An efficient algorithm to satisfy ℓ_1 and ℓ_2 constraints

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Résumé. Dans ce papier, un algorithme efficace de projection sous contraintes de normalisation et de parcimonie est proposé. Cet algorithme a été confronté à des méthodes à l'état de l'art (recherche dichotomique et POCS) et a permis des améliorations significatives en terme de temps de calcul. Son déploiement dans l'algorithme associé à l'Analyse Canonique Généralisée Sparse (SGCCA) a motivé ce travail.

Mots-clés. SGCCA, parcimonie, Optimisation.

Abstract. An efficient projection enforcing both normalization and sparsity is proposed in this paper. The algorithm has been compared to state of the art methods (binary search and POCS) and provides valuable runtime improvements. Its application within the algorithm associated to Sparse Generalized Canonical Correlation Analysis (SGCCA) has motivated this work.

Keywords. SGCCA, sparsity, Optimization.

1 Introduction

We consider the non-convex set $\mathcal{X} = \left\{\mathbf{x} \in \mathbb{R}^p \mid \|\mathbf{x}\|_2 = 1 \text{ and } \|\mathbf{x}\|_1 \leq \tau \text{ with } \tau \in \mathbb{R}_+^*\right\}$ and $\mathbf{a} \in \mathbb{R}^p$. The optimization problem that is considered is :

$$\begin{aligned} \underset{\mathbf{x}\in\mathcal{X}}{\operatorname{argmin}} \ \|\mathbf{x}-\mathbf{a}\|_2^2 &= \underset{\mathbf{x}\in\mathcal{X}}{\operatorname{argmin}} \ \|\mathbf{x}\|_2^2 + \|\mathbf{a}\|_2^2 - 2\mathbf{a}^\top\mathbf{x} \\ &= \underset{\mathbf{x}\in\mathcal{X}}{\operatorname{argmax}} \ \mathbf{a}^\top\mathbf{x} \end{aligned} \tag{1}$$

According to (Witten, 2009), the solution of the optimization problem (1) satisfies $\mathbf{u} = S(\mathbf{a}, \lambda)/\|S(\mathbf{a}, \lambda)\|_2$; where S is a softh-thresholding operator defined by $S(a, \lambda) = \max(0, |a| - \lambda)$ applied componentwise. The parameter $\lambda = 0$ if $\|\mathbf{u}\|_1 \leq \tau$ and λ is chosen such that $\|\mathbf{u}\|_1 = \tau$ otherwise. λ is usually determined by binary search or by Projection On Convex Set algorithm (POCS), also known as alternating projection method (Boyd &

Dattorro, 2003). In this paper, we proposed a new algorithm similar to the one for projecting a point onto the ℓ_1-ball which was described in (van den Berg et al., 2008). This approach is summarized in the next section.

2 Efficient projection onto the ℓ_1-ball

Let $\tilde{\mathbf{a}}$ be the absolute value of $\mathbf{a}$ with its elements sorted in decreasing order. Further, we define the function $\varphi(\lambda) = \|S(\mathbf{a}, \lambda)\|_1$ which is continuous, piecewise linear and decreasing from $\varphi(0) = \|\tilde{\mathbf{a}}\|_1$ to $\varphi(\tilde{a}_1) = 0$. Therefore, if $\|\mathbf{a}\|_1 \geq \tau$, as φ is continuous, it exists λ such that $\varphi(\lambda) = \tau$. Hence, this projection algorithm onto the ℓ_1-ball reduces to 4 steps :

1. Take the absolute value of $\mathbf{a}$ and sort its elements in decreasing order to get $\tilde{\mathbf{a}}$.
2. Find i such that $\varphi(\tilde{a}_i) \leq \tau < \varphi(\tilde{a}_{i+1})$.
3. Find δ such that $\varphi(\tilde{a}_i - \delta) = \tau$. As $\varphi(\tilde{a}_i - \delta) = \sum_{j=1}^{i} \tilde{a}_j - i(\tilde{a}_i - \delta) = \varphi(\tilde{a}_i) + i\delta$ then $\delta = \frac{\tau - \varphi(\tilde{a}_i)}{i}$.
4. Compute $S(\mathbf{a}, \lambda) = \text{sign}(\mathbf{a}) \max(|\mathbf{a}| - \lambda, 0)$ with $\lambda = \tilde{a}_i - \delta$.

Similar algorithm was proposed by (Candès, 2005), (Daubechies, 2007) and (Duchi, 2008).

