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Wavelets and multiresolution : from NMR spectroscopy to motion analysis

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Wavelets and multiresolution : from NMR spectroscopy to motion analysis

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WARM-UP : WAVELET ANALYSIS OF 1D SIGNALS

Introduction

Traditional tool of signal processing : Fourier transform

$$s(x) \quad \leftrightarrow \quad \widehat{s}(\xi) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} e^{-i\xi x} s(x)\, \mathrm{d}x$$

- in principle, applies only to stationary signals
- but, in real life, signals are mostly nonstationary (e.g. finite duration)
- no time localization : when does the $\widehat{s}(\xi)$ component occur ?
- very uneconomical : (almost) flat signal (no information!) requires summation of infinite series or calculation of integral
- very unstable : tiny perturbation $\Rightarrow$ Fourier spectrum completely perturbed (FT is global)
- Conclusion : Fourier analysis is not sufficient, sometimes even misleading !

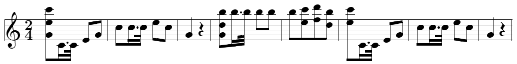
Time-frequency representation

- Solution : Time-frequency representation
- Two parameters are needed :
  - frequency : which one ? $\longleftarrow$ a
  - time : when ? $\longleftarrow$ b
- General linear time-frequency transform :

$$s(x) \mapsto S(b,a) = \int_{-\infty}^{\infty} \overline{\psi_{b,a}(x)}\, s(x)\, \mathrm{d}x,$$

where $\psi_{b,a}$ is the analyzing function.

- Example : Musical score !



A traditional time-frequency representation of a signal (from Mozart's Don Giovanni, Act 1)

- Popular solutions :
  - Windowed Fourier transform or Gabor transform
  - Wavelet transform

Three stages of WT

- Continuous WT (CWT)

$$S(b,a) = |a|^{-1/2} \int_{-\infty}^{\infty} \overline{\psi\left(\frac{x-b}{a}\right)}\, s(x)\,\mathrm{d}x, \quad a \neq 0,\ b \in \mathbb{R}$$

. a = scaling, b = translation
. all values of a and b : useful for feature detection (often $a > 0$)

- Discretization of CWT

. discretization needed for numerical implementation
. choice of sampling grid
. no orthonormal bases, only frames (redundant representation)

- Discrete WT (DWT)

. preselected grid (dyadic)
. (bi)orthonormal bases from multiresolution analysis
. good for data compression

- Note : (discretized) CWT incompatible with DWT, totally different philosophies
- Analogy :

CWT	⇔	Fourier integral
discretized CWT	⇔	Fourier series
DWT	⇔	discrete FT

The Continuous WT in 1-D

- Basic formulas

$$S(b,a) = \langle \psi_{b,a} | s \rangle = |a|^{-1/2} \int_{-\infty}^{\infty} \overline{\psi\left(\frac{x-b}{a}\right)}\, s(x)\,\mathrm{d}x$$

$$= |a|^{1/2} \int_{-\infty}^{\infty} \overline{\widehat{\psi}(a\xi)}\, \widehat{s}(\xi)\, e^{i\xi b}\,\mathrm{d}\xi$$

$a \neq 0$, $b \in \mathbb{R}$: time-scale plane $\mathbb{R}^2_*$ (often $a > 0$)

- Conditions on analyzing wavelet ψ

(i) $\psi,\ \widehat{\psi} \in L^2$

(ii) ψ admissible : $c_\psi \equiv 2\pi \int_{-\infty}^{\infty} \frac{|\widehat{\psi}(\xi)|^2}{|\xi|}\,\mathrm{d}\xi < \infty$

$\Rightarrow$ zero mean condition : $\widehat{\psi}(0) = 0 \iff \int_{-\infty}^{\infty} \psi(x)\,\mathrm{d}x = 0$

