PENDANTSS: PEnalized Norm-ratios Disentangling Additive Noise, Trend and Sparse Spikes [1]

Paul Zheng(1)3, Emilie Chouzenoux1, Laurent Duval2

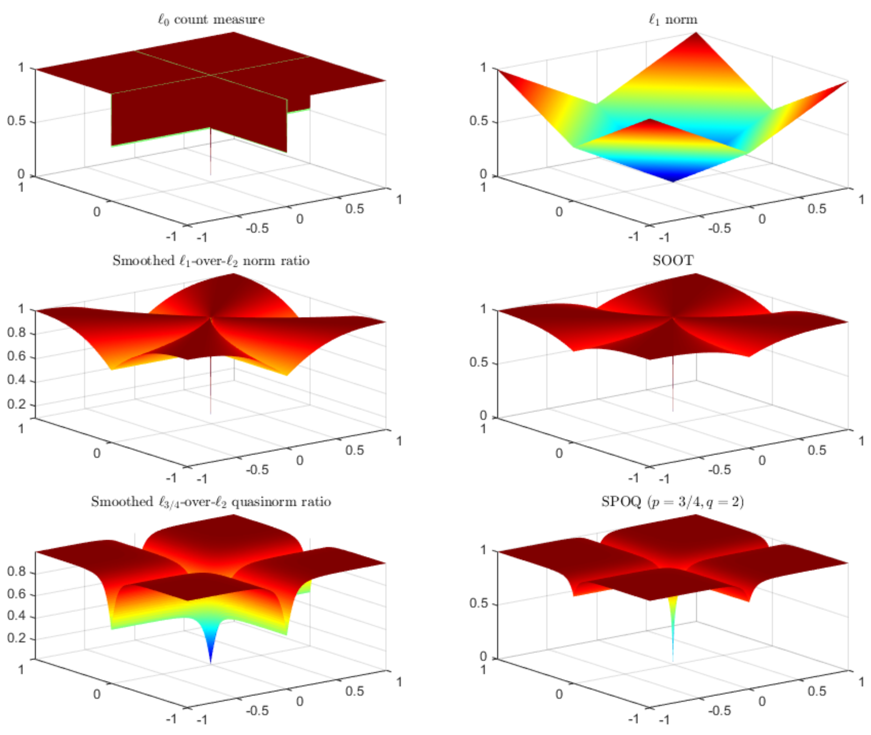
1 Univ. Paris-Saclay, CentraleSupélec, CVN, Inria, Gif-sur-Yvette; 2 IFP Energies nouvelles, Rueil-Malmaison; 3 RWTH Aachen University, Germany

Background & Inspiration

- BEADS (Baseline Estimation And Denoising using Sparsity) [2]
- SOOT ℓ_1/ℓ_2, SPOQ ℓ_p/ℓ_q (Smooth One-Over-Two/p-Over-q norm/quasi-norm ratios) [3, 4]

→ **PENDANTSS** (PEnalized Norm-ratios Disentangling Additive Noise, Trend and Sparse Spikes) [1]

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



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

Proposed Optimization Method

Block Coordinate Variable Metric Forward-Backward (BC-VMFB) [5] using trust-region (TR):

- Data fidelity $\rho(\boldsymbol{s},\boldsymbol{\pi}) \triangleq \frac{1}{2}\|\boldsymbol{H}(\boldsymbol{y}-\boldsymbol{\pi}*\boldsymbol{s})\|^2$ **Lipschitz-smooth** w.r.t. $\boldsymbol{s}$ (resp. $\boldsymbol{\pi}$), with constants $\Lambda_1(\boldsymbol{\pi})$ (resp. $\Lambda_2(\boldsymbol{s})$). Denote $f(\boldsymbol{s},\boldsymbol{\pi}) \triangleq \rho(\boldsymbol{s},\boldsymbol{\pi}) + \lambda\Psi(s)$ the differentiable part.
- **Diagonal MM metric** for f w.r.t. $\boldsymbol{s}$ (for all $\boldsymbol{\pi}$), denoting $\chi_{q,\rho} = (q-1)/(\eta^q+\rho^q)^{2/q}$,
$$\boldsymbol{A}_{1,\rho}(\boldsymbol{s},\boldsymbol{\pi}) = (\Lambda_1(\boldsymbol{\pi}) + \lambda\chi_{q,\rho})\mathbf{Id}_N + \frac{\lambda}{\ell^p_{p,\alpha}(\boldsymbol{s})+\beta^p}\mathrm{Diag}((s_n^2+\alpha^2)^{p/2-1})_{1\le n\le N};$$
- **Local majoration** valid only for $\boldsymbol{s} \in \overline{\mathcal{B}}_{q,\rho} = \{\boldsymbol{s} = (s_n)_{1\le n\le N} \in \mathbb{R}^N \mid \sum_{n=1}^N |s_n|^q \ge \rho^q\}$;

