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Greedy algorithms for nonnegativity-constrained simultaneous sparse recovery

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ABSTRACT

This work proposes a family of greedy algorithms to jointly reconstruct a set of vectors that are (i) nonnegative and (ii) simultaneously sparse with a shared support set. The proposed algorithms generalize previous approaches that were designed to impose these constraints individually. Similar to previous greedy algorithms for sparse recovery, the proposed algorithms iteratively identify promising support indices. In contrast to previous approaches, the support index selection procedure has been adapted to prioritize indices that are consistent with both the nonnegativity and shared support constraints. Empirical results demonstrate for the first time that the combined use of simultaneous sparsity and nonnegativity constraints can substantially improve recovery performance relative to existing greedy algorithms that impose less signal structure.

1. Introduction

We consider the following inverse problem: given data matrix $\mathbf{Y} \in \mathbb{R}^{M \times K}$ (possibly noisy), observation/dictionary matrix $\mathbf{\Phi} \in \mathbb{R}^{M \times N}$, and noiseless linear measurement model $\mathbf{Y} = \mathbf{\Phi}\mathbf{X}$, we seek to recover the unknown matrix $\mathbf{X} \in \mathbb{R}^{N \times K}$ by solving the optimization problem:

$$\hat{\mathbf{X}} = \arg\min_{\mathbf{X} \in \Omega} \|\mathbf{Y} - \mathbf{\Phi}\mathbf{X}\|_F^2, \qquad (\mathrm{P}\Omega)$$

where $\Omega \subseteq \mathbb{R}^{N \times K}$ is an appropriate constraint set. We are primarily concerned with the case of $K > 1$, which is called the multiple measurement vector (MMV) formulation.

Estimation of $\mathbf{X}$ is relatively easy whenever the matrix $\mathbf{\Phi}$ has a full column-rank and good condition number, in which case the standard unconstrained linear least squares (LLS) solution will be both stable and accurate. However, in many scenarios of interest, the matrix $\mathbf{\Phi}$ is poorly conditioned, and the choice of Ω can have a dramatic impact on the quality of the estimated $\hat{\mathbf{X}}$. For example, in the underdetermined case where there are fewer measurements than unknowns (i.e., $M < N$), there are infinitely many optimal solutions to P_Ω if no constraints are applied (i.e., setting $\Omega = \mathbb{R}^{N \times K}$). For this case, there will not be a unique solution to P_Ω unless Ω is refined, and different choices of Ω could lead to very different estimates $\hat{\mathbf{X}}$.

In this work, we propose new greedy algorithms for solving P_Ω under two specific constraints: the columns of $\mathbf{X}$ are both *nonnegative* (NN) and *simultaneously sparse* (SS). Specifically, we derive combined NN and SS (NNS) extensions of the following existing greedy algorithms for sparse recovery: orthogonal matching pursuit (OMP) [1–4], subspace pursuit (SP) [5], CoSaMP [6], and hard thresholding pursuit (HTP) [7]. The proposed extensions are also easily generalized to other greedy sparse algorithms like iterative hard thresholding (IHT) [8] which are based on similar principles. Applications where these constraints and algorithms may prove useful include magnetic resonance relaxometry [9,10], kinetic parameter

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estimation in dynamic positron emission tomography [11], spectral unmixing [12], and sparse NN matrix factorization [13].

Existing work has already demonstrated that combining sparsity constraints with NN constraints leads to improved reconstruction results, both when using convex relaxations [14] and when using greedy algorithms [15]. Extensions of greedy sparse recovery algorithms such as OMP, SP, and HTP to the SS context also already exist [16–24]. However, to the best of our knowledge, there are no previously proposed algorithms for combining NN with SS. This paper fills that gap by proposing a new family of greedy NNS algorithms, and by demonstrating empirically that combined NNS constraints can substantially improve recovery performance relative to the individual use of NN, sparsity, or SS constraints.

This paper is organized as follows. Prior work related to NN constraints and SS constraints is discussed in Section 2. The details of our proposed NNS greedy algorithms are described in Section 3. Theoretical considerations for the proposed algorithms are discussed in Section 4. The simulations we use to evaluate the proposed algorithms are described in Section 5, while the corresponding results are presented and analyzed in Section 6. An application example is described in Section 7. Finally, we provide additional discussion in Section 8 and conclusions in Section 9.