(iii) ψ and $\widehat{\psi}$ well localized : $\psi \in L^1 \cap L^2$ or better
$\Rightarrow$ good bandpass filtering in x and ξ

(iv) Vanishing moments: $\int_{-\infty}^{\infty} x^n\, \psi(x)\,\mathrm{d}x = 0,\ n = 0, 1, \ldots N$

$\Rightarrow$ ψ blind to polynomials of degree $\leqslant N$ (smooth part of signal)
$\Rightarrow$ better detection of singularities

(v) ψ progressive : $\widehat{\psi}$ real and $\widehat{\psi}(\xi) = 0$ for $\xi < 0$ (analytic signal)

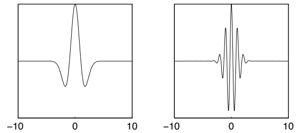
Two common wavelets

The Mexican hat wavelet

$$\psi_H(x) = (1 - x^2)\, e^{-\frac{1}{2}x^2}$$

$$\widehat{\psi}_H(\xi) = \xi^2\, e^{-\frac{1}{2}\xi^2}$$

. real
. admissible
. not progressive
. 2 vanishing moments $n = 0, 1$



(left) Mexican hat or Marr wavelet;
(right) Real part of the Morlet wavelet, for $\xi_o = 5.6$

The Morlet wavelet

$$\psi_M(x) = e^{i\xi_o x}\, e^{-x^2/2\sigma_o^2} + h(x)$$

$$\widehat{\psi}_M(\xi) = \sigma_o\, e^{-[(\xi - \xi_o)\sigma_o]^2/2} + \widehat{h}(\xi)$$

. complex
. admissible with correction term
. correction term negligible for $\sigma_o \xi_o \geqslant 5.5$
. not progressive

Localization properties and interpretation

- Localization properties :
  - $a \gg 1$ $\Rightarrow$ sensitive to low frequencies (rough analysis)
  - $a \ll 1$ $\Rightarrow$ sensitive to high frequencies (small details)
- Consequence :

WT = zero mean filter (convolution) + localization properties $\Rightarrow$

  - CWT = local filtering in time (b) and scale (a)

$$S(b,a) \not\approx 0 \iff \psi_{b,a}(x) \approx s(x)$$

  - CWT = mathematical microscope
    optics ψ, position b, magnification $1/a$
  - CWT works at constant relative bandwidth : $\Delta\xi/\xi$ = const

$\Rightarrow$ CWT = singularity detector and analyzer

Mathematical properties

For ψ admissible, the CWT $W_\psi : s(x) \mapsto S(b,a)$ is a linear map, with the following properties:

- Covariance under translation and dilation

$$W_\psi : s(x - x_o) \mapsto S(b - x_o, a)$$

$$W_\psi : \frac{1}{\sqrt{a_o}}\, s\left(\frac{x}{a_o}\right) \mapsto S\left(\frac{b}{a_o}, \frac{a}{a_o}\right)$$

- Energy conservation

$$\int_{-\infty}^{\infty} |s(x)|^2 \, \mathrm{d}x = c_\psi^{-1} \iint_{\mathbb{R}^2_*} |S(b,a)|^2 \, \frac{\mathrm{d}a\,\mathrm{d}b}{a^2}$$

$\Rightarrow$ $|S(b,a)|^2$ = energy density in half-plane

$\Longleftrightarrow$ W_ψ = isometry from space of signals $L^2(\mathbb{R})$ onto closed subspace $\mathcal{H}_\psi$ of $L^2(\mathbb{R}^2_*, \mathrm{d}a\,\mathrm{d}b/a^2)$ = space of transforms

$\Rightarrow$ W_ψ invertible on its range $\mathcal{H}_\psi$ by adjoint map, i.e.

