Signaux bivariés, polarisation et quaternions

ANR Ricochet – kick-off

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CNRS, CRAN, Université de Lorraine

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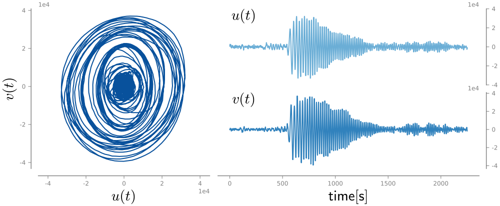
joint work with Nicolas Le Bihan, Pierre Chainais, Sebastian Miron, David Brie

Bivariate signals in nature

polarized
seismic waves



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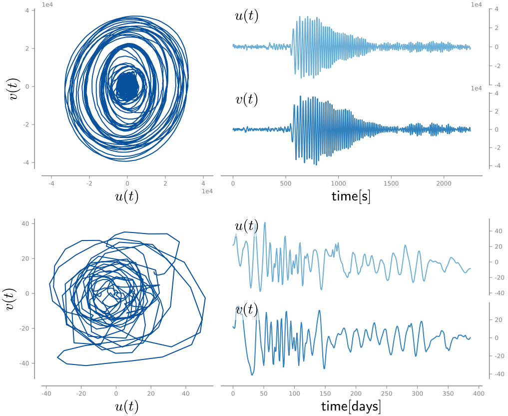

Bivariate signals in nature

polarized
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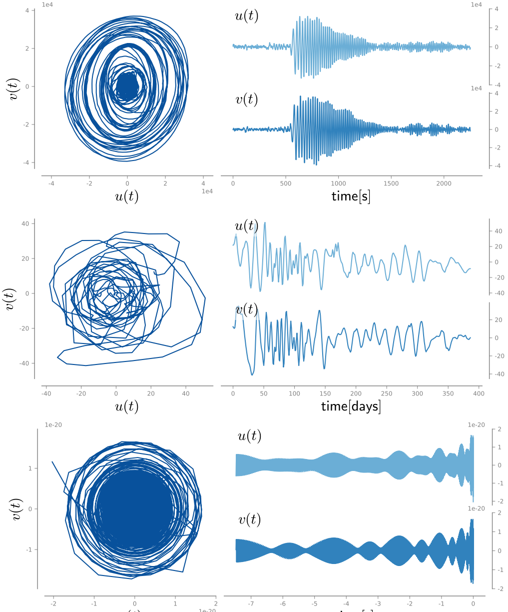
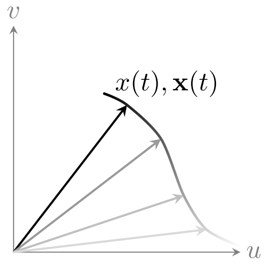
velocities

gravitational waves in
precessing binaries



Different but equivalent representations

vector $\mathbf{x}(t) = \begin{bmatrix} u(t) \\ v(t) \end{bmatrix}$ complex $x(t) = u(t) + \boldsymbol{i} v(t)$



bivariate signal processing

$\longleftrightarrow$

tools for the joint analysis / processing of 2 components $u(t)$ and $v(t)$

Vector representation of bivariate signals

$$\boxed{\mathbf{x}(t) = [u(t), v(t)]^\top \in \mathbb{R}^2}$$

- Special case of analysis of multivariate vector signals

  Hannan (1970), Priestley (1981)

- Polarization in optics

  Born and Wolf (1980), Goodman (1984), Mandel and Wolf (1995)

- Jones matrix-vector calculus

  Jones (1941), Azzam and Bashara (1978)

- Instantaneous polarization attributes in seismology

  Diallo et al. (2005), Roueff et al. (2006)

Complex representation of bivariate signals

$$\boxed{x(t) = u(t) + \boldsymbol{i}v(t) \in \mathbb{C}}$$

- Circularity of random complex signals (rotational invariance)

  Picinbono (1994), Amblard et al. (1996)

- Augmented representations ${}_{\uparrow}\mathbf{x}(t) = [x(t), \overline{x(t)}]^\top$

  Schreier and Scharf (2003, 2010), Adalı et al. (2011)

- Rotary components $x \equiv \sum \circlearrowleft + \sum \circlearrowright$

  Blanc-Lapierre and Fortet (1953), Gonella (1972), Walden (2013)

- Instantaneous ellipse description for nonstationary bivariate signals

  deterministic Lilly and Olhede (2010) random Schreier (2008)

  EMD Rilling et al. (2007)

The need for interpretability

existing approaches: no straightforward physical descriptions

feature	$\mathbf{x}(t) \in \mathbb{R}^2$	$x(t) \in \mathbb{C}$	desired
direct ellipse parametrization	✗	✗	✓
positive frequencies	✓	✗	✓
interpretable filtering relations	✗	✗	✓

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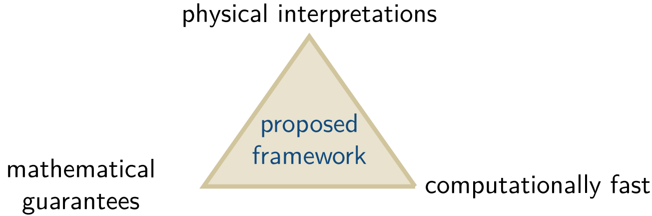

$\Downarrow$

efficient, relevant generalization of ubiquitous signal processing tools

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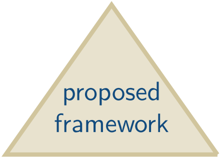
interpretable filtering relations	✗	✗	✓

physical interpretations

mathematical guarantees

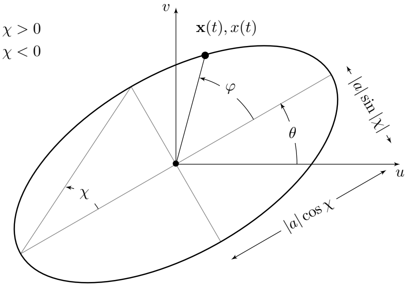


computationally fast

$\Downarrow$

efficient, relevant generalization of ubiquitous signal processing tools

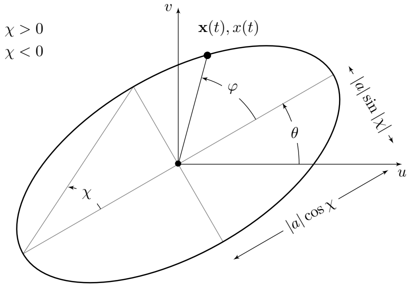
Monochromatic bivariate signal representation



