T),\tag{4}$$

which ensures that the solution is smooth over the graph, promoting similarity between connected nodes.

3.3 Graph and Rank Regularized Matrix Recovery (GRMR)

GRMR combines these regularization techniques within a singular framework. By adopting the proximal splitting method, the GRMR problem is expressed as minimizing the sum of two functions:

$$f(X) = ||y - A(X)||_2^2 + \beta \text{tr}(XLX^T),$$
(5)

$$g(X) = ||X||_*.$$
 (6)

The solution is iteratively approached using the proximal gradient method, which updates the matrix X in a manner that respects both the acquired data and the assumed low-rank, smooth graph structure.

So, the final minimization problem that this method is trying to solve is the one below:

$$\underset{X}{\text{minimize}} f(X) + g(X) \tag{7}$$

In the analysis that have been done, and by the definition of functions f(X) (5) and g(X) (6), the minimization problem in (7) is equivalently expressed as

minimize
$$||X||_* + \frac{1}{2}||A(X) - Y||_2^2 + \beta \operatorname{tr}(XLX^T)$$
 (8)

The solution to the minimization in (7) can be obtained by the proximal gradient method, an iterative approach where each iteration is given by

$$X^{t+1} = \operatorname{prox}_{\lambda g} \left(X^t - \lambda \nabla f(X^t) \right) \tag{9}$$

In the context of the GRMR framework, the computation of the gradient of $f(X^t)$ as indicated in equation (4), involves a combination of the derivative with respect to the ℓ_2 norm and the contribution from the trace term. Explicitly, this gradient can be represented as follows:

$$\nabla f(X^t) = A^*(A(X^t) - y) + \beta X^t L^T$$
(10)

Here, A^* denotes the adjoint of the linear operator A, and L is a matrix that encodes certain structure or constraints on the solution. The term β is a regularization parameter that balances the fit of the model to the data and the complexity of the model.

To address the minimization problem involving the nuclear norm as specified in equation (5), authors utilize a thresholding technique on the singular values of the matrix X. There are two primary variants of this thresholding: the soft version and the hard version. The soft-thresholding operation is described as:

$$D_r(X) = U\Sigma_r V^T, \quad D_r(\Sigma) = \operatorname{diag}(\max(\sigma_i - \tau, 0))$$
 (11)

where Σ_r is the diagonal matrix of singular values after soft-thresholding, τ is the thresholding

parameter, and the operation $\max(\sigma_i - \tau, 0)$ ensures that each singular value is either reduced by τ or set to zero if it is less than τ .

Authors of the paper have selected the hard-thresholding approach due to its specific properties:

$$H_r(X) = UH_r(\Sigma)V^T, \quad H_r(\Sigma) = \begin{cases} \sigma_i & \text{if } i \le r \\ 0 & \text{otherwise} \end{cases}$$
 (12)

This hard-thresholding operation retains only the r largest singular values and sets all others to zero. As a result, the rank of the resulting matrix X is effectively limited to r, allowing us to construct matrices with a predetermined rank. This is particularly useful in scenarios where a low-rank approximation of the data is desirable for reasons such as dimensionality reduction, noise suppression, or data compression.

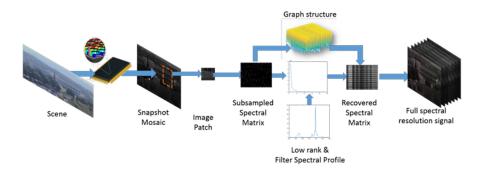


Figure 2: Process flow of the Spectral Imaging system illustrating the transformation from the scene capture to the full spectral resolution signal. The flow begins with the scene being captured as a snapshot mosaic, which is then sectioned into image patches. These patches are used to form a subsampled spectral matrix that, after applying the low rank and filter spectral profile constraints and leveraging the graph structure, is processed to recover the spectral matrix. The final output is the full spectral resolution signal.

3.4 The Algorithm

So the final algorithm, based on the previous discussions and the mathematical framework established, is detailed below.

Algorithm 1 Graph and Rank Regularized Matrix Recovery (GRMR)

Input: The sampled measurements matrix M, the regularization parameter β and rank estimate k, the maximum number of iterations limit or variation less than δ between successive iterations.

