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# TWO-DIMENSIONAL NMR SIGNAL ANALYSIS
# WITH AN ADAPTED SUBBAND
# DECOMPOSITION

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Abstract: This paper presents a methodology allowing to estimate the parameters of two-dimensional damped/undamped sinusoids from high complexity noisy signals, which is the case in 2-D nuclear magnetic resonance spectroscopy. The proposed approach performs an adaptive subband decomposition combined with a classical frequency estimator based on the Prony model. At each node resulting from the decomposition, a stopping rule is computed in order to decide whether the decomposition must be continued or not. The rule is a measure of flatness of residuals resulting from the estimation step. The method is demonstrated using simulated signals.

Keywords: Magnetic resonance spectroscopy, subband decomposition, 2-D frequency estimation, subspace methods.

## 1. INTRODUCTION

Since the discovery in 1945 of the magnetic resonance spectroscopy (NMR) phenomenon, this technique became a powerful and very successful tool to study structures and molecular interactions Canet et al. [2002]. The multidimensional NMR has widened the field of investigation to the study of macromolecules structures by allowing the detection and interpretation of interactions which are impossible to analyze along a single dimension (see e.g. Bax and Lerner [1986], Bax [1985], Canet et al. [2002]).

In this paper, we consider the problem of estimating the parameters of two-dimensional NMR signals modeled as a sum of two-dimensional damped exponentials (also called modes or resonances). For this issue, several high-resolution methods have been developed such as 2-D IQML in Clark and Scharf [1994], 2-D MUSIC in Li et al. [1998], TLS-Prony by Sacchini et al. [1993], Matrix Pencil by Hua [1992], etc. Nevertheless, whatever the method is used, its numerical implementation is problematical. Indeed, in the case of high complexity signals (large number of samples and/or modes), the algorithms have to handle with very large matrices that must be inverted and with possible large order polynomial rooting, resulting in prohibitive calculation cost and memory capacities requested. So, in such cases it is preferable to perform a subband decomposition before the estimation process itself. This enables one to transform a complex estimation problem into a set of subproblems, each much simpler and more favorable from a numerical point of view since the estimation is focused on small spectral regions. Moreover, it is known that such decomposition procedures may enhance the performances

of the spectral estimator used (e.g. Quirk and Liu [1983], Rao and Pearlman [1996]). The purpose of this work is to present a subband decomposition approach combined with a frequency estimator, suitable to the analysis of two-dimensional damped/undamped sinusoidal signals. This technique is a generalization from 1-D to 2-D of the approach proposed in Djermoune et al. [2004].

The paper is organized as follows. In the next section, the model of a 2-D NMR signal is given, together with an estimation technique. In section 3, we describe the proposed approach based on an adaptive subband decomposition. This method is then demonstrated in section 4 by using simulation signals. Finally, conclusions are given in section 5.

## 2. SIGNAL MODELING AND PARAMETER ESTIMATION

The model of the signals considered here is a combination of a certain number $I$ of two-dimensional distinct damped complex exponentials, also called resonances in NMR spectroscopy:

$$d(n, m) = \sum_{i=1}^{I} h_i z_i^n w_i^m + e(n, m), \qquad (1)$$

for $n = 0, ..., N - 1$ and $m = 0, ..., M - 1$. Here, $z_i = \exp(-\alpha_i^x + j\omega_i^x)$ and $w_i = \exp(-\alpha_i^y + j\omega_i^y)$ are the components of the mode $(z_i, w_i)$ with amplitude $h_i$ ($\alpha_i^x \geqslant 0$ and $\alpha_i^y \geqslant 0$). The error term $e(n, m)$ is representative of measurement noise. It is assumed to be spatially and temporally uncorrelated. The problem is to estimate the number of modes $I$ and the set of parameters $\{z_i, w_i, h_i\}_{i=1}^{I}$, given the noisy measurements $d(n, m)$.

There are several methods that may be used to solve this problem. Most of them are derived from the well known one-dimensional Prony method which is a linear prediction-based technique. The reader is referred to Ying et al. [1996] and the references therein for performance comparison between some of these methods. Without loss of generality, here we choose to use the 2-D TLS-Prony method developed in Sacchini et al. [1993] and which is now briefly recalled.