  → **TR radius backtracking**.
- **BC-VMFB updates:**
$$\forall k\in\mathbb{N},\ \forall i \in \{1,\dots,\mathcal{I}\},\ \begin{cases} \boldsymbol{s}_{k,i} = \mathrm{Proj}_{C_1}\left(\boldsymbol{s}_k - \gamma_{s,k}\boldsymbol{A}_{1,\rho_{k,i}}(\boldsymbol{s}_k,\boldsymbol{\pi}_k)^{-1}\nabla_1 f(\boldsymbol{s}_k,\boldsymbol{\pi}_k)\right), \\ \boldsymbol{\pi}_{k+1} = \mathrm{Proj}_{C_2}\left(\boldsymbol{\pi}_k - \gamma_{\pi,k}\Lambda_2(\boldsymbol{s}_{k+1})^{-1}\nabla_2 f(\boldsymbol{s}_{k+1},\boldsymbol{\pi}_k)\right). \end{cases}$$
- **Theorem:** $(\boldsymbol{s}_k,\boldsymbol{\pi}_k)_{k\in\mathbb{N}}$ converges to $(\widehat{\boldsymbol{s}},\widehat{\boldsymbol{\pi}})$ critical point of [1, Eq.5].

Problem, Hypotheses & Notations

Denoising, detrending, deconvolution: traditionally decoupled, ill-posed problem:
$$\boldsymbol{y} = \overline{\boldsymbol{s}} * \overline{\boldsymbol{\pi}} + \overline{\boldsymbol{t}} + \boldsymbol{n}\,.$$

- $\boldsymbol{y} \in \mathbb{R}^N$: 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*;
- $\overline{\boldsymbol{x}} = \overline{\boldsymbol{s}} * \overline{\boldsymbol{\pi}} \in \mathbb{R}^N$: *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 estimation using a low-pass filter $\boldsymbol{L} = \mathbf{Id}_N - \boldsymbol{H}$:
$$\widehat{\boldsymbol{t}} = \boldsymbol{L}(\boldsymbol{y} - \widehat{\boldsymbol{\pi}} * \widehat{\boldsymbol{s}}). \qquad \text{([1, Eq. 3])}$$

- Constraint: $(\widehat{\boldsymbol{s}},\widehat{\boldsymbol{\pi}}) \in (C_1 \times C_2)$ some closed, non-empty and convex sets;
- Sparsity prior on signal through penalty: $\Psi(\boldsymbol{s}) = \log\left(\frac{(\ell^p_{p,\alpha}(\boldsymbol{s})+\beta^p)^{1/p}}{\ell_{q,\eta}(\boldsymbol{s})}\right)$

  with $\ell^p_{p,\alpha}(\boldsymbol{s}) = \left(\sum_{n=1}^N \left((s_n^2+\alpha^2)^{p/2} - \alpha^p\right)\right)^{1/p}$, and $\ell_{q,\eta}(\boldsymbol{s}) = \left(\eta^q + \sum_{n=1}^N |s_n|^q\right)^{1/q}$.