Polarization ellipse parameters

- $a \geq 0$ intensity
- $\theta \in [-\pi/2, \pi/2]$ orientation
- $\chi \in [-\pi/4, \pi/4]$ ellipticity
- $\varphi \in [0, 2\pi)$ phase

Monochromatic bivariate signal representation



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Jones vector: Vector representation (optics, seismology)

$$\mathbf{x}(t) = \begin{bmatrix} A_u \cos(2\pi\nu_0 t + \Phi_u) \\ A_v \cos(2\pi\nu_0 t + \Phi_v) \end{bmatrix} \quad \theta, \chi \leftarrow f(A_u, A_v, \Phi_u, \Phi_v)$$

Rotary components: Complex representation (oceanography, SPTM)

$$x(t) = A_+ e^{\boldsymbol{i}\theta_+} e^{\boldsymbol{i}2\pi\nu_0 t} \qquad \theta \leftarrow g_1(\theta_+, \theta_-)$$

$$+ A_- e^{-\boldsymbol{i}\theta_-} e^{-\boldsymbol{i}2\pi\nu_0 t} \qquad \chi \leftarrow g_2(A_+, A_-)$$

Today's agenda

Outline

Framework

Ingredient $\#1$ bivariate signal as complex signal embedded in $\mathbb{H}$

$$x(t) = u(t) + \boldsymbol{i}v(t) \in \mathbb{C}_{\boldsymbol{i}} \subset \mathbb{H}$$

alike embedding a signal $x(t) \in \mathbb{R}$ into $\mathbb{C}$

Quaternions

4D algebra $\quad \boldsymbol{i}^2 = \boldsymbol{j}^2 = \boldsymbol{k}^2 = -1 \quad$ ⚠ $\boldsymbol{ij} = \boldsymbol{k},\ \boldsymbol{ij} = -\boldsymbol{ji}$ ⚠

complex subfields of $\mathbb{H}$: $\mathbb{C}_{\boldsymbol{i}} = \mathrm{Span}\left\{1, \boldsymbol{i}\right\}$, $\mathbb{C}_{\boldsymbol{j}} = \mathrm{Span}\left\{1, \boldsymbol{j}\right\}$, $\ldots$

polar forms, 3D and 4D geometry, etc.

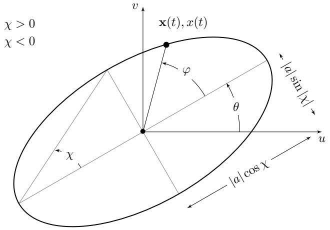
Ingredient #2 adapt Fourier transform

Quaternion Fourier Transform (QFT)

$$X(\nu) = \int \underbrace{x(t)}_{\in \mathbb{C}_{\boldsymbol{i}}} \underbrace{e^{-\boldsymbol{j}2\pi\nu t}}_{\in \mathbb{C}_{\boldsymbol{j}}} \mathrm{d}t \in \mathbb{H}$$

Monochromatic polarized signal

polar form by Bülow and Sommer (2001)



$$x(t) = \mathrm{Proj}_{\mathbb{C}_{\boldsymbol{i}}}\left\{a e^{\boldsymbol{i}\theta} e^{-\boldsymbol{k}\chi} e^{\boldsymbol{j}(2\pi\nu_0 t + \varphi)}\right\}$$

$\updownarrow$ QFT

$$X(\nu) = a e^{\boldsymbol{i}\theta} e^{-\boldsymbol{k}\chi} e^{\boldsymbol{j}\varphi} \delta_{\nu_0}(\nu) + \text{sym.}$$

polar form $\leftrightarrow$ physical parameters

QFT properties

Existence for L^1, L^2 functions Jamison Ph.D. thesis (1970)
Easy to compute

$$x(t) = u(t) + \boldsymbol{i}v(t) \xleftrightarrow{\text{QFT}} X(\nu) = \underbrace{U(\nu)}_{1,\boldsymbol{j}} + \underbrace{\boldsymbol{i}V(\nu)}_{\boldsymbol{i},\boldsymbol{k}}$$

For bivariate signals keep $\nu \geq 0$ only (***i**-Hermitian symmetry*)

$$X(-\nu) = -\boldsymbol{i}X(\nu)\boldsymbol{i}, \quad \text{for } x(t) \in \mathbb{C}_{\boldsymbol{i}}$$

2 invariants for finite energy signals (QFT Parseval theorem)

$$\int_{-\infty}^{+\infty} |x(t)|^2 \, \mathrm{d}t = \int_{-\infty}^{+\infty} |X(\nu)|^2 \, \mathrm{d}\nu \qquad \text{(energy)}$$

$$\boxed{\int_{-\infty}^{+\infty} x(t)\boldsymbol{j}\overline{x(t)} \, \mathrm{d}t = \int_{-\infty}^{+\infty} \underbrace{X(\nu)\boldsymbol{j}\overline{X(\nu)}}_{\in \operatorname{span}\{\boldsymbol{i},\boldsymbol{j},\boldsymbol{k}\}} \, \mathrm{d}\nu \qquad \text{(geometry)}}$$

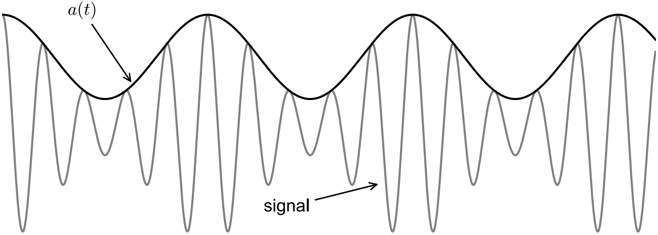
JF, NLB, PC, 2017

Fundamental property: Hermitian symmetry of FT of real signals

Analytic signal of a real signal — Gabor (1946), Ville (1948)

One to one corresp. between a real signal and its analytic signal

$$x(t) \in \mathbb{R} \longleftrightarrow x_+(t) \in \mathbb{C}$$
$$a(t)\cos[\varphi(t)] \longleftrightarrow a(t)e^{\boldsymbol{i}\varphi(t)}$$



Amplitude Modulation

Quaternion embedding of bivariate signals

$x(t) = u(t) + \boldsymbol{i}v(t) \qquad X(-\nu) = -\boldsymbol{i}X(\nu)\boldsymbol{i}$ ($\boldsymbol{i}$-Hermitian symmetry)

