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# A Novel Smoothed Norm Ratio for Sparse Signal Restoration Application to Mass Spectrometry

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**Abstract**—We propose a new smoothed  $\ell_p$ -Over- $\ell_q$  norm ratio for sparse signal reconstruction. A trust-region Variable Metric Forward-Backward is proposed to solve efficiently the resulting non-convex minimization problem. Numerical experiments in the context of mass spectrometry (MS) illustrate the benefits of the novel penalty.

## I. PROBLEM STATEMENT

We consider the linear observation model  $\mathbf{y} = \mathbf{H}\mathbf{x} + \mathbf{n}$  where  $\mathbf{y} = (y_m)_{1 \leq m \leq M} \in \mathbb{R}^M$  represents the degraded measurements related to the original signal  $\mathbf{x} = (x_n)_{1 \leq n \leq N} \in \mathbb{R}^N$  through the observation matrix  $\mathbf{H} \in \mathbb{R}^{M \times N}$  and some additive acquisition noise  $\mathbf{n} \in \mathbb{R}^M$ . In this work, we focus on the inverse problem aiming at recovering signal  $\mathbf{x}$  from  $\mathbf{y}$  and  $\mathbf{H}$ , under the assumption that the sought signal is sparse, *i.e.*, has few non-zero entries. An efficient strategy is to employ a penalized approach, which defines an estimate  $\hat{\mathbf{x}} \in \mathbb{R}^N$  of  $\mathbf{x}$  as the solution of the following constrained minimization problem

$$\underset{\mathbf{x} \in S}{\text{minimize}} \Psi(\mathbf{x}) \quad \text{with} \quad S = \{\mathbf{x} \in \mathbb{R}^N \mid \|\mathbf{H}\mathbf{x} - \mathbf{y}\| \leq \xi\}. \quad (1)$$

Function  $\Psi: \mathbb{R}^N \rightarrow ]0, +\infty]$  is a regularization function used to enforce sparsity on the solution. Moreover,  $\xi > 0$  is a parameter depending on the noise characteristics. The choice of the regularization function  $\Psi$  is important to reach satisfactory results.

## II. PROPOSED APPROACH

The  $\ell_1$  norm has probably been the most frequently used regularizer for sparse signal restoration. Special cases of quasi-norm ratios have also served as sparse penalties, for instance the  $\ell_1/\ell_2$  ratio [1] or  $\ell_4/\ell_2$  [2], with the advantage of limiting scale biases. In this work, we propose a new Smoothed  $p$ -Over- $q$  (SPOQ) penalty defined as:

$$(\forall \mathbf{x} \in \mathbb{R}^N) \quad \Psi(\mathbf{x}) = \log \left( \frac{(\ell_{p,\alpha}^p(\mathbf{x}) + \beta^p)^{1/p}}{\ell_{q,\eta}(\mathbf{x})} \right), \quad (2)$$

where  $p \in ]0, 2[$  and  $q \in [2, +\infty[$ . We denote by  $\ell_{p,\alpha}$  and  $\ell_{q,\eta}$  the smoothed versions of  $\ell_p$  and  $\ell_q$  norms respectively given by  $\ell_{p,\alpha}(\mathbf{x}) = \left( \sum_{n=1}^N \left( (x_n^2 + \alpha^2)^{p/2} - \alpha^p \right) \right)^{1/p}$  and  $\ell_{q,\eta}(\mathbf{x}) = \left( \eta^q + \sum_{n=1}^N |x_n|^q \right)^{1/q}$  for every  $\mathbf{x} \in \mathbb{R}^N$  and  $(\alpha, \eta) \in ]0, +\infty[^2$ . In (2), the parameter  $\beta \in ]0, +\infty[$  is introduced to account for the fact that the log function is not defined at 0.