Optimization Problem:
$$\underset{\boldsymbol{s}\in\mathbb{R}^N,\,\boldsymbol{\pi}\in\mathbb{R}^L}{\text{minimize}}\ \tfrac{1}{2}\|\boldsymbol{H}(\boldsymbol{y}-\boldsymbol{\pi}*\boldsymbol{s})\|^2 + \iota_{C_1}(\boldsymbol{s}) + \iota_{C_2}(\boldsymbol{\pi}) + \lambda\Psi(\boldsymbol{s}). \qquad \text{([1, Eq. 5])}$$

Algorithm

Algorithm 1: TR-BC-VMFB to solve [1, Eq. 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 [1, Eq.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 $k = 0, 1, \dots$ **do**

Update of the signal

for $i = 1, \dots, \mathcal{I}$ **do**

Set TR radius $\rho_{k,i}$ using backtracking [1, Eq.16] with parameter θ;

Construct diagonal MM metric $\boldsymbol{A}_{1,\rho_{k,i}}(\boldsymbol{s}_k,\boldsymbol{\pi}_k)$ using [1, Eq.15];

BC-VMFB update: Find $\boldsymbol{s}_{k,i} \in C_1$ such that [1, Eq.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

BC-VMFB update: Find $\boldsymbol{\pi}_{k+1} \in C_2$ such that [1, Eq.19] holds.

Stopping criterion

if $\|\boldsymbol{s}_k - \boldsymbol{s}_{k+1}\| \le \varepsilon$ *or* $k \ge K_{\max}$ **then**

Stop loop

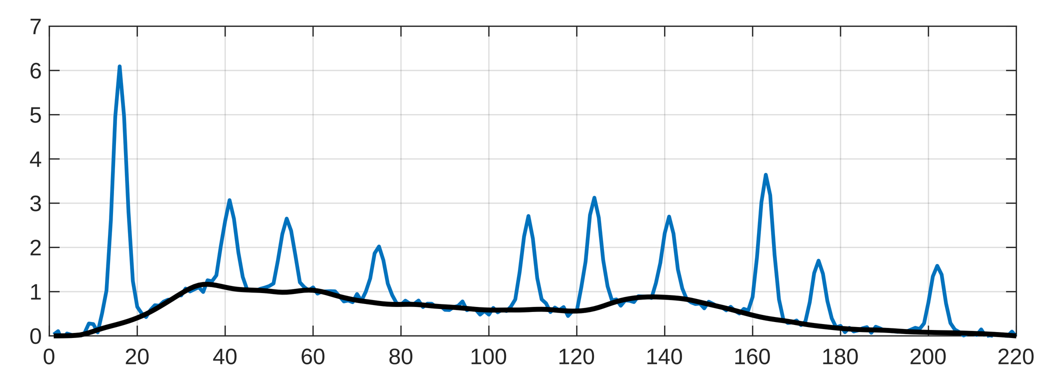
end

end

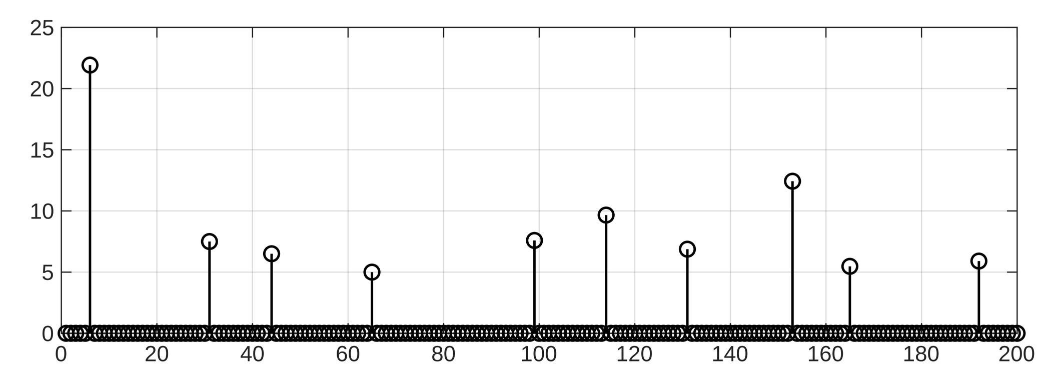
$(\widehat{\boldsymbol{s}},\widehat{\boldsymbol{\pi}}) = (\boldsymbol{s}_{k+1},\boldsymbol{\pi}_{k+1})$ and $\widehat{\boldsymbol{t}}$ given by [1, Eq.3];

Result: $\widehat{\boldsymbol{s}}, \widehat{\boldsymbol{\pi}}, \widehat{\boldsymbol{t}}$

