From the modeling of direct problems in image processing to the resolution of inverse problems

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Contents

From modeling to resolution

$$\boxed{\begin{array}{c}\text{Object of interest}\\ y\end{array}} \longrightarrow \boxed{\begin{array}{c}\text{System}\\ \mathcal{D}_\alpha\end{array}} \longrightarrow \boxed{\begin{array}{c}\text{Observation}\\ z = \mathcal{D}_\alpha(y)\end{array}}$$

From modeling to resolution

α - system parameters (e.g. noise)

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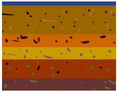

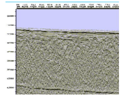

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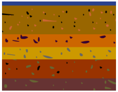

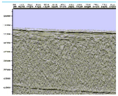

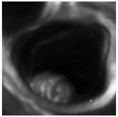

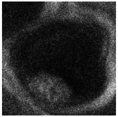

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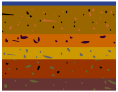

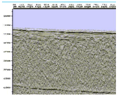
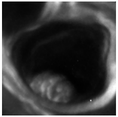


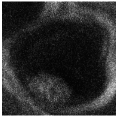
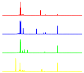
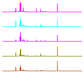

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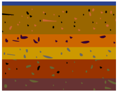

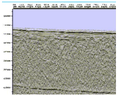
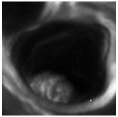

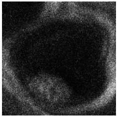
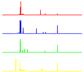

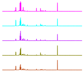

How? $\rightarrow$ Solving inverse problems

From modeling to resolution

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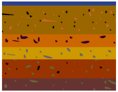
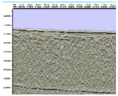
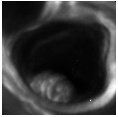
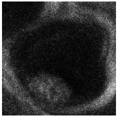
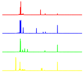
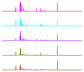




method parameters (e.g. regularization)

How? → Solving inverse problems

Inverse problem formulation

What?

Recovering the original (unknown data) from distorded observations.

How?

Formulating the inverse problem as a minimization problem

- Variational approach;
- Statistical approach (MAP).

And so

$$\underset{y}{\text{minimize}} \quad \underbrace{f_1(y)}_{\text{Fidelity}} \quad + \quad \underbrace{f_2(y)}_{\text{Regularization}}$$

Minimization problems

- Standard problem:

$$\underset{y\in\mathbb{R}^N}{\text{minimize}} \quad \underbrace{f_1(y)}_{\text{Fidelity}} \quad + \quad \underbrace{f_2(y)}_{\text{Regularization}} \quad .$$

- Taking into account several regularizations ($P-1$ terms):

$$\underset{y\in\mathbb{R}^N}{\text{minimize}} \; f_1(y) + \sum_{p=2}^{P} f_p(y).$$

- Introducing linear operators $(F_p)_{p\in\{1,\dots,P\}}$:

$$\underset{y\in\mathbb{R}^N}{\text{minimize}} \; \sum_{p=1}^{P} f_p(F_p y).$$

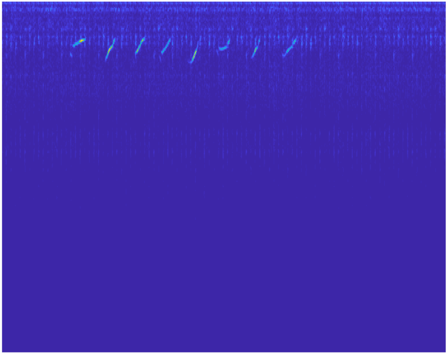
- For large size problem or for other reasons, can be interesting to work on data blocks $y^{(p)}$ of size L_p ($y = (y^{(p)})_{p=1}^{P}$)

$$\underset{y\in\mathbb{R}^N}{\text{minimize}} \; \sum_{p=1}^{P} f_p(y^{(p)}).$$

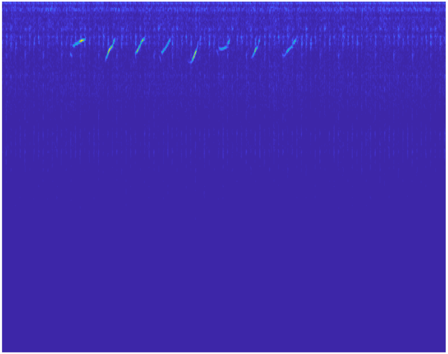
Some proximal approaches

- *Parallel ProXimal Algorithm + (PPXA+)* [Pesquet, Pustelnik, 2012]
- Generalized Forward-Backward [Raguet et al., 2012]
- M+SFBF [Briceño-Arias, Combettes, 2011]
- M+LFBF [Combettes, Pesquet, 2011]
- FB based algorithms [Chambolle, Pock, 2011],[Vũ,2013],[Condat,2013]
- Proximal Alternating Linearized Minimization (PALM) [Bolte et al., 2014]
- An accelerated projection gradient based algorithm [Zhang et al., 2016]
- Block-Coordinate Variable Metric Forward-Backward (BC-VMFB) algorithm [Chouzenoux et al., 2016]

Motivation



Motivation



Inpainting problem

$$\min_{\mathbf{Y}\in\mathbb{C}^{F\times T}} \frac{1}{2}\|\mathbf{M}\odot(\mathbf{X}-\mathbf{Y})\|_F^2+\lambda\|\mathbf{Y}\|_*, \text{ where } \lambda>0.$$

Initial point

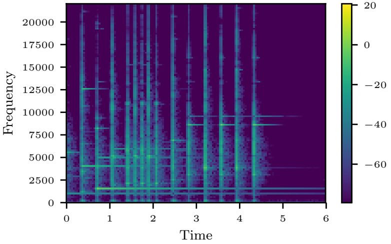


Figure: Spectrogram of the *Glockenspiel*, composed of about 50 spectral peaks distributed on 15 occurrences of 8 notes.

- How the intuitions of the low-rankness of the spectrograms can be extended to complex-valued time-frequency matrices ?
- What is a rank-one matrix, or more generally a rank-r matrix, in the time-frequency plane?
- Do time-frequency matrices of real-world sounds have good low-rank approximations?