Quaternion embedding

One-to-one correspondence

$$\text{bivariate signal} \longleftrightarrow \text{quaternion embedding}$$
$$x(t) \in \mathbb{C}_{\boldsymbol{i}} \longleftrightarrow x_+(t) \in \mathbb{H}$$

Polar form: instantaneous attributes

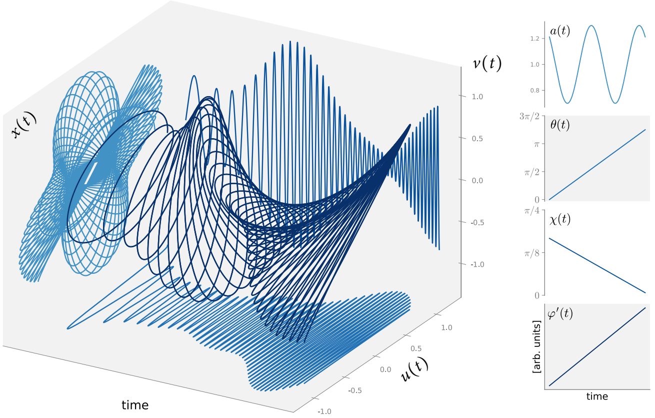
$$x_+(t) = \underbrace{a(t)}_{\text{amplitude}} \times \underbrace{e^{\boldsymbol{i}\theta(t)}e^{-\boldsymbol{k}\chi(t)}}_{\text{geometry}} \times \underbrace{e^{\boldsymbol{j}\varphi(t)}}_{\text{phase}}$$

$a(t) \geq 0$
$\theta(t) \in [-\pi/2, \pi/2]$
$\chi(t) \in [-\pi/4, \pi/4]$
$\varphi(t) \in [-\pi, \pi]$

Canonical quadruplet

Bivariate AM-FM signal model

$$x(t) = \mathrm{Proj}_{\mathbb{C}_{\boldsymbol{i}}}\{x_+(t)\} = a(t)e^{\boldsymbol{i}\theta(t)}\left[\cos\chi(t)\cos\varphi(t) + \boldsymbol{i}\sin\chi(t)\sin\varphi(t)\right]$$



bivariate linear chirp w/ amplitude, orientation and ellipticity modulation

justifies a posteriori Lilly and Olhede's (2010) parametric model

Physical interpretation

Instantaneous Stokes parameters

Born and Wolf (1980)

Common description of polarization properties in optics

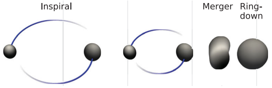
$$
\begin{aligned}
S_0(t) &= |a(t)|^2 \\
S_1(t) &= |a(t)|^2 \cos 2\chi(t) \cos 2\theta(t), \\
S_2(t) &= |a(t)|^2 \cos 2\chi(t) \sin 2\theta(t), \\
S_3(t) &= |a(t)|^2 \sin 2\chi(t).
\end{aligned}
$$

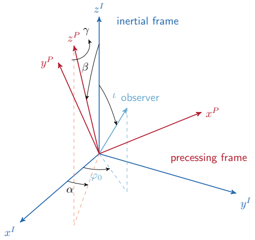
Basic quaternion calculus shows that:

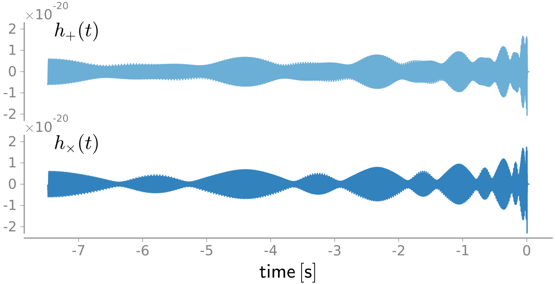
$$
|x_+(t)|^2 = S_0(t), \quad x_+(t)\boldsymbol{j}\overline{x_+(t)} = \boldsymbol{i}S_3(t) + \boldsymbol{j}S_1(t) + \boldsymbol{k}S_2(t)
$$

QFT Parseval invariants $\longleftrightarrow$ Stokes parameters

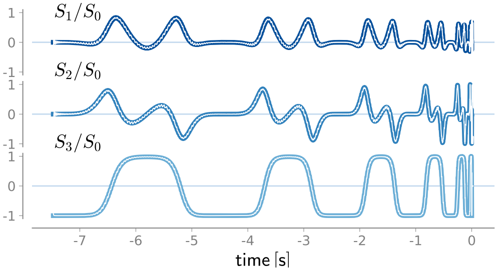
Gravitational waves and precessing binaries







GW strain $h(t) = h_+(t) - \boldsymbol{i}\, h_\times(t)$



nonparametric diagnostic of precession

more in Cyril's presentation tomorrow !

Quaternion spectrogram

Quaternion Short Term Fourier Transform

Extend the STFT to the QFT setting

$$\mathrm{F}_x^g(\tau,\nu) = \int \underbrace{x(t)}_{\in\mathbb{C}_{\boldsymbol{i}}} \underbrace{g(t-\tau)}_{\in\mathbb{R}} \underbrace{\exp(-\boldsymbol{j}2\pi\nu t)}_{\in\mathbb{C}_{\boldsymbol{j}}} \mathrm{d}t$$

Theorems $\begin{cases} \text{inversion} \\ \text{conservation: energy} \quad \text{geometry/polarization} \end{cases}$

$|\mathrm{F}_x^g(\tau,\nu)|^2 \rightarrow$ Time-frequency energy density (S_0)

$\mathrm{F}_x^g(\tau,\nu)\boldsymbol{j}\overline{\mathrm{F}_x^g(\tau,\nu)} \rightarrow$ Time-frequency-polarization features (S_1, S_2, S_3)

new interpretable time-frequency-polarization representation

Q-STFT theorem

Theorem: inversion formula and energy/polarization conservation

Let $x \in L^2(\mathbb{R}; \mathbb{H})$. Then the inversion formula reads

$$x(t) = \int_{-\infty}^{+\infty} \int_{-\infty}^{+\infty} \mathrm{F}_x^g(\tau, \nu) g(t-\tau) e^{\boldsymbol{j} 2\pi \nu t} \mathrm{d}\nu \mathrm{d}\tau,$$