Dataset A

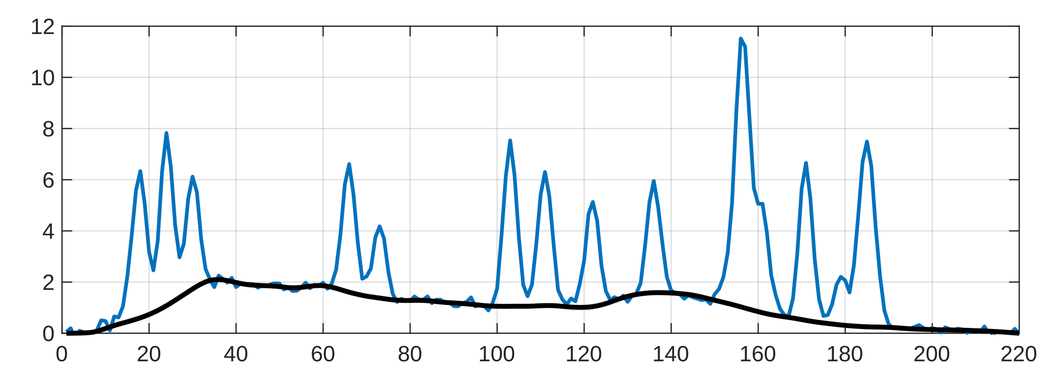


Observation $\boldsymbol{y}$ (blue) and baseline $\overline{\boldsymbol{t}}$ (black) for dataset A.

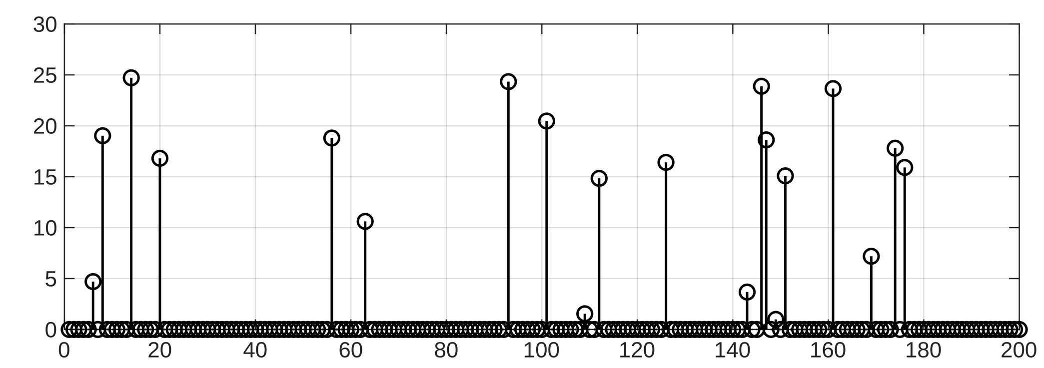


Unknown sparse signal $\overline{\boldsymbol{s}}$. Signal A has 10 spikes (5.0 % of sparsity).

Dataset B



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



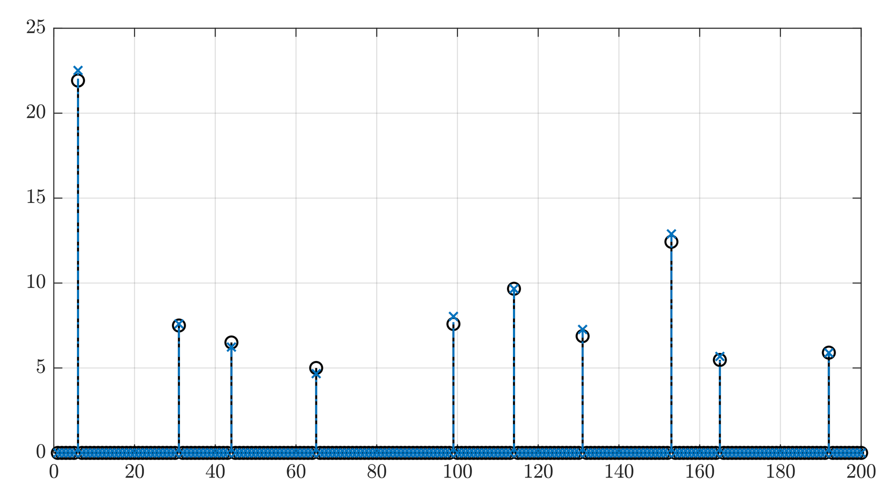
Unknown sparse signal $\overline{\boldsymbol{s}}$. Signal B has 20 spikes (10.0 % of sparsity).