STFT definitions

$(K \times N)$-STFT, band-pass convention

$$\mathbf{S}_{\mathrm{BP}}^{(K\times N)}\left[k,n\right] = \sum_{m} \mathbf{s}\left[t_n + m\right] \mathbf{w}\left[m\right] e^{-2i\pi\nu_k m}$$

$(K \times N)$-STFT, low-pass convention

$$\mathbf{S}_{\mathrm{LP}}^{(K\times N)}\left[k,n\right] = \sum_{m} \mathbf{s}\left[m\right] \mathbf{w}\left[m - t_n\right] e^{-2i\pi\nu_k m}.$$

where $\left(\mathbf{w}\left[m\right]\right)_{m\in[\![L]\!]} \in \mathbb{C}^L$ denotes the window, $\nu_k, k \in [\![K]\!]$ is a discrete frequency and $t_n, n \in [\![N]\!]$ a discrete time.

Relation between conventions

$\forall k \in [\![K]\!], n \in \mathbb{Z}, \mathbf{S}_{\mathrm{LP}}\left(k,n\right) = \mathbf{S}_{\mathrm{BP}}\left(k,n\right) \times e^{-2i\pi\nu_k t_n}$

Factorization of STFT matrices

$(L \times L)$-STFT (full redundancy $K = L = N$)

$$\forall k, n, \mathbf{S}_{\mathrm{BP}}[k, n] = \sum_m \mathbf{s}[n+m]\,\mathbf{w}[m]\,e^{-2i\pi\frac{km}{L}}$$

$$\forall k, n, \mathbf{S}_{\mathrm{LP}}[k, n] = \sum_m \mathbf{s}[m]\,\mathbf{w}[m-n]\,e^{-2i\pi\frac{km}{L}}.$$

For any signal $\mathbf{s} \in \mathbb{C}^L$ and window $\mathbf{w} \in \mathbb{C}^L$, we have

$$\mathbf{S}_{\mathrm{BP}} = \mathbf{E}\,\mathrm{diag}(\mathbf{w})\,\mathbf{E}^{-1}\,\mathrm{diag}(\widehat{\mathbf{s}})\,\mathbf{E}$$

and

$$\mathbf{S}_{\mathrm{LP}} = \mathbf{E}\,\mathrm{diag}(\mathbf{s})\,\mathbf{E}^{-1}\,\mathrm{diag}(\widehat{\mathbf{w}})\,\mathbf{E}$$

where

$$\boxed{\mathbf{E} = \left(e^{-2i\pi\frac{kt}{L}}\right)_{k\in[\![L]\!],t\in[\![L]\!]}}$$

Rank-r STFT matrices

Band-pass convention

If $\mathbf{w} \in \mathbb{C}^L$ is a window that does not vanish, i.e., $\forall k \in [\![L]\!], \mathbf{w}[k] \neq 0$,
then $\operatorname{rank}(\mathbf{S}_{\mathrm{BP}}) = \|\widehat{\mathbf{s}}\|_0$.

$\Rightarrow$ *The set of rank-r STFT matrices in the band-pass convention is composed of the signals that are a sum of r pure complex exponentials at Fourier frequencies.*

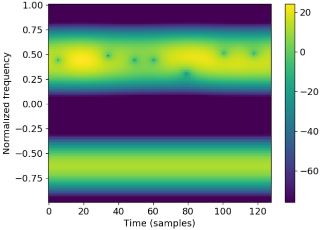
Low-pass convention

If $\mathbf{w} \in \mathbb{C}^L$ is a window such that $\widehat{\mathbf{w}}$ does not vanish, i.e., $\forall k \in [\![L]\!], \widehat{\mathbf{w}}[k] \neq 0$,
then $\operatorname{rank}(\mathbf{S}_{\mathrm{LP}}) = \|\mathbf{s}\|_0$.

$\Rightarrow$ *The set of rank-r STFT matrices in the low-pass convention is composed of the signals that are a sum r diracs at integer times.*

Analysis of low-rank STFT matrices

Context : Signal with length $L = 128$ composed of a sum of $N_c = 6$ complex sinusoids at exact Fourier frequencies (5 closed frequencies and 1 isolated frequency).



Results : $\text{rank}\,(\mathbf{S}_{\text{BP}}) = Nc$ while $\text{rank}\,(\mathbf{S}_{\text{LP}})$ is higher.

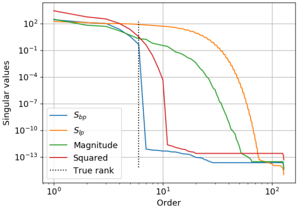


Figure: Analysis with a Gaussian window: singular values of STFT matrices, magnitude and energy spectrograms.

Analysis of low-rank STFT matrices

Context: rank vs. number of components N_c (frequencies drawn randomly at exact Fourier frequencies), signal length $L = 64$.

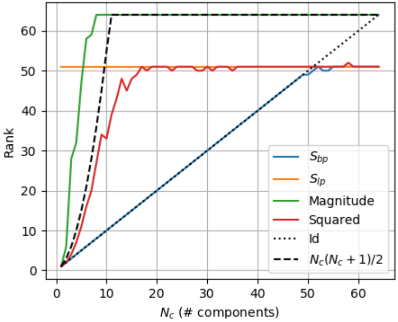


Figure: Rank of several types of time-frequency matrices vs. number of sinusoids in the signal.

Results: $\mathrm{rank}\left(\mathbf{S}_{\mathrm{BP}}\right) = N_c$ while $\mathrm{rank}\left(\mathbf{S}_{\mathrm{LP}}\right)$ is higher.

rg STFT matrix $<$ related spectrograms.