3 Main contribution

The novelty of this paper is to extend the algorithm described previously to the function $\psi(\lambda) = \|S(\tilde{\mathbf{a}}, \lambda)\|_1 / \|S(\tilde{\mathbf{a}}, \lambda)\|_2$ in order to solve optimization problem (1).

Proposition 1. *For $\lambda \in [0; \tilde{a}_1[$, $\psi(\lambda) = \dfrac{\|S(\tilde{\mathbf{a}}, \lambda)\|_1}{\|S(\tilde{\mathbf{a}}, \lambda)\|_2}$ verifies the 3 following properties:*

(i) ψ is continuous and decreasing.

(ii) Let n_{max} be the number of element equal to $\tilde{a}_1$, the maximum of $\tilde{\mathbf{a}}$.
For $\tau \in [\sqrt{n_{max}}; \sqrt{p}]$ it exists $i \in [\![1; p]\!]$ and $\delta \in [0; \tilde{a}_i - \tilde{a}_{i+1}[$ such that $\psi(\tilde{a}_i - \delta) = \tau$.

(iii) δ is solution of a second degree polynomial equation.

Proof. **(i).** The numerator and denominator of ψ are continuous as composition of continuous functions. Moreover, for $\lambda \in [0; \tilde{a}_1[$, $\|S(\tilde{\mathbf{a}}, \lambda)\|_2 \neq 0$. Therefore, ψ is continuous as quotient of 2 non-null continuous functions.
Assuming $\tilde{a}_{p+1} = 0$, for $\lambda \in [0; \tilde{a}_1[$ it exists $k \in [\![1; p]\!]$ such that $\tilde{a}_{k+1} \leq \lambda < \tilde{a}_k$. For this specific λ, we have:

$$\|S(\tilde{\mathbf{a}}, \lambda)\|_1 = \left[\sum_{j=1}^{k} \tilde{a}_j\right] - k\lambda \tag{2}$$

$$\|S(\tilde{\mathbf{a}},\lambda)\|_2^2 = \sum_{j=1}^{k}(\tilde{a}_j-\lambda)^2 = \left[\sum_{j=1}^{k}\tilde{a}_j^2\right] - 2\lambda\left[\sum_{j=1}^{k}\tilde{a}_j\right] + k\lambda^2 \tag{3}$$

From equations (2) and (3), the derivate of ψ is :

$$\psi'(\lambda) = \frac{1}{\|S(\tilde{\mathbf{a}},\lambda)\|_2^2}\left(\frac{\|S(\tilde{\mathbf{a}},\lambda)\|_1^2}{\|S(\tilde{\mathbf{a}},\lambda)\|_2} - k\|S(\tilde{\mathbf{a}},\lambda)\|_2\right) = \frac{1}{\|S(\tilde{\mathbf{a}},\lambda)\|_2}(\psi(\lambda)^2-k) \tag{4}$$

Moreover, the number of non-null elements of $S(\tilde{\mathbf{a}},\lambda)$ is equal to k. Therefore, from Cauchy-Schwarz, the inequality $\|S(\tilde{\mathbf{a}},\lambda)\|_1 \leq \sqrt{k}\|S(\tilde{\mathbf{a}},\lambda)\|_2$ holds, implying $\psi'(\lambda) \leq 0$.

(ii). For $\nu \in [\tilde{a}_2;\tilde{a}_1[$, $\psi(\nu) = \frac{n_{max}(\tilde{a}_1-\nu)}{\sqrt{n_{max}}(\tilde{a}_1-\nu)} = \sqrt{n_{max}}$. Thus, ψ is decreasing from $\psi(0) = \|\mathbf{a}\|_1/\|\mathbf{a}\|_2 \leq \sqrt{p}$ (Cauchy-Schwarz) to $\psi(\nu) = \sqrt{n_{max}}$. It implies that for $\tau \in [\sqrt{n_{max}};\sqrt{p}]$, it exists $i \in [\![1;p]\!]$ such that $\psi(\tilde{a}_i) \leq \tau < \psi(\tilde{a}_{i+1})$. Finally, as ψ is continuous, it exists $\delta \in [0;\tilde{a}_i - \tilde{a}_{i+1}[$ such that $\psi(\tilde{a}_i-\delta) = \tau$.