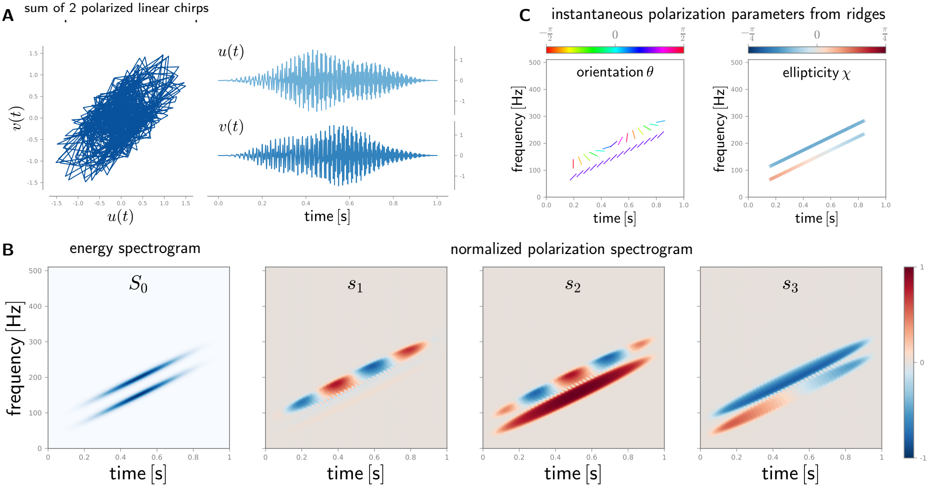
and the energy of x is conserved,

$$\int_{-\infty}^{+\infty} |x(t)|^2 \mathrm{d}t = \int_{-\infty}^{+\infty} \int_{-\infty}^{+\infty} |\mathrm{F}_x^g(\tau, \nu)|^2 \mathrm{d}\tau \mathrm{d}\nu,$$

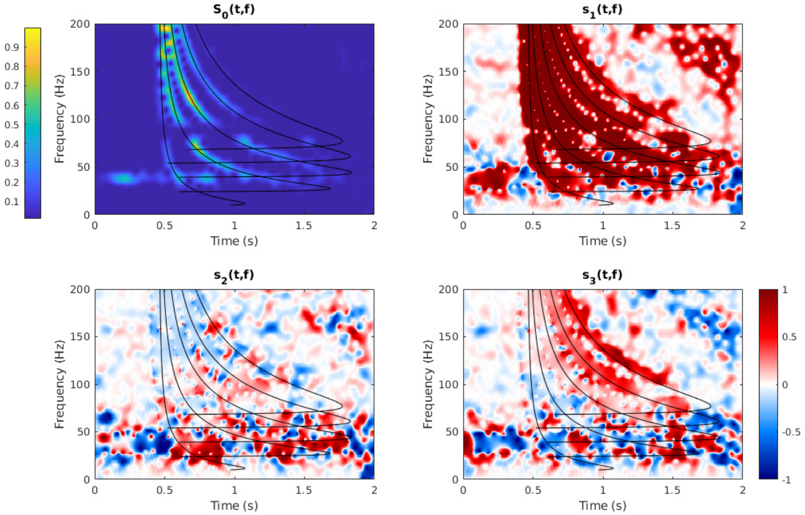
as well as the polarization properties of x:

$$\boxed{\int_{-\infty}^{+\infty} x(t) \boldsymbol{j} \overline{x(t)} \mathrm{d}t = \int_{-\infty}^{+\infty} \int_{-\infty}^{+\infty} \mathrm{F}_x^g(\tau, \nu) \boldsymbol{j} \overline{\mathrm{F}_x^g(\tau, \nu)} \mathrm{d}\tau \mathrm{d}\nu.}$$

Quaternion spectrogram: sum of two linear chirps



Polarization of normal modes in underwater acoustics



particular velocity data from SBCEX17 experiment

Bonnel et al. 2021

Novel and general approach to time-frequency-polarization analysis

✓ novel representations ✓ theorems ✓ numerically efficient

- Quaternion embedding $x(t) \in \mathbb{C}_{\boldsymbol{i}} \longleftrightarrow x_+(t) \in \mathbb{H}$
- Time-frequency-polarization analysis Q-STFT $\mathrm{F}_x^g(\tau, \nu)$
- Time-scale-polarization analysis Q-CWT $\mathrm{W}_x(\tau, s)$

JF, NLB, PC, 2017

Some open questions

- robust estimation of ridges and instantaneous parameters
- new observables: theory of instantaneous moments?
- advanced TF analysis: reassignment, synchrosqueezing?
- nonstationary random signals?

1. Quaternion Fourier transform for bivariate signals
2. Time-frequency analysis of bivariate signals
3. Quaternion non-negative matrix factorization
   - Extending the NMF to polarized data
   - Uniqueness properties
   - A practical algorithm
4. Conclusions and outlook

Back to Stokes parameters

natural observables for bivariate signals borrowed from polarimetry

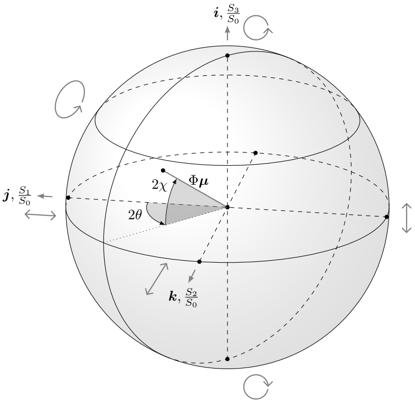
General definition

$$S_0 = a^2$$
$$S_1 = a^2\Phi \cos 2\theta \cos 2\chi$$
$$S_2 = a^2\Phi \sin 2\theta \cos 2\chi$$
$$S_3 = a^2\Phi \sin 2\chi$$

degree of polarization $0 \leq \Phi \leq 1$

deterministic signals $\Phi = 1$
(fully polarized)

random signals $\Phi \leq 1$
(partially polarized in general)



Poincaré sphere

Polarization: physical constraints and multiple diversities

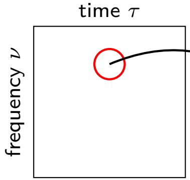
Stokes parameters as experimental observables

S_0	S_1	S_2	S_3
intensity	$\leftrightarrow$ $\updownarrow$	⤢ ⤡	↺ ↻

$S_0 \geq 0$ physical constraints $\mathcal{S}$ $S_1^2 + S_2^2 + S_3^2 \leq S_0^2$

