DÉMÉLANGE, DÉCONVOLUTION ET DÉBRUITAGE CONJOINTS D'UN MODÈLE CONVOLUTIF PARCIMONIEUX AVEC DÉRIVE INSTRUMENTALE, PAR PÉNALISATION DE RAPPORTS DE NORMES OU QUASI-NORMES LISSÉES (PENDANTSS)

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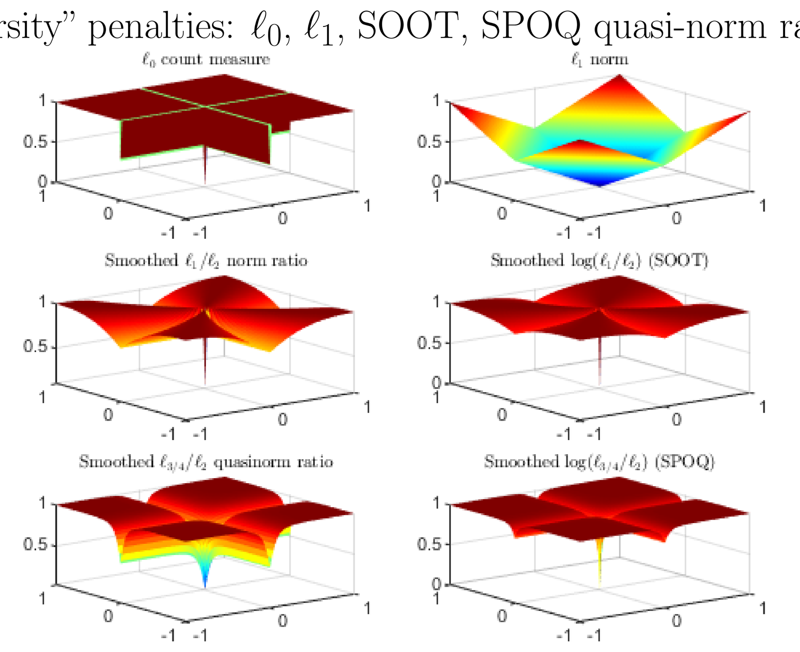
PENDANTSS, a GRETSI history

- GRETSI 2011 (Bordeaux): inspired by Vincent Mazet's *backcor* [1]
- GRETSI 2015 (Lyon): BEADS (Baseline Estimation And Denoising using Sparsity) [2]
- GRETSI 2019 (Lille): SOOT ℓ_1/ℓ_2, SPOQ ℓ_p/ℓ_q (Smooth One-Over-Two/p-Over-q norm/quasi-norm ratios) [3, 4]
- GRETSI 2023 (Grenoble): PENDANTSS (PEnalized Norm-ratios Disentangling Additive Noise, Trend and Sparse Spikes) [5]

"Sparsity" penalties: ℓ_0, ℓ_1, SOOT, SPOQ quasi-norm ratios



`https://github.com/paulzhengfr/PENDANTSS`

Problem, hypotheses & notations

Denoising, detrending, deconvolution: traditionally decoupled, complex ill-posed:

$$\boldsymbol{y} = \overline{\boldsymbol{s}} * \overline{\boldsymbol{\pi}} + \overline{\boldsymbol{t}} + \boldsymbol{n}.$$

- $\boldsymbol{y} \in \mathbb{R}^N$: single observation;
- $\overline{\boldsymbol{s}} \in \mathbb{R}^N$: *sparse spikes* (impulses, events, "diracs", spectral lines);
- $\overline{\boldsymbol{\pi}} \in \mathbb{R}^L$: peak-shaped, short-support *kernel*;
- $\overline{\boldsymbol{x}} = \overline{\boldsymbol{s}} * \overline{\boldsymbol{\pi}} \in \mathbb{R}^N$: peak-signal;
- $\overline{\boldsymbol{t}} \in \mathbb{R}^N$: *trend* (offset, reference, baseline, background, continuum, drift, wander);
- $\boldsymbol{n} \in \mathbb{R}^N$: *noise* (stochastic residuals).