Mathematical properties

- Reconstruction formula

$$s(x) = c_\psi^{-1} \iint_{\mathbb{R}^2_*} \psi_{b,a}(x)\, S(b,a)\, \frac{\mathrm{d}a\,\mathrm{d}b}{a^2}$$

$\Rightarrow$ linear superposition of wavelets $\psi_{b,a}$ with coefficients $S(b,a)$

- Projection $P_\psi : L^2(\mathbb{R}^2_*, \mathrm{d}a\,\mathrm{d}b/a^2) \to \mathcal{H}_\psi$ is an integral operator, with kernel

$$K(b', a'; b, a) = c_\psi^{-1} \langle \psi_{b',a'} | \psi_{b,a} \rangle$$

K = autocorrelation function of ψ, reproducing kernel

$\Rightarrow$ $f \in L^2(\mathbb{R}^2_*, \mathrm{d}a\,\mathrm{d}b/a^2)$ is the WT of a certain signal iff it satisfies the reproduction property

$$f(b', a') = c_\psi^{-1} \iint_{\mathbb{R}^2_*} \langle \psi_{b',a'} | \psi_{b,a} \rangle\, f(b,a)\, \frac{\mathrm{d}a\,\mathrm{d}b}{a^2}$$

$\Rightarrow$ the CWT is a highly redundant representation !

$\Rightarrow$ Full information contained is small subset of half-plane :

- Lines of local maxima : ridges = lines of local maxima
- Discrete subset $\Rightarrow$ frames

Applications of the 1D CWT - 1

Main usage : analyzing transient phenomena, detecting abrupt changes in a signal or comparing it with a given pattern

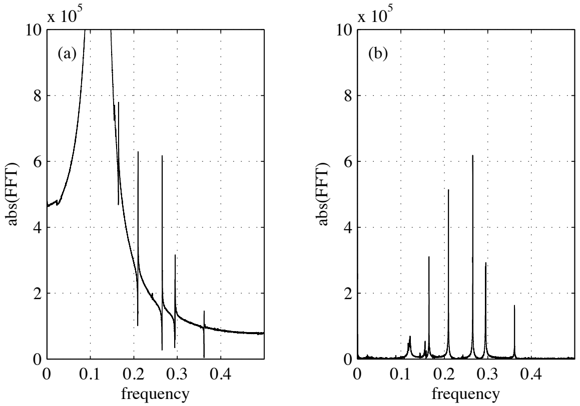
- Sound and acoustics
  musical synthesis, speech analysis, disentangling of an underwater refracted wave
- Geophysics, meteorology
  analysis of various long time series of geophysical origin: gravimetry, geomagnetism, astronomy (Solar physics), analysis of meteorological radar data . . .
- Fractals
  artificial (diffusion limited aggregates) or natural (arborescent growth phenomena) fractals
- Turbulence, fluid mechanics
  identification of coherent structures and hierarchical structure, detection of intermittency
- Atomic physics
  analysis of high order harmonic generation, controlled emission of ultrashort light pulses, in the 10^{-18}s (attosecond) range

Applications of the 1D CWT -2

- Spectroscopy
  subtraction of unwanted spectral lines or filtering out of background noise, e.g. in NMR spectroscopy
- Analysis of local singularities
  detection of singularities in a signal, fine characterization of their strengths
- Quantum cosmology
  wavelet quantization regularizes the gravitational singularity in a Friedmann-Lemaître universe
- Edge detection and shape characterization
  take contour of an object as a complex curve in the plane, then apply CWT
- Medical and biological applications
  analyzing or monitoring various electrical or mechanical phenomena in the brain (EEG, VEP), the heart (ECG) or the visual system, statistical analysis of correlations in DNA sequences
- Engineering and applied science
  monitoring of nuclear, electrical or mechanical installations (detection of anomalies)
- Economy
  detection of trends or correlations in data from financial markets

