Proximity operators for a class hybrid sparsity + entropy priors.

Application to DOSY NMR signal reconstruction.

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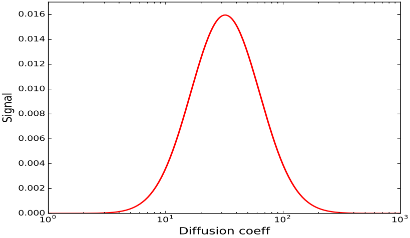
Motivation



Original data

$\overline{x} \in \mathbb{R}^N$

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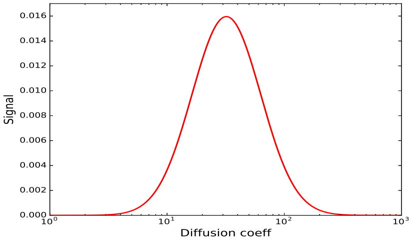

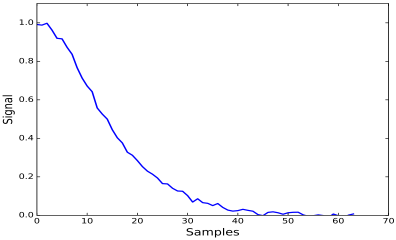

Original data
$\overline{x} \in \mathbb{R}^N$

Measurements
$y = \mathcal{T}(\boldsymbol{K}\overline{x}) \in \mathbb{R}^M$

- $\boldsymbol{K} \in \mathbb{R}^{M \times N}$: Measurement operator
- $\mathcal{T} : \mathbb{R}^M \to \mathbb{R}^M$: Noise degradation operator

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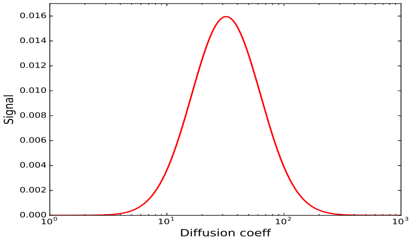

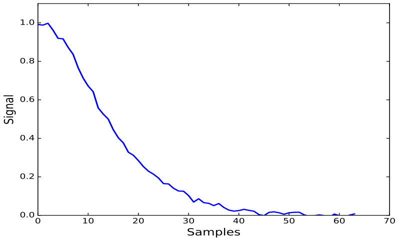

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Goal

Find a good estimate $\hat{x}$ of $\overline{x}$ from the observations y, using some **a priori** knowledge on $\overline{x}$ and on the **noise** characteristics.

Problematic (1/2)

DOSY NMR

Diffusion **O**rdered **S**pectroscop**Y**, an application in the **N**uclear **M**agnetic **R**esonance field *[Delsuc and Malliavin, 1998]*.

Measure model

$$I(q) = \int_{D_{\min}}^{D_{\max}} X(D) exp(-D\Delta q^2) dD$$

with :

- D : Diffusion coefficient
- Δ : Diffusion time
- $q = \gamma\delta g$: Measure of the phase dispersion
- γ : Gyromagnetic ratio
- δ : Duration of the Pulsed field gradients (PFG)
- g : Intensity of the PFG

Problematic (2/2)

Discrete model

$$y = \boldsymbol{K}x + w$$

- $y = (y_1, ..., y_M) \in \mathbb{R}^M$: measurement signal
- $x = (x_1, ..., x_N) \in \mathbb{R}^N$: original signal
- $\boldsymbol{K} = (K_{m,n})_{m \in \mathbb{N}, n \in \mathbb{N}} \in \mathbb{R}^{M \times N}$: measurement matrix **with positive entries**
- $w = (w_1, ..., w_M) \in \mathbb{R}^M$: noise signal

where

$$K_{m,n} = \exp(-D_n \Delta q_m^2)$$

Problematic (2/2)

▶ Discrete model

$$y = \boldsymbol{K}x + w$$

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▶ Measure operator ?

$\boldsymbol{K}$: Laplace matrix : unstable operator $\rightsquigarrow$ ill-conditioned matrix
$M < N$ $\rightsquigarrow$ ill-posed problem

Existing methods (1/2)

- Constrained formulation

$$\underset{x\in\mathbb{R}^N}{\text{minimize}} \quad \Psi(x) \quad \text{subject to} \quad \frac{1}{2}\|\boldsymbol{K}x - y\|_2^2 \leq \tau$$

where $\tau > 0$: noise characteristic parameter
Ψ : regularization function.