$S_i = S_i(\text{time, frequency, space, wavelength, etc. })$

Example: time-frequency analysis of bivariate signals



$$\mathrm{F}_x^g(\tau,\nu) = S_0(\tau,\nu) + \boldsymbol{i}S_3(\tau,\nu) + \boldsymbol{j}S_1(\tau,\nu) + \boldsymbol{k}S_2(\tau,\nu) \in \mathbb{H}$$

Polarization: physical constraints and multiple diversities

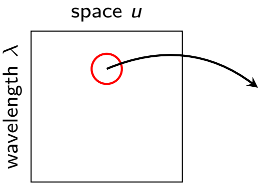
Stokes parameters as experimental observables

S_0	S_1	S_2	S_3
intensity	$\leftrightarrow \quad \updownarrow$	$\nearrow\!\!\!\swarrow \quad \nwarrow\!\!\!\searrow$	$\circlearrowleft \quad \circlearrowright$

$S_0 \geq 0$ physical constraints $\mathcal{S}$ $S_1^2 + S_2^2 + S_3^2 \leq S_0^2$

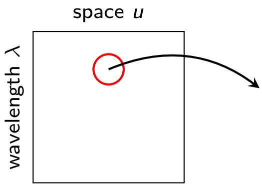
⚠ $S_i = S_i(\text{time, frequency, space, wavelength, etc. })$ ⚠

Example: spectro-polarimetric imaging astrophysics, non-destructive control, etc.



$$X(u,\lambda) = S_0(u,\lambda) + \boldsymbol{i}S_3(u,\lambda) + \boldsymbol{j}S_1(u,\lambda) + \boldsymbol{k}S_2(u,\lambda) \in \mathbb{H}$$

Blind polarized source separation



$$X(u,\lambda) = S_0(u,\lambda) + \boldsymbol{i}S_3(u,\lambda) + \boldsymbol{j}S_1(u,\lambda) + \boldsymbol{k}S_2(u,\lambda)$$

P polarized sources linear mixture model

$$X(u,\lambda) = w_1(\lambda)h_1(u) + w_2(\lambda)h_2(u) + \ldots + w_P(\lambda)h_P(u)$$

Stokes vector $\in \mathbb{H}$

activations ≥ 0

Comments

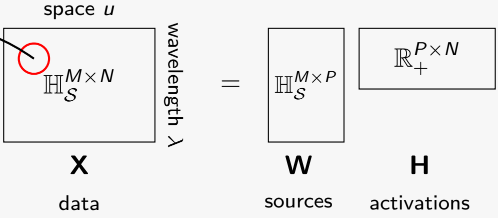
- assume incoherent superposition of Stokes vectors
- generalizes the classical linear mixing model to polarized data

how to solve this Stokes vector source separation problem?

Our proposition: QNMF

Quaternion Non-negative Matrix Factorization (QNMF)

$$X(u,\lambda) = S_0(u,\lambda) + \boldsymbol{i}S_3(u,\lambda) + \boldsymbol{j}S_1(u,\lambda) + \boldsymbol{k}S_2(u,\lambda)$$



$P \ll M, N$: low-rank representation of Stokes parameter data

2 key ingredients:

1. algebraic representation of Stokes parameters using quaternions $\mathbb{H}$
2. “non-negativity” constraint $\mathcal{S}$ on Stokes parameters

Physical admissibility constraints for Stokes parameters

Ensure correct physical interpretation of Stokes parameters

Ingredient 2: "non-negativity" constraint on Stokes parameters

$$(\mathcal{S}) \qquad \underset{\text{intensity}}{S_0 \geq 0} \qquad \text{and} \qquad \underset{\text{polarization}}{\boxed{S_1^2 + S_2^2 + S_3^2 \leq S_0^2}}$$

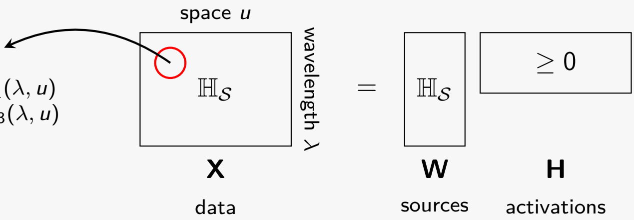
$$\iff \boldsymbol{\Sigma} = \frac{1}{2}\begin{bmatrix} S_0 + S_1 & S_2 + \boldsymbol{i}S_3 \\ S_2 - \boldsymbol{i}S_3 & S_0 - S_1 \end{bmatrix} \text{ is nonnegative definite}$$

comment

- $\boldsymbol{\Sigma}$ is nonnegative definite $\iff \operatorname{tr}\boldsymbol{\Sigma} \geq 0$ and $\det \boldsymbol{\Sigma} \geq 0$
- nonnegativity of Stokes parameters arises from definition of $\boldsymbol{\Sigma}$ as the covariance matrix of the complex electric field

QNMF generalizes NMF to polarized data

$$\begin{aligned}&\mathbf{x}(\lambda, u)\\ &= S_0(\lambda, u) + \boldsymbol{i}S_1(\lambda, u)\\ &+\boldsymbol{j}S_2(\lambda, u) + \boldsymbol{k}S_3(\lambda, u)\end{aligned}$$

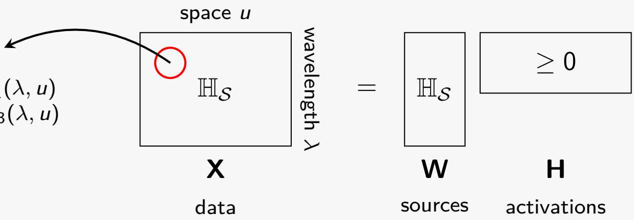


QNMF as co-factorization problem with common activations **H**

$$\mathbf{X} = \mathbf{W}\mathbf{H} \iff \begin{cases} \mathrm{Re}\,\mathbf{X} = \mathrm{Re}[\mathbf{W}]\mathbf{H} & (\text{NMF on } S_0 \geq 0) \\ \mathrm{Im}\,\mathbf{X} = \mathrm{Im}[\mathbf{W}]\mathbf{H} & (\text{polarization, } S_1, S_2, S_3) \end{cases}$$

QNMF generalizes NMF to polarized data

$$\begin{aligned}&\mathbf{x}(\lambda, u)\\ &= S_0(\lambda, u) + \boldsymbol{i}S_1(\lambda, u)\\ &+\boldsymbol{j}S_2(\lambda, u) + \boldsymbol{k}S_3(\lambda, u)\end{aligned}$$