Trend can be estimated from peak-less signal with a low-pass filter $\boldsymbol{L} = \mathbf{Id}_N - \boldsymbol{H}$:

$$\widehat{\boldsymbol{t}} = \boldsymbol{L}(\boldsymbol{y} - \widehat{\boldsymbol{\pi}} * \widehat{\boldsymbol{s}}), \qquad ([5, \text{Eq. } 3])$$

Reformulation:

- Sets C_1 and C_2: closed, non-empty and convex;
- $\ell_{p,\alpha}(\boldsymbol{s}) = \left(\sum_{n=1}^N \left((s_n^2 + \alpha^2)^{p/2} - \alpha^p\right)\right)^{1/p}$, $\ell_{q,\eta}(\boldsymbol{s}) = \left(\eta^q + \sum_{n=1}^N |s_n|^q\right)^{1/q}$, $\Psi(\boldsymbol{s}) = \log\left(\frac{(\ell_{p,\alpha}^p(\boldsymbol{s}) + \beta^p)^{1/p}}{\ell_{q,\eta}(\boldsymbol{s})}\right)$.

$$\underset{\boldsymbol{s}\in\mathbb{R}^N,\, \boldsymbol{\pi}\in\mathbb{R}^L}{\text{minimize}} \ \frac{1}{2}||\boldsymbol{H}(\boldsymbol{y} - \boldsymbol{\pi} * \boldsymbol{s})||^2 + \iota_{C_1}(\boldsymbol{s}) + \iota_{C_2}(\boldsymbol{\pi}) + \lambda\Psi(\boldsymbol{s}).$$

Trust-region (TR):

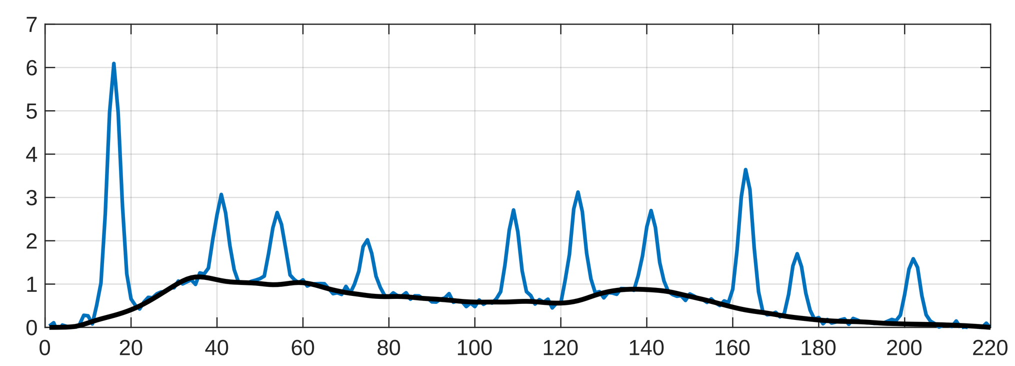
- ℓ_q-ball complement set: $\bar{\mathcal{B}}_{q,\rho} = \{\boldsymbol{s} = (s_n)_{1\le n\le N} \in \mathbb{R}^N \mid \sum_{n=1}^N |s_n|^q \ge \rho^q\}$,
- TR radius: $\rho_{k,i} = \begin{cases} \sum_{n=1}^N |s_{n,k}|^q & \text{if } i = 1\,, \\ \theta\rho_{k,i-1} & \text{if } 2 \le i \le \mathcal{I} - 1\,, \\ 0 & \text{if } i = \mathcal{I}\,. \end{cases}$

Algorithm

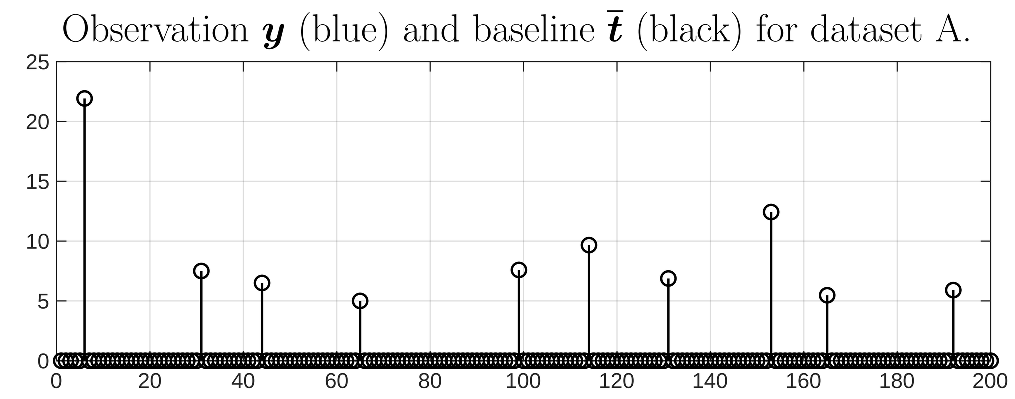
Novel Trust-Region block alternating variable metric forward-backward approach. Equations numbers are consistent with those in [5].

