Proceedings of International Joint Conference on Neural Networks, Montreal, Canada, July 31 - August 4, 2005

An Algorithm for Automatic Assignment of Artifact-Related Independent Components in Biomedical Signal Analysis

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Abstract— **In this work an automatic assignment tool for estimated independent components within an independent component analysis is presented. The tool is applied to the problem of removing the water resonance and related artifacts from multi-dimensional proton NMR spectra. The algorithm uses local PCA to approximate the water artifact and defines a suitable cost function which is optimized using simulated annealing. The blind extraction of artifact-related source signals is effected by a recently developed algorithm called dAMUSE.**

I. Introduction

Blind Source Separation (BSS) methods consider the separation of observed sensor signals into their underlying source signals knowing neither these source signals nor the mixing process. Considering biomedical applications, BSS methods are especially valuable to remove artifacts from the sensor signals recorded. In many biomedical applications quite a number of independent components have to be determined with ICA algorithms and it is not *a priori* clear how many components should be assigned to signals representing artifacts. This is especially obvious in proton NMR spectra of biomolecules, where a prominent water artifact distorts the recorded spectra considerably [1]. Many efforts have been undertaken to remove it. As a consequence of the experimental pulse protocol, the water artifact is strongly phase distorted in the various component spectra belonging to deliberately incremented evolution periods within the pulse sequence. This, however, prohibits any simple analytical or wavelet-based fitting of the water artifact and subsequent subtraction from the recorded spectrum. As experimental means are also unable to suppress the artifact sufficiently, only computational signal processing techniques may be able to solve the problem satisfactorily. Recently artifact removal was considered using BSS techniques based on a generalized eigenvalue decomposition (GEVD) of a matrix pencil [2], [3]. The latter techniques have been extended recently [4], [5] by projecting the sensor data to a high-dimensional feature space of delayed coordinates to achieve BSS and denoising simultaneously, with the newly developed algorithm dAMUSE. But the artifact-related components estimated usually have to be assigned by hand. With more than 100 estimated components this turns out to become a rather tedious undertaking prone to be biased by subjective judgements of the assignment criteria.

In this work we propose a local PCA approximation to the free induction decay (FID) related with the water artifact in protein proton NMR and to use simulated annealing [6] to identify those uncorrelated components, estimated with dAMUSE, which have to be assigned to the water artifact.

The following section will provide a very brief summary of the algorithm dAMUSE [4] and then introduce the new algorithm AutoAssign. To illustrate the proposed method, an application is discussed comprising theoretical 2D NOESY NMR spectra with added noise and an experimental water resonance added as well.

II. Theory

A. BSS model

Given N complex sensor signals $x(t_{1,n}, t_{2,l}) \equiv x_n[l]$ sampled at L discrete time instances, and arranged in a data matrix $\mathbf{X}_{N\times L}$. In each row the L columns of the data matrix contain samples of complex interferograms, which represent superpositions of 1-dim free induction decays (FIDs) of each nuclear species in the probe. The N rows then correspond to discrete evolution times $t_{1,n} \equiv [n]$, $n = 1, ..., N$ of the 2D NOESY experiment. Blind source separation (BSS) then relies on the following linear mixing model

$$\mathbf{x}[l] = \mathbf{A}\mathbf{s}[l] + \epsilon[l] \tag{1}$$

where $l = 0, ..., L-1$ and $\mathbf{x}[l] = (x_1[l], \ldots, x_N[l])^T$ designates the observed signals sampled at time instance l, $\mathbf{s}[l]$ the underlying uncorrelated source signals, $\mathbf{A}$ the stationary mixing matrix and $\epsilon[l]$ an additional zero mean white Gaussian noise term which is independent of the source signals.

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B. The algorithm dAMUSE

A generalized eigenvalue decomposition (GEVD) technique [2] using congruent matrix pencils (GEVD-MP) [3] may be used to separate the water artifact from 2D NOESY NMR spectra of proteins as has been shown recently [7]. Later the GEVD-MP algorithm [8] has been extended to data embedded in a high-dimensional feature space of delayed coordinates, resulting in the algorithm dAMUSE [4]. It provides a means to perform BSS and denoising simultaneously [5]. The method uses the concept of a trajectory matrix borrowed from singular spectral analysis (SSA)(see [9] for a recent review). The algorithm dAMUSE will be used in the following, hence a short summary will be presented.

