ON THE UNIQUENESS OF NON-NEGATIVE SPARSE REDUNDANT REPRESENTATIONS

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ABSTRACT

We consider an underdetermined linear system of equations $\mathbf{Ax} = \mathbf{b}$ with non-negative entries in $\mathbf{A}$ and $\mathbf{b}$, and seek a non-negative solution $\mathbf{x}$. We generalize known equivalence results for the basis pursuit, for an arbitrary matrix $\mathbf{A}$, and an arbitrary monotone element-wise concave penalty replacing the ℓ_1-norm in the objective function. This result is then used to show that if there exists a sufficiently sparse solution to $\mathbf{Ax} = \mathbf{b},\ \mathbf{x} \geq 0$, it is necessarily unique.

***Index Terms*—** Sparse representation, redundancy, non-negative, uniqueness, basis pursuit, matching pursuit.

1. INTRODUCTION

We consider an underdetermined linear system of equations of the form $\mathbf{Ax} = \mathbf{b}$, where the entries of $\mathbf{A} \in \mathbb{R}^{n\times k}$ and $\mathbf{b} \in \mathbb{R}^n$ are all non-negative, and seek non-negative solutions $\mathbf{x} \in \mathbb{R}^k$ to this system. Such a problem is frequently encountered in signal and image processing, in handling of multi-spectral data, considering non-negative factorization for recognition, and more (see [6, 7, 8, 9] for representative work).

When considering an underdetermined linear system (i.e. $k > n$), with a full rank matrix $\mathbf{A}$, the removal of the non-negativity requirement $\mathbf{x} \geq 0$ leads to an infinite set of feasible solutions. How is this set reduced when we further require non-negativity? Assuming there could be several possible solutions, the common practice is the definition of an optimization problem of the form

$$(P_f): \quad \min_{\mathbf{x}} f(\mathbf{x}) \text{ subject to } \mathbf{Ax} = \mathbf{b} \text{ and } \mathbf{x} \geq 0, \qquad (1)$$

where $f(\cdot)$ measures the quality of the candidate solutions. Possible choices for this penalty could be various entropy measures, or the general ℓ_p-norm for various p in the range $[0, \infty)$. Popular choices are $p = 2$, $p = 1$, and $p = 0$ (enforcing sparsity). For example, recent work reported in [10] proved that the $p = 0$ and $p = 1$ choices lead to the same result, provided that this result is sparse enough. This work also provides bounds on the required sparsity that guarantees such equivalence, but in a different setting.

Clearly, if the set $\{\mathbf{x}|\ \mathbf{Ax} = \mathbf{b} \text{ and } \mathbf{x} \geq 0\}$ contains only one element, then all the above choices of $f(\cdot)$ lead to the same result. In such a case, the above-discussed ℓ_0-ℓ_1 equivalence becomes an example of a much wider phenomenon. Surprisingly, this is exactly what happens when a sufficiently sparse solution exists. The main result shown of this paper proves such a uniqueness of sparse solutions, and provides a bound on $\|\mathbf{x}\|_0$ below which such a uniqueness takes place.

There are several known results reporting an interesting behavior of sparse solutions of a general under-determined linear system of equations, when minimum of ℓ_1-norm is imposed on the solution (the Basis Pursuit algorithm) [2, 3]. For the case where the columns of $\mathbf{A}$ have a unit ℓ_2-norm, these results state that the minimal ℓ_1-norm solution coincides with the sparsest one for sparse enough solutions. As mentioned above, a similar claim is made in [10] for non-negative solutions, leading to stronger bounds.

In this work we extend the basis pursuit analysis, presented in [2, 3], to the case of a matrix with arbitrary column norms and an arbitrary monotone element-wise concave penalty replacing the ℓ_1-norm objective function. A generalized theorem of the same flavor is obtained. Using this result, we get conditions of uniqueness of sparse solution of non-negative system of equations, as mentioned above. Interestingly, there is no need to use an ℓ_1 penalty – non-negativity constraints are sufficient to lead to the unique (and sparsest) solution in such cases.

The structure of this paper is as follows: In Section 2 we extend the basis pursuit analysis to the case of arbitrary monotone element-wise concave penalty and matrix $\mathbf{A}$ with arbitrary column norms. This analysis relies on a special definition of coherence measure of the matrix $\mathbf{A}$. We also introduce preconditioning that improves this coherence. In Section 3 we develop the main theoretical result in this paper, claiming that a sufficiently sparse solution of $\{\mathbf{Ax} = \mathbf{b}, \mathbf{x} \geq 0\}$ is unique. More details on the practical implications of this paper's results are given in [1].