The starting point of the TLS-Prony method is the following form of equation (1) Sacchini et al. [1993]:

$$d(n, m) = \sum_{k=1}^{K} \sum_{l=1}^{L_k} a_{k,l} p_{x_k}^n p_{y_{k,l}}^m + e(n, m) \qquad (2)$$

$$= \sum_{k=1}^{K} c_{k,m} p_{x_k}^n + e(n, m), \qquad (3)$$

where

$$c_{k,m} = \sum_{l=1}^{L_k} a_{k,l} p_{y_{k,l}}^m, \qquad (4)$$

$p_{x_k}$ is the $k$th $x$-mode ($x$-component of 2-D exponential), $p_{y_{k,l}}$ is the $k, l$th $y$-mode, $a_{k,l}$ is the $k, l$th amplitude coefficient and $L_k$ is the number of $y$-modes corresponding to the $k$th $x$-mode. In order to estimate the 2-D signal parameters, the idea is to perform a set of 1-D estimation procedures using equations (3) and (4). Indeed, it is clear from equation (3) that the sequence obtained for a fixed value of $m$ is a 1-D exponential signal whose parameters may be estimated with a 1-D high-resolution technique.

The TLS-Prony algorithm for 2-D frequency estimation in Sacchini et al. [1993] consists in the following four steps.

(1) Using Eq. (3), form the backward linear prediction system given in Eq. (6), where $p \geqslant K$ is the prediction order. By performing the singular value decomposition (SVD) of the matrix $S$, one can estimate the number of $x$-modes $\hat{K}$ using a theoretical information criterion, such as MDL or AIC (see Wax and Kailath [1985]). Then, Eq. (6) should be solved in the total least squares (TLS) sense Rahman and Yu [1987] with an SVD truncation to obtain $\hat{b}$. Finally, the estimated $x$-modes are found by

$$\hat{p}_{x_k} = \frac{1}{\text{zero}_k(\hat{B}(z))}, \quad k = 1, 2, ..., \hat{K}, \quad (5)$$

where $B(z) = 1 + b_1 z + ... + b_p z^p$ (the $p - \hat{K}$ zeros of $\hat{B}(z)$ lying inside the unit circle must be discarded).

(2) For each time index $m = 0, ..., M - 1$, compute the $x$-amplitude coefficients $\hat{c}_{k,m}$ in the least squares sense using Eq. (3) and the estimated modes $\hat{p}_{x_k}$.

(3) For each $x$-mode $\hat{p}_{x_k}$, $k = 1, ..., \hat{K}$, obtain the corresponding $\hat{L}_k$ $y$-modes $\hat{p}_{y_{k,l}}$ from Eq. (4) using once again the 1-D TLS-Prony approach (here the prediction equations are made over the $m$ index, for a fixed $k$).

(4) Compute the amplitude coefficients $\hat{a}_{k,l}$ for $k = 1, ..., \hat{K}$ by solving the set of Vandermonde equations obtained from Eq. (4) in the least squares sense.

Finally, the 2-D signal parameters $(\hat{z}_i, \hat{w}_i)$ with amplitudes $\hat{h}_i$ correspond to the set of couples $(\hat{p}_{x_k}, \{\hat{p}_{y_{k,l}}\}_{l=1}^{\hat{L}_k})$ with amplitudes $\{\hat{a}_{k,l}\}_{l=1}^{\hat{L}_k}$. The total number of estimated modes is then:

$$\hat{I} = \sum_{k=1}^{\hat{K}} \hat{L}_k. \qquad (7)$$

Generally speaking, the use of the so-called high-resolution techniques to estimate the parameters

$$
\begin{bmatrix}
d(0,0) & d(1,0) & \cdots & d(p,0) \\
d(1,0) & d(2,0) & \cdots & d(p+1,0) \\
\vdots & \vdots & & \vdots \\
d(N-p-1,0) & d(N-p,0) & \cdots & d(N-1,0) \\
\hline
d(0,1) & d(1,1) & \cdots & d(p,1) \\
d(1,1) & d(2,1) & \cdots & d(p+1,1) \\
\vdots & \vdots & & \vdots \\
d(N-p-1,1) & d(N-p,1) & \cdots & d(N-1,1) \\
\hline
\vdots & & & \\
\hline
d(0,M-1) & d(1,M-1) & \cdots & d(p,M-1) \\
d(1,M-1) & d(2,M-1) & \cdots & d(p+1,M-1) \\
\vdots & \vdots & & \vdots \\
d(N-p-1,M-1) & d(N-p,M-1) & \cdots & d(N-1,M-1)
\end{bmatrix}
\begin{bmatrix} 1 \\ b_1 \\ \vdots \\ b_p \end{bmatrix} \approx 0 \Rightarrow S \begin{bmatrix} 1 \\ b \end{bmatrix} \approx 0. \qquad (6)
$$