Considering a sensor signal component $x_n[l]$, a trajectory matrix $\mathbf{X}_n^e$ is constructed with each row containing delayed versions $x_n(l+(M-m)K)$ of the given signal component [10], where K denotes the delay in number of sampling intervals between consecutive rows and M gives the dimension of the embedding space. Using a set of L samples and M delayed versions of the signal $x_n[l+(M-m)K]$, $l = 0,...,L-1$, $m = 0,....,M-1$, the following component trajectory matrix $\mathbf{X}_n^e$ results

$$\mathbf{X}_n^e = \begin{bmatrix} x_n[(M-1)K] & \cdots & x_n[L-1] \\ x_n[(M-2)K] & \cdots & x_n[L-1-K] \\ \vdots & \ddots & \vdots \\ x_n[2K] & \cdots & x_n[L-1-(M-3)K] \\ x_n[K] & \cdots & x_n[L-1-(M-2)K] \\ x_n[0] & \cdots & x_n[L-1-(M-1)K] \end{bmatrix} \quad (2)$$

The total trajectory matrix $\mathbf{X}^e$ of all N signals is formed by concatenating the component trajectory matrices $\mathbf{X}_n^e$ according to:

$$\mathbf{X}^e = [\mathbf{X}_1^e \mathbf{X}_2^e \ldots \mathbf{X}_N^e]^T \quad (3)$$

After embedding, the instantaneous mixing model can be written as $\mathbf{X}^e = \mathbf{A}^e\mathbf{S}^e$ where $\mathbf{S}^e$ represents the corresponding source signal trajectory matrix, $\mathbf{A}^e = \mathbf{A}_n \otimes \mathbf{I}_{M\times M}$ is a block matrix and $\mathbf{I}_{M\times M}$ denotes the identity matrix. Then, if $\mathbf{A}_n$ is an invertible matrix, it follows that $\mathbf{A}^e$ is also invertible as it is obtained via a *Kronecker* product of two invertible matrices. Next a matrix pencil $(\mathbf{R}_x, \mathbf{R}_z)$ is computed with the sensor signals $\mathbf{x}[l]$ and filtered versions $mathbfz[l]$ thereof. The $\mathbf{R}_j$, $j = x, z$ denote corresponding correlation matrices of zero mean data according to

$$\begin{aligned} \mathbf{R}_x &= \langle \mathbf{X}^e (\mathbf{X}^e)^H \rangle \\ \mathbf{R}_z &= \langle \mathbf{Z}^e (\mathbf{Z}^e)^H \rangle \end{aligned} \quad (4)$$

using the trajectory matrix $\mathbf{X}^e$ and a filtered version $\mathbf{Z}^e = \mathbf{X}^e\mathbf{F}^H$ of it with $\mathbf{F}$ representing a circular convolution matrix and H denoting the Hermitian conjugate [8]. A GEVD of the sensor pencil then provides a solution to the BSS problem [3] and is given by

$$\mathbf{R}_x\mathbf{E} = \mathbf{R}_z\mathbf{E}\mathbf{\Lambda} \quad (5)$$

where $\mathbf{E}$ represents an *unique* eigenvector matrix if the diagonal matrix $\mathbf{\Lambda}$ has *distinct* eigenvalues λ_i. This sensor pencil is congruent [3] with a corresponding source pencil, hence the respective eigenvectors are related by $\mathbf{E}_s^H = \mathbf{E}^H\mathbf{A}^e$. Assuming that the source signals and their filtered versions are uncorrelated, the matrix $\mathbf{E}_s$ is block-diagonal, with block size $(M \times M)$. The solution of the GEVD problem yields a linearly transformed trajectory matrix then

$$\mathbf{Y}^e = \mathbf{E}^H\mathbf{X}^e = \mathbf{E}^H\mathbf{A}^e\mathbf{S}^e = \mathbf{E}_s^H\mathbf{S}^e \quad (6)$$

which contains filtered versions of the estimated source signals.