Result: Comparative Table

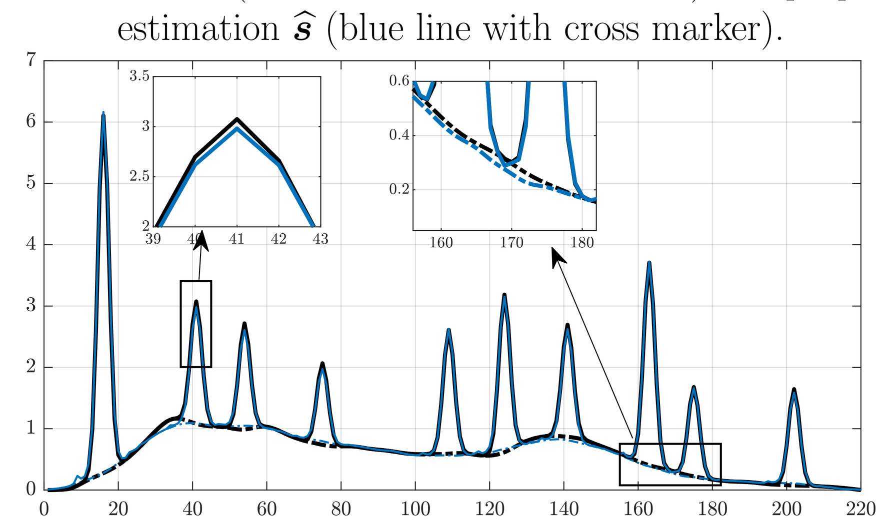
		Dataset A		Dataset B	
	Noise level σ (% of $x_{\max}$)	0.5 %	1.0 %	0.5 %	1.0 %
SNR_s	backcor[6]+SOOT	29.2±0.7	28.5±1.9	14.9±4.0	11.5±4.7
	backcor[6]+SPOQ	29.2±0.7	29.3±1.3	12.9±3.5	11.3±4.4
	PENDANTSS (1, 2)	32.9±1.5	30.9±2.2	22.3±8.2	17.5±8.4
	PENDANTSS (0.75, 2)	33.2±2.3	31.0±4.2	15.9±4.5	12.9±4.6
TSNR_s	backcor[6]+SOOT	29.2±0.7	29.3±1.3	16.6±3.5	13.4±4.3
	backcor[6]+SPOQ	29.2±0.7	29.3±1.3	15.1±3.0	13.7±3.7
	PENDANTSS (1, 2)	34.1±1.4	32.2±2.1	24.9±8.0	19.2±7.7
	PENDANTSS (0.75, 2)	35.4±1.7	32.6±3.8	17.7±4.0	14.5±4.1
SNR_t	backcor[6]+SOOT	20.5±0.2	20.3±0.4	15.5±0.5	14.8±0.8
	backcor[6]+SPOQ	20.5±0.2	20.3±0.4	15.5±0.5	14.8±0.8
	PENDANTSS (1, 2)	26.9±0.5	26.0±0.8	22.0±0.4	21.6±1.0
	PENDANTSS (0.75, 2)	26.9±0.6	26.0±1.0	24.6±0.6	19.6±3.9
SNR_π	backcor[6]+SOOT	36.3±1.3	33.9±1.7	30.3±1.3	28.5±1.8
	backcor[6]+SPOQ	36.3±1.3	34.0±1.7	33.1±1.9	31.2±2.1
	PENDANTSS (1, 2)	41.3±2.0	34.4±2.4	38.3±1.9	33.6±2.2
	PENDANTSS (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, second best performing method.

Dataset A (result)