(iii). Using the notations $l_1 = \|S(\tilde{\mathbf{a}},\tilde{a}_i)\|_1$ and $l_2 = \|S(\tilde{\mathbf{a}},\tilde{a}_i)\|_2$:

$$\|S(\tilde{\mathbf{a}},\tilde{a}_i-\delta)\|_1 = \sum_{j=1}^{i}[\tilde{a}_j-(\tilde{a}_i-\delta)] = \sum_{j=1}^{i}[\tilde{a}_j-\tilde{a}_i] + i\delta = \|S(\tilde{\mathbf{a}},\tilde{a}_i)\|_1 + i\delta = l_1 + i\delta \tag{5}$$

$$\|S(\tilde{\mathbf{a}},\tilde{a}_i-\delta)\|_2^2 = \sum_{j=1}^{i}[\tilde{a}_j-(\tilde{a}_i-\delta)]^2 = \sum_{j=1}^{i}[(\tilde{a}_j-\tilde{a}_i)^2 + 2\delta(\tilde{a}_j-\tilde{a}_i)+\delta^2] = l_2^2 + 2\delta l_1 + i\delta^2 \tag{6}$$

Moreover, as $\psi(\tilde{a}_i-\delta) = \tau = \|S(\tilde{\mathbf{a}},\tilde{a}_i-\delta)\|_1/\|S(\tilde{\mathbf{a}},\tilde{a}_i-\delta)\|_2$, the following equality holds:

$$\|S(\tilde{\mathbf{a}},\tilde{a}_i-\delta)\|_1^2 = \tau^2\|S(\tilde{\mathbf{a}},\tilde{a}_i-\delta)\|_2^2 \tag{7}$$

Incorporating (5) and (6) in (7) gives:

$$\delta^2[i^2 - i\tau^2] + 2\delta l_1[i-\tau^2] + l_1^2 - \tau^2 l_2^2 = 0 \tag{8}$$

The goal is now to find the positive root of this second degree polynomial equation. The discriminant Δ is equal to $4\tau^2[\tau^2-i][l_1^2 - il_2^2]$. It remains to show that Δ is positive.
First, the number of non-null elements of $S(\tilde{\mathbf{a}},\tilde{a}_{i+1})$ is equal to i and the Cauchy-Schwartz inequality yields $\|S(\tilde{\mathbf{a}},\tilde{a}_{i+1})\|_1 \leq \sqrt{i}\|S(\tilde{\mathbf{a}},\tilde{a}_{i+1})\|_2$. Second, $\psi(\tilde{a}_{i+1}) = \dfrac{\|S(\tilde{\mathbf{a}},\tilde{a}_{i+1})\|_1}{\|S(\tilde{\mathbf{a}},\tilde{a}_{i+1})\|_2} > \tau$ so $\|S(\tilde{\mathbf{a}},\tilde{a}_{i+1})\|_1 > \tau\|S(\tilde{\mathbf{a}},\tilde{a}_{i+1})\|_2$. Combining the two previous inequalities yields $(i-\tau^2)\|S(\tilde{\mathbf{a}},\tilde{a}_{i+1})\|_1 > 0$ which implies that $i-\tau^2 > 0$. Third, from $\psi(\tilde{a}_i) = l_1/l_2 \leq \tau < \sqrt{i}$, we deduce that $l_1^2 - il_2^2 \leq 0$ which ensures that Δ is positive.
To conclude, the sign of $\dfrac{l_1^2-\tau^2 l_2^2}{i^2-i\tau^2}$ corresponds to the sign of the product of the 2 roots. As

this term is negative, the 2 roots have opposite signs. The single solution of $\psi(\tilde{a}_i - \delta) = \tau$ is:

$$\delta = \frac{-2l_1(i-\tau^2) + \sqrt{\Delta}}{2i(i-\tau^2)} = \frac{-2l_1(i-\tau^2) + 2\tau\sqrt{[\tau^2 - i][l_1^2 - il_2^2]}}{2i(i-\tau^2)} = -\frac{l_1}{i} + \frac{\tau}{i}\sqrt{\frac{il_2^2 - l_1^2}{i-\tau^2}}.$$

Using the fact that $\psi(\tilde{a}_i) = l_1/l_2$, the previous equation can be simplified as

$$\delta = \frac{\|S(\tilde{\mathbf{a}}, \tilde{a}_i)\|_2}{i}\left(\tau\sqrt{\frac{i-\psi(\tilde{a}_i)^2}{i-\tau^2}} - \psi(\tilde{a}_i)\right). \tag{9}$$

□

Remark. $\tau < \sqrt{i}$ implies that if you know the number of non-null elements you want to keep, then τ is in $[\sqrt{n_{max}}; \sqrt{i}]$.