The eigenvalues and eigenvectors of a matrix pencil can be obtained via standard eigenvalue decompositions (EVD) applied in two consecutive steps. Starting with the sensor pencil $(\mathbf{R}_x, \mathbf{R}_z)$ the following steps are performed within dAMUSE:

- Compute a standard eigenvalue decomposition of the symmetric positive definite correlation matrix

$$\mathbf{R}_x = \mathbf{V}\mathbf{\Lambda}\mathbf{V}^H \quad (7)$$

  where $(\mathbf{v}_i)$ represents the eigenvectors and (λ_i) the corresponding eigenvalues and organize the eigenvalues in descending order $(\lambda_1 > \lambda_2 > .... > \lambda_q .... > \lambda_{NM})$.
- For *denoising* purposes, a variance criterion has been established to retain only the q largest eigenvalues exceeding a threshold parameter Θ [4].
- A transformation matrix can then be computed using the q largest eigenvalues and respective eigenvectors

$$Q = \mathbf{\Lambda}^{-\frac{1}{2}}\mathbf{V}^H \quad (8)$$

  where $\mathbf{Q}$ is an $q \times NM$ matrix.
- Compute the transformed correlation matrix of the filtered sensor signals

$$\tilde{\mathbf{R}} = \mathbf{Q}\mathbf{R}_z\mathbf{Q}^H = \mathbf{U}\mathbf{D}_z\mathbf{U}^H \quad (9)$$

  and its standard eigenvalue decomposition: the eigenvector matrix $\mathbf{U}$ and eigenvalue matrix $\mathbf{D}_z$

The eigenvectors of the pencil $(\mathbf{R}_x, \mathbf{R}_y)$ form the columns of the eigenvector matrix

$$\mathbf{E} = \mathbf{Q}^H\mathbf{U} = \mathbf{V}\mathbf{\Lambda}^{-\frac{1}{2}}\mathbf{U} \quad (10)$$

which can be used to compute the output signals as described above.

C. The algorithm AutoAssign

Applying the BSS algorithms above to 2D NOESY NMR spectra to separate the water artifact and related artifacts from the protein spectra, the most tedious task is to assign the uncorrelated components estimated to the water signal. Because of erratic phase relations during signal aquisition, up to 160 out of 512 estimated components need to be assigned to the water resonance. Hence an automated and objective assignment procedure deemed necessary and will be proposed in the following section.

The idea is to embed the signal in a high-dim feature space of delayed coordinates and to apply a cluster analysis to the columns of the corresponding trajectory matrix. Within each cluster a local PCA is then performed to obtain a low-dim approximation to the signals using only the most important principal components to approximate the signals. The latter are then feed into a suitable cost function which is optimized with simulated annealing.

Consider a signal (here one column vector of a component trajectory matrix)

$$\mathbf{x}_n[l] = (x_n[l], x_n[l+1], \ldots, x_n[l+(M-1)])^T \quad (11)$$

embedded in an M-dim feature space. Divide the feature space in k_c subsets $\mathcal{N}^{(k)}$ using *k-means* clustering of the embedded signal vectors $\mathbf{x}_n[l]$ and center the signals in each cluster locally by subtracting the cluster mean:

$$\bar{\mathbf{x}}_n^{(i)} = |\mathcal{N}^{(i)}|^{-1} \sum_{\mathbf{x}_n[l] \in \mathcal{N}^{(i)}} \mathbf{x}_n[l], \quad i = 1, ..., k_c \quad (12)$$

Next a principal component analysis (PCA) is performed on each cluster separately, and a local approximation to the time domain signal is computed using only the eigenvectors $\mathbf{w}_j^{(i)}$ corresponding to the $p(i)$ largest eigenvalues

$$\tilde{\mathbf{x}}_n[l] = \sum_{j=1}^{p(i)} \alpha_j[l] \mathbf{w}_j^{(i)} + \bar{\mathbf{x}}_n^{(i)} \quad (13)$$

with $\alpha_j[l] = \mathbf{x}_n[l] \cdot \mathbf{w}_j^{(i)}$ and $\mathbf{x}_n[l] \in \mathcal{N}^{(i)}$. This yields a new trajectory matrix, the entries of which represent local PCA approximations of the original signals

$$\tilde{\mathbf{X}}_n = \begin{bmatrix} \tilde{x}_n[M-1] & \tilde{x}_n[M] & \ldots & \tilde{x}_n[L-1] \\ \tilde{x}_n[M-2] & \tilde{x}_n[M-1] & \ldots & \tilde{x}_n[L-2] \\ \tilde{x}_n[M-3] & \tilde{x}_n[M-2] & \ldots & \tilde{x}_n[L-3] \\ \vdots & \vdots & \ddots & \vdots \\ \tilde{x}_n[0] & \tilde{x}_n[1] & \ldots & \tilde{x}_n[(L-1)-(M-1)] \end{bmatrix} \quad (14)$$