of a 2-D signal leads to good performances in terms of resolution as compared to that obtained with the classical Fourier transform. Unfortunately, when the number of measurements and/or the number of the signal parameters are large, it is often difficult to take advantage of these performances because of implementation problems. For instance, the dimension of matrix $S$ in Eq. (6) is approximately $N.M \times p$, which is directly proportional to the number of samples ($N$ or $M$) and the number of parameters expressed by the prediction order $p$. So it is clear that, in this case, it becomes necessary to reduce the underlaying problem complexity by using some separation techniques such as subband decomposition.

## 3. SUBBAND DECOMPOSITION

The concept of subband decomposition is used in various fields of investigation. In the particular domain of spectral analysis, the advantages of a subband decomposition approach, have been emphasized by several authors Steedly et al. [1994], Rao and Pearlman [1996], Tkacenko and Vaidyanathan [2001], Djermoune et al. [2004]. This idea enables to transform a complex estimation problem into a set of sub-problems, each being much simpler than the original.

The decomposition being achieved classically through filtering and decimation stages, the problem which arises is about the endpoint of the decomposition. At first, a tradeoff must be reached between two alternatives. To improve frequency resolution, it is necessary to increase the decimation factor, but the number of data samples reduces as the decimation gets deeper. Secondly, it would be desirable to stop the decomposition as soon as all the information is retrieved. These remarks suggest to use adaptive forms of decomposition rather than simple uniform ones. In this case, the decimation is carried out according to the spectral content of the subbands encountered, but the problem is

then to establish a stop-criterion that determines an optimal decomposition tree (in some sense).

For instance, in van den Branden Lambrecht and Karrakchou [1995], the selection of the optimal decomposition is made by maximizing the number of modes over the whole decomposition tree. The number of modes lying in some band being unknown, it has to be estimated using, say, the minimum description length (MDL) criterion Wax and Kailath [1985]. The problem which arises with such an approach is that it does not ensure that all the spectral information has been retrieved, because order criteria are not always reliable. As an alternative, we propose to use a stop-criterion that reflects the quality of the estimation in a given subband, that is a measure of whiteness of the corresponding residuals. Unlike adaptive decompositions using order criteria, the decision about stopping or following up the decomposition is made after the estimation process. This allows one to minimize the number of possible missed components.

### 3.1 Decomposition of a 2-D signal

The subband decomposition is achieved by successive filtering and decimation stages as illustrated in figure 1. In each subband (node), the model of the 2-D signal is still a sum of a (reduced) number of modes which can be estimated by the TLS-Prony method presented in the previous section.

Let $d'(n,m)$ be the sub-signal corresponding to a given node in the decomposition tree, constituted of $I'$ 2-D damped exponentials:

$$d'(n,m) = \sum_{i=1}^{I'} h'_i z_i'^n w_i'^m + e'(n,m). \qquad (8)$$

Assume that $\hat{I}'$ modes are detected and estimated by the TLS-Prony approach, and define the estimation residuals by the difference between the true sub-signal and the reconstructed one:
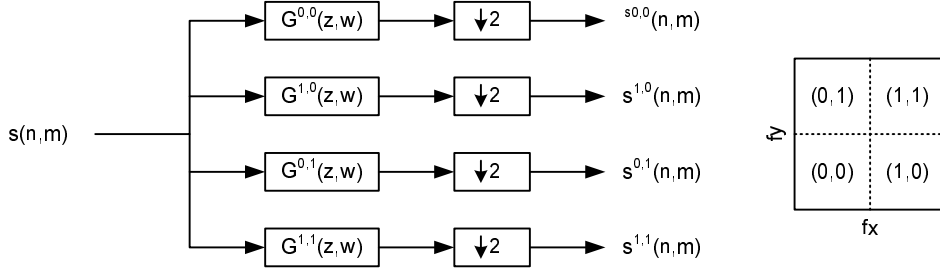
Fig. 1. Principle of decomposition of a 2-D signal $s(n, m)$ into four subbands. $G^{i,k}(z, w)$ are the frequency responses of bandpass filters.