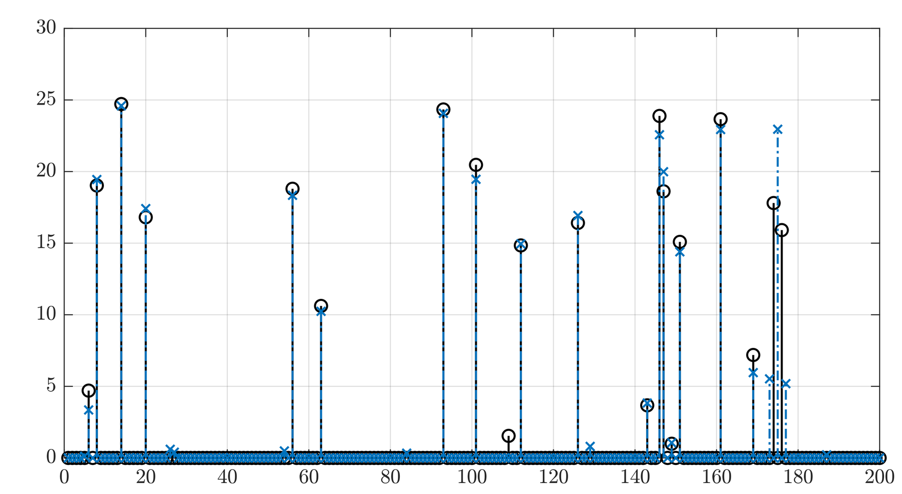


Ground truth $\overline{\boldsymbol{s}}$ (black line with circle marker) and proposed estimation $\widehat{\boldsymbol{s}}$ (blue line with cross marker).

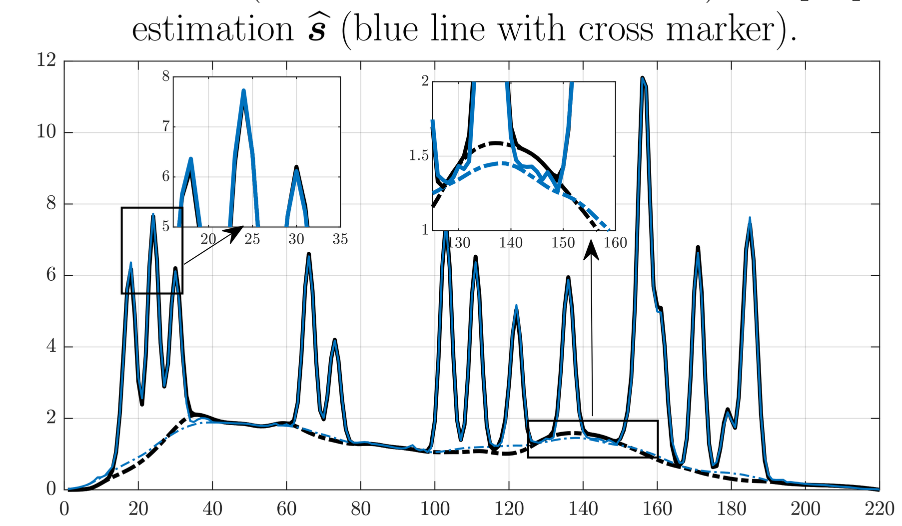


Ground truth (black line) and proposed estimation results (blue line), for the baseline $\boldsymbol{t}$ (dashed dot) and the signal $\boldsymbol{s}*\boldsymbol{\pi}$ (continuous).

Dataset B (result)



Ground truth $\overline{\boldsymbol{s}}$ (black line with circle marker) and proposed estimation $\widehat{\boldsymbol{s}}$ (blue line with cross marker).



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

Conclusions

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

References

[1] 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.

[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.

[3] A. Repetti, M. Q. Pham, L. Duval, E. Chouzenoux, and J.-C. Pesquet. Euclid in a taxicab: Sparse blind deconvolution with smoothed ℓ_1/ℓ_2 regularization. *IEEE Signal Process. Lett.*, 22(5):539–543, May 2015.

[4] A. Cherni, E. Chouzenoux, L. Duval, and J.-C. Pesquet. SPOQ ℓ_p-over-ℓ_q regularization for sparse signal recovery applied to mass spectrometry. *IEEE Trans. Signal Process.*, 68, 6070–6084, 2020.

[5] E. Chouzenoux, J.-C. Pesquet, and A. Repetti, A block coordinate variable metric forward-backward algorithm. *J. Glob. Optim.*, 66, 457-485, 2016.

[6] V. Mazet, C. Carteret, D. Brie, J. Idier, and B. Humbert. Background removal from spectra by designing and minimising a non-quadratic cost function, *Chemometr. Intell. Lab. Syst.*, vol. 76, no. 2, pp. 121-133, 2005

Github code

PENDANTSS Tunes (YouTube)

Support: European Research Council Starting Grant MAJORIS ERC-2019-STG-850925.