After reverting the clustering process, the final global approximation $\langle \tilde{\mathbf{x}}_n[l] \rangle_{[l]}$, $l = M-1, ..., L-1$ is obtained by averaging all entries at the same time instance $[l]$ (which lie along diagonals).

As the water signal provides the dominant contribution to each FID observed, the PCA approximation can be simplified further by retaining only the principal component to the largest eigenvalue, i.e.

$$\tilde{\mathbf{x}}_n[l] = \alpha_1[l] \mathbf{w}_1^{(i)} + \bar{\mathbf{x}}_n^{(i)} \quad (15)$$

This approximation to the observed FID supposedly contains the contribution from the water signal almost exclusively.

This local PCA approximation to the FID related with the water artifact is then used to define a cost function

$$\mathcal{E}(\boldsymbol{\beta}) = \sum_{l=0}^{L-1} (\mathbf{x}_{n,\boldsymbol{\beta}}[l] - \langle \tilde{\mathbf{x}}_n[l] \rangle_{[l]})^2 \quad (16)$$

to be minimized with simulated annealing [6]. The BSS approximation to the water signal using the uncorrelated components estimated with the GEVD-MP or the dAMUSE algorithm is obtained as

$$\mathbf{x}_{n,\boldsymbol{\beta}}[l] = \sum_j \mathbf{a}_{nj} \beta_j s_j[l] \quad (17)$$

where a configuration is represented by a vector $\boldsymbol{\beta}$ which contains as many components β_j as there are sources $\mathbf{s}_j$. To each source one element of $\boldsymbol{\beta}$ is assigned which can take on the values $\beta_j \in \{0, 1\}$ only. A new configuration $\boldsymbol{\beta}$ is generated by changing any $\beta_j \in \{0, 1\}$ randomly. Each configuration thus consists oft those sources, whose corresponding element in $\boldsymbol{\beta}$ has the value 1. In addition each source is weighted with the corresponding entry of the mixing matrix $\mathbf{A}$. The difference in the values of the cost function for the current and the new configuration

$$\Delta\mathcal{E} = \mathcal{E}(\beta_{new}) - \mathcal{E}(\beta_{old}) \quad (18)$$

determines the probability of acceptance of the new configuration in the simulated annealing algorithm using Metropolis sampling [6] according to

$$P[\beta_{old} \rightarrow \beta_{new}] = \min \left\{ 1, \exp\left(-\frac{\Delta\mathcal{E}}{k_B T} \right) \right\} \quad (19)$$

After convergence of the simulated annealing algorithm, the configuration which best fits to the local PCA approximation of the water signal is obtained. Nullifying these components deliberately, the water-artifact-free protein spectrum $\mathbf{x}_n^\dagger$ can be reconstructed using the remaining estimated source signals $\mathbf{s}_n^\dagger$ via $\mathbf{x}_n^\dagger = \mathbf{A}\mathbf{s}_n^\dagger$.