$$r(n, m) = d'(n, m) - \sum_{i=1}^{\hat{I}'} \hat{h}'_i \hat{z}'^n_i \hat{w}'^m_i. \qquad (9)$$

for $n = 0, ..., N' - 1$ and $m = 0, ..., M' - 1$. Ideally, if all subband modes are correctly retrieved (i.e. $\hat{I}' = I'$), the residuals are close to a white noise. If one or more modes are missed, then the signal $r(n, m)$ is no more white. The stopping rule described below is based on this observation.

### 3.2 The measure of spectral flatness

The stopping rule of the decomposition is based on the measure of whiteness of the subband residuals. Assume that $r(n, m)$ is a wide sense stationary Gaussian sequence. Its power spectral density is estimated by the periodogram defined by:

$$\hat{P}'(\omega_1, \omega_2) =$$

$$\frac{1}{N'M'} \left| \sum_{n=0}^{N'-1} \sum_{m=0}^{M'-1} r(n, m) e^{-jn\omega_1} e^{-jm\omega_2} \right|^2. \qquad (10)$$

The test of whiteness developed in Drouiche [2000] is a spectral flatness measure of a 1-D sequence. If we denote by $\hat{Q}(\omega)$ the periodogram of a 1-D sequence of length $L$, then the measure of whiteness is defined by:

$$\hat{W} = \log \frac{1}{2\pi} \int_{-\pi}^{\pi} \hat{Q}(\omega) d\omega$$
$$- \frac{1}{2\pi} \int_{-\pi}^{\pi} \log \hat{Q}(\omega) d\omega - \gamma, \qquad (11)$$

where $\gamma = 0.57721$ denotes the Euler constant. It can be shown that $\hat{W} \approx 0$ for a white noise and $\hat{W} \rightarrow \infty$ if the sequence is maximally correlated. In practice, we reject the whiteness hypothesis if $\hat{W} > t_\alpha$, where $t_\alpha$ is a threshold obtained using a false alarm rate $\alpha$:

$$t_\alpha = \frac{\sqrt{2}\nu_0}{\sqrt{L}} \text{erf}^{-1}(1 - 2\alpha), \qquad (12)$$

where $\nu_0 = \sqrt{\pi^2/6 - 1}$, and $\text{erf}^{-1}(x)$ is the inverse of the standard error function

$$\text{erf}(x) = \frac{2}{\sqrt{\pi}} \int_0^x e^{-t^2} dt. \qquad (13)$$

Table 1. Parameters of signal 1.

| $i$ | 1 | 2 | 3 | 4 | 5 | 6 | 7 |
|---|---|---|---|---|---|---|---|
| $f_i^x$ | -.15 | -.15 | .10 | .10 | .15 | .40 | .40 |
| $f_i^y$ | -.10 | .10 | .10 | .40 | .08 | .20 | .40 |
| $\alpha_i^x$ | .05 | .05 | .05 | .05 | .10 | .10 | .08 |
| $\alpha_i^y$ | .05 | .05 | .05 | .05 | .10 | .10 | .08 |
| $h_i$ | 1 | .5 | .5 | 1 | 1 | 1 | 1 |

In this paper, we fixed $\alpha = 5\%$. In order to test for the whiteness of the 2-D signal $r(n, m)$, we apply the previous measure on the two marginals of $\hat{P}'(\omega_1, \omega_2)$ along the two dimensions to obtain $\hat{W}_1$ and $\hat{W}_2$. The signal $r(n, m)$ is a white noise only if the two measures are less than a threshold.

Finally, the stopping rule of the decomposition can be expressed as:

$$\begin{cases} \text{if } \hat{W}_1 \leqslant t_\alpha \text{ and } \hat{W}_2 \leqslant t_\alpha, \text{ then stop}, \\ \text{if } \hat{W}_1 > t_\alpha \text{ or } \hat{W}_2 > t_\alpha, \text{ then continue}. \end{cases} \qquad (14)$$

## 4. EXPERIMENTS

In this section, we present two experiments made on simulated signals of increasing complexity.