Output: The estimated spectral measurements matrix X.

- 1: initialization
- 2: Initialize $X^{(0)}$ from interpolation, t = 0
- 3: Calculate the Degree and Weight matrix from $X^{(0)}$ and estimate the Laplacian matrix L according to Eq. (12)
- 4: **while** t < limit or $||X^{(t+1)} X^{(t)}||_2 \ge \delta$ **do**
- 5: Estimate update parameter μ_t according to Eq. (24)
- 6: Estimate intermediate variable $Z^{(t)}$
- 7: $Z^{(t)} = X^{(t)} \mu_t (A^*(A(X^{(t)}) y)) \beta X^{(t)} L^T$
- 8: Obtain the updated estimate of matrix $X^{(k+1)}$:
- 9: $(U, \Sigma, V) = \text{SVD}(Z^{(t)})$
- 10: $X^{(t+1)} = UH_k(\Sigma)V^T$
- 11: set $t \leftarrow t + 1$
- 12: end while

The GRMR algorithm works as follows:

- 1. **Input:** Subsampled measurements matrix M, regularization parameter β , rank estimate k, maximum iterations *limit* or convergence threshold δ .
- 2. **Initialization:** Interpolate to initialize spectral measurements matrix $X^{(0)}$, set iteration t=0.
- 3. **Degree and Weight Matrix Calculation:** Calculate Degree and Weight matrix from $X^{(t)}$ and estimate the Laplacian matrix L.
- 4. Iterative Update:
 - (a) Estimate intermediate variable $Z^{(t)}$ using current $X^{(t)}$, sampling operator A, measurements matrix y, and Laplacian L.
 - (b) Apply regularization involving graph structure and rank penalty.
- 5. **Matrix Update:** Update X using SVD of $Z^{(t)}$, retaining only k largest singular values and vectors
- 6. Convergence Check: Repeat until $||X^{(t+1)} X^{(t)}||_F \le \delta$ or iteration count exceeds *limit*.
- 7. **Output:** Final spectral measurements matrix X after convergence.

4 Methodological Enhancement (sGRMR)

The Graph and Rank Regularized Matrix Recovery (GRMR) method innovatively recovers high-dimensional data matrices from undersampled measurements. This approach primarily leverages rank and graph regularizations. The optimization area chosen for enhancement involves the rank selection process within the hard-thresholding operator used in GRMR. By introducing a stochastic element—tossing a coin to decide the rank of retained singular values—we aim to navigate around the potential rigidity and limitations of a fixed rank determination. This stochastic approach to rank determination allows the method to adapt more flexibly to the data's structure, which can be particularly beneficial in handling noisy or incomplete data, common in real-world scenarios. The resulting sGRMR (stochastic GRMR) method is hypothesized to be more robust and yield more accurate reconstructions by avoiding overfitting and better capturing the underlying data distribution.

The approach integrates a stochastic element into the previously deterministic algorithm for Graph and Rank Regularized Matrix Recovery (GRMR), tentatively named "Stochastic GRMR" (sGRMR). The introduction of stochasticity aims to avoid potential pitfalls of deterministic algorithms, such as getting trapped in local minima, and to explore a broader solution space that could lead to better overall results.

Here's a detailed breakdown of the sGRMR approach:

- 1. Stochastic Hard-thresholding Operator: Instead of consistently applying a fixed rank r for the hard-thresholding operator $H_r(X)$, sGRMR employs a randomized approach. This randomization is enacted through a coin toss to determine whether to use the conventional hard-thresholding with rank r or a random rank r' where r' < r.
- 2. **Coin Toss Mechanism**: The algorithm incorporates a coin toss to add randomness to each iteration, with a 50% chance to proceed with the standard method or invoke the stochastic method.
 - If heads, the algorithm continues as the standard GRMR, retaining the top r singular values
 - If tails, the algorithm selects a random integer r' such that $r' \leq r$, retaining the top r' singular values.
- 3. **Stochastic Thresholding Effects**: Introducing stochasticity in the thresholding step allows the algorithm to potentially escape local optima and sample different subspaces of the solution space by varying the number of singular values retained.
- 4. **Exploration vs. Exploitation**: The original GRMR algorithm exploits known information about the data's structure with a deterministic rank r. In contrast, sGRMR balances exploitation with exploration by occasionally exploring matrices of lower rank than the best-known rank r.