Application to NMR spectroscopy - 1

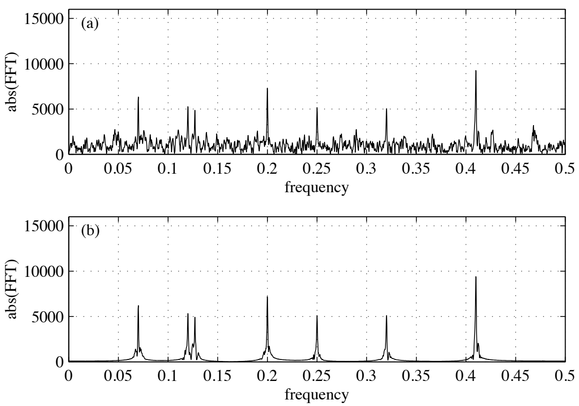
- Subtraction of an unwanted peak



(a) The original spectrum
(b) The spectrum reconstructed after subtraction of the water peak.

Application to NMR spectroscopy - 2

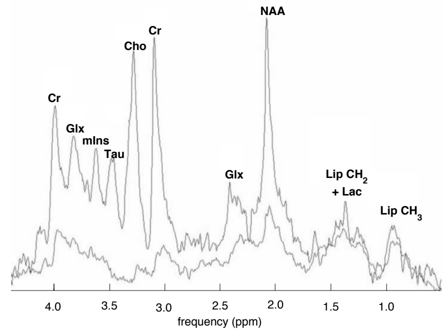
- Noise filtering



(a) The original spectrum
(b) The spectrum reconstructed after noise removal.

Application to NMR spectroscopy - 3

- Disentangling of metabolites



Signal: *In vivo* short-echo time MRS spectrum acquired at 4.7T in a mouse brain, superimposed on a measured *in vivo* macromolecular spectrum
Aim: to detect the presence of different metabolites and to measure their relative abundance

Application to NMR spectroscopy - 3

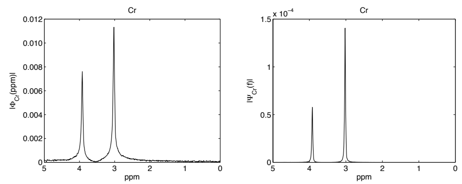
- Detecting the presence of a given metabolite in a mixture

Technique : design metabolite-based wavelets

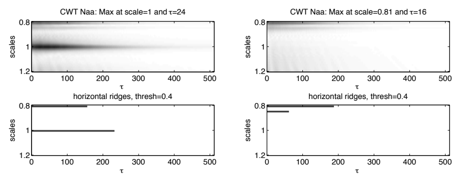
- Acquire profile $s(X)$ of a given metabolite X
- Autocorrelation of $s(X)$ = wavelet ψ_X adapted to the metabolite X
- Analyze composed signal with ψ_X
  - If CWT of $s(X)$ has a strong horizontal ridge at $a = 1 \Rightarrow X$ is present in the mixture
  - Otherwise $\Rightarrow X$ is not present in the mixture