### 4.1 Signal 1

The first simulated signal is composed of 7 complex modes given in table 1. The number of samples in both dimensions is 64 and the noise variance is fixed to $10^{-4}$ (i.e. 40 dB for a mode with unitary amplitude).

The results achieved with the method developed using a prediction order $p = 6$ in all subbands are presented in figure 2. Figure 2(a) shows the final spectral decomposition together with the number of estimated modes in each subband. We can observe that the subband decomposition is sufficient at this level since all the modes have been retrieved. Figures 2(b) and 2(c) represent the power spectra of subband signals corresponding to the frequency ranges $[0, .25] \times [0, .25]$ and $[.25, .5] \times [0, .25]$, respectively. The estimated modes are represented by filled circles. In both subbands, the estimated positions of the modes are close to the theoretical ones.
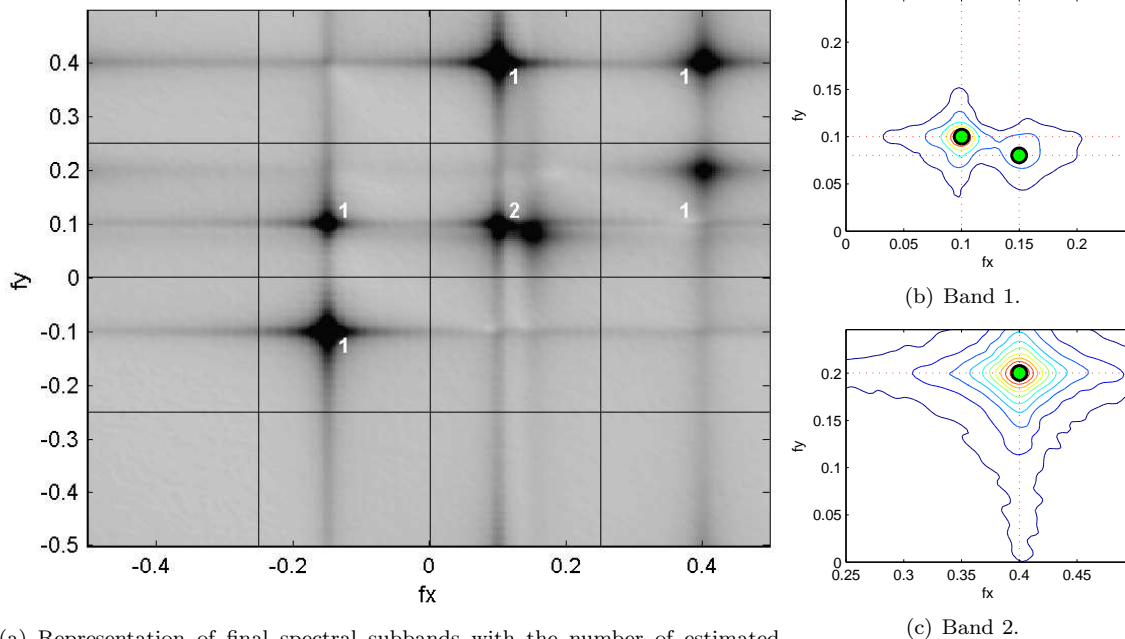
(a) Representation of final spectral subbands with the number of estimated modes.

(b) Band 1.

(c) Band 2.

Fig. 2. Some results achieved on signal 1. Band 1 and Band 2 correspond to the frequency ranges $[0, .25] \times [0, .25]$ and $[.25, .5] \times [0, .25]$, respectively.
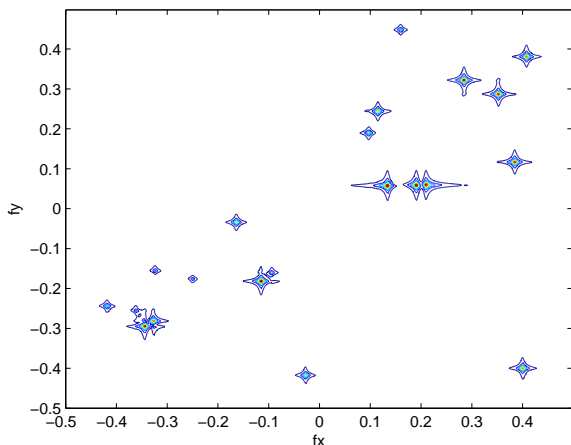


Fig. 3. Power spectrum of signal 2.