Formulation of phase inpainting problem

Gabor atoms (STFT): $\mathbf{a}_{t,\nu} = \mathbf{w}[n - th]e^{2\imath\pi\frac{\nu}{F}n}$ for $\begin{cases} t \in \{0, \dots, T-1\} \\ \nu \in \{0, \dots, F-1\} \\ \mathbf{w} : \text{window} \\ h : \text{hop size} \end{cases}$

Known binary mask: $\boldsymbol{m} \in \{0, 1\}^{F \times T}$

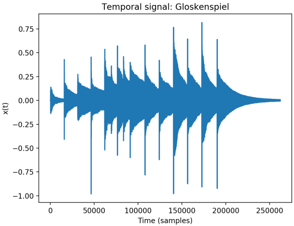
Observations: $\mathbf{b} \in \mathbb{C}^{F \times T}$ $\begin{cases} \mathbf{b}(\boldsymbol{m}) \text{ fully known ceofficients} \\ \mathbf{b}(\neg\boldsymbol{m}) \text{ known magnitudes} \end{cases}$

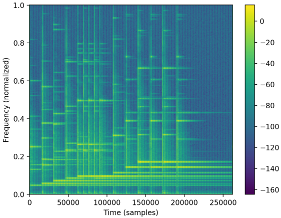
Proposition

$$\textit{Find } \mathbf{x} \in \mathbb{C}^N \textit{ s.t. } \begin{cases} \langle \mathbf{x}, \mathbf{a}_{t,\nu} \rangle & = \mathbf{b}[t, \nu], \forall t, \nu \in \operatorname{supp}(\boldsymbol{m}) \ (\textit{our contribution}) \\ |\langle \mathbf{x}, \mathbf{a}_{t,\nu} \rangle| & = \mathbf{b}[t, \nu], \forall t, \nu \in \operatorname{supp}(\neg\boldsymbol{m}) \end{cases}$$

STFT with some missing data

- Missing data in TF plane = Missing phases ie magnitudes assumed to be known.
- What about the quality of the reconstructed signal with 30% of missing phases in its spectrogram ?





Original glockenspiel Reconstructed signal

- What about putting random phases ?

RPI reconstruction:

STFT with some missing data

- Missing data in TF plane = Missing phases ie magnitudes assumed to be known.
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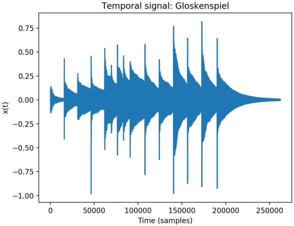
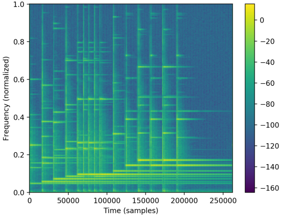


Original glockenspiel



Reconstructed signal

- What about putting random phases ?

RPI reconstruction:

- $\boxed{\text{Phases are very important}}$

Algorithm 1 Griffin and Lim for phase inpainting (GLI)

Require: $\begin{cases} \mathbf{b} : \text{observations} , \boldsymbol{m} : \text{binary mask} \\ n_{\text{iter}} : \text{number of iterations} \\ \text{STFT}_{\mathbf{x}} \text{ and } \text{STFT}^{-1} : \text{operators related to } \{a_{t,\nu}\} \end{cases}$

Random initialization φ_0 of missing phases:

$$\varphi \leftarrow \boldsymbol{m} \circ \angle \mathbf{b} + (1 - \boldsymbol{m}) \circ \varphi_0 \quad \text{and} \quad \mathbf{y}^{(0)} \leftarrow \mathbf{b} \circ \exp(\imath \varphi)$$

for $i \in \{1, 2, \ldots, n_{\text{iter}}\}$ **do**

$\mathbf{z}^{(i)} \leftarrow \text{STFT}_{\mathbf{x}} \left(\text{STFT}^{-1} \left(\mathbf{y}^{(i-1)} \right) \right)$

$\varphi^{(i)} \leftarrow \boldsymbol{m} \circ \angle \mathbf{b} + (1 - \boldsymbol{m}) \circ \angle \mathbf{z}^{(i)}$

$\mathbf{y}^{(i)} \leftarrow \mathbf{b} \circ \exp(\imath \varphi^{(i)})$

end for

return $\text{STFT}^{-1}(\mathbf{y}^{(n_{\text{iter}})})$

Original signal: RPI reconstruction: GLI reconstruction:

PhaseLift for phase inpainting (PLI)

Phase inpainting problem (non-convex)

$$\text{Find } \mathbf{x} \in \mathbb{C}^N \text{ s.t. } \begin{cases} \langle \mathbf{x}, \mathbf{a}_{t,\nu} \rangle & = \mathbf{b}[t,\nu], \forall t,\nu \in \text{supp}\,(\boldsymbol{m}) \\ |\langle \mathbf{x}, \mathbf{a}_{t,\nu} \rangle| & = \mathbf{b}[t,\nu], \forall t,\nu \in \text{supp}\,(\neg \boldsymbol{m}) \end{cases}$$

$$\Big\downarrow \ \textbf{lifting} \quad \mathbf{X} = \mathbf{x}\mathbf{x}^H$$

$$\min_{\mathbf{X} \in \mathbb{C}^{N \times N}} \text{Rank}(\mathbf{X}) \text{ s.t. } \begin{cases} \text{Trace}(\mathbf{A}_{(t,\nu),(t',\nu')}\mathbf{X}) = \mathbf{b}[t',\nu']\bar{\mathbf{b}}[t,\nu], & \forall\ (t,\nu) \in \text{supp}(\boldsymbol{m}) \\ \text{Trace}(\mathbf{A}_{(t',\nu')(t',\nu')}\mathbf{X}) = \mathbf{b}^2[t',\nu'], & \forall\ (t',\nu') \in \text{supp}\,(\neg \boldsymbol{m}) \\ \mathbf{X} \succeq 0 \quad \text{(positive semidefinite matrix (PSD))} \end{cases}$$

$$\Big\downarrow \ \textbf{relaxation}$$

$$\min_{\mathbf{X} \in \mathbb{C}^{N \times N}} \text{Trace}(\mathbf{X}) \text{ s.t. } \begin{cases} \text{Trace}(\mathbf{A}_{(t,\nu),(t',\nu')}\mathbf{X}) = \mathbf{b}[t',\nu']\bar{\mathbf{b}}[t,\nu], & \forall\ (t,\nu) \in \text{supp}(\boldsymbol{m}) \\ \text{Trace}(\mathbf{A}_{(t',\nu')(t',\nu')}\mathbf{X}) = \mathbf{b}^2[t',\nu'], & \forall\ (t',\nu') \in \text{supp}(\neg \boldsymbol{m}) \\ \mathbf{X} \succeq 0 \end{cases}$$

1

[1] TFOCS: Templates for convex cone problems with applications to sparse signal recovery, S. Becker , E.J. Candès and M. Grant, 2010.