2. BASIS PURSUIT: AN EXTENDED RESULT

In this section we develop a theorem claiming that a sufficiently sparse solution of a general under-determined linear system $\mathbf{Dz} = \mathbf{b}$ is necessarily a minimizer of a separable concave function. Note that we use a different notation for the linear system – the reason for this change will be clarified in the next section.

The result we are about to present and prove extends Theorem 7 in [2] in the following ways:

- It does not assume normalization of the columns in $\mathbf{D}$ (and thus it is more general);
- It relies on a different (weaker) feature of the matrix $\mathbf{D}$ – a one-sided coherence measure; and
- The objective function is more general than the ℓ_1-norm used in [2]. In fact, it is similar to the one proposed by Gribonval and Nielsen in [5], but due to the above changes, the analysis is rather different.

The results presented in this section form the grounds for the main result of this paper - the analysis of non-negative linear systems, as discussed in Section 3.

2.1. The One-Sided Coherence and Its Use

For an arbitrary $n \times k$ matrix $\mathbf{D}$ with columns $\mathbf{d}_i$ we define its one-sided coherence as

$$\rho(\mathbf{D}) = \max_{i,j;j\neq i} \frac{|\mathbf{d}_i^T \mathbf{d}_j|}{\|\mathbf{d}_i\|_2^2}. \tag{2}$$

Defining the Gram matrix $\mathbf{G} = \mathbf{D}^T\mathbf{D}$, its elements satisfy

$$\frac{|G_{ij}|}{G_{ii}} \le \rho(\mathbf{D}) \quad \forall i, j \neq i. \tag{3}$$

This measure tends to behave like $1/\sqrt{n}$ for random matrices, very much like the regular *mutual-coherence* as defined in [2].

Lemma 1 *Any vector δ from the null-space of $\mathbf{D}$ satisfies*

$$\|\delta\|_\infty \le t_{\mathbf{D}} \|\delta\|_1, \tag{4}$$

where we denote $t_{\mathbf{D}} = \frac{\rho(\mathbf{D})}{1+\rho(\mathbf{D})}$.

Proof: Multiplying the null-space condition $\mathbf{D}\delta = 0$ by $\mathbf{D}^T$, and using $\mathbf{G} = \mathbf{D}^T\mathbf{D}$, we get $\mathbf{G}\delta = 0$. The i-th row of this equation,

$$G_{ii}\delta_i + \sum_{j\neq i} G_{ij}\delta_j = 0, \quad 1 \le i \le k, \tag{5}$$

gives us

$$\delta_i = -\sum_{j\neq i} \frac{G_{ij}}{G_{ii}} \delta_j, \quad 1 \le i \le k. \tag{6}$$

Taking absolute value of both sides, we obtain

$$|\delta_i| = \left| \sum_{j\neq i} \frac{G_{ij}}{G_{ii}} \delta_j \right| \le \sum_{j\neq i} \left| \frac{G_{ij}}{G_{ii}} \right| |\delta_j| \le \rho(\mathbf{D}) \sum_{j\neq i} |\delta_j|, \tag{7}$$

where the last inequality is due to (3). Adding a term $\rho(\mathbf{D})|\delta_i|$ to both sides, we get

$$(1 + \rho(\mathbf{D}))|\delta_i| \le \rho(\mathbf{D})\|\delta\|_1, \quad 1 \le i \le k, \tag{8}$$

implying

$$|\delta_i| \le \frac{\rho(\mathbf{D})}{1 + \rho(\mathbf{D})} \|\delta\|_1 = t_{\mathbf{D}} \|\delta\|_1, \quad 1 \le i \le k. \tag{9}$$

Thus, $\|\delta\|_\infty \le t_{\mathbf{D}}\|\delta\|_1$, as the Lemma claims. □

2.2. Sparsity Guarantees Unique Global Optimality

In the following analysis we shall use a non-trivial (i.e., non-zero) concave and increasing semi-monotonic scalar function $\varphi : \mathbb{R}_+ \to \mathbb{R}$. Concavity implies that $\forall\ 0 \le t_1 < t_2$, the line stretched between the points $(t_1, \varphi(t_1))$ and $(t_2, \varphi(t_2))$ is below the function for $x \in [t_1, t_2]$, and above it otherwise, i.e.,

$$\frac{\varphi(t_2) - \varphi(t_1)}{t_2 - t_1}(x - t_1) + \varphi(t_1) : \begin{cases} \ge \varphi(x) & \text{for } x \notin [t_1, t_2] \\ \le \varphi(x) & \text{for } x \in [t_1, t_2] \end{cases}.$$

The monotonicity means that $\forall\ 0 \le t_1 < t_2$ we have that $\varphi(t_2) \ge \varphi(t_1)$.