### 4.2 Signal 2

The second signal is intended to demonstrate the capability of the proposed approach to track the spectral subbands in which information is localized. The signal contains 21 modes. Ten modes are positioned randomly in the lower-left quarter of the frequency plane (i.e. in the frequency range $[-.5, 0] \times [-.5, 0]$), and ten other modes in the upper-right quarter. The last one is located at $(.4, -.4)$. All damping factors are equal to $0.02$ and the amplitudes are generated randomly in the interval $[0.5, 3.5]$. As before, the variance of the additive noise is fixed to $10^{-4}$. The generated samples form a data matrix of dimension $256 \times 256$, whose Fourier transform is shown on figure 3.

The results obtained with a prediction order $p = 6$ are shown on figure 4. One can observe on figure 4(a) that the decomposition is generally deeper in the spectral regions where several modes are located. On the other hand, for remote modes, the decomposition is stopped at lower decimation levels. This is the case for instance for mode $(.4, .4)$. So the method is able to adapt the decomposition on the local complexity of a signal, allowing one to reduce the calculation time as compared to a uniform decomposition in which several small subbands should be analyzed.

## 5. CONCLUSION

We have proposed in this paper an adaptive subband decomposition approach for the analysis of 2-D NMR data. This method uses a stopping rule based on a spectral flatness measure of the subband residuals. If the test for whiteness fails in a given node, then the decomposition is carried on, otherwise the decomposition is stopped. The results obtained points out the advantage the method over a global estimation and a uniform decomposition.

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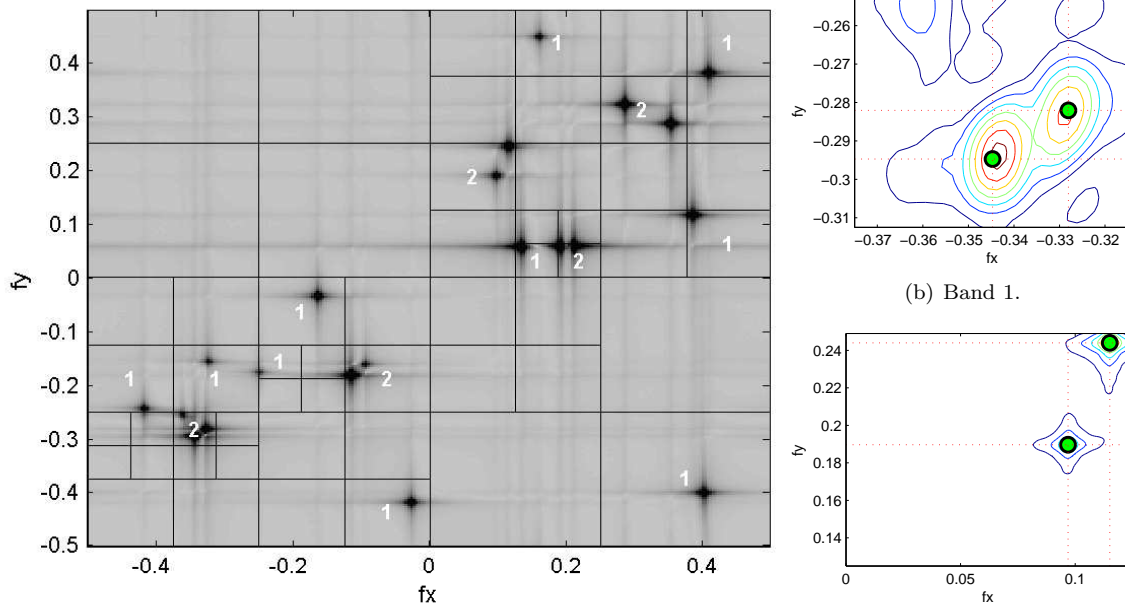
(a) Representation of final spectral subbands with the number of estimated modes.

(b) Band 1.

(c) Band 2.

Fig. 4. Some results achieved on signal 2. Band 1 and Band 2 have different sizes and correspond to the frequency ranges $[-.375, -.3125] \times [-.3125, -.25]$ and $[0, .125] \times [.125, .25]$, respectively. Note that one small mode is missed in Band 1.

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