2. Background

2.1. Nonnegativity constraints

Formally, we define the set of NN signals as

$$\Omega_+ \triangleq \left\{ \mathbf{X} \in \mathbb{R}^{N\times K} : x_{nk} \geq 0, \quad \begin{array}{l} n = 1,\ldots,N \\ k = 1,\ldots,K \end{array} \right\}, \tag{1}$$

where x_{nk} is the entry in the nth row and kth column of $\mathbf{X}$. NN signals are encountered in a variety of applications, due to the fact that certain physical and mathematical quantities are inherently NN. For instance, Euclidean distances, image intensities, signal powers, probabilities, photon counts, and volume fractions are all examples of positive-valued quantities, with negative values being unphysical and difficult to interpret. The use of NN constraints is therefore essential in certain applications, and has a long history: see [25] for a review. Interestingly, it has been demonstrated theoretically that NN constraints alone can lead to unique and robust solutions to P_Ω when $\mathbf{\Phi}$ is underdetermined, under appropriate additional conditions on $\mathbf{\Phi}$ and $\mathbf{Y}$ [26–28]. In addition, the NN least squares (NNLS) problem (the common name for P_Ω combined with constraint set Ω_+) is a simple convex optimization problem for which efficient algorithms already exist [25].

2.2. Sparsity and simultaneous sparsity constraints

Single measurement vector (SMV) sparsity (i.e., sparsity for the case when $K=1$) has also emerged as a popular constraint for solving P_Ω in underdetermined settings. This popularity is based on three main observations: (i) most real-world signals possess structure that allows them to be sparsely represented in an appropriate basis or frame; (ii) if $\mathbf{X}$ is sufficiently sparse and the underdetermined $\mathbf{\Phi}$ matrix has appropriate subspace structure, then various sparsity-constrained solutions to P_Ω are theoretically guaranteed to yield stable and accurate estimates of $\mathbf{X}$ [29]; and (iii) even when theoretical guarantees are not applicable, the use of appropriate sparsity constraints allows valuable prior information to be incorporated into the estimation process, generally yielding better results than an unconstrained reconstruction would.

We define the set of S-sparse SMV signals as

$$\Omega_S \triangleq \left\{ \mathbf{X} \in \mathbb{R}^{N\times 1} : |\Lambda_S(\mathbf{X})| \leq S \right\}, \tag{2}$$

where the *support set* $\Lambda_S(\mathbf{X})$ is defined as

$$\Lambda_S(\mathbf{X}) \triangleq \{ n \in \{1,\ldots,N\} : x_{n1} \neq 0 \} \tag{3}$$

and $|\Lambda_S(\mathbf{X})|$ denotes its cardinality. The cardinality of this set equals the number of nonzeros in $\mathbf{X}$, such that Ω_S is the set of all vectors that possess no more than S nonzero entries.

Rather than just considering standard SMV sparsity, this work focuses on SS, a specific form of structured MMV sparsity (SS is also sometimes called joint sparsity, group sparsity, or multi-channel sparsity). In SS, it is assumed that the columns of $\mathbf{X}$ are each sparse and share a common support set. Formally, we define the set of simultaneously S-sparse signals as

$$\Omega_{SS} \triangleq \left\{ \mathbf{X} \in \mathbb{R}^{N\times K} : |\Lambda_{SS}(\mathbf{X})| \leq S \right\}, \tag{4}$$

where the *shared support set* $\Lambda_{SS}(\mathbf{X})$ is defined as

$$\Lambda_{SS}(\mathbf{X}) \triangleq \left\{ n \in \{1,\ldots,N\} : x_{nk} \neq 0 \text{ for some } k \right\}. \tag{5}$$

The cardinality of $\Lambda_{SS}(\mathbf{X})$ is equal to the number of rows of $\mathbf{X}$ that are not identically zero, such that Ω_{SS} is the set of all matrices $\mathbf{X} \in \mathbb{R}^{N\times K}$ possessing no more than S nonzero rows. Unsurprisingly, methods that impose SS are empirically more powerful than methods that solely impose sparsity without enforcing structured sparsity information [30].

Unlike the easy-to-solve NNLS optimization problem,[1] sparsity-constrained optimization problems generally have combinatorial complexity. As a result, it is common in the literature to either consider greedy algorithms [16–20,22–24] or convex/nonconvex relaxations of the sparsity constraint [17,18,32–35]. We focus on greedy approaches.

2.3. Greedy sparse algorithms

While greedy optimization algorithms can potentially be trapped at suboptimal local minima, they are frequently less computationally demanding than relaxation-based algorithms, and several have optimality guarantees under

[1] Interestingly, the classical active-set NNLS algorithm of Lawson and Hansen [31] has strong algorithmic similarities to NN-OMP [15], a greedy algorithm designed for solving P_Ω with $\Omega = \Omega_+ \cap \Omega_S$. However, while the active-set NNLS algorithm is guaranteed to optimally solve P_Ω, the optimality of the result produced by NN-OMP depends on the characteristics of $\mathbf{\Phi}$.

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