Settings: $K_{\max} > 0$, $\varepsilon > 0$, $\mathcal{I} > 0$, $\theta \in]0, 1[$, $(\gamma_{s,k})_{k\in\mathbb{N}} \in [\underline{\gamma}, 2 - \overline{\gamma}]$ and $(\gamma_{\pi,k})_{k\in\mathbb{N}} \in [\underline{\gamma}, 2 - \overline{\gamma}]$ for some $(\underline{\gamma}, \overline{\gamma}) \in]0, +\infty[^2$, $(p, q) \in]0, 2[\times[2, +\infty[$ satisfying (9), convex sets $(C_1, C_2) \subset \mathbb{R}^N \times \mathbb{R}^L$.
Initialize: $\boldsymbol{s}_0 \in C_1$, $\boldsymbol{\pi}_0 \in C_2$
for $k = 0, 1, \ldots$ **do**
 Update of the signal
 for $i = 1, \ldots, \mathcal{I}$ **do**
  Set TR radius $\rho_{k,i}$ using (16) with parameter θ;
  Construct MM metric $\boldsymbol{A}_{1,\rho_{k,i}}(\boldsymbol{s}_k, \boldsymbol{\pi}_k)$ using (15);
  Find $\boldsymbol{s}_{k,i} \in C_1$ such that (17) holds.
  if $\boldsymbol{s}_{k,i} \in \overline{\mathcal{B}}_{q,\rho_{k,i}}$ **then**
   Stop loop
  end
 end
 $\boldsymbol{s}_{k+1} = \boldsymbol{s}_{k,i}$;
 Update of the kernel
 Find $\boldsymbol{\pi}_{k+1} \in C_2$ such that (19) holds.
 Stopping criterion
 if $\|\boldsymbol{s}_k - \boldsymbol{s}_{k+1}\| \le \varepsilon$ *or* $k \ge K_{\max}$ **then**
  Stop loop
 end
end
$(\widehat{\boldsymbol{s}}, \widehat{\boldsymbol{\pi}}) = (\boldsymbol{s}_{k+1}, \boldsymbol{\pi}_{k+1})$ and $\widehat{\boldsymbol{t}}$ given by (3);
Result: $\widehat{\boldsymbol{s}}, \widehat{\boldsymbol{\pi}}, \widehat{\boldsymbol{t}}$

Dataset A

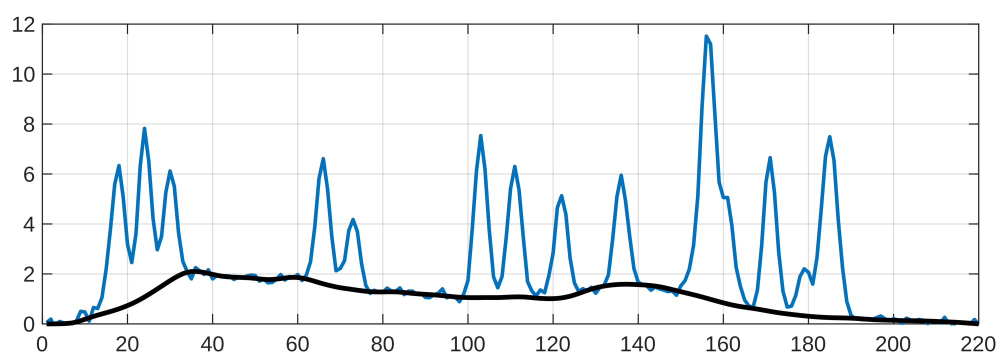


Observation $\boldsymbol{y}$ (blue) and baseline $\overline{\boldsymbol{t}}$ (black) for dataset A.