- Examples

$s(Cr)$ ψ_{Cr}



ψ_{NAA} + signal with NAA

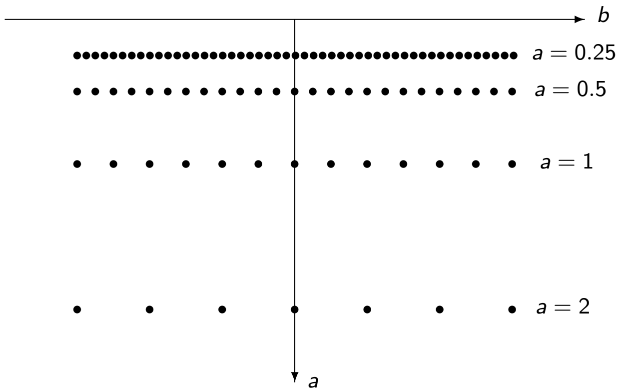


ψ_{NAA} + signal without NAA

Discretization of CWT

- CWT must be discretized for numerical implementation
- Choice of sampling grid: discrete lattice $\Gamma = \{a_j, b_{j,k}, j, k \in \mathbb{Z}\}$ yields good discretization if
$$s = \sum_{j,k\in\mathbb{Z}} \langle \psi_{jk}, s\rangle \widetilde{\psi}_{jk}$$
with $\psi_{jk} \equiv \psi_{b_{j,k},a_j}$ and $\widetilde{\psi}_{jk}$ explicitly constructible from ψ_{jk}
- Common choice : dyadic grid $a_j = 2^{-j}$, $b_{j,k} = k \cdot 2^{-j}$
$$\psi_{jk}(x) = 2^{j/2}\psi(2^j\, x - k), \quad j, k \in \mathbb{Z}$$
- Usually leads to frames, not bases

The dyadic lattice



The discrete WT (DWT)

- Multiresolution analysis of $L^2(\mathbb{R})$ = increasing sequence of closed subspaces
$$\ldots \subset V_{-2} \subset V_{-1} \subset V_0 \subset V_1 \subset V_2 \subset \ldots$$
with $\bigcap_{j\in\mathbb{Z}} V_j = \{0\}$ and $\bigcup_{j\in\mathbb{Z}} V_j$ dense in $L^2(\mathbb{R})$, and such that
  (1) $f(x) \in V_j \Leftrightarrow f(2x) \in V_{j+1}$
  (2) There exists a function $\phi \in V_0$, called a scaling function, such that the family $\{\phi(x-k), k \in \mathbb{Z}\}$ is an orthonormal basis of V_0.
  $\Rightarrow \{\phi_{jk}(x) \equiv 2^{j/2}\phi(2^j x - k), k \in \mathbb{Z}\}$ = orthonormal basis of V_j
- Define the spaces W_j by the relation $V_j \oplus W_j = V_{j+1}$
  - V_j = approximation space at resolution 2^j (at level j)
  - W_j = additional details 2^j to 2^{j+1} (called wavelet spaces)
$$\Rightarrow\ L^2(\mathbb{R}) = \bigoplus_{j\in\mathbb{Z}} W_j = V_{j_o} \oplus \left(\bigoplus_{j=j_o}^{\infty} W_j\right) \qquad (j_o = \text{lowest resolution level})$$
- Main result : $\exists$ function ψ, explicitly computable from ϕ, such that
$$\{\psi_{jk}(x) \equiv 2^{j/2}\psi(2^j x - k), j \in \mathbb{Z}\} = \text{orthonormal basis of } W_j$$
$$\{\psi_{jk}(x) \equiv 2^{j/2}\psi(2^j x - k), j, k \in \mathbb{Z}\} = \text{orthonormal basis of } L^2(\mathbb{R})$$
  $\Rightarrow$ orthonormal wavelets
- Examples : Haar wavelets, B-splines, Daubechies wavelets

Discretized CWT vs. DWT

- Question: CWT (discretized) or DWT?
- Answer: Depends on the application
  - CWT for feature detection (no *a priori* choice for a, b) : more flexible, more robust to noise, but only frames in general
  - DWT for large amount of data, data compression : bases, faster, but more rigid (need generalizations)
- Generalizations
  - Biorthogonal wavelets
  - Wavelet packets
  - Continuous wavelet packets (integrated wavelets)
  - Redundant WT (on a rectangular lattice)
  - "Second generation" wavelets (lifting scheme)

WAVELET ANALYSIS OF 2D IMAGES

Wavelet analysis of 2D images- 1

- Geometric transformations in the plane $\mathbb{R}^2$:

  (i) translation by $\vec{b} \in \mathbb{R}^2 : \vec{x} \mapsto \vec{x}' = \vec{x} + \vec{b}$