QNMF as co-factorization problem with common activations **H**

$$\mathbf{X} = \mathbf{WH} \iff \begin{cases} \mathrm{Re}\mathbf{X} = \mathrm{Re}[\mathbf{W}]\mathbf{H} & \text{(NMF on } S_0 \geq 0\text{)} \\ \mathrm{Im}\mathbf{X} = \mathrm{Im}[\mathbf{W}]\mathbf{H} & \text{(polarization, } S_1, S_2, S_3\text{)} \end{cases}$$

Fundamental questions

- uniqueness conditions on **W** and **H**? (interpretability)
- existence of an efficient algorithm? (applicability)

QNMF uniqueness

non-uniqueness of QNMF factors $(\mathbf{W}, \mathbf{H})$

$$\mathbf{X} = \mathbf{WH} = (\mathbf{WT})(\mathbf{T}^{-1}\mathbf{H}) \qquad \mathbf{T} \in \mathbb{R}^{P \times P}$$

As with NMF, **T** can always represent trivial ambiguities

scale $\quad \mathbf{T} = \mathrm{diag}(\lambda_1, ..., \lambda_p), \quad \lambda_i > 0$

permutation $\quad \mathbf{T} = \mathrm{perm}_\pi, \quad \pi : \{1, 2, ..., P\} \to \{1, 2, ..., P\}$ is one-to-one

Definition

QNMF is said unique iff the only indeterminacies are scale and permutation

QNMF uniqueness

non-uniqueness of QNMF factors $(\mathbf{W}, \mathbf{H})$

$$\mathbf{X} = \mathbf{W}\mathbf{H} = (\mathbf{W}\mathbf{T})(\mathbf{T}^{-1}\mathbf{H}) \qquad \mathbf{T} \in \mathbb{R}^{P \times P}$$

As with NMF, $\mathbf{T}$ can always represent trivial ambiguities

$$\begin{aligned} \text{scale} \quad & \mathbf{T} = \mathrm{diag}(\lambda_1, ..., \lambda_p), \quad \lambda_i > 0 \\ \text{permutation} \quad & \mathbf{T} = \mathrm{perm}_\pi, \quad \pi : \{1, 2, ..., P\} \to \{1, 2, ..., P\} \text{ is one-to-one} \end{aligned}$$

Definition

QNMF is said unique iff the only indeterminacies are scale and permutation

NMF-based uniqueness for QNMF

If the NMF $\mathrm{Re}\mathbf{X} = \mathrm{Re}\,[\mathbf{W}]\,\mathbf{H}$ is unique, then $\mathbf{X} = \mathbf{W}\mathbf{H}$ is unique

▶ QNMF encompasses known sufficient NMF uniqueness conditions (e.g. separability or sufficiently scattered assumptions)

QNMF uniqueness: going beyond NMF

Sufficient condition for uniqueness ($P = 2$ sources)

- $\exists$ 2 wavelengths λ_1, λ_2 (not necessarily different)

$$\begin{cases} w_1(\lambda_1) \text{ is fully polarized, } \mathrm{Re}\, w_1(\lambda_1) \geq c\mathrm{Re}\, w_2(\lambda_1), c \in [0, 1] \\ w_2(\lambda_1) \text{ is polarized differently} \\ +\text{reciprocal for } \lambda_2 \end{cases}$$

- $\exists$ 2 locations u_1, u_2 s.t.

$$\begin{cases} h_1(u_1) > 0 \text{ and } h_2(u_1) = 0 \\ h_2(u_2) > 0 \text{ and } h_1(u_1) = 0 \end{cases}$$

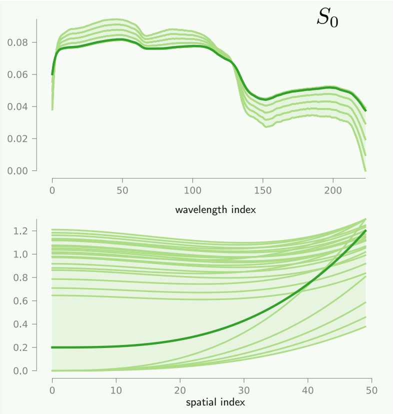
Source uniqueness conditions are stated in terms of polarization properties

QNMF without uniqueness?

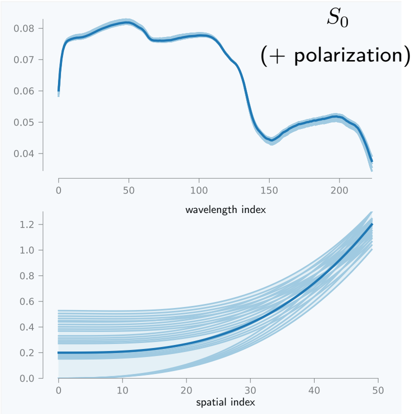
polarization information still plays a key role in QNMF model identifiability

Range of admissible solutions ($P = 2$)

NMF



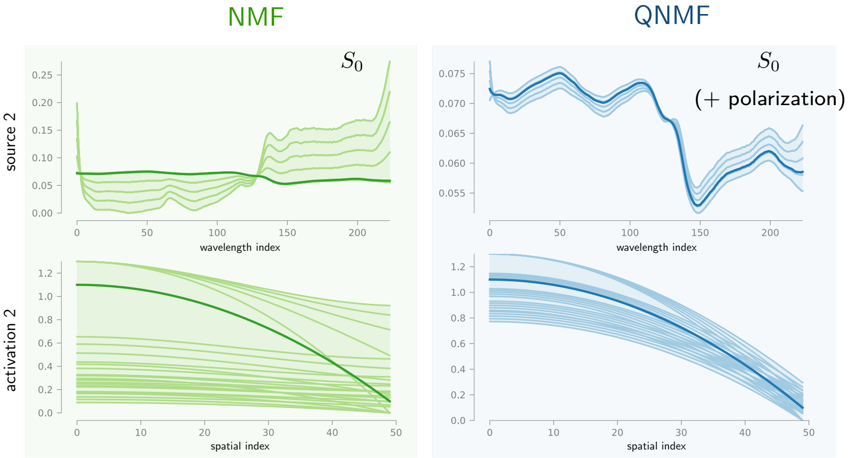
QNMF



Relation between NMF and QNMF

$$\mathbf{X} = \mathbf{W}\mathbf{H} \iff \begin{cases} \mathrm{Re}\mathbf{X} = \mathrm{Re}[\mathbf{W}]\mathbf{H} & \text{(NMF)} \\ \mathrm{Im}\mathbf{X} = \mathrm{Im}[\mathbf{W}]\mathbf{H} & \text{(polarization)} \end{cases}$$

Range of admissible solutions ($P = 2$)



polarization information → significantly improves model identifiability

QNMF uniqueness: general case

Necessary uniqueness conditions for QNMF are looser than NMF

no zero-pattern condition on $\mathbf{W}$!