PhaseCut for phase inpainting (PCI)

$$\text{Find } \mathbf{x} \in \mathbb{C}^N \text{ s.t. } \begin{cases} \langle \mathbf{x}, \mathbf{a}_{t,\nu} \rangle & = \mathbf{b}[t,\nu], \forall t,\nu \in \operatorname{supp}(\boldsymbol{m}) \\ |\langle \mathbf{x}, \mathbf{a}_{t,\nu} \rangle| & = \mathbf{b}[t,\nu], \forall t,\nu \in \operatorname{supp}(\neg \boldsymbol{m}) \end{cases}$$

$$\Big\downarrow \textbf{splitting}$$

$$\text{Find } \mathbf{x} \in \mathbb{C}^N, \mathbf{u} \in \mathbb{C}^{F\times T} \text{ s.t. } \begin{cases} \mathbf{A}\mathbf{x} & = \operatorname{Diag}(\mathbf{c})\mathbf{u} \\ \mathbf{u}[t,\nu] & = e^{\imath \angle \mathbf{b}[t,\nu]} \ \forall t,\nu \in \operatorname{supp}(\boldsymbol{m}) \\ |\mathbf{u}[t,\nu]| & = 1 \ \forall t,\nu \end{cases}$$

$$\Big\downarrow \textbf{lifting and relaxation}$$

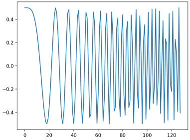
$$\min_{\mathbf{U} \in \mathbb{C}^{(F\times T)^2}} \operatorname{Trace}(\mathbf{U}\boldsymbol{\Gamma}) \text{ s.t. } \begin{cases} \operatorname{Diag}(\mathbf{U}) = \mathbb{1} \\ \mathbf{U}[(t,\nu),(t',\nu')] = \frac{\mathbf{b}[t,\nu]}{|\mathbf{b}[t,\nu]|} \frac{\bar{\mathbf{b}}[t',\nu']}{|\mathbf{b}[t',\nu']|}, \forall (t,\nu),(t',\nu') \in \operatorname{supp}(\boldsymbol{m}) \\ \mathbf{U} \succeq 0 \end{cases}$$

2

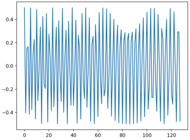
[2] Block coordinate descent methods for semidefinite programming. Wen, Z. and Goldfarb, D. and Scheinberg, K. 2012.

Data

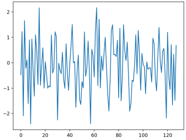
- A signal composed of a mixture of 3 signals: s = (a) +(b) + (c)



(a) chirp $\nearrow$

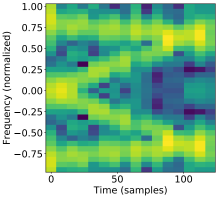


(b) Chirp $\searrow$



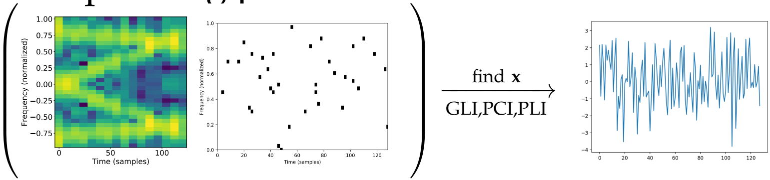
(c)

$\|$

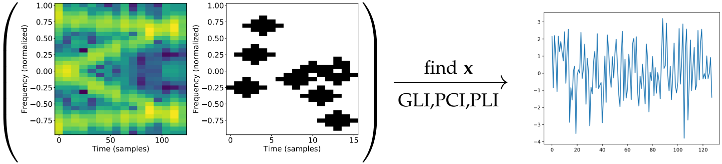


- Signal spectrogram ($T = 16$ and $F = 32$)

Phase inpainting problem



Reconstruction from a random mask with holes of **width one**.

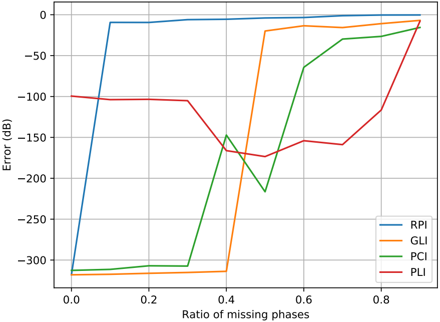


Reconstruction from a random mask with **larger holes**.

Reconstruction error up to a global phase:

$$E_{dB}(\mathbf{x}, \tilde{\mathbf{x}}) = 20 \log_{10} \min_{\theta} \frac{\|\mathbf{x} - e^{\imath\theta}\tilde{\mathbf{x}}\|_2}{\|\mathbf{x}\|_2}$$

Reconstruction error: random holes of size one

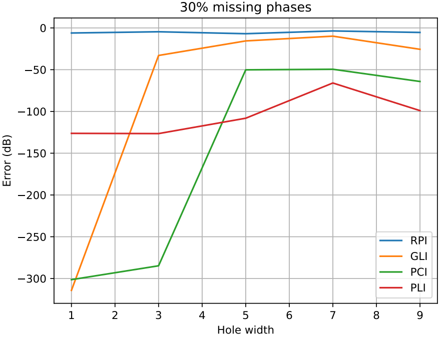


- Perfect reconstruction below 40% by GLI and PCI

- PLI works very well but not perfect

- >= 40% PLI and PCI perform better than GLI, but the performance is even better for PLI

Reconstruction error: large randomly distributed holes

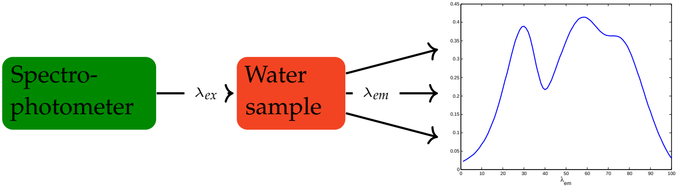


- Bad reconstruction of GLI

- Good performance for SDP methods: PLI and PCI

3D fluorescence spectroscopy

- **Problem**: identifying dissolved fluorescent substances in water solutions
- **Method**: fluorescence spectroscopy technique
- **Data acquisition:**