III. Results and Discussion

The algorithms discussed above will be applied to artificial 2D NOESY proton NMR spectra of proteins dissolved in water. Every data set comprises 512 or 1024 FIDs $S(t_1, t_2) \equiv x_n[l]$, with $L = 2048$ samples each, which correspond to $N = 128$ or $N = 256$ evolution periods $t_1 \equiv [n]$. To each evolution period belong four FIDs with different phase modulations, hence only FIDs with equal phase modulations have been considered for analysis. A BSS analysis, using the algorithm dAMUSE, was applied to the FIDs collected in the data matrix $\mathbf{X}$. Filtering was done in the frequency domain for convenience. Hence, all FIDs have been Fourier transformed with respect to the sampling time $t_2 \equiv [l]$ to obtain 1D spectra $\hat{S}(t_1, \omega_2) \equiv \hat{\mathbf{x}}_n(\omega)$, $0 < n \leq 128$ or $0 < n \leq 256$. Filtered versions of the data were obtained by applying a Gaussian filter $\hat{\mathbf{f}}[\omega]$ with width $\sigma = 1$, centered near the water resonance, to each row of the data matrix $\hat{\mathbf{X}}$ in the frequency domain. After filtering the data have been back-transformed to the time domain to calculate the corresponding correlation matrices of the pencils. The automatic assignment of the uncorrelated components, estimated with dAMUSE, which belong to the water resonance was achieved using the proposed algorithm

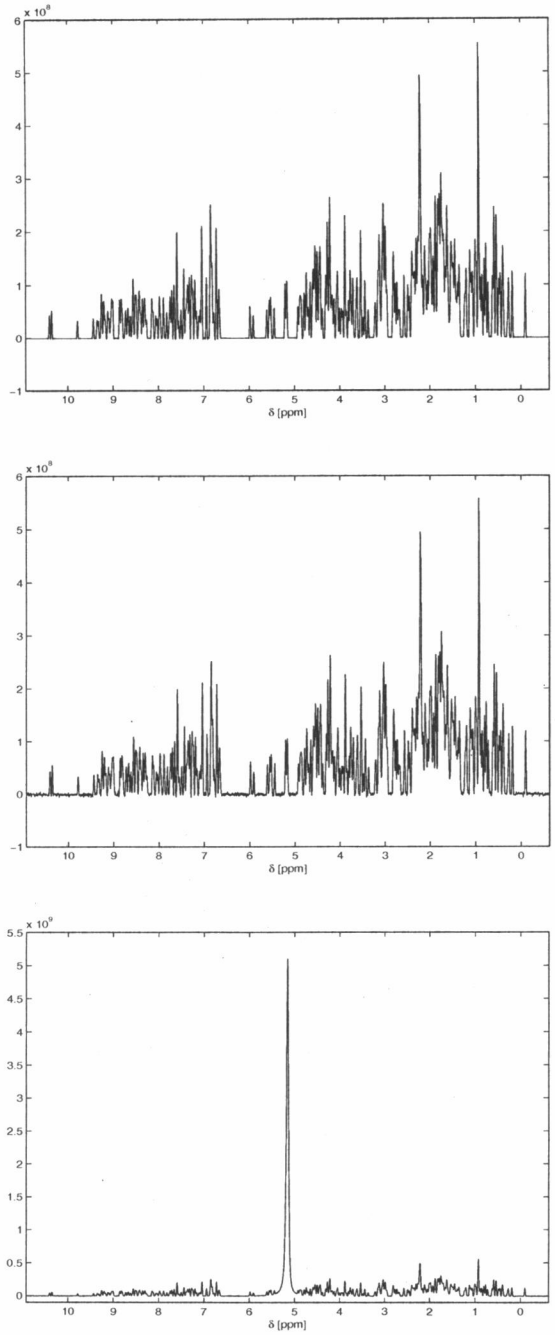

Fig. 1. (a)- Theoretical protein spectrum, (b)- Theoretical protein spectrum with Gaussian noise, (c)- Theoretical spectrum with Gaussian noise and an experimentally recorded water resonance

AutoAssign which is based on a local PCA and a simulated annealing optimization.

For test purposes, a theoretical 2D NOESY proton NMR spectrum of the cold-shock protein of the bacterium *Thematoga maritima*, containing only protein resonances, was used. The spectrum was obtained through reverse calculation using the algorithm RELAX [11]. Gaussian white noise with realistic amplitude as well as an experimentally recorded water resonance were added to the theoretical spectrum (see Fig. 1). The BSS was done with the algorithm dAMUSE [4] using $K = 1$. The second correlation matrix $\mathbf{R}_{x2}$ of the pencil was computed with the theoretical spectrum with added noise taken as the filtered version of the original spectrum. An approximation of the water artifact dominating the time domain FIDs was obtained with the local PCA algorithm. As the experimental pure water FID was available also, both could be compared to access the quality of the approximation. To perform local PCA, each sample of the data was projected into a $M = 40$ dimensional feature space and *k-means* clustering was used to divide the projected data into $k = 2$ cluster. Only the largest principal component was considered to approximate the water signal.