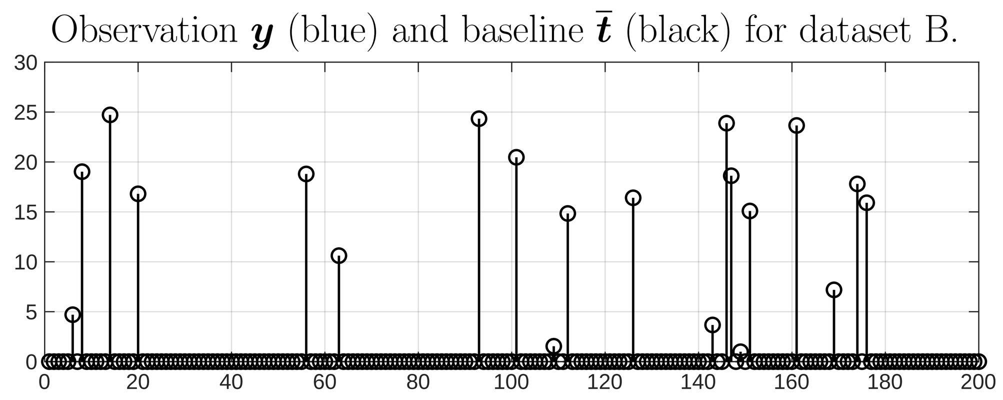


Unknown sparse signal $\overline{\boldsymbol{s}}$. Signal A has 10 spikes (5.0 % of sparsity).

Dataset B



Observation $\boldsymbol{y}$ (blue) and baseline $\overline{\boldsymbol{t}}$ (black) for dataset B.



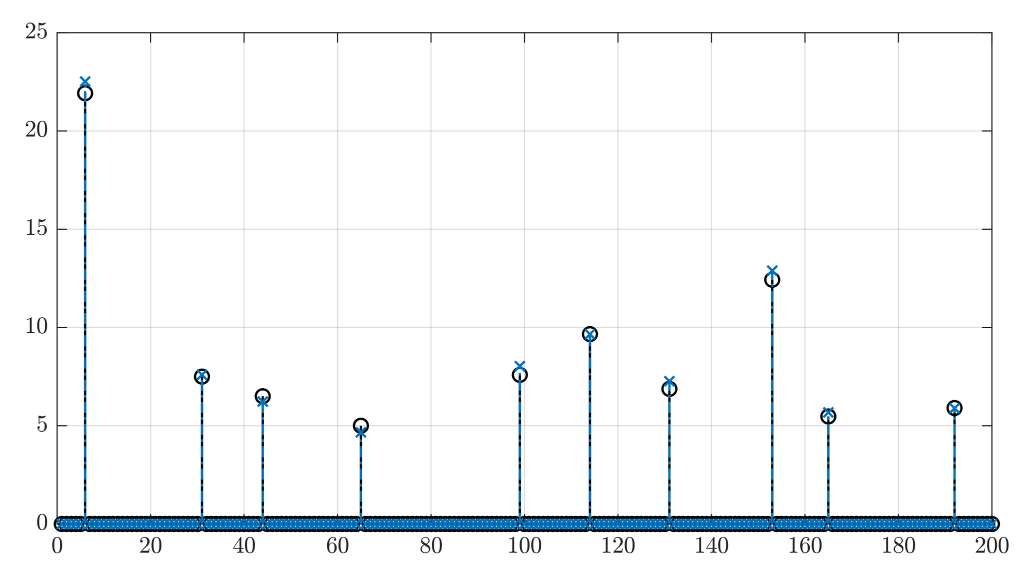
Unknown sparse signal $\overline{\boldsymbol{s}}$. Signal B has 20 spikes (10.0 % of sparsity).