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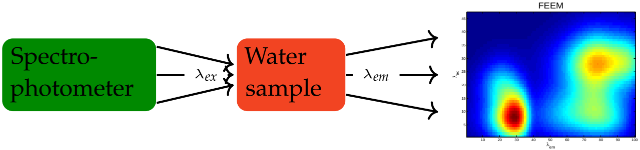

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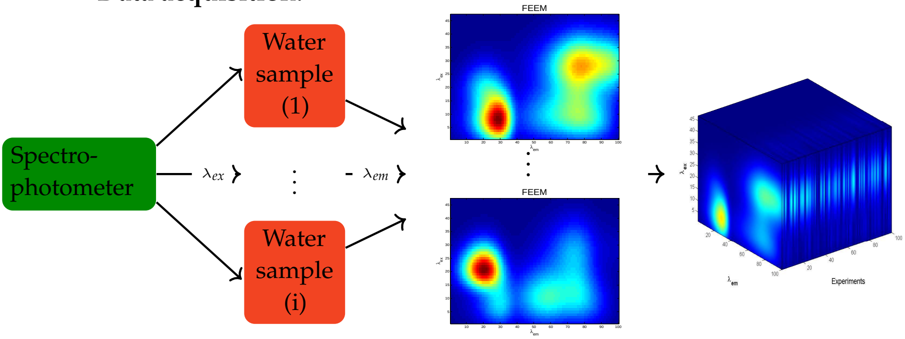

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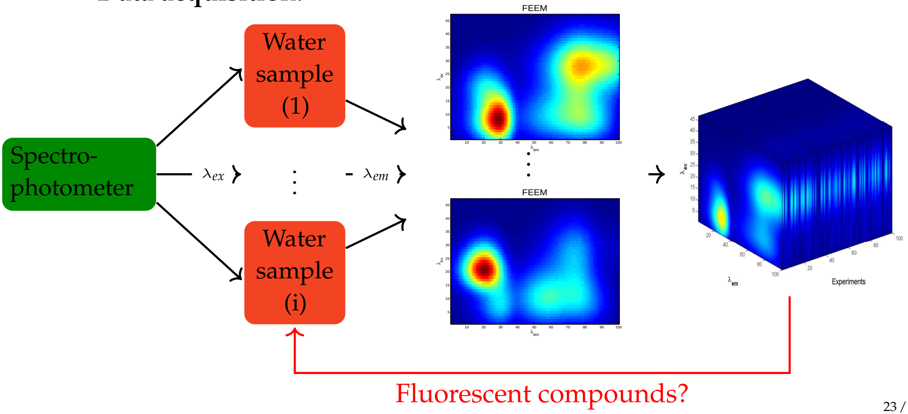
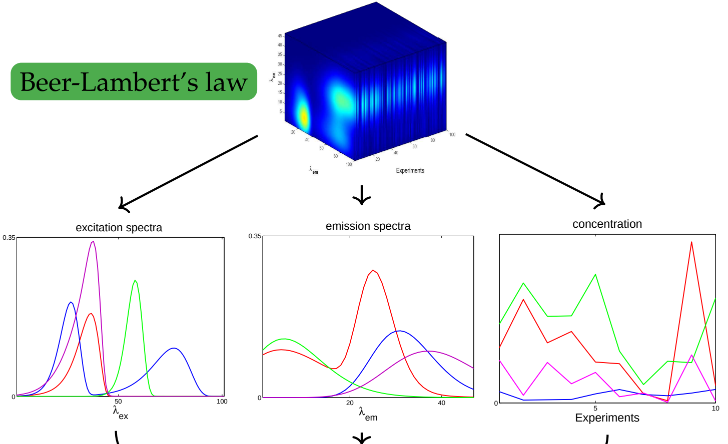


3D fluorescence spectroscopy and tensors



$$\overline{\mathcal{T}} = \sum_{r=1}^{\overline{R}} \bar{\mathbf{a}}_r^{(1)} \circ \bar{\mathbf{a}}_r^{(2)} \circ \bar{\mathbf{a}}_r^{(3)}$$

$\circ$: outer product

(Canonical) Polyadic Decomposition (CPD)

Tensor form: [Harshman1927]

$$\overline{\mathcal{T}} = \sum_{r=1}^{\overbrace{\overline{R}}^{\text{Tensor rank}}} \underbrace{\bar{\mathbf{a}}_r^{(1)} \circ \bar{\mathbf{a}}_r^{(2)} \circ \ldots \circ \bar{\mathbf{a}}_r^{(N)}}_{\text{Rank-1 tensor}} = [\![\bar{\mathbf{A}}^{(1)}, \bar{\mathbf{A}}^{(2)}, \ldots, \bar{\mathbf{A}}^{(N)}]\!]$$

Loading vectors: $\bar{\mathbf{a}}_r^{(n)}$

Loading matrices: $\bar{\mathbf{A}}^{(n)}$

$\forall n \in \{1, 2, \ldots, N\}$, $\bar{\mathbf{a}}_r^{(n)} \in \mathbb{R}^{I_n}$ and $\bar{\mathbf{A}}^{(n)} \in \mathbb{R}^{I_n \times \overline{R}}$

Canonical Polyadic Decomposition (CPD) (2)

Scalar form:

$$\bar{t}_{i_1 \dots i_N} = \sum_{r=1}^{\overline{R}} \bar{a}^{(1)}_{i_1 r} \bar{a}^{(2)}_{i_2 r} \dots \bar{a}^{(N)}_{i_N r}$$

Matrix form: [Cichocki2009]

$$\overline{\mathbf{T}}^{(n)}_{I_n, I_{-n}} = \bar{\mathbf{A}}^{(n)} (\overline{\mathbf{Z}}^{(-n)})^\top, \quad n \in \{1, \dots, N\},$$

$\overline{\mathbf{T}}^{(n)}_{I_n, I_{-n}} \in \mathbb{R}_+^{I_n \times I_{-n}}$: the matrix obtained by unfolding $\overline{\mathcal{T}}$ in the n-th mode, $I_{-n} = I_1 \dots I_N / I_n$; for all $n \in \{1, \dots, N\}$,

$$\boxed{\overline{\mathbf{Z}}^{(-n)} = \bar{\mathbf{A}}^{(N)} \odot \dots \bar{\mathbf{A}}^{(n+1)} \odot \bar{\mathbf{A}}^{(n-1)} \odot \bar{\mathbf{A}}^{(1)} \in \mathbb{R}_+^{I_{-n} \times \overline{R}}}$$

$\odot$: Khatri-Rao product.