Theorem 1 *Consider the following optimization problem*

$$\min_{\mathbf{z}} \sum_{i=1}^{k} \varphi(|z_i|) \quad \textit{subject to } \mathbf{Dz} = \mathbf{b} \tag{10}$$

with a scalar function φ as defined above. A feasible solution $\bar{\mathbf{z}}$ (i.e. $\mathbf{D}\bar{\mathbf{z}} = \mathbf{b}$) is a unique global optimum of (10) if $\|\bar{\mathbf{z}}\|_0 < \frac{1}{2t_{\mathbf{D}}}$.

Proof: Adding a constant to the objective function does not change the solution. Therefore, without loss of generality, we shall assume hereafter that $\varphi(0) = 0$. We intend to show that under the conditions of the theorem, any feasible non-zero deviation vector $\delta \in \mathbb{R}^k$ of $\bar{\mathbf{z}}$ (i.e. $\bar{\mathbf{z}} + \delta$) necessarily leads to an increase in the objective function, namely

$$\sum_{i=1}^{k} \varphi(|\bar{z}_i + \delta_i|) > \sum_{i=1}^{k} \varphi(|\bar{z}_i|). \tag{11}$$

Feasibility of the deviation vector means $\mathbf{D}(\bar{\mathbf{z}} + \delta) = \mathbf{b}$, implying $\mathbf{D}\delta = \mathbf{0}$. Thus, by Lemma 1 we can state:

$$|\delta_i| \le t_{\mathbf{D}}\|\delta\|_1 \equiv \delta_{\text{tol}}, \quad 1 \le i \le k. \tag{12}$$

Among all vectors δ of fixed total amplitude satisfying $\|\delta\|_1 = \delta_{\text{tol}}/t_{\mathbf{D}}$ satisfying inequalities (12), we shall try to compose one that reduces the objective function. For this, we separate the summation of the objective function into two parts – the on-support elements (i.e. those with $|\bar{z}_i| > 0$), and the off-support ones (where $\bar{z}_i = 0$). We denote the support of $\bar{\mathbf{z}}$ as Γ and write

$$\sum_{i=1}^{k} \varphi(|\bar{z}_i + \delta_i|) = \sum_{i\in\Gamma} \varphi(|\bar{z}_i + \delta_i|) + \sum_{i\notin\Gamma} \varphi(|\delta_i|). \tag{13}$$

We consider first the on-support term. Taking into account monotonicity and concavity of $\varphi(\cdot)$, a maximal decrease of the objective function would be possible for the choice

$$\delta_i = \begin{cases} -\delta_{\text{tol}} \cdot \text{sign}(\bar{z}_i) & |\bar{z}_i| \ge \delta_{\text{tol}} \\ -\bar{z}_i & 0 < |\bar{z}_i| < \delta_{\text{tol}} \end{cases}. \tag{14}$$

For this assignment, the descent in the objective function is given by

$$\begin{aligned} E_\Gamma &= \sum_{i\in\Gamma}\varphi(|\bar z_i|) - \sum_{i\in\Gamma}\varphi(|\bar z_i+\delta_i|) \\ &= \sum_{i\in\Gamma}\varphi(|\bar z_i|) - \sum_{i\in\Gamma}\varphi(|\bar z_i|-\delta_i) \\ &= \sum_{i\in\Gamma}\varphi(|\bar z_i|) - \sum_{i\in\Gamma}\varphi\left(\max\{|\bar z_i|-\delta_{\text{tol}},0\}\right) \\ &\le |\Gamma|\cdot\varphi(\delta_{\text{tol}}). \end{aligned} \tag{15}$$

The last inequality is a direct consequence of the zero-bias ($\varphi(0)=0$), monotonicity, and the concavity of the function $\varphi(\cdot)$.