Comparative table

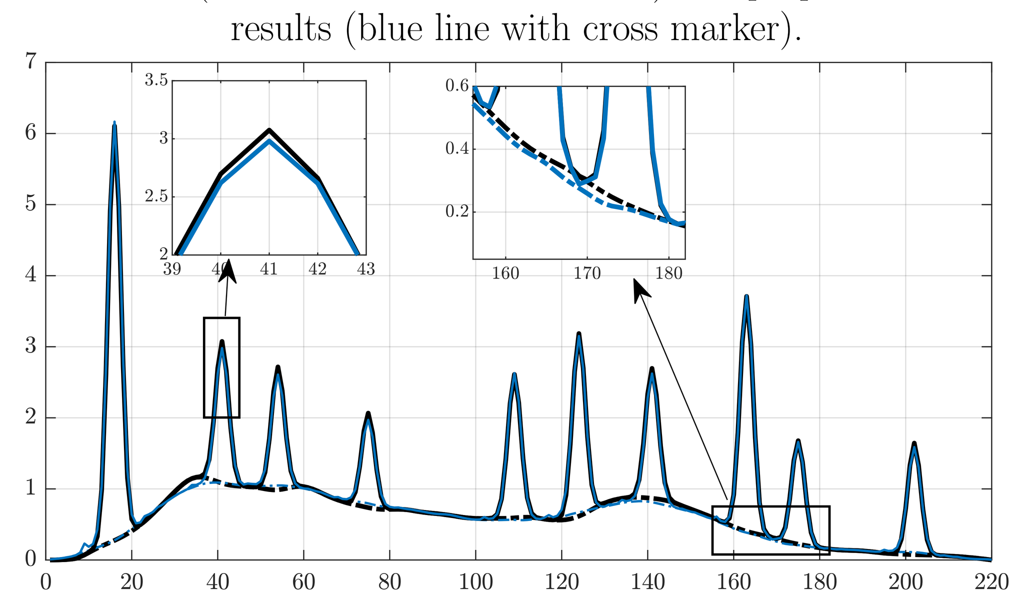
		Dataset A		Dataset B	
Noise level σ (% of $x_{\max}$)		0.5 %	1.0 %	0.5 %	1.0 %
$\text{SNR}_{\boldsymbol{s}}$	backcor+SOOT	29.2±0.7	28.5±1.9	14.9±4.0	11.5±4.7
	backcor+SPOQ	29.2±0.7	29.3±1.3	12.9±3.5	11.3±4.4
	PENDANTS (1, 2)	32.9±1.5*	30.9±2.2*	22.3±8.2**	17.5±8.4**
	PENDANTS (0.75, 2)	33.2±2.3**	31.0±4.2**	15.9±4.5*	12.9±4.6*
$\text{TSNR}_{\boldsymbol{s}}$	backcor+SOOT	29.2±0.7	29.3±1.3	16.6±3.5	13.4±4.3
	backcor+SPOQ	29.2±0.7	29.3±1.3	15.1±3.0	13.7±3.7
	PENDANTS (1, 2)	34.1±1.4*	32.2±2.1*	24.9±8.0**	19.2±7.7**
	PENDANTS (0.75, 2)	35.4±1.7**	32.6±3.8**	17.7±4.0*	14.5±4.1*
$\text{SNR}_{\boldsymbol{t}}$	backcor+SOOT	20.5±0.2	20.3±0.4	15.5±0.5	14.8±0.8
	backcor+SPOQ	20.5±0.2	20.3±0.4	15.5±0.5	14.8±0.8
	PENDANTS (1, 2)	26.9±0.5**	26.0±0.8**	22.0±0.4*	21.6±1.0**
	PENDANTS (0.75, 2)	26.9±0.6**	26.0±1.0**	24.6±0.6**	19.6±3.9*
$\text{SNR}_{\boldsymbol{\pi}}$	backcor+SOOT	36.3±1.3	33.9±1.7	30.3±1.3	28.5±1.8
	backcor+SPOQ	36.3±1.3	34.0±1.7	33.1±1.9	31.2±2.1*
	PENDANTS (1, 2)	41.3±2.0**	34.4±2.4**	38.3±1.9**	33.6±2.2**
	PENDANTS (0.75, 2)	41.3±2.0**	34.2±2.5*	35.7±1.5*	25.4±5.5

Numerical results on datasets A and B. SNR quantities in dB, averaged over 30 random realizations. Best performing method followed by **, second by *.

Dataset A (details)