Conjecture

If $\mathbf{W}$ exhibits a fully polarized pattern and $\mathbf{H}$ obeys the separability conditions, then $\mathbf{X} = \mathbf{WH}$ is unique

✓ $P = 2$ sources

? $P > 2$ sources

finding general QNMF uniqueness conditions remains an open problem

Solving QNMF

Goal

$$(\mathbf{W}, \mathbf{H}) = \min \|\mathbf{X} - \tilde{\mathbf{W}}\tilde{\mathbf{H}}\|_F^2 \quad \text{s.t. } \tilde{\mathbf{W}} \in \mathbb{H}_{\mathcal{S}}^{M \times P}, \tilde{\mathbf{H}} \in \mathbb{R}_+^{P \times N}$$

non-convex in (**W**, **H**) but convex in **W**, **H** individually

Alternating minimization scheme

After initialization, at iteration $r > 0$

$$\mathbf{H}_{r+1} \leftarrow \underset{\mathbf{H} \in \mathbb{R}_+^{P \times N}}{\arg\min} \|\mathbf{X} - \mathbf{W}_r \mathbf{H}\|_F^2$$

$$\mathbf{W}_{r+1} \leftarrow \underset{\mathbf{W} \in \mathbb{H}_{\mathcal{S}}^{M \times P}}{\arg\min} \|\mathbf{X} - \mathbf{W}\mathbf{H}_{r+1}\|_F^2$$

and repeat until convergence

Convergence to a stationary point is guaranteed provided that subproblems can be solved exactly !

Quaternion Alternating Least Squares (Q-ALS)

Q-ALS is an approximation to exact alternating minimization scheme

After initialization, at iteration $r > 0$

$$\mathbf{H}_{r+1} \leftarrow \Pi_{\mathbb{R}_+}\left[\underset{\mathbf{H}\in\ \mathbb{R}^{P\times N}}{\arg\min} \|\mathbf{X} - \mathbf{W}_r\mathbf{H}\|_F^2\right]$$

$$\mathbf{W}_{r+1} \leftarrow \Pi_{\mathbb{H}_\mathcal{S}}\left[\underset{\mathbf{W}\in\ \mathbb{H}^{M\times P}}{\arg\min} \|\mathbf{X} - \mathbf{W}\mathbf{H}_{r+1}\|_F^2\right]$$

repeat until some exit criterion is satisfied

Key questions

1. Projections operators $\Pi_{\mathbb{R}_+}$ and $\Pi_{\mathbb{H}_\mathcal{S}}$?
2. Closed-form quaternion updates?

Q-ALS in practice: computing projections

Imposing non-negativity constraints?

- non-negativity constraint on activations $\mathbf{H}$:

$$[\Pi_{\mathbb{R}^+}(\mathbf{H})]_{pn} = \max(0, (\mathbf{H})_{pn}) \quad \forall \text{ entries}$$

set to zero any negative entries in $\mathbf{H}$

- constraint $(\mathcal{S})$ on sources $\mathbf{W}$:
  for $W_{mp} = w_0 + \boldsymbol{i}w_1 + \boldsymbol{j}w_2 + \boldsymbol{k}w_3 \in \mathbb{H}$

$$W_{mp} \in \mathbb{H}_{\mathcal{S}} \iff \boldsymbol{\Sigma} = \frac{1}{2}\begin{bmatrix} w_0 + w_1 & w_2 + \boldsymbol{i}w_3 \\ w_2 - \boldsymbol{i}w_3 & w_0 - w_1 \end{bmatrix} \text{ is nonnegative definite}$$

keep the nonnegative eigenvalues of Σ, zero out the others and identify projected Stokes parameters

Example

$$\Pi_{\mathbb{H}_{\mathcal{S}}}(1 + \boldsymbol{i} + 0.5\boldsymbol{j} + 0.5\boldsymbol{k}) = \frac{5}{4} + \boldsymbol{i}\frac{5}{6} + \boldsymbol{j}\frac{5}{6} + \boldsymbol{k}\frac{5}{12}$$

Q-ALS in practice: explicit updates

Explicit use of generalized $\mathbb{HR}$-derivatives

[Xu et al., 2015]

Consider the $\mathbf{W}$ subproblem:

$$\underset{\mathbf{W}\in\ \mathbb{H}^{M\times P}}{\arg\min}\ \|\mathbf{X}-\mathbf{W}\mathbf{H}_{r+1}\|_F^2$$

$\mathbf{W}$ is optimal iff only its conjugated quaternion gradient vanishes:

$$\nabla_{\overline{\mathbf{W}}}\|\mathbf{X}-\mathbf{W}\mathbf{H}_{r+1}\|_F^2=0 \underset{\mathbb{HR}\text{-calculus tables}}{\Longleftrightarrow} -\frac{1}{2}(\mathbf{X}-\mathbf{W}\mathbf{H}_{r+1})\mathbf{H}_{r+1}^\top=0$$

A similar approach is taken for $\mathbf{H}$ using standard real-derivatives, with special care due to the quaternion nature of $\mathbf{W}$ and $\mathbf{X}$.

