A novel sparsity and clustering regularization

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Abstract

We propose a novel SPARsity and Clustering (SPARC) regularizer, which is a modified version of the previous octagonal shrinkage and clustering algorithm for regression (OSCAR), where, the proposed regularizer consists of a $K$-sparse constraint and a pair-wise $\ell_\infty$ norm restricted on the $K$ largest components in magnitude. The proposed regularizer is able to separate sparsity and encourage the non-zeros to be in equal magnitude. Moreover, it can accurately group the features without shrunk their magnitude. In fact, SPARC is closely related to OSCAR, so that the proximity operator of the former can be efficiently computed based on that of the latter, allowing using proximal splitting algorithms to solve problems with SPARC regularization. Experiments on synthetic data and with benchmark breast cancer data show that SPARC is a competitive group-sparsity inducing regularizer for regression and classification.

1. Introduction

In recent years, much attention has been paid not only to sparsity but also to structured/group sparsity. Several group-sparsity-inducing regularizers have been proposed, including group LASSO (gLASSO), fused LASSO (fLASSO), elastic net (EN) [6], octagonal shrinkage and clustering algorithm for regression (OSCAR) [5], and several others, not listed here due to space limitations (see review in [6]). However, gLASSO (and its many variants and descendants [6]) require prior knowledge about the structure of the groups, which is a strong requirement in many applications, while fLASSO depends on a given order of variables; these two classes of approaches are thus better suited to signal processing applications than to variable selection and grouping in machine learning problems, such as regression or classification (where the order of the variables is often meaningless). In contrast, EN and OSCAR were proposed for regression problems and do not rely on any ordering of the variables or knowledge about group structure. The OSCAR regularizer (shown in [10] to outperform EN in feature grouping) is defined as

$$\phi_{\text{OSCAR}}(x) = \lambda_1 \|x\|_1 + \lambda_2 \sum_{i,j} \max \{ |x_i|, |x_j| \}$$

where $\lambda_1$ and $\lambda_2$ are non-negative parameters (which, in practice, can be chosen, for example, by cross validation [10]). The $\ell_1$ norm and the pairwise $\ell_\infty$ penalty simultaneously encourage the components to be sparse and equal in magnitude, respectively. However, it may happen that components with small magnitude that should be shrunk to zero by the $\ell_1$ norm are also penalized by the pairwise $\ell_\infty$ term, which may prevent accurate grouping; moreover, components with large magnitude that should simply be grouped by the pairwise $\ell_\infty$ norm are also shrunk by the $\ell_1$ norm (see Figure 1). In this paper, to overcome these drawbacks, we propose the SPARsity-and-Clustering (SPARC) regularizer, where the cardinality of the support of the solution is restricted and the pairwise $\ell_\infty$ penalty is applied only to the non-zero elements (see Figure 1). We also show how to compute the proximity operator of the SPARC regularizer, which allows using proximal splitting algorithms to problems with this regularizer.

2. Proposed Formulation and Approach

A linear regression problem (with design matrix $A \in \mathbb{R}^{n \times p}$) under SPARC regularization is formulated as

$$\min_{x \in \mathbb{R}^p} \frac{1}{2} \| y - Ax \|^2 + \ell_\infty(x) + \lambda \sum_{i,j \in \Omega_k(x), i < j} \max \{ |x_i|, |x_j| \}$$

where $\ell_\infty$ denotes the indicator of set $C$ ($\ell_\infty(x) = 0$, if $x \in C$; $\ell_\infty(x) = +\infty$, if $x \notin C$), $\Sigma_K = \{ x : \|x\|_0 \leq K \}$ is the set of $K$-sparse vectors, and $\Omega_k(x) = \text{supp}(P_{\Sigma_k}(x))$ (where $P_{\Sigma_k}(x)$ is the projection on $\Sigma_k$, and $\text{supp}(v) = \{i : v_i \neq 0\}$) is the set of indices of the $K$ largest components of $x$ (in magnitude). This regularizer enforces $K$-sparsity and encourages the non-zeros to be in equal magnitude.

Applying proximal splitting algorithms to address (1) requires the proximity operator

$$\text{prox}_{\psi_{\text{SPARC}}}^\lambda(y) = \arg\min_x \left( \psi_{\text{SPARC}}^\lambda(x) + \frac{1}{2} \| x - y \|^2 \right),$$

where $x \in \Sigma_K \Rightarrow \psi_{\text{SPARC}}^\lambda(x) = \psi_{\text{OSCAR}}^\lambda(x_{\Omega_k(x)}),$ where $x_{S} \in \mathbb{R}^{|S|}$ is the sub-vector of $x$ indexed by an index subset $S \subseteq \{1, \ldots, p\}$. Combining this with properties of proximity operators and ideas from [6] allows showing (naturally, details are omitted here) that $z = \text{prox}_{\psi_{\text{SPARC}}}^\lambda(x)$ can be computed as follows:

$$z_{\Omega_k}(x) = \text{prox}_{\psi_{\text{OSCAR}}}^\lambda(x_{\Omega_k}(x)),$$

where $0$ is a vector of zeros, $\Omega_k(x) = \{1, \ldots, p\} \setminus \Omega_k(x),$ and $\text{prox}_{\psi_{\text{SPARC}}}^\lambda(x)$ can be obtained using the algorithm proposed in [10]. Therefore, we can solve (1) by proximal splitting algorithms, such as FISTA [3], TWIST [4], or SpaRSA [8], which is the algorithm adopted in our experiments. SpaRSA (which stands for sparse reconstruction by separable approximation [8]) is a fast proximal splitting algorithm, based on the step-length selection method of Barzilai and Borwein [2]. It application to SPARC leads to the following algorithm:

\textbf{Algorithm SpaRSA for solving (1)}

1. Set $k = 1$, $\gamma > 1$, $\alpha_0 = \alpha_{\text{max}} > 0$, $\alpha_{\text{max}} < \alpha_{\text{min}}$, and $x_0$.
2. $y_0 = x_0 - A^T (Ax_0 - y) / \alpha_0$.
3. $x_1 = \text{prox}_{\psi_{\text{SPARC}}}^\lambda(y_0)$.
4. repeat
5. $\alpha_k = \max \{ \alpha_{\text{min}}, \min \{ \alpha_k, \alpha_{\text{max}} \} \}$
6. $\alpha_k = \gamma \alpha_k$
7. $y_k = x_k - A^T (Ax_k - y) / \alpha_k$
8. $x_{k+1} = \text{prox}_{\psi_{\text{SPARC}}}^\lambda(y_k)$
9. $\alpha_k \leftarrow \frac{1}{\alpha_k}$
10. until $x_{k+1}$ Satisfies an acceptance criterion.
11. $k \leftarrow k + 1$
12. until some stopping criterion is satisfied.

In this algorithm, the acceptance criterion in Line 10 may be used to enforce the objective function to decrease; see [8] for details.
3 Experiments

In this section, we report results of experiments with synthetic data and with the breast cancer benchmark data, aimed at comparing the SPARC with the LASSO, EN and OSCAR. In order to measure their performances, we employ the following six metrics defined on an estimate $e$ of an original vector $x^*$:

- Mean absolute error: $\text{MAE} = \|A(x^*-e)\|_1$;
- Mean square error: $\text{MSE} = \|A(x^*-e)\|_2^2$;
- Selection error rate: $\text{SER} = \|x^* - e\|_1 / p$;
- Degrees of freedom (DoF): the number of unique non-zero coefficients of $e$;
- Classification accuracy (CLA): the number of correct classifications of $e$;
- Number of non-zero features (NNZ).

3.1 Synthetic data

We consider a regression problem where $y = Ax + w$, where the true parameters

$$x^* = [3, \ldots, 3, 0, \ldots, 0]^T$$

and the design matrix $A$ is generated as

$$a_i = z_i + \varepsilon_i^x, z_i \sim N(0,1), i = 1, \ldots, 5;$$
$$a_i = z_i + \varepsilon_i^z, z_i \sim N(0,1), i = 6, \ldots, 10;$$
$$a_i = z_i + \varepsilon_i^z, z_i \sim N(0,1), i = 11, \ldots, 15;$$
$$a_i \sim N(0,1), i = 16, \ldots, 40$$

where $\varepsilon_i$ are independent identically distributed $N(0,0.16)$, $i = 1, \ldots, 15$. Then $A = [a_1, a_2, \ldots, a_{40}]^T$ is further normalized, the noise variance of $w$ is 0.01. The number of samples for training, cross validation and testing are 20, 40 and 200, respectively. Notice that it is an ill-posed training problem, since the number of samples is less than the dimension of $x$ ($20 < 40$).

3.2 Breast cancer data

In this section, we report experiments with the breast cancer benchmark data, which contains 8141 genes in 295 tumors, where 300 genes that are most correlated with the responses. 50%, 30% and 20% of the data are then randomly chosen for training, cross validation, and testing, respectively. The results averaged over 50 repetitions are show in Table 2. We can observe that SPARC is a competitive group-sparsity-inducing regularizer for classification in terms of CLA, and it is able to select features with lower degrees of freedom than LASSO, EN, and OSCAR.

| Metrics   | LASSO | EN   | OSCAR | SPARC |
|-----------|-------|------|-------|-------|
| MAE       | 27.067| 29.438| 66.239| 25.747|
| MSE       | 7.6614| 7.6939| 36.8120| 5.2904|
| DoF       | 15.64 | 25.28 | 4.56  | 4.02  |
| SER       | 14.50%| 25.75%| 8.95% | 5.50% |

Table 2: Results of the metrics on synthetic data

From Figure 2 and Table 1, the SPARC outperforms the LASSO, EN and OSCAR, showing it is a promising approach to feature selection and grouping in regression.

4 Conclusions

We have proposed the SPARsity and Clustering (SPARC) regularizer for regression and classification. We have shown that the proposed SPARC is able to separably enforce $K$-sparsity and encourage the non-zeros to be equal in magnitude, thus accurately grouping the features without parameter shrinkage, outperforming the LASSO, the elastic net, and the octagonal shrinkage and clustering algorithm for regression (OSCAR). Future work will involve considering faster algorithms to solve problems with SPARC regularization.

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