Turning to the off-support term in Equation (13), any assignment of $\delta_i \neq 0$ implies an ascent. Of the original deviation vector δ, we are left with a total amplitude of at least $\|\delta\|_1 - |\Gamma|\cdot\delta_{\text{tol}} = \|\delta\|_1\cdot(1-t_{\mathbf{D}}|\Gamma|)$, to be assigned to the off-support elements. Again, due to the concavity of $\varphi(\cdot)$, this remaining energy leads to the smallest possible ascent if the assignment chosen is δ_{tol} to as few as possible elements. Thus, the obtained ascent becomes

$$E_{\bar\Gamma} = \frac{\|\delta\|_1 - |\Gamma|\cdot\delta_{\text{tol}}}{\delta_{\text{tol}}}\cdot\varphi(\delta_{\text{tol}}) = \frac{1-t_{\mathbf{D}}|\Gamma|}{t_{\mathbf{D}}|\Gamma|}\cdot\varphi(\delta_{\text{tol}}). \tag{16}$$

In order for $\bar{\mathbf{z}}$ to be a unique global minimizer of the problem posed in Equation (10), the change of the objective function should be positive – i.e., $E_\Gamma < E_{\bar\Gamma}$, implying

$$\frac{1-t_{\mathbf{D}}|\Gamma|}{t_{\mathbf{D}}|\Gamma|}\cdot\varphi(\delta_{\text{tol}}) > |\Gamma|\cdot\varphi(\delta_{\text{tol}}). \tag{17}$$

which is always satisfied if $|\Gamma| \equiv \|\bar{\mathbf{z}}\|_0 < \frac{1}{2t_{\mathbf{D}}}$, as claimed. □

3. NON-NEGATIVE SYSTEMS OF EQUATIONS

We now turn to the main result of this paper, showing that if a linear system with non-negativity constraint has a sufficiently sparse solution, then this solution is unique. Afterwards, we show how to preconditioning of the linear system can be used to strengthen this theorem.

3.1. Main Result

Suppose that we are given a system of linear of equations with non-negativity constraints

$$\mathbf{A}\mathbf{x} = \mathbf{b},\ \ \mathbf{x}\ge 0, \tag{18}$$

with non-negative $\mathbf{A}\in\mathbb{R}^{n\times k}$ and $\mathbf{b}\in\mathbb{R}^n$. In order to simplify the exposition, we re-scale the problem to have unit column sums of the coefficients. Let $\mathbf{W}$ be a diagonal matrix with the entries $W_{jj} = \sum_i A_{ij}$. We assume that there are no zero columns of in $\mathbf{A}$, and thus $\mathbf{W}$ is invertible. The equivalent system is

$$\mathbf{A}\mathbf{W}^{-1}\mathbf{W}\mathbf{x} = \mathbf{b},\ \ \mathbf{x}\ge 0. \tag{19}$$

Denoting $\mathbf{D}\equiv\mathbf{A}\mathbf{W}^{-1}$ and $\mathbf{z}\equiv\mathbf{W}\mathbf{x}$, we get the normalized system with $\sum_i D_{ij}=1$:

$$\mathbf{D}\mathbf{z} = \mathbf{b},\ \ \mathbf{z}\ge 0. \tag{20}$$

Denote $\mathbf{1}_n$ a column vector of n ones. Multiplying the last equation with $\mathbf{1}_n^T$, and using the fact that $\mathbf{1}_n^T\mathbf{D} = \mathbf{1}_k^T$, we obtain $\mathbf{1}_k^T\mathbf{z} = \mathbf{1}_n^T\mathbf{b} = c$, where c denotes the sum of the entries in $\mathbf{b}$.

Theorem 2 *Suppose that we are given a system of linear equations with non-negativity constraints $\mathbf{D}\mathbf{z}=\mathbf{b},\ \ \mathbf{z}\ge 0$, such that all its solutions satisfy $\mathbf{1}^T\mathbf{z}=c$, where c is some constant. If a vector $\bar{\mathbf{z}}$ is a sparse solution of this system with $\|\bar{\mathbf{z}}\|_0 < \frac{1}{2t_{\mathbf{D}}}$, then it is a unique solution of this problem.*

Proof: Taking into account non-negativity of $\mathbf{z}$, we can rewrite the condition $\mathbf{1}^T\mathbf{z}=c$ differently, as

$$\|\mathbf{z}\|_1 = c. \tag{21}$$

The vector $\bar{\mathbf{z}}$ is a sparse (with less than $1/2t_{\mathbf{D}}$ non-zeros) feasible solution of the linear programming problem

$$\min_{\mathbf{z}}\ \|\mathbf{z}\|_1 \ \ \text{subject to}\ \ \mathbf{D}\mathbf{z}=\mathbf{b}. \tag{22}$$

Notice that we do not specify the constraint $\mathbf{1}_k^T\mathbf{z}=c$ because any feasible solution of this problem must satisfy this condition anyhow. Also, we do not add a non-negativity constraint – the problem is defined as described above, and we simply observe that $\bar{\mathbf{z}}$ is a feasible solution.

