Sparse modal estimation of 2-D NMR signals

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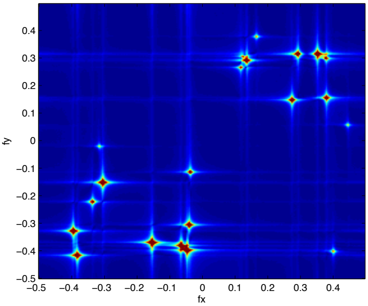
Modal estimation of 2-D NMR signals



– 2-D NMR spectroscopy
$\Rightarrow$ detection of complex chemical interactions
$\Rightarrow$ study of macromolecules

– Superposition of 2-D damped complex sinusoids (2-D case)

– Amplitude spectrum $\Rightarrow$ superposition of 2-D Lorentzian peaks

– Modal estimation : determination of the 2-D frequencies and dampings

– TLS-Prony, MEMP, 2-D Esprit, IMDF

Sparse approximation approach for modal estimation

- Sparse approximations for 1-D modal estimation [Goodwin1999, Malioutov 2005, Stoica 2011]
- (Very) high resolution $\Rightarrow$ (Very) large dictionary
- [Sahnoun 2012] : multigrid sparse approximation $+$ R-D extension
  1-D case : very effective approach (accuracy, computation cost)
  $R \geq 2$: computational burden is untractable for large signals (dictionary size)

How to process large size signals ?

- Same idea as TLS-Prony, MEMP
- 2-D estimation $= 2 \times 1$-D estimation $+$ mode pairing

2-D modal signal model

Superposition of 2-D exponentially decaying sinusoids in noise

$$y(m_1, m_2) = \sum_{i=1}^{F} c_i a_i^{m_1-1} b_i^{m_2-1} + e(m_1, m_2)$$

with :

- Number of sample $m_1 = 1, \ldots, M_1$ (1st dimension), $m_2 = 1, \ldots, M_2$ (2nd dimension)
- Modes : $a_i = e^{-\alpha_{a,i}+j2\pi f_{a,i}}$ (1st dimension), $b_i = e^{-\alpha_{b,i}+j2\pi f_{b,i}}$ (2nd dimension)
- Complex amplitudes $\{c_i\}_{i=1}^{F}$
- Noise $e(m_1, m_2)$

Matrix form

$\mathbf{Y}$ noise-free data matrix containing the samples $y(m_1, m_2)$

$$\mathbf{Y} = [\mathbf{y}_1, \mathbf{y}_2, \cdots, \mathbf{y}_{M_2}] = \left[\sum_{i=1}^{F} c_i \mathbf{a}_i \quad \sum_{i=1}^{F} c_i b_i \mathbf{a}_i \quad \cdots \quad \sum_{i=1}^{F} c_i b_i^{M_2-1} \mathbf{a}_i \right]$$

with $\mathbf{a}_i = [1, a_i, \ldots, a_i^{M_1-1}]^T$. Defining $\mathbf{h}_i = [c_i, c_i b_i, \cdots, c_i b_i^{M_2-1}]$

$$\mathbf{Y} = [\mathbf{a}_1 \cdots \mathbf{a}_F][\mathbf{h}_1 \cdots \mathbf{h}_F]^T = \mathbf{A}\mathbf{H}_b$$

Noisy data :

$$\mathbf{Y} = \mathbf{A}\mathbf{H}_b + \mathbf{E}$$

Important remark :

$$\mathbf{Y}^T = \mathbf{B}\mathbf{H}_a + \mathbf{E}^T$$

A last writing :

$$\mathbf{Y} = \mathbf{A} \; diag(\mathbf{c}) \; \mathbf{B}^T + \mathbf{E}$$

Sparse approximation

For each column of the data matrix $\mathbf{y}_{m_2}, m_2 = 1, \ldots, M_2$,

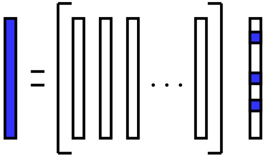
Dictionnary $\mathbf{Q}_a$

- $\mathbf{a}(\alpha, f) = [1, e^{(-\alpha+j2\pi f)}, \ldots, e^{(-\alpha+j2\pi f)(M_1-1)}]^T$
- $\mathbf{q}(\alpha, f) = \mathbf{a}(\alpha, f)/||\mathbf{a}(\alpha, f)||_2$
- Discretization of the (α, f) plane

Sparse modal estimation

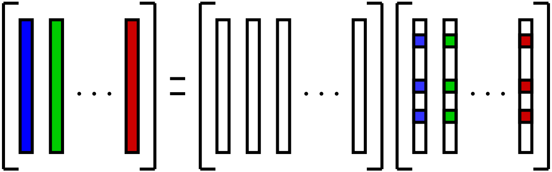
$$\mathbf{x}_{m_2} = \min_{\mathbf{x}} \|\mathbf{x}\|_0$$

$$\text{subject to} \quad \|\mathbf{y}_{m_2} - \mathbf{Q}_a\mathbf{x}\|_2^2 \leq \epsilon$$