The SPOQ penalty is non-convex, which makes problem (1) challenging. It can however be shown that it is Lipschitz-differentiable on  $\mathbb{R}^N$ . Moreover, we established that  $\Psi$  presents a local majorization property. Let us define  $\mathcal{B}_{q,\rho} = \{\mathbf{x} \in \mathbb{R}^N \mid \sum_{n=1}^N |x_n| \geq \rho^q\}$ . Then, for every  $(\mathbf{x}, \mathbf{x}') \in \mathcal{B}_{q,\rho}^2$ ,  $\Psi(\mathbf{x}) \leq \Psi(\mathbf{x}') + \nabla \Psi(\mathbf{x}')^\top (\mathbf{x} - \mathbf{x}') + \frac{1}{2} (\mathbf{x} - \mathbf{x}')^\top \mathbf{A}_{q,\rho}(\mathbf{x}') (\mathbf{x} - \mathbf{x}')$  where, for every  $\mathbf{x} \in \mathcal{B}_{q,\rho}$ ,

$$\begin{aligned} \mathbf{A}_{q,\rho}(\mathbf{x}) &= \frac{1}{\ell_{p,\alpha}^p(\mathbf{x}) + \beta^p} \text{Diag} \left( (x_n^2 + \alpha^2)^{p/2-1} \right)_{1 \leq n \leq N} \\ &\quad + \frac{q-1}{(\eta^q + \rho^q)^{2/q}} \mathbf{I}_N. \end{aligned}$$

We thus propose to solve (1) using the novel trust-region Variable Metric Forward Backward algorithm described below. It can be viewed as an extension of [3], where a trust-region strategy has been introduced in order to keep the iterates inside the sets fulfilling the majorization.

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$$\begin{aligned} &\mathbf{x}_0 \in \mathbb{R}^N, \quad B \in \mathbb{N}^*, \quad \theta \in ]0, 1[, \quad (\gamma_k)_{k \in \mathbb{N}} \in ]0, 2[ \\ &\text{For } k = 0, 1, \dots : \\ &\quad \text{For } i = 1, \dots, B : \\ &\quad \quad \text{If } i = 1, \quad \rho_{k,1} = \sum_{n=1}^N |x_{n,k}|^q. \\ &\quad \quad \text{If } i \in \{2, \dots, B-1\}, \quad \rho_{k,i} = \theta \rho_{k,i-1}. \\ &\quad \quad \text{Else } \rho_{k,B} = 0. \\ &\quad \quad \text{Construct } \mathbf{A}_{k,i} = \mathbf{A}_{q,\rho_{k,i}}(\mathbf{x}_k) \\ &\quad \quad \mathbf{z}_{k,i} = \text{P}_{\mathbf{A}_{k,i}, S} \left( \mathbf{x}_k - \gamma_k (\mathbf{A}_{k,i})^{-1} \nabla \Psi(\mathbf{x}_k) \right) \\ &\quad \quad \text{If } \mathbf{z}_{k,i} \in \mathcal{B}_{q,\rho_{k,i}} : \text{ Stop loop} \\ &\quad \mathbf{x}_{k+1} = \mathbf{z}_{k,i} \end{aligned}$$


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Hereabove,  $\text{P}_{\mathbf{A},S}$  denotes the projection onto  $S$  in the metric induced by  $\mathbf{A}$  [3]. In this case, this projection cannot be explicitly expressed. We thus propose to compute it using the dual forward backward method [4]. Under mild assumptions, we proved that  $(\mathbf{x}_k)_{k \in \mathbb{N}}$  converges to a critical point of Problem (1).

## III. APPLICATION TO MASS SPECTROMETRY DATA ANALYSIS

We illustrate the usefulness of our proposed SPOQ penalty in the context of mass spectrometry (MS) data processing. MS is a fundamental technology of analytical chemistry widely used in structural biology [5], chemistry [6], pharmaceutical analysis [7], clinical drug development [8], etc. We have recently proposed a dictionary-based approach in [9] for proteins characterization in MS data. This method aimed at solving Problem (1) where  $\Psi$  is the  $\ell_1$  norm. We propose here to follow the same dictionary-based approach and to compare the results obtained by solving (1) using various choices of  $\Psi$ , namely the proposed SPOQ penalty for given  $p$  and  $q$ , the  $\ell_1$  norm, and the Cauchy and Welsh non-convex penalties [10].

Two synthetic signals A and B, with size  $N = 1000$  and sparsity degree  $P$  are tested (Fig. 1 (top)). The associated MS spectra  $\mathbf{y}$  are built with  $\mathbf{H}$  being the MS average dictionary [11], and  $\mathbf{n}$  a zero-mean Gaussian noise with standard deviation  $10^{-2}$  (Fig. 1 (bottom)). Tab. I displays the means and standard deviations, on 10 noise realizations, for three metrics: SNR =  $20 \log_{10}(\|\mathbf{x}\|/\|\mathbf{x} - \hat{\mathbf{x}}\|)$ , TSNR defined as the SNR computed only on the support of the sought sparse signal, and sparsity, *i.e.* the number of entries of the restored signals greater (in absolute value) than a given threshold (here,  $10^{-4}$ ). We can observe that SPOQ is superior to the three other penalties with respect to all metrics. In particular,  $p = 0.25$  and  $q = 2$  seem to provide an optimal choice in terms of estimation accuracy.