5. **Convergence and Output**: The algorithm follows a convergence criterion based on the Frobenius norm of the difference between successive iterations or a maximum number of iterations. The output is the final spectral measurements matrix *X* upon convergence, which has undergone a combination of deterministic and stochastic updates.

This stochastic approach could lead to a solution that generalizes better or finds a more global optimum. However, the introduction of variability in the results means that the performance may depend on the problem nature, the distribution of ranks r', and the specific dataset. The balance between the increased computational complexity due to randomness and the quality of the obtained solution would need to be empirically evaluated.

4.1 Stochastic Rank Regularization

In sGRMR, the rank regularization does not solely focus on minimizing the nuclear norm as a proxy for the rank. Instead, it incorporates a random element in the selection of singular values to retain, which is determined by a stochastic process akin to a coin toss:

- With a probability of 0.5, the algorithm performs the usual hard-thresholding by retaining the top r singular values.
- With the remaining probability, a random integer r', where $r' \leq r$, is chosen, and only the top r' singular values are retained.

4.2 Graph Regularization in sGRMR

Just like the original GRMR algorithm, sGRMR also employs graph regularization to exploit the intrinsic geometry of the data represented by a graph. The graph Laplacian L, which captures the manifold structure and penalizes the solution based on the graph's topology, remains a core component. The graph regularization term, represented by the trace of the product of X, L, and X^T , encourages smoothness across connected nodes in the graph, thereby respecting the underlying data manifold.

In the context of sGRMR, the graph regularization works in tandem with the stochastic rank regularization to ensure that the recovered matrix X is not only of low rank but also exhibits smoothness over the graph. This dual regularization approach is particularly powerful as it allows for the incorporation of domain-specific knowledge through the graph structure while also providing a mechanism to escape potential local minima through stochastic rank selection.

4.3 Stochastic Graph and Rank Regularized Matrix Recovery (sGRMR)

The sGRMR algorithm solves the following optimization problem:

minimize
$$||X||_* + \frac{1}{2}||A(X) - Y||_2^2 + \beta \operatorname{tr}(XLX^T),$$
 (13)

where $||X||_*$ denotes the nuclear norm of X, A(X) represents the measurements acquired through a linear operator A, Y is the matrix of sampled measurements, L is the graph Laplacian matrix, and β is the regularization parameter.

The stochastic aspect is introduced in the hard-thresholding step, where the selection between the standard hard-thresholding operator and a stochastic variant is determined by a random process:

$$X^{t+1} = \begin{cases} UH_k(\Sigma)V^T, & \text{with probability 0.5,} \\ UH_{r'}(\Sigma)V^T, & \text{with probability 0.5,} \end{cases}$$
(14)

where (U, Σ, V) is the Singular Value Decomposition (SVD) of X, H_k and $H_{r'}$ are the hard-thresholding operators retaining the top k and r' singular values, respectively, and r' is a random integer such that $r' \leq k$.

The stochastic hard-thresholding operator is defined as:

$$H_r(\Sigma) = \begin{cases} \sigma_i, & \text{if } i \le r, \\ 0, & \text{otherwise,} \end{cases}$$
 (15)

and the selection of r' is done by a uniform random choice from the set $\{1, 2, \dots, k\}$.

4.4 The Enhanced Algorithm

Algorithm 2 Stochastic Graph and Rank Regularized Matrix Recovery (sGRMR)

Require: The sampled measurements matrix M, the regularization parameter β , and rank estimate k, the maximum number of iterations *limit* or convergence threshold δ .