Objective: tensor decomposition

- **Input**: Observed tensor $\mathcal{T}$
- **Output**: Estimated loading factors $\widehat{\mathbf{a}}_r^{(n)}$ for all $n \in \{1, \ldots, N\}$

Constraint:

- Loading factors $\bar{\mathbf{a}}_r^{(n)}$ entrywise nonnegative

Difficulties:

- Large dimension tensors
- Rank $\overline{R}$ unknown $\rightarrow$ needs to be estimated (overestimation problems)

Proximal algorithm for CP decomposition

$$\overline{\mathcal{T}} = \sum_{r=1}^{\overline{R}} \bar{\mathbf{a}}_r^{(1)} \circ \ldots \circ \bar{\mathbf{a}}_r^{(N)} = [\![\bar{\mathbf{A}}^{(1)}, \ldots, \bar{\mathbf{A}}^{(N)}]\!].$$

Tensor structure: naturally leads to consider N blocks corresponding to the loading matrices $\mathbf{A}^{(1)}, \ldots, \mathbf{A}^{(N)}$

Proposed optimization problem

$$\underset{\mathbf{A}^{(n)} \in \mathbb{R}^{I_n \times R},\, n \in \{1,\ldots,N\}}{\text{minimize}} \quad \mathcal{F}(\mathbf{A}^{(1)}, \ldots, \mathbf{A}^{(N)}) + \mathcal{R}_1(\mathbf{A}^{(1)}) + \ldots + \mathcal{R}_N(\mathbf{A}^{(N)})$$

Proximal algorithm for tensor decomposition

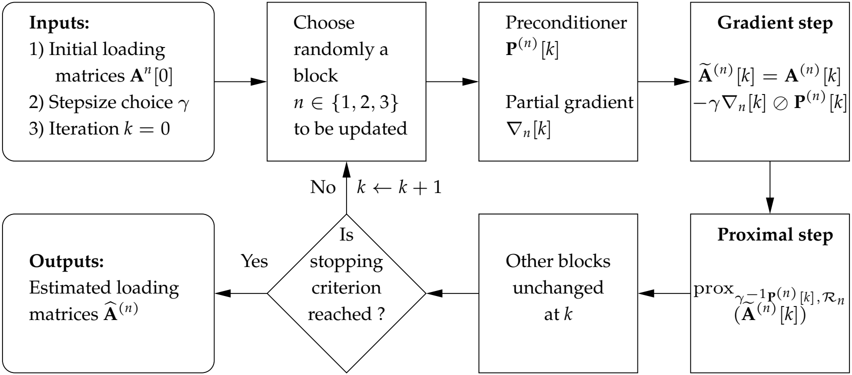


Figure: BC-VMFB algorithm for CPD.

Fidelity term

- $\mathcal{F}(\mathbf{A}^{(1)}, \dots, \mathbf{A}^{(N)})$: quadratic data fidelity term

$$\begin{aligned}\mathcal{F}(\mathbf{A}^{(1)}, \dots, \mathbf{A}^{(N)}) &= \frac{1}{2}\|\mathcal{T} - [\![\mathbf{A}^{(1)}, \dots, \mathbf{A}^{(N)}]\!]\|_F^2 \\ &= \frac{1}{2}\|\mathbf{T}^{(n)}_{I_n, I_{-n}} - \mathbf{A}^{(n)}\mathbf{Z}^{(-n)^\top}\|_F^2\end{aligned}$$

- Gradient matrices of $\mathcal{F}$ with respect to $\mathbf{A}^{(n)}, \forall n = 1, \dots, N$

$$\boxed{\nabla_n \mathcal{F}(\mathbf{A}^{(1)}, \dots, \mathbf{A}^{(N)}) = -(\mathbf{T}^{(n)}_{I_n, I_{-n}} - \mathbf{A}^{(n)}\mathbf{Z}^{(-n)^\top})\mathbf{Z}^{(-n)}}$$

Regularization terms

- $\mathcal{R}_n(\mathbf{A}^{(n)})$: block dependent penalty terms enforcing sparsity and nonnegativity

$$\mathcal{R}_n(\mathbf{A}^{(n)}) = \sum_{i_n=1}^{I_n} \sum_{r=1}^{R} \rho_n(a_{i_n r}^{(n)}) \qquad \forall n \in \{1, \dots, N\}$$

where loading matrices $\mathbf{A}^{(n)} = (a_{i_n r}^{(n)})_{(i_n, r) \in \{1,\dots,I_n\} \times \{1,\dots,R\}}$

$$\boxed{\rho_n(\omega) = \begin{cases} \alpha^{(n)} |\omega|^{\pi^{(n)}} & \text{if } \eta_{\min}^{(n)} \leq \omega \leq \eta_{\max}^{(n)} \\ +\infty & \text{otherwise} \end{cases}}$$

$\alpha^{(n)} \in]0, +\infty[$, $\pi^{(n)} \in \mathbb{N}^*$, $\eta_{\min}^{(n)} \in [-\infty, +\infty[$ and $\eta_{\max}^{(n)} \in [\eta_{\min}^{(n)}, +\infty]$
$\Rightarrow$ block dependent but constant within a block regularization parameters

Preconditioning

- Preconditioner matrix $\mathbf{P}$ for the n-th block, $\forall n \in \{1, \ldots, N\}$

$$\boxed{\mathbf{P}^{(n)}(\mathbf{A}^{(1)}, \ldots, \mathbf{A}^{(N)}) = \mathbf{A}^{(n)}(\mathbf{Z}^{(-n)^{\top}}\mathbf{Z}^{(-n)}) \oslash \mathbf{A}^{(n)}}$$

$\forall n \in \{1, \ldots, N\}$, $\mathbf{A}^{(n)}$ must be non zero
$\oslash$: Hadamard entry-wise division
(Preconditioning: extension of the one used in NMF [Lee and Seung, 2001])