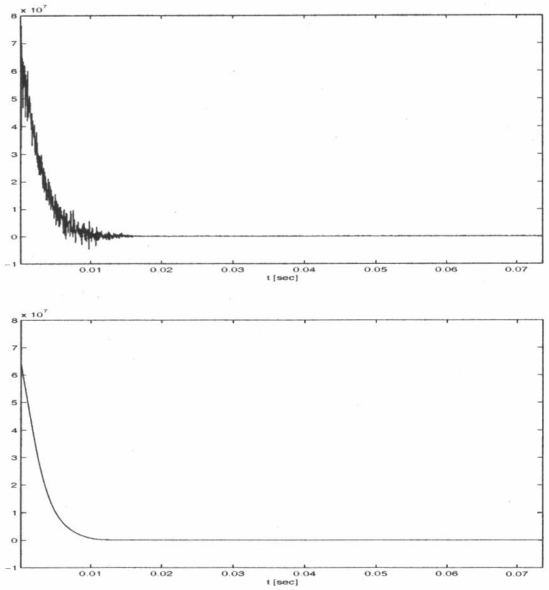

Fig. 2. Free Induction Decays (FID) of a)-the total FID of the protein signal plus additive noise plus an experimental water FID, b)-local PCA approximation of the total FID

Fig. 2-a) compares the total FID corresponding to the shortest evolution period with the local PCA approximation (Fig. 2-b)) of the latter. It is immediately obvious that the water artifact dominates the total FID. It is seen that local PCA provides a very good approximation to the water artifact. This can be corroborated by subtracting the approximate water FID from the total FID and transforming the resulting FID into the frequency domain. The resulting protein spectrum contains only small remnants of the huge water artifact as can be seen in Fig. 3. The spectra thus obtained will henceforth be called *approximated spectra*.

This indicates that it should be possible to use the local PCA approximation of the water artifact as a reference signal in a cost function to be minimized with a simulated annealing algorithm. This is confirmed by analyzing the theoretical protein spectra plus noise plus water artifact (see Fig. 1-b)) with the dAMUSE algorithm to extract the uncorrelated

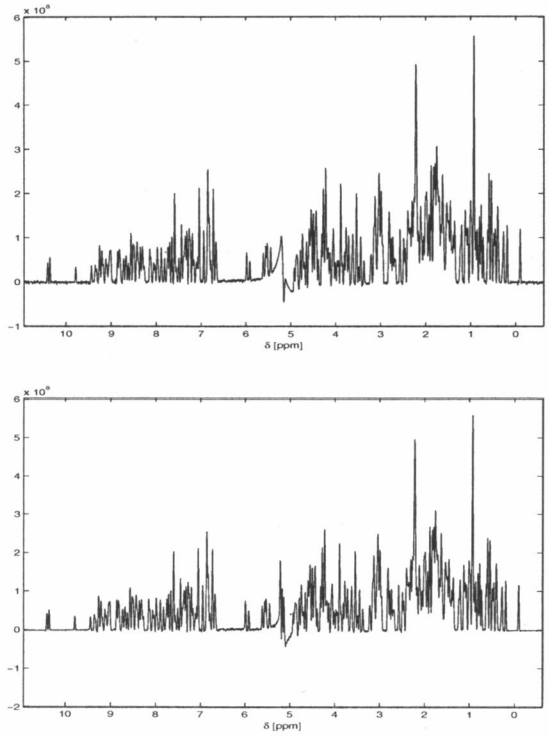

Fig. 3. a)-Protein spectrum obtained after subtracting the approximated water FID from the total FID and Fourier transformation of the difference FID, b)-Reconstructed protein spectrum obtained with dAMUSE.