The proposed algorithm reduces to 4 steps:

1. Take the absolute value of $\mathbf{a}$ and sort its elements in decreasing order to get $\tilde{\mathbf{a}}$.
2. Find i such that $\psi(\tilde{a}_i) \leq \tau < \psi(\tilde{a}_{i+1})$.
3. $\delta = \frac{\|S(\tilde{\mathbf{a}}, \tilde{a}_i)\|_2}{i}\left(\tau\sqrt{\frac{i-\psi(\tilde{a}_i)^2}{i-\tau^2}} - \psi(\tilde{a}_i)\right)$.
4. Compute $S(\mathbf{a}, \lambda) = \text{sign}(\mathbf{a})\max(|\mathbf{a}| - \lambda, 0)$ with $\lambda = \tilde{a}_i - \delta$.

Remark. Sorting the elements in step 1 implies that the time complexity is at least in $\mathcal{O}(p \ln p)$ with p the dimension of $\mathbf{a}$. In (Thom & Palm, 2013) a similar algorithm is proposed where they avoid the sorting step which reduces the time complexity to $\mathcal{O}(p)$.

This algorithm is freely available within the RGCCA package (Tenenhaus & Guillemot, 2017).

4 Applications

Runtime. The runtime performances of the proposed algorithm (Proj_l1_l2) are compared to the binary search (Binary) algorithm, POCS algorithm and the projection onto the ℓ_1-ball (Proj_l1) algorithm. Figure 1(a) shows that Proj_l1_l2 is almost 10 times faster than Binary and POCS and performs similarly to Proj_l1. Moreover, Figure 1(b) reports the runtime of the four methods as a function of the dimension p.

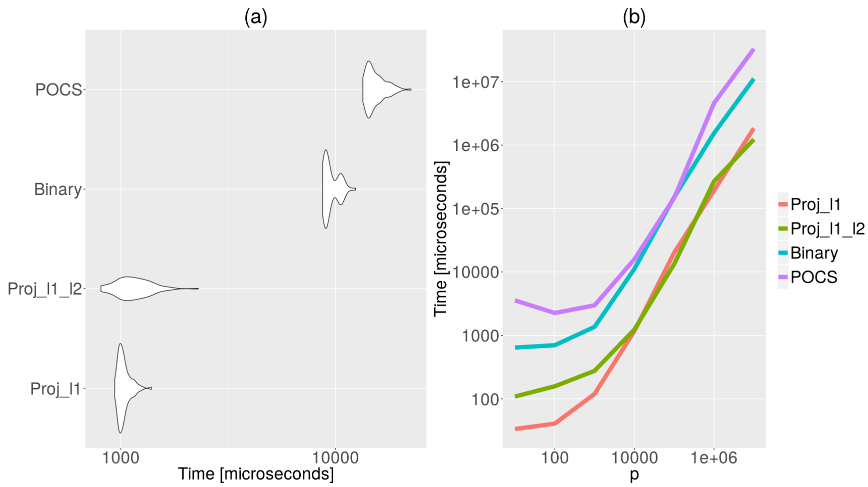

Figure 1: (a): Violin plots of the runtime of POCS, Binary, Proj_l1_l2 and Proj_l1 throughout 100 runs for a vector of length p =10.000. (b): Log-log plot of the runtime average over 20 runs for POCS, Binary, Proj_l1_l2 and Proj_l1 for different value of p. For all the experiments, the vector was drawn from a standardized normal distribution and τ was set to 2.3.

SGCCA. This work was motivated by its application to Sparse Generalized Canonical Correlation Analysis (SGCCA), a multiblock component method. This method, fully described in (Tenenhaus et al., 2014), is based on block relaxation to maximize a specific cost function. At each block relaxation substep, an optimization problem similar to (1) needs to be solved. Our algorithm (Proj_l1_l2) has been embedded within the SGCCA algorithm and has been compared to the original implementation with binary search. For this experiment, we applied SGCCA to a 3-block dataset which combine gene expression (p_1 = 15702), comparative genomic hybridization (p_2 = 1229), and a qualitative phenotype (p_3 = 3) measured on a set of 53 children with glioma. The Glioma dataset is freely available at `http://biodev.cea.fr/sgcca/`. For each of these two algorithms SGCCA was run 20 times and converged in average at 10.48 (resp. 7.62s) with a standard deviation of 0.60s (resp. 0.29s) for binary search (resp. Proj_l1_l2) on midrange laptop computer. We mention that the two implementations of the SGCCA algorithm converged to the same solution.

5 Conclusion

We proposed a computationally efficient alternative to binary search and POCS algorithm to solve optimization problem (1). This algorithm was then applied in the frame of SGCCA.

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