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- Lagrangian formulation

$$\underset{x\in\mathbb{R}^N}{\text{minimize}} \quad \frac{1}{2}\|\boldsymbol{K}x - y\|_2^2 + \lambda\Psi(x)$$

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- Regularization choice

$$(\forall x \in \mathbb{R}^N) \quad \Psi(x) = \sum_{n=1}^{N} \psi(x_n)$$

Existing methods (2/2)

- Most used regularization functions
  - Shannon entropy *[Nityananda and Narayan, 1982]*

$$(\forall x \in \mathbb{R}^N) \quad \Psi(x) = \sum_{n=1}^{N} \psi(x_n)$$

where :

$$(\forall x \in \mathbb{R}) \quad \psi(x) = \begin{cases} -x \log x & \text{if} \quad x > 0 \\ 0 & \text{if} \quad x = 0 \\ +\infty & \text{elsewhere.} \end{cases}$$

  - ℓ_1 norm *[Candes, 2008]*

$$(\forall x \in \mathbb{R}^N) \quad \Psi(x) = \ell_1(x) = \sum_{n=1}^{N} |x_n|$$

Outline

- **Introduction**
- **Proposed approach**
  - Hybrid regularization
  - Proximity operators
- **Application to DOSY NMR**
- **Conclusion**

Sparse + Entropy regularization

$$(\forall x \in \mathbb{R}^N, \alpha \geq 0, \beta \geq 0) \qquad \Psi(x) = \underbrace{\alpha \Psi_1(x)}_{\text{Entropy prior}} + \underbrace{\beta \Psi_2(x)}_{\text{Sparsity prior}}$$

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Entropy prior ψ_1	
$x \log(x) + \iota_{[0,+\infty)}(x)$	*Shannon*
$-\log(x) + \iota_{[0,+\infty)}(x)$	*Burg*

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Sparsity prior ψ_2	
$\|x\|^0$	ℓ_0
$\|x\|$	ℓ_1
$\log(1+\|x\|)$	*log-sum*
$\log(1+x^2)$	*Cauchy*

Proximity operator

Definition

Let $\Psi : \mathbb{R} \rightarrow]-\infty, +\infty]$ a lower semi continuous (lsc) and proper function. The proximity operator of Ψ is defined as *[Hiriart-Urruty and Lemaréchal, 1993, Bauschke and Combettes, 2011]*

$$\begin{aligned} \mathrm{prox}_{\Psi} : &\mathbb{R}^{\mathbb{N}} \rightarrow \mathbb{R}^{\mathbb{N}} \\ &x \rightarrow \underset{y \in \mathbb{R}^{\mathbb{N}}}{\mathrm{Argmin}} \left(\Psi(y) + \frac{1}{2} \|y - x\|^2 \right) \end{aligned}$$

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Separability

For every $n \in \{1, \ldots, N\}$ and $x = (x_1, \ldots, x_N)$:

$$\mathrm{prox}_{\Psi}(x) = (p_n(x_n))_{1 \leq n \leq N}$$

$$\text{with :} \quad p_n(x_n) = \mathrm{prox}_{\alpha\psi_1 + \beta\psi_2}(x_n)$$

Proximity operators for hybrid sparse + entropy prior (1/2)

▶ Case of Shannon entropy (ψ_1)

ψ_2	$\text{prox}_{\alpha\psi_1+\beta\psi_2}(x) \quad / \; x \in \mathbb{R}$
$\beta = 0$	$\alpha W\left((1/\alpha)\exp\left((x/\alpha) - 1\right)\right)$
ℓ_1	$\alpha W\left((1/\alpha)\exp\left((x-\beta)/\alpha - 1\right)\right)$
ℓ_0	$\begin{cases} p & \text{if} \quad \beta < \overline{\beta} \\ \{0, p\} & \text{if} \quad \beta = \overline{\beta} \\ 0 & \text{elsewhere} \end{cases}$ where $p = \alpha W\left((1/\alpha)\exp\left((1/\alpha) - 1\right)\right)$ and $\overline{\beta} = (1/2)p^2 + \alpha p \in]0, +\infty[$
log-sum	$\underset{p \in]0,+\infty[\text{ s.t. } \varphi(p)=0}{\text{Argmin}} \left((1/2)(x-p)^2 + \psi(p)\right)$ with $\varphi(p) = p^2 + (\delta - x + \alpha)p + \alpha(\delta + p)\log(p) + \delta(\alpha - x) + \beta$
Cauchy	$\underset{p \in]0,+\infty[\text{ s.t. } \varphi(p)=0}{\text{Argmin}} \left((1/2)(x-p)^2 + \psi(p)\right)$ with $\varphi(p) = p^3 + (\alpha - x)p^2 + (\delta + 2\beta)p + \alpha(\delta + p^2)\log(p) + \delta(\alpha - x)$

W(.) denotes the Lambert function *[Corless et al., 1996]*.