components and using simulated annealing (SA) to automatically assign those components related with the water artifact. The SA-algorithm identifies the same 9 components irrespective whether the experimental water FID or its local PCA approximation has been used in the cost function. Without denoising, the reconstructed protein spectrum resembles the original noisy spectrum (Fig. 1-b)) except for a much enhanced noise level. Calculating the signal-to-noise ratio (SNR) via $SNR(\mathbf{x}, \mathbf{x}_{noise})[dB] = 20 \log_{10} \frac{\|\mathbf{x}\|}{\|\mathbf{x}-\mathbf{x}_{noise}\|}$ where $\mathbf{x}$ denotes the theoretical spectrum, $\mathbf{x}_{noise}$ its noisy counterpart, the theoretical spectrum plus gaussian noise shows a SNR of $24.5dB$, whereas the reconstructed protein spectrum only yields a SNR of $10.1dB$. Denoising can be accomplished elegantly with the dAMUSE algorithm which achieves blind source separation and denoising simultaneously. The water related components extracted are automatically assigned with the algorithm AutoAssign using a local PCA approximation to the water artifact. The optimal number M of delays as well as the optimal size of the time lag have been determined by the best minimum to the cost function obtained with the SA algorithm. A minimum of the cost function has been obtained with using one time-delayed FID, a lag of one sampling interval and by retaining 158 eigenvectors (out of $2 \cdot 128$) after the first step of the algorithm dAMUSE. The result of the dAMUSE denoising is shown in Fig. 3, the SNR achieved amounts to $SNR = 22.1\ dB$.

IV. Conclusions

The separation of artifacts from biomedical signal recordings is one of the more prominent applications of blind source separation techniques using independent component analysis. The assignment of the artifact-related independent components estimated is, however, not a trivial task and often done by hand. In this work we presented an automatic assignment tool, called AutoAssign, which uses local PCA to approximate the prominent water artifact in 2D NOESY protein NMR spectra and defines a suitable cost function to be optimized by simulated annealing.

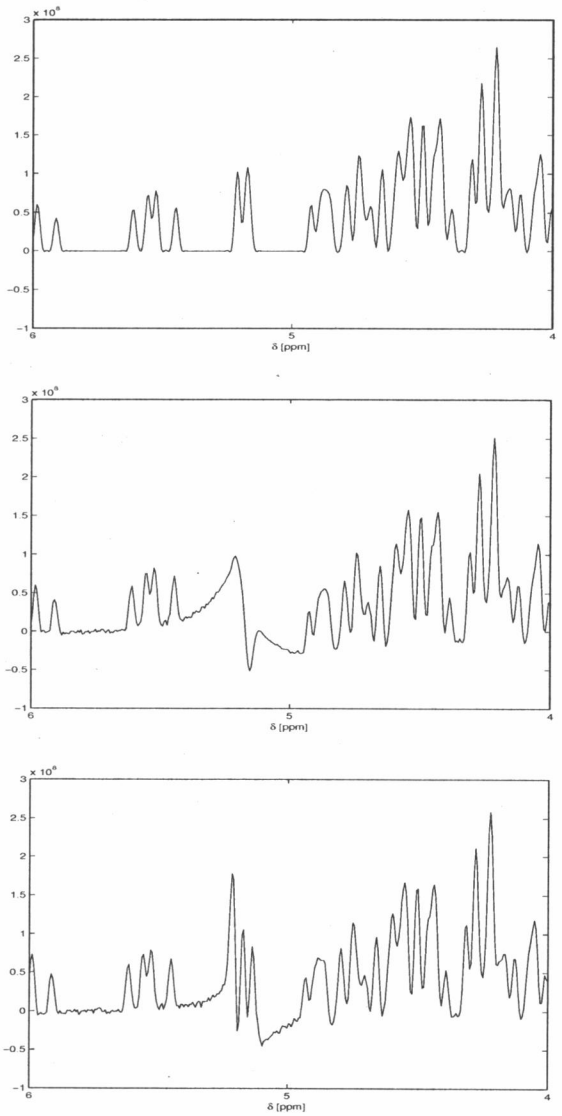

Fig. 4. Theoretical protein spectrum: a)- expanded region of the original spectrum corresponding to Fig. 1, b)- expanded region of the approximated spectrum corresponding to Fig. 3, c)- expanded region of the theoretical spectrum reconstructed with dAMUSE and AutoAssign corresponding to Fig. **??**-b)