Q-ALS in summary

Q-ALS explicit updates:

After initialization, at iteration r, repeat until convergence:

$$\mathbf{H}_{r+1} \leftarrow \Pi_{\mathbb{R}_+}\left[\left(\mathrm{Re}\left[\mathbf{W}_r^\top \overline{\mathbf{W}_r}\right]\right)^{-1} \mathrm{Re}\left[\mathbf{W}_r^\top \overline{\mathbf{X}}\right]\right]$$

$$\mathbf{W}_{r+1} \leftarrow \Pi_{\mathbb{H}_{\mathcal{S}}}\left[\mathbf{X}\mathbf{H}_{r+1}^\top \left(\mathbf{H}_{r+1}\mathbf{H}_{r+1}^\top\right)^{-1}\right]$$

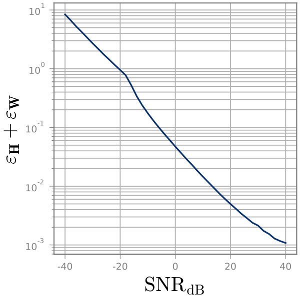
simple, efficient iterates with good practical performances despite no guarantee of convergence to a stationary point

Reconstruction error performance of Q-ALS

$$\mathbf{X} = \mathbf{W}_0\mathbf{H}_0 + \mathbf{N}, \quad N_{ij} \sim \mathcal{N}_{\mathbb{H}}(0, \sigma^2)$$

$P = 3$ sources, uniqueness checked exp.
100 independent runs for each SNR value,
30 iterations max. to converge

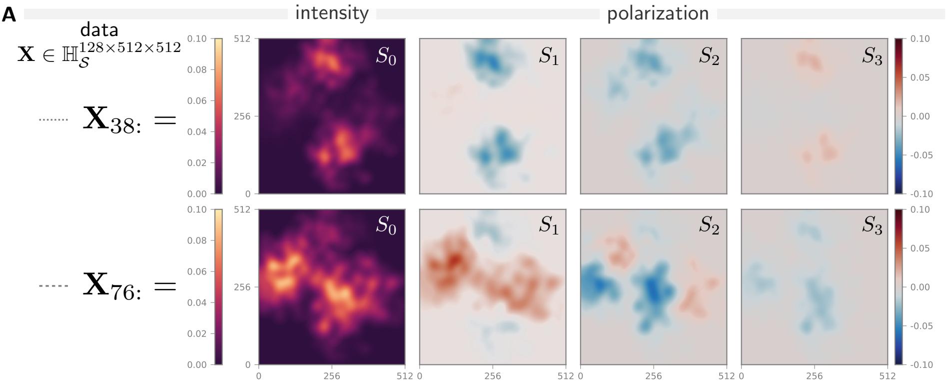
$$\varepsilon_{\mathbf{H}} = \|\hat{\mathbf{H}} - \mathbf{H}_0\|_2, \quad \varepsilon_{\mathbf{W}} = \|\hat{\mathbf{W}} - \mathbf{W}_0\|_2$$



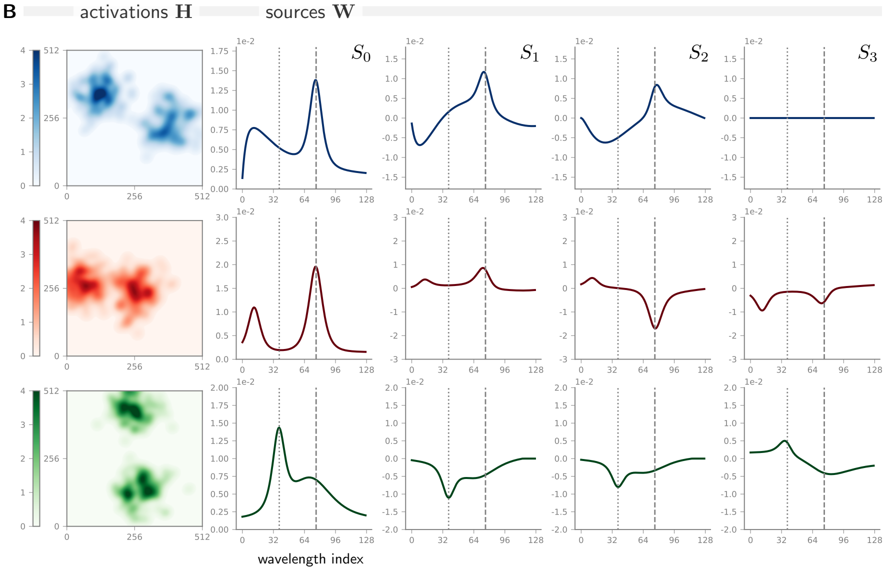
Simulation results

simulated spectro-polarimetric data $\mathbf{X}$ with $P = 3$ sources

512×512 spatial locations $\times$ 128 wavelengths $\times$ 4 Stokes parameters

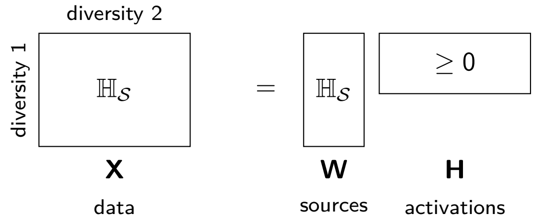


Simulation results



Take home message

QNMF $\mathbf{X} = \mathbf{WH}$



a new tool for low-rank approximations with Stokes data

✓very generic ✓broad unicity ✓simple algorithm

JF, SM, DB, 2020

Perspectives

- **Uniqueness**: sufficient conditions (w/ polarization) for $P \geq 2$
- **Algorithms**: polarization distances / regularizations,
- **Applications**: time-frequency-polarization source separation?

Outline

quaternion spectral representation
of bivariate signals

$$X(\nu) = \int \underbrace{x(t)}_{\in \mathbb{C}_{\boldsymbol{i}}} \underbrace{e^{-\boldsymbol{j}2\pi\nu t}}_{\in \mathbb{C}_{\boldsymbol{j}}} \mathrm{d}t \in \mathbb{H}$$

✓ general signal processing framework
✓ straightforward geometric and physical interpretations
✓ computationally efficient

- spectral analysis — TSP 2017
  random stationary signals · spectral densities · nonparametric spectral estimation
- linear time-invariant filtering — TSP 2018
  unitary/hermitian filters · Wiener filtering · original decompositions
- time-frequency analysis — ACHA 2017
  quaternion embedding · spectrograms · scalograms

+ `BiSPy Python toolbox`
+ QNMF for bivariate source separation

… but many more are yet to be explored

- simple parametric models are still lacking

  what is a basic, yet physically meaningful bivariate signal?

- new tools and models based on quaternion representations

  are quaternions sustainable in modern signal processing, i.e. compatible with constrained optimization problems or large scale Bayesian inference?

- exploiting the geometry of polarization to design meaningful priors / cost functions

  how to leverage the different geometric representations of polarization? (Poincaré sphere, PSD matrices, etc.)

- demonstrate the relevance of such a framework in challenging real-world applications

  GWs seismology underwater acoustics

Fortunately, we have RICOCHET !

thank you for your attention