Proximity operator

Proximity operator of $\mathcal{R}_n$ associated with $\mathbf{P}^{(n)}$

$$\operatorname{prox}_{\gamma[k]^{-1}\mathbf{P}^{(n)}[k],\mathcal{R}_n}(y) = \left(\operatorname{prox}_{\gamma[k]^{-1}p_i^{(n)}[k],\rho_n}(y^{(i)})\right)_{i\in\{1,\ldots,RI_n\}}$$

$(\forall y = (y^{(i)})_{i\in\{1,\ldots,RI_n\}} \in \mathbb{R}^{RI_n})$, where $(\forall i \in \{1, \ldots, RI_n\})$, $(\forall v \in \mathbb{R})$

$$\boxed{\operatorname{prox}_{\gamma[k]^{-1}p_i^{(n)},\rho_n}(v) = \min\left\{\eta_{\max}^{(n)}, \max\left\{\eta_{\min}^{(n)}, \operatorname{prox}_{\gamma[k]\alpha^{(n)}(p_i^{(n)}[k])^{-1}|\,.\,|^{\pi^{(n)}}}(v)\right\}\right\}}$$

(separable structure, diagonal preconditioning matrices, componentwise calculation)

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Proximity operator of $\mathcal{R}_n$ associated with $\mathbf{P}^{(n)}$

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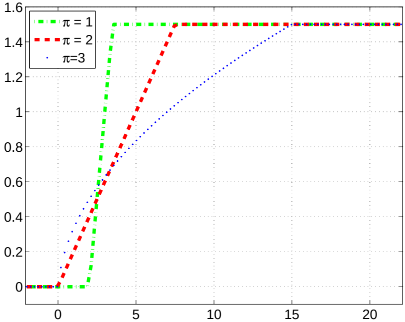
Example:

$\mathrm{prox}_{\rho_n}(v)$ where $v \in [-2, 22]$,
$[\eta^{(n)}_{\min}, \eta^{(n)}_{\max}] = [0, 1.5]$, $\alpha^{(n)} = 2$ and

1) $\pi^{(n)} = 1$

2) $\pi^{(n)} = 2$

3) $\pi^{(n)} = 3$



Experiments on simulated data

- Simulated tensor $\overline{\mathcal{T}}$: (uni or bimodal type) emission and excitation spectra, $\overline{R} = 5$
- Simulated observed tensor: $\mathcal{T} = \overline{\mathcal{T}} + \mathcal{B}$, $\mathcal{B}$: white Gaussian noise
- 2 considered cases:
  1. **3D tensor**: $\overline{\mathcal{T}} \in \mathbb{R}_+^{100\times100\times100}$
     + Noiseless case: no noise added, $\widehat{R} = 6$ (overestimation)
  2. **4D tensor**: $\overline{\mathcal{T}} \in \mathbb{R}_+^{100\times100\times100\times100}$
     + Noisy case: SNR $= 18.46$ dB, $\widehat{R} = 7$ (overestimation)
- Error measure:
  1. Signal to Noise Ratio defined as $\mathsf{SNR} = 20\log_{10}\frac{\|\overline{\mathcal{T}}\|_F}{\|\widehat{\mathcal{T}}-\overline{\mathcal{T}}\|_F}$
  2. Estimation error: $E_1 = 10\log_{10}\left(\frac{\sum_{n=1}^{N}\|\widehat{\mathbf{A}}^{(n)}(1{:}\overline{R}) - \bar{\mathbf{A}}^{(n)}\|_1}{\sum_{n=1}^{N}\|\bar{\mathbf{A}}^{(n)}\|_1}\right)$
  3. Over-factoring error $E_2 = 10\log_{10}\left(\|\sum_{r=\overline{R}+1}^{\widehat{R}}\widehat{\mathbf{a}}_r^{(1)}\circ\ldots\circ\widehat{\mathbf{a}}_r^{(N)}\|_1\right)$

Numerical results - 3D tensor

Noisy case

Elapsed time (s)	BC-VMFB	N-way	fast HALS
For 50 iterations	0.2	11	0.5
To reach stopping conditions ($\mathbf{E}_1$, $\mathbf{E}_2$) dB	75 (-11.2, -409)	8 (-12.5, 30.6)	8 (-12.5, 30.6)

Noiseless case

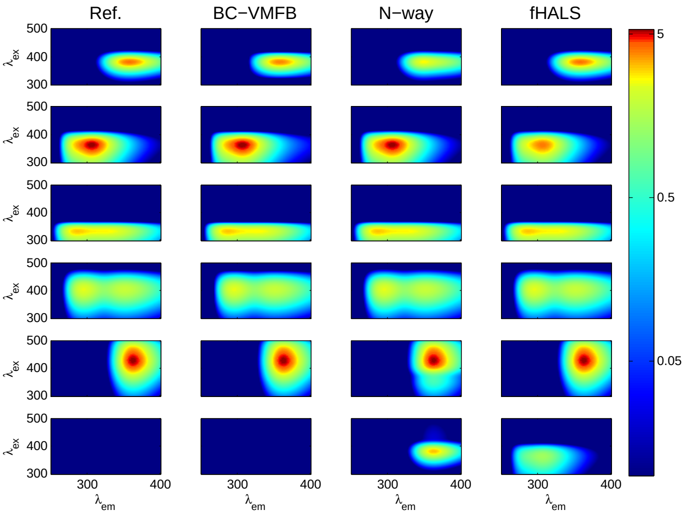
Elapsed time (s)	BC-VMFB	N-way	fast HALS
To reach stopping conditions ($\mathbf{E}_1$, $\mathbf{E}_2$) dB	74 (-15, -409)	80 (-8.7, 31.7)	3.7 (-6.1, 31.7)

Computation time comparison: BC-VMFB (with penalty), N-way [Bro, 1997], fast HALS [Phan et al., 2013] using the same initial value

BC-VMFB:

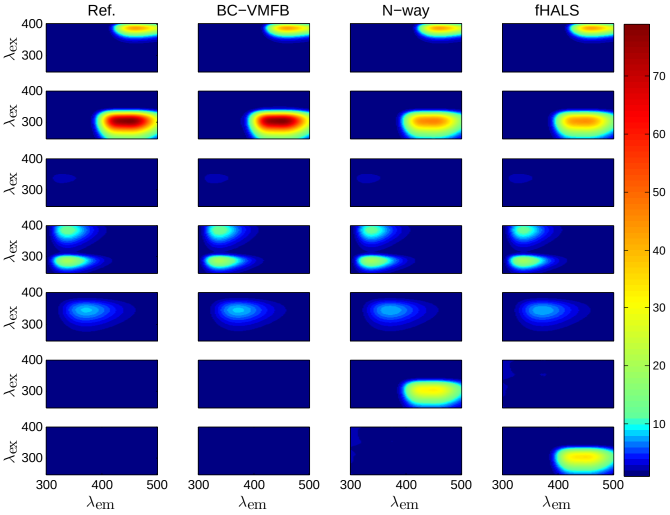
+ Fastest computation time / iteration
+ Smallest estimation error E_1 (noisy case), overestimation error E_2 (both cases)

Visual results: 3D tensor, noiseless case



Penalized BC-VMFB $\alpha = 0.05$

Visual results: 4D tensor, noisy case



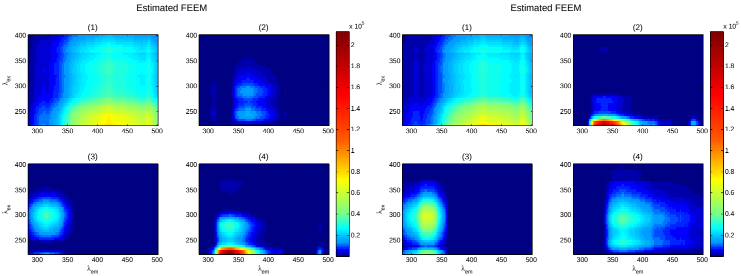
Computer simulation: real experimental data - water monitoring to detect pollutants

- Data were acquired automatically every 3 minutes, during a 10 days monitoring campaign performed on water extracted from an urban river $\Rightarrow$ tensor of size $36 \times 111 \times 2594$.
- The excitation wavelengths range from 225nm to 400nm with a 5nm bandwidth, whereas the emission wavelengths range from 280nm to 500nm with a 2nm bandwidth.
- The FEEM have been pre-processed using the Zepp's method (negative values were set to 0).

Contamination

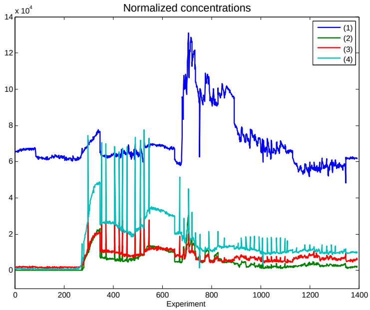
During this experiment, a contamination with diesel oil appeared 7 days after the beginning of the monitoring.

Results: assuming that $\widehat{R} = 4$



penalized BC-VMFB algorithm | Bro's *N*-way algorithm

Results: concentrations



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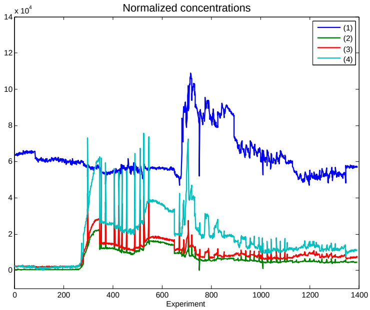
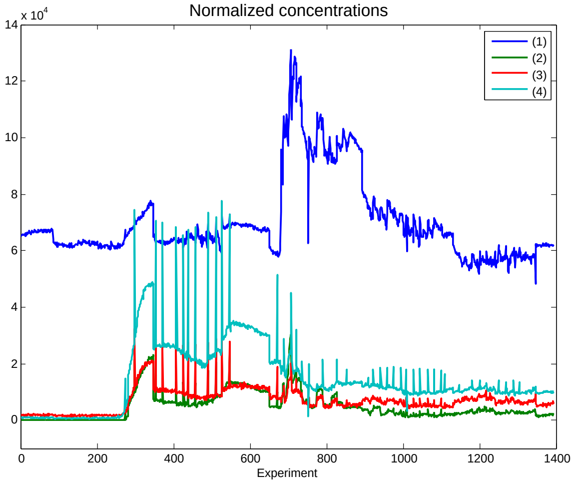


Bro's N-way algorithm

Case $\widehat{R} = 4$

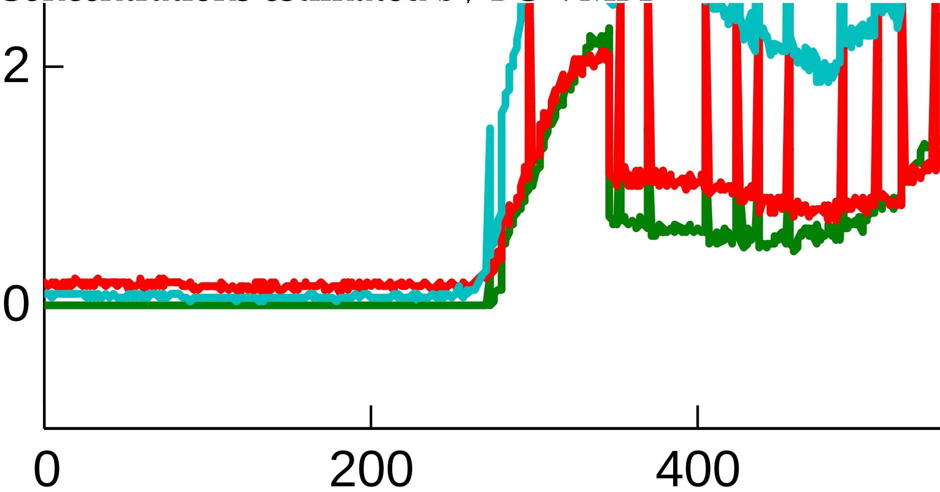
Concentrations estimated by BC-VMFB



↑ Day 7

Case $\widehat{R} = 4$

Concentrations estimated by BC-VMFB



Conclusions and perspectives

- Inverse problems study from model to resolution through parameterization.
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- Elaboration of efficient methods based on wavelets, optimization, proximal algorithms.

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Thank you !