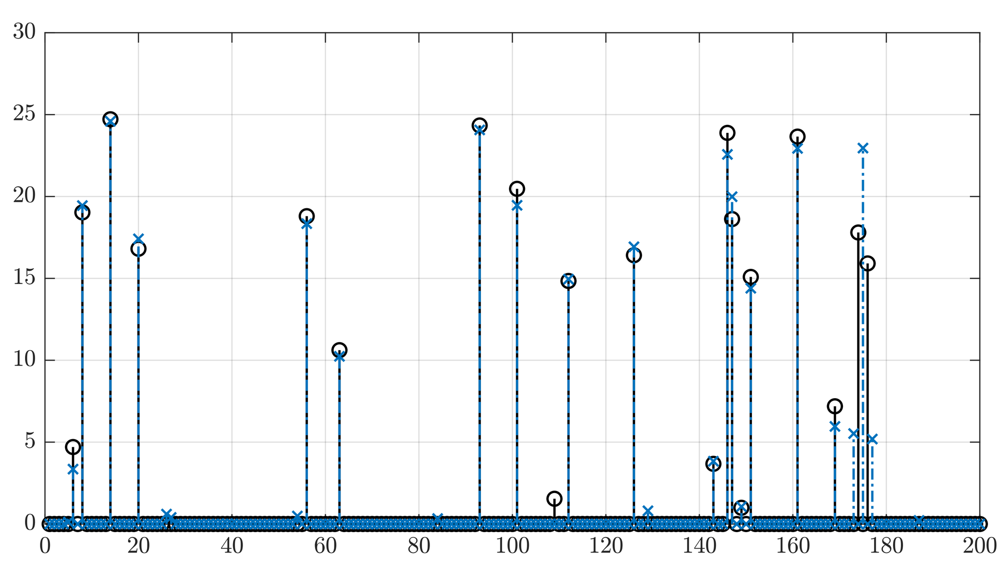


Ground truth (black line with circle marker) and proposed estimation results (blue line with cross marker).

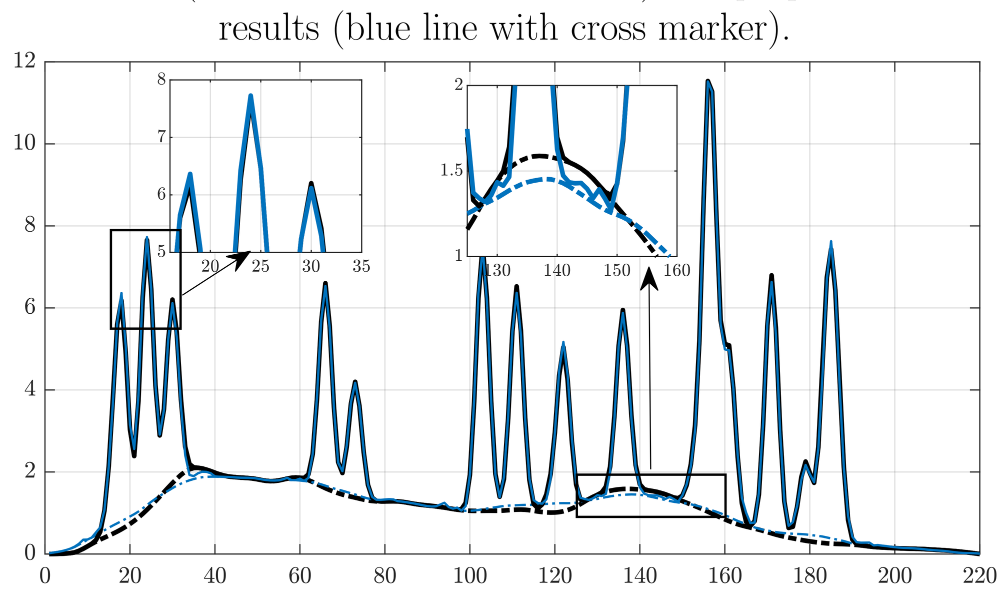


Ground truth (thick black line) and proposed estimation results (thin blue line), and the baseline $\boldsymbol{t}$ (dashed dot) and the signal $\boldsymbol{s} * \boldsymbol{\pi}$ (continuous).

Dataset B (details)



Ground truth (black line with circle marker) and proposed estimation results (blue line with cross marker).



Ground truth (thick black line) and proposed estimation results (thin blue line), and the baseline $\boldsymbol{t}$ (dashed dot) and the signal $\boldsymbol{s} * \boldsymbol{\pi}$ (continuous).

Conclusions

- Complicated joint blind deconvolution with additive trend,
- New block alternating algorithm: TR acceleration, convergence,
- Appropriate parameters to investigate (sparsity, separability),
- PENDANTSS Matlab code available.

References

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[2] X. Ning, I. W. Selesnick, and L. Duval. Chromatogram baseline estimation and denoising using sparsity (BEADS). *Chemometr. Intell. Lab. Syst.*, 139:156–167, Dec. 2014.

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[5] P. Zheng, E. Chouzenoux, and L. Duval. PENDANTSS: PEnalized Norm-ratios Disentangling Additive Noise, Trend and Sparse Spikes. *IEEE Signal Process. Lett.*, 30, 215–219, 2023.

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