By Theorem 1, the vector $\bar{\mathbf{z}}$ is necessarily a unique global minimizer of (22), i.e. any other feasible vector $\mathbf{z} : \mathbf{D}\mathbf{z} = \mathbf{b}$ has a larger value of $\|\mathbf{z}\|_1$; hence, being non-negative, it cannot satisfy $\mathbf{1}^T\mathbf{z}=c$, and therefore it can not be a solution of $\mathbf{D}\mathbf{z}=\mathbf{b},\ \ \mathbf{z}\ge 0$. □

Before leaving this sub-section, we add the following two comments:

- Here is a brief discussion to get more intuition on the above theorem. Assume that a very sparse vector $\bar{\mathbf{z}}$ has been found to be a feasible solution of $\mathbf{D}\mathbf{z}=\mathbf{b},\ \ \mathbf{z}\ge 0$. At least locally, if we aim to find other feasible solutions, we must use a deviation vector that lies in the null-space of $\mathbf{D}$, i.e., $\mathbf{D}\delta = \mathbf{0}$. Positivity of the alternative solution $\bar{\mathbf{z}}+\delta$ forces us to require that at the off-support of $\bar{\mathbf{z}}$, all entries of δ are non-negative. Thus, the above theorem is parallel to the claim that such constrained vector is necessarily the trivial zero one.

- We started the discussion in this section by requiring that $\mathbf{A}$ is non-negative. The only place that used this property is the normalization by $\mathbf{W}$ in Equation (19), requiring that $\mathbf{W}$ is invertible. Thus, any matrix $\mathbf{A}$ that leads to an invertible positive weight matrix $\mathbf{W}$ is adequate for our analysis.

3.2. Better Bounds via Preconditioning

The problem (10) can be rewritten in an equivalent form

$$\min_{\mathbf{z}} \sum_i \varphi(|z_i|) \quad \text{subject to} \quad \mathbf{PDz} = \mathbf{Pb}, \tag{23}$$

where the "preconditioner" matrix $\mathbf{P}$ is any invertible $n \times n$ matrix. Therefore the statement of the Theorem 1 remains valid if we change $\rho(\mathbf{D})$ and $t_{\mathbf{D}}$ by $\rho(\mathbf{PD})$ and $t_{\mathbf{PD}}$. This gives us a useful degree of freedom in the analysis of problem (10): In order to relax the requirement on the number of non-zeros, one can try to find such $\mathbf{P}$ that reduces $\rho(\mathbf{PD})$. The same is valid for problem posed in (20).

In the case of positive matrix $\mathbf{D}$, an efficient preconditioning can be obtained just by subtracting the mean of each column $\mathbf{d_i}$ from its entries:

$$\mathbf{Pd}_i = \mathbf{d}_i - \text{mean}(\mathbf{d}_i)\mathbf{1}_n = \left(\mathbf{I} - \frac{1}{n}\mathbf{E}\right)\mathbf{d_i}, \tag{24}$$

where $\mathbf{E}$ is $n \times n$ matrix of ones and $\mathbf{I}$ is the identity matrix of the same size. Such preconditioner typically reduces correlation between columns. For example, when the columns are normalized, $\sum_k d_{kl} = 1$,

$$(\mathbf{Pd}_i)^T(\mathbf{Pd}_j) = \mathbf{d_i}^T \left(\mathbf{I} - \frac{1}{n}\mathbf{E}\right)\mathbf{d_i} = \mathbf{d}_i^T\mathbf{d}_j - \frac{1}{n}.$$

This usually leads to a smaller coherence constant $\rho(\mathbf{PD})$. Note that the matrix $(\mathbf{I} - \frac{1}{n}\mathbf{E})$ is singular (and thus non-invertible); therefore we use $(\mathbf{I} - \frac{1-\epsilon}{n}\mathbf{E})$ instead, with ϵ being a small positive constant $0 < \epsilon << 1$.

We should note again that this preconditioning does not change the solution of the original linear system; it just improves our worst-case forecast of uniqueness versus sparsity. On the other hand, as shown in [1], it improves significantly the behavior of the orthogonal matching pursuit algorithm [4], targeting the above problem.

4. CONCLUSIONS

Non-negative linear systems of equations come up often in many applications in signal and image processing. Solving such systems is usually done by adding conditions such as minimal ℓ_2 length, maximal entropy, maximal sparsity, and so on. In this work we have shown that if a sparse enough solution exists, then it is the only one, implying that all the mentioned measures lead to the same solution. We also have proposed an effective preconditioning for improving the chances of such linear system to be handled well by greedy algorithms. Future work on this front could consider ways to optimize the preconditioning operator, suggest ways improve the proposed bound by probabilistic means, and attempt to exploit this uniqueness for compressed sensing and other applications.

5. REFERENCES

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