Local PCA tries to approximate the water related component to the measured free induction decay (FID) which then can

be subtracted from the total FID observed. This is done only for the FIDs corresponding to the shortest evolution period where the latter is most prominent. This approximation is then used within a simulated annealing procedure to assign those estimated ICs which most closely resemble the approximated water FID from the local PCA approximation. It is then assumed that this assignment of the estimated ICs also holds with all other evolution periods where no local PCA approximations have been determined. Doing so would result in a computational effort which seems prohibitive. The FID resulting from the local PCA approximation can be Fourier transformed to yield an almost artifact-free protein spectrum. The results obtained look very convincing from a visual inspection of the spectra. However, they remove any signal in the spectral region of the water peak. Hence all information about protein peaks in that area is inevitably lost (see Fig. 4).

A much more versatile analysis method is based on the recently proposed algorithm dAMUSE in combination with AutoAssign. A close inspection of the results obtained with the theoretical spectra of *Tm*CSP demonstrate convincingly that AutoAssign in combination with dAMUSE retains information about spectral features in the region of the water artifact where the local PCA approximation erases all features whatsoever. This is clearly visible in Fig. 4 in the region between 5 ppm and 5.5 ppm where a doublet is hidden under the water resonance but can be recovered by the algorithm dAMUSE in combination with AutoAssign, but not with the local PCA approximation. Furthermore, baseline artifacts are cured with dAMUSE and AutoAssign in all cases. With the local PCA approximation alone, often severe baseline distortions remain which hampers the subsequent structure determination considerably. Hence a more robust method is needed to reliably extract the water artifacts. The algorithms dAMUSE in combination with AutoAssign seem a promising tool for an automatic assignment and removal of artifacts in biomedical signal recordings. Further investigations concerning other biomedical signals are under way in our laboratories.

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APPENDIX

Pseudocode of the algorithm dAMUSE:

- Compute the trajectory matrix $\mathbf{X}^e$ of the embedded signals
- Compute the trajectory matrix $\mathbf{Z}^e$ of the filtered signals
- Compute correlation matrices $\mathbf{R}_x = \langle \mathbf{X}^e (\mathbf{X}^e)^H \rangle$ and $\mathbf{R}_z = \langle \mathbf{Z}^e (\mathbf{Z}^e)^H \rangle$
- Compute an EVD of $\mathbf{R}_x = \mathbf{V}\mathbf{\Lambda}\mathbf{V}^H$
- Compute the transformation matrix $\mathbf{Q} = \mathbf{\Lambda}^{-1/2}\mathbf{V}^H$
- Compute an EVD of $\tilde{\mathbf{R}} = \mathbf{Q}\mathbf{R}_z\mathbf{Q}^H = \mathbf{U}\mathbf{D}_z\mathbf{U}^H$
- Compute the eigenvector matrix $\mathbf{E} = \mathbf{V}\mathbf{\Lambda}^{-1/2}\mathbf{U}$ of the pencil
- Calculate filtered versions of the source signals $\mathbf{Y}^e = \mathbf{E}^H\mathbf{X}^e$

Pseudocode of the algorithm AutoAssign:

- Cluster feature space vectors $\mathbf{x}_n[l]$ into k_c clusters using *k-means*
- Perform a PCA on each cluster locally
- Represent each FID using the principal component(s) corresponding to the largest (in general $p(i)$ largest) eigenvalue(s) $\tilde{\mathbf{x}}_n[l] = \alpha_1[l]\mathbf{w}_1^{(i)} + \bar{\mathbf{x}}_n^{(i)}$
- Compute an approximation to the water artifact related BSS component $x_{n,\beta}[l] = \sum_j a_{nj}\beta_j s_j[l]$
- Compute the cost function $\mathcal{E}(\boldsymbol{\beta}) = \sum_{l=0}^{L-1}(x_{n,\beta}[l] - \langle \tilde{x}_n[l] \rangle)^2$
- Minimize the cost function using simulated annealing employing Metropolis sampling $P[\beta_{old} \rightarrow \beta_{new}] = \min\left\{1, \exp\left(-\frac{\Delta\mathcal{E}}{k_B T}\right)\right\}$
- Nullify the components of the dAMUSE algorithm which best fit to the local PCA approximation of the water artifact
- Reconstruct the artifact-free signal