  (ii) dilation by a factor $a > 0 : \vec{x} \mapsto \vec{x}' = a\vec{x}$

  (iii) rotation by an angle $\theta : \vec{x} \mapsto \vec{x}' = r_\theta(\vec{x})$

$$r_\theta \equiv \begin{pmatrix} \cos\theta & -\sin\theta \\ \sin\theta & \cos\theta \end{pmatrix}, \; 0 \leqslant \theta < 2\pi, \text{ rotation matrix}$$

- Action on finite energy signals

$$\left[U(\vec{b}, a, \theta)s\right](\vec{x}) \equiv s_{\vec{b},a,\theta}(\vec{x}) = a^{-1} s(a^{-1}\, r_{-\theta}(\vec{x} - \vec{b}))$$

Wavelet analysis of 2-D images - 2

- Basic formulas for CWT : from CS formalism, as in 1-D

$$S(\vec{b}, a, \theta) = \langle \psi_{\vec{b},a,\theta} | s \rangle = a^{-1} \int_{\mathbb{R}^2} \overline{\psi(a^{-1}\, r_{-\theta}(\vec{x} - \vec{b}))}\, s(\vec{x})\, d^2\vec{x}$$
$$= a \int_{\mathbb{R}^2} e^{i\vec{b}\cdot\vec{k}}\, \overline{\widehat{\psi}(a r_{-\theta}(\vec{k}))}\, \widehat{s}(\vec{k})\, d^2\vec{k}$$

- Admissibility of wavelet ψ : $\quad c_\psi \equiv (2\pi)^2 \int_{\mathbb{R}^2} \frac{|\widehat{\psi}(\vec{k})|^2}{|\vec{k}|^2}\, d^2\vec{k} < \infty$

- Necessary condition : $\widehat{\psi}(\vec{0}) = 0 \iff \int_{\mathbb{R}^2} \psi(\vec{x})\, d^2\vec{x} = 0.$

- Energy conservation

$$c_\psi^{-1} \iiint_{\mathrm{SIM}(2)} |S(\vec{b}, a, \theta)|^2\, d^2\vec{b}\, \frac{da}{a^3}\, d\theta = \int_{\mathbb{R}^2} |s(\vec{x})|^2\, d^2\vec{x}$$

  i.e., isometry from space of signals $L^2(\mathbb{R}^2)$ onto closed subspace of $L^2(\mathrm{SIM}(2))$ = space of wavelet transforms

- Reconstruction formula

  Inversion of CWT by adjoint map :

$$s(\vec{x}) = c_\psi^{-1} \iiint_{\mathrm{SIM}(2)} \psi_{\vec{b},a,\theta}(\vec{x})\, S(\vec{b}, a, \theta)\, d^2\vec{b}\, \frac{da}{a^3}\, d\theta$$

  i.e., decomposition of the signal in terms of the analyzing wavelets $\psi_{\vec{b},a,\theta}$, with coefficients $S(\vec{b}, a, \theta)$

Wavelet analysis of 2-D images - 3

- Reproduction property (reproducing kernel)

$$S(\vec{b}', a', \theta') = c_\psi^{-1} \iiint_{\mathrm{SIM}(2)} \langle \psi_{\vec{b}',a',\theta'} | \psi_{\vec{b},a,\theta} \rangle\, S(\vec{b}, a, \theta)\, d^2\vec{b}\, \frac{da}{a^3}\, d\theta$$

- WT is covariant under translations, dilations and rotations : the correspondence $W_\psi : s(\vec{x}) \mapsto S(\vec{b}, a, \theta)$ implies the following ones

$$\begin{aligned} s(\vec{x} - \vec{b}_o) &\mapsto S(\vec{b} - \vec{b}_o, a, \theta) \\ a_o^{-1} s(a_o^{-1}\vec{x}) &\mapsto S(a_o^{-1}\vec{b}, a_o^{-1} a\theta) \\ s(r_{\theta_o}(\vec{x})) &\mapsto S(r_{-\theta_o}(\vec{b}), a, \theta - \theta_o) \end{aligned}$$

- Note: translation covariance ("shift invariance") is lost in the standard formulation of the discrete WT, based on multiresolution

  ⇒ problems in pattern recognition, e.g.