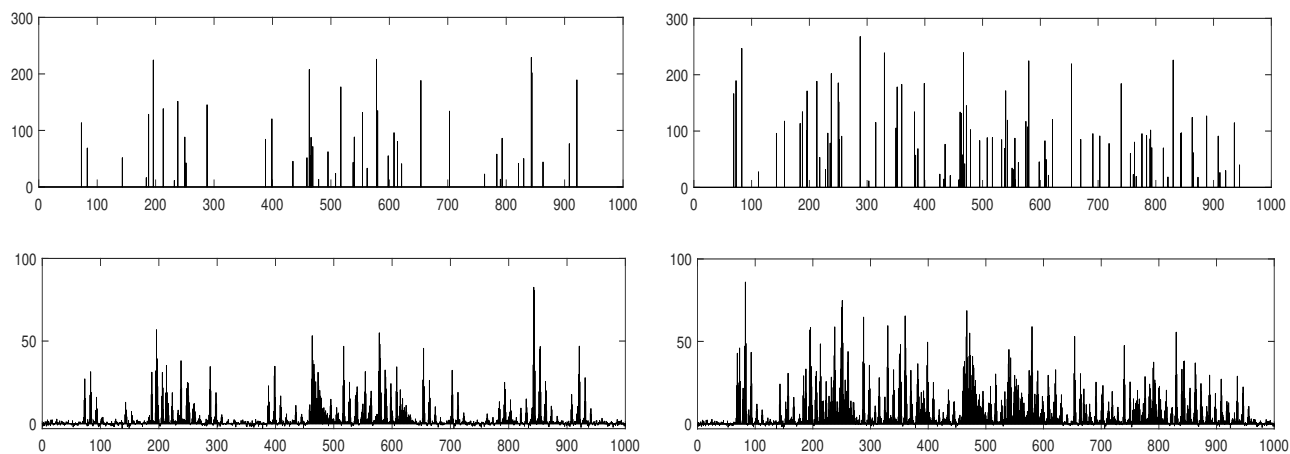


Figure 1. Original sparse signals and associated MS spectra for dataset A (left,  $N = 1000$ ,  $P = 48$ ) and dataset B (right,  $N = 1000$ ,  $P = 94$ ) (top: synthetic data, bottom: noisy MS spectra).

		$P$	$\ell_{0.25}/\ell_2$	$\ell_{0.5}/\ell_2$	$\ell_1/\ell_2$	$\ell_1$	Cauchy	Welsh
Signal A	SNR	48	<b>46.28</b>	41.91	40.91	43.16	42.84	27.54
			0.497	0.436	0.910	0.654	0.572	0.461
	TSNR	48	46.55	<b>47.71</b>	46.24	43.94	43.53	29.12
			0.571	1.136	1.660	0.679	0.532	0.501
	Sparsity	48	<b>49</b>	129	365	80	883	259
			1.32	11.85	10.13	9.46	10.57	8.08
Signal B	SNR	94	<b>45.56</b>	42.74	41.31	43.02	42.71	30.99
			0.538	1.266	1.298	1.260	1.194	0.488
	TSNR	94	<b>47.26</b>	46.88	45.11	44.17	43.68	33.39
			0.639	1.495	1.654	1.138	0.961	0.507
	Sparsity	94	<b>111</b>	216	410	165	952	342
			3.54	12.43	11.03	17.41	6.66	11.72

Table I

MEANS/STDS OF SNR, TRUNCATED SNR AND SPARSITY LEVEL OF THE RESTORED SIGNALS. COMPUTED ON 10 NOISE REALIZATIONS FOR DATASETS A AND B AND VARIOUS PENALTIES.

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<sup>1</sup><https://www.i2m.univ-amu.fr/project/bifrost>

<sup>2</sup><http://www.syscom.univ-mlv.fr/~chouzeno/MajIC>