Proximity operators for hybrid sparse + entropy prior (2/2)

▶ Case of Burg entropy (ψ_1)

ψ_2	$\text{prox}_{\alpha\psi_1+\beta\psi_2}(x)$
$\beta = 0$	$(x + \sqrt{x^2 + 4\alpha})/2$
ℓ_1	$(x - \beta + \sqrt{(\beta - x)^2 + 4\alpha})/2$
ℓ_0	$(x + \sqrt{x^2 + 4\alpha})/2$
log-sum	$\underset{p\in]0,+\infty[\text{ s.t. } \varphi(p)=0}{\text{Argmin}} \left(\frac{1}{2}(x-p)^2 + \psi(p)\right)$ with $\varphi(p) = p^3 + (\delta - x)p^2 + p(\beta - \delta x - \alpha) - \delta\alpha$
Cauchy	$\underset{p\in]0,+\infty[\text{ s.t. } \varphi(p)=0}{\text{Argmin}} \left(\frac{1}{2}(x-p)^2 + \psi(p)\right)$ with $\varphi(p) = p^4 - xp^3 + (\delta + 2\beta - \alpha)p^2 - \delta xp - \delta\alpha$

Application to DOSY NMR

- **Prior function**

$\Psi = \alpha \,\mathrm{ent} + (1-\beta)\ell_1$
$\alpha = 1 - \beta \in [0,1]$

- **Minimization**

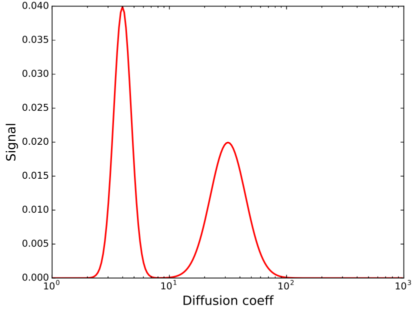
PPXA+ : Parallel Proximal Algorithm *[Pesquet and Pustelnik, 2012]*

- **Resulting algorithm**

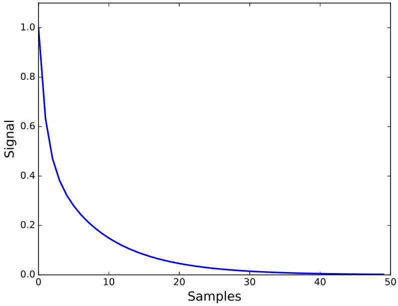
PALMA : **P**roximal **A**lgorithm for ℓ_1 combined with **MA**xent prior.
Code available at http://palma.labo.igbmc.fr

Numerical results (1/3)

- $M = 50,\ N = 200,\ Dmin = 1,\ Dmax = 103$



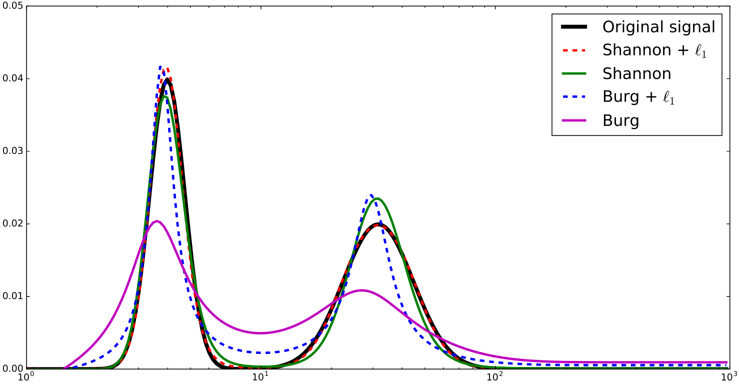
Original signal



Measured data

Numerical results (2/3)

- Results with $\sigma = 10^{-5}$ (noise level), and $\tau = 7.14\,10^{-5}$.



Recovered signal with different regularizations

Numerical results (3/3)

- Results for different noise levels

σ	Shannon prior	Shannon $+\ell_1$	Burg prior	Burg $+\ell_1$
10^{-2}	12.45	**13.16**	12.92	**12.92**
10^{-3}	18.16	**20.86**	12.11	**13.44**
10^{-4}	20.87	**25.95**	12.03	**15.53**

Quality reconstruction in dB for various choices of the penalization function

$\leadsto$ Optimal case : **Shannon + ℓ_1 prior**

Conclusion & perspectives

$\surd$ New proximity operators combining entropy and sparsity promoting terms.

$\surd$ Great approach to solve DOSY NMR problem reconstruction.

$\surd$ The proposed novel proximity operators can be applied in a variety of proximal algorithms, in the convex or the non-convex case.

Conclusion & perspectives

√ New proximity operators combining entropy and sparsity promoting terms.
√ Great approach to solve DOSY NMR problem reconstruction.
√ The proposed novel proximity operators can be applied in a variety of proximal algorithms, in the convex or the non-convex case.

- Test with complex data in spectrometry field.
- Hybrid regularization in blind signal restoration problems.

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Thank you for your attention !

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