- Interpretation of CWT : exactly as in 1-D
  - localization properties of ψ + convolution with zero mean function ⇒ local filtering in $\vec{b}, a, \theta$

    ⇒ CWT = mathematical directional microscope

    (optics ψ, global magnification $1/a$, orientation tuning parameter θ)

Localization properties and interpretation

- support properties of $\psi \Rightarrow$ analysis with constant relative bandwidth: $\Delta k/k =$ const, $\quad k = |\vec{k}|$

  $\Rightarrow$ analysis is most efficient at high spatial frequencies or small scales

  $\Rightarrow$ good detection of discontinuities in images :

  . point singularities (contours, corners)

  . directional features (edges, segments) . . .).

  $\Rightarrow$ CWT = detector and analyzer of singularities

  (edges, contours, corners, . . .)

- Possible additional requirements :
  - restrictions on the support of ψ and of $\widehat{\psi}$
  - vanishing moments, up to order $N \geqslant 1$ ($N = 0$: admissibility) :

$$\int d^2\vec{x}\, x^\alpha\, y^\beta\, \psi(\vec{x}) = 0, \quad \vec{x} = (x, y), \quad 0 \leqslant \alpha + \beta \leqslant N$$

  $\Rightarrow$ improved efficiency at detecting singularities in the signal : transform is blind to smoothest part of the signal,i.e., polynomial of degree up to N (less interesting, in general)

  Example : if $N = 1$, the transform erases any linear trend in the signal, such as a linear gradient of luminosity

Group-theoretical justification in one dimension

- Dilation + translation = affine transformation of the line

$$y = (b, a)x \equiv ax + b, \quad a \neq 0, \; b \in \mathbb{R}, \; x \in \mathbb{R}$$

- Composition rule : $(b, a)(b', a') = (b + ab', aa')$

  $\Rightarrow \{(b, a)\} \equiv G_{\rm aff} \simeq \mathbb{R}^2_* =$ affine group

- Action of (b, a) on the signal : $\psi \mapsto U(b, a)\psi$

$$(U(b, a)\psi)(x) = |a|^{-1/2}\psi\left(\frac{x-b}{a}\right) \qquad (*)$$

  and U = unitary irreducible representation of $G_{\rm aff}$ in $L^2(\mathbb{R})$

- U is square integrable

$$\psi \text{ admissible} \iff \iint_{G_{\rm aff}} |\langle U(b, a)\psi|\psi\rangle|^2 \, \frac{{\rm d}b\,{\rm d}a}{a^2} < \infty$$

- Note : Restricting to $a > 0$, one gets the connected affine group $G^+_{\rm aff}$ (or $ax + b$ group) and $(*)$ is a UIR of it in $L^2(\mathbb{R}^+)$

In two dimensions

- Dilations + translations + rotations

  = similitude group of the plane : SIM(2) $= \mathbb{R}^2 \rtimes (\mathbb{R}^+_* \times {\rm SO}(2))$

$$\vec{y} = (\vec{b}, a, \theta)\vec{x} \equiv a r_\theta \vec{x} + \vec{b},$$

- Action on finite energy signals

$$\left[U(\vec{b}, a, \theta)s\right](\vec{x}) = a^{-1}s(a^{-1}\, r_{-\theta}(\vec{x} - \vec{b}))$$

  and U = unitary irreducible representation of SIM(2) in $L^2(\mathbb{R}^2)$

- U is square integrable

$$\psi \text{ admissible} \iff \iiint_{{\rm SIM}(2)} \left|\langle U(\vec{b}, a, \theta)\psi|\psi\rangle\right|^2 \, d^2\vec{b}\,\frac{da}{a^3}\, d\theta < \infty$$

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