Ensure: The estimated spectral measurements matrix X.

```
1: initialization
2: Initialize X^{(0)} from interpolation, t=0
3: Calculate the Degree and Weight matrix from X^{(0)} and estimate the Laplacian matrix L ac-
    cording to Eq. (12)
4: while t < limit or ||X^{(t+1)} - X^{(t)}||_F \ge \delta do
        Estimate update parameter \mu_t according to Eq. (24)
5:
        Estimate intermediate variable Z^{(t)}
6:
        Z^{(t)} = X^{(t)} - \mu_t(A^*(A(X^{(t)}) - y)) - \beta X^{(t)}L^T
7:
        Obtain the updated estimate of matrix X^{(k+1)}:
8:
        (U, \Sigma, V) = \text{SVD}(Z^{(t)})
9:
        Generate a random number p \in [0, 1]
10:
        if p < 0.5 then
11:
             X^{(t+1)} = UH_k(\Sigma)V^T
                                                                              \triangleright Retain top k singular values
12:
13:
        else
            Choose a random integer r' \leq k
14:
             X^{(t+1)} = UH_{r'}(\Sigma)V^T
                                                                              \triangleright Retain top r' singular values
15:
16:
        end if
        set t \leftarrow t + 1
17:
18: end while
```

5 Results Comparison on GRMR and sGRMR

The comparison of algorithmic performance on the CAVE and SENTINEL datasets reveals insightful trends in spectral image reconstruction efficacy. We utilized two metrics for this comparative study: the Peak Signal-to-Noise Ratio (PSNR) and the Spectral Angle Mapper (SAM), which collectively provide a measure of image quality and spectral fidelity.

5.1 Analysis on the CAVE Dataset

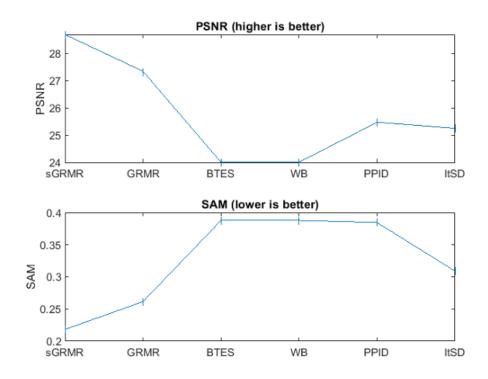


Figure 3: Performance comparison of different algorithms on the CAVE dataset using PSNR and SAM metrics.

For the CAVE dataset, as depicted in Figure 3, the sGRMR algorithm stands out with the highest PSNR values, indicating superior performance in terms of image reconstruction quality. Concurrently, sGRMR achieves the lowest SAM values, which suggests it also maintains the best spectral fidelity among the methods evaluated.

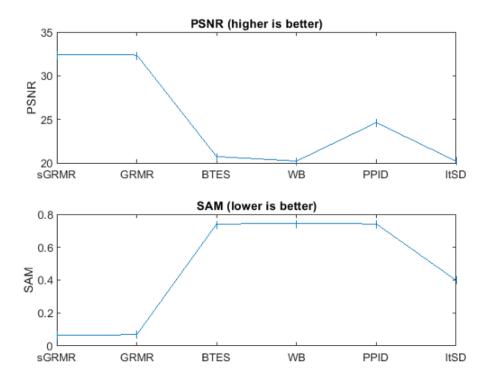


Figure 4: Performance comparison of different algorithms on the SENTINEL dataset using PSNR and SAM metrics.

5.2 Analysis on the SENTINEL Dataset

The SENTINEL dataset results, shown in Figure 4, indicate that sGRMR continues to lead in terms of PSNR. However, the margin of improvement over other methodologies is not as marked as observed in the CAVE dataset. The SAM metric for SENTINEL exhibits greater variability, with sGRMR not achieving the lowest values but still showing competitive performance.

5.3 Conclusions

In summary, while the sGRMR algorithm demonstrates improved performance over the original GRMR in terms of PSNR and SAM on the CAVE dataset, its enhancements on the SENTINEL dataset are modest. This observation points towards the need for further optimization of the sGRMR algorithm to better cater to the complexities of various datasets.

References

[1] G. Tsagkatakis, B. Geelen, M. Jayapala, P. Tsakalides, et al., "Graph and Rank Regularized Matrix Recovery for Snapshot Spectral Image Demosaicing," *IEEE Transactions on Computational Imaging*, vol. 4, no. 4, pp. 530–544, 2018.