Simultaneous sparse approximation

Each column of the data matrix is a 1-D signal generated by the **same modes** but with **different amplitudes** $\Rightarrow$ **Simultaneous sparse approximation**



$$\min_{\mathbf{X}} \|\mathbf{X}\|_{2,0} \quad \text{subject to} \quad \|\mathbf{Y} - \mathbf{Q}_a\mathbf{X}\|_f^2 \leq \epsilon$$

where

$$\|\mathbf{Y} - \mathbf{Q}_a\mathbf{X}\|_f^2 = \|\text{vec}(\mathbf{Y} - \mathbf{Q}_a\mathbf{X})\|_2^2$$
$$\|\mathbf{X}\|_{2,0} = \left\| \begin{bmatrix} \|\mathbf{X}[1,:]\|_2 & \cdots & \|\mathbf{X}[N,:]\|_2 \end{bmatrix}^T \right\|_0$$

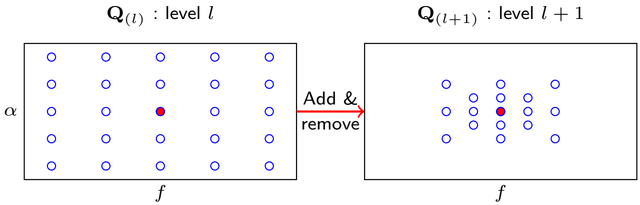
and $\mathbf{X}[n,:]$ stands for the nth row of $\mathbf{X}$.

Algorithm : Simultaneous OMP [Tropp 2006]

Multigrid dictionary

High-resolution modal estimation

- high resolution dictionary ⇒ prohibitive computational burden.
- multi-grid scheme [Sahnoun2012]
- signal dependent dictionary



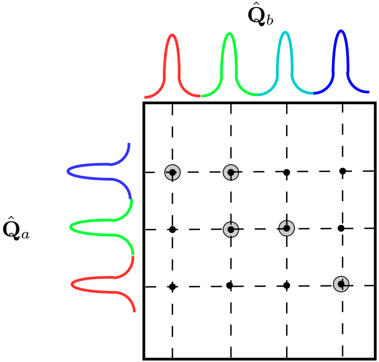
Mode pairing

Simultaneous sparse approximations

$$\mathbf{Y} \Rightarrow \hat{\mathbf{Q}}_a = [\hat{\mathbf{a}}_1, \hat{\mathbf{a}}_2, \dots, \hat{\mathbf{a}}_{F_a}]$$
$$\mathbf{Y}^T \Rightarrow \hat{\mathbf{Q}}_b = [\hat{\mathbf{b}}_1, \hat{\mathbf{b}}_2, \dots, \hat{\mathbf{b}}_{F_b}]$$

Low dimension dictionary

$$\hat{\mathbf{Q}} = \hat{\mathbf{Q}}_a \otimes \hat{\mathbf{Q}}_b.$$



Selection of the pairs of 2-D modes ⇒ sparse approximation

$$\min_{\mathbf{x}} \|\mathbf{x}\|_0 \quad \text{subjet to} \quad \|\mathbf{y} - \hat{\mathbf{Q}}\mathbf{x}\|^2 \leq \epsilon.$$

Greedy algorithm : OMP, SBR

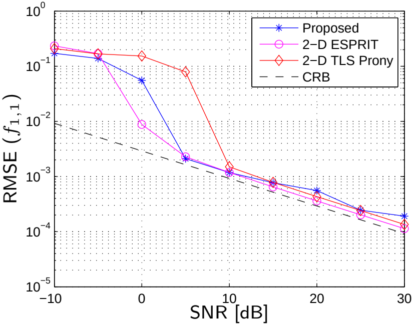
Algorithm summary

1. Perform the SVD of $\mathbf{Y}$ and take its low rank approximation
2. Apply the multi-grid algorithm combined with S-OMP on matrix $\mathbf{Y}$ to obtain the modes a_i (first dimension)
3. Repeat step 2 using $\mathbf{Y}^T$ to estimate the modes b_i (second dimension)
4. Form the 2-D modes using the pairing procedure

Numerical simulations

Comparison with 2-D ESPRIT and TLS-Prony

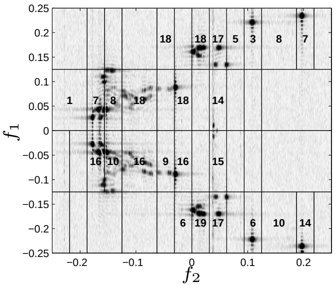
- Signal size 30×30
- 3 modes
- Initial dictionary : 40 frequency points uniformly distributed over the interval $[0, 1[$, and 4 damping factors $\alpha \in \{0, 0.025, 0.05, 1\}$
- 30 levels of resolution

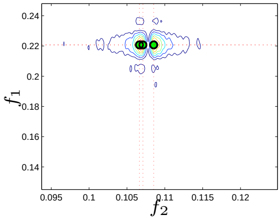


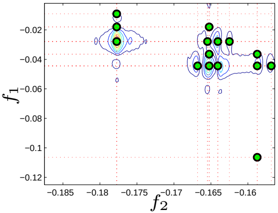
Accuracy similar to 2D-ESPRIT
Lower computational burden than TLS-Prony
$\Rightarrow$ processing of large signals possible

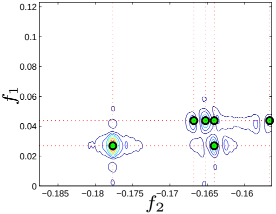
2-D NMR signal analysis

- Signal size 64×2024
- Sub-bands decomposition [Djermoune 2008]
- Same setting for Multigrid S-OMP









Conclusions

- Sparse modal estimation adapted to large signals
- Performances similar to 2D-ESPRIT
- Computation time lower than TLS-Prony
- Application to other NMR modalities
- Extension to the $R > 2$ case