# SORTING TECHNIQUES FOR PERMUTATED PARAMETERS OF FITTING BASED ALGORITHMS

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## ABSTRACT

This paper is focused on the new concepts of postprocessing methods applicable on evaluated parameters of model fitting based methods. These methods was developed especially for signals of Nuclear Magnetic Resonance (NMR), which are not sometimes passed properly even when using professional sophisticated nonlinear algorithms for parametric estimations such as AMARES, VARPRO or linear LPSVD. A sorting techniques based on two sorting criterias with suppression of redundant signal components is presented.

## 1 INTRODUCTION

As signal processing of biomedical signals have risen in recent years and gained more significance, development of new methods and algorithms is necessary to treat and understand signals on focus properly. Especially parametric estimation and quantition of signals of Nuclear Magnetic Resonance (NMR) is on focus today [1]. New versions of robust nonlinear approaches are evaluated and presented for more accurate and stable parameter estimation in the presence of high noise.

This contribution deals with the new postprocessing method applicable on evaluated parameters of linear / nonlinear fitting algorithms. The problem that needs to be solved is variance of estimated parameters at statistical realizations. It is not guaranteed that estimated parameters of the same physical meaning will hold the same position in the output parameter vector regardless of realization. That is the reason that makes it difficult to orientate in results. Introduced sorting approaches combine power criteria at the first procesing stage and additional criteria at the second processing stage. Sorting algorithm is applied on estimated individual NMR signal components called FIDs (Free Induction Decays). These FIDs are composed from estimated parameters inserted into proper signal models.

First, we need model parameters to be processed. Parameters are produced by linear or nonlinear algorithms, most often used are linear LPSVD (Linear Prediction Singular Value Decomposition), nonlinear AMARES (Advanced Method for Accurate, Robust and Efficient Spectral fitting) or nonlinear VARPRO (VARiable PROjectional) [2]. Output parameters are solution to least squares fitting problem, where are minimize the sum of squared residuas

between noisy input signal NMR and its model. NMR signal is often described by the sum of damped complex sinusoids in the presence of noise, called Lorentz model:

$$y_k = \sum_{m=1}^{M} (A_m \exp(\alpha_m .k.T) \exp(i(\omega_m .k.T + \varphi_m))) + e_k \quad (1)$$

where $\boldsymbol{y}$ is the observable signal NMR, $\boldsymbol{A}$ stands for amplitude, $\boldsymbol{\alpha}$ means damping parameter, $\boldsymbol{\omega}$ represents angular frequency and $\boldsymbol{\varphi}$ stands for initial phase – these four variables are parameters we are trying to find by nonlinear or linear signal processing. In addition $\boldsymbol{e}$ represents noise and mismatch of Lorentz model with signal NMR, $T$ means sampling interval, $k$ represens sample index. $M$ denotes number of decayed complex sinusoids composing signal NMR, $m$ is their index. Each component created by parameters $\{A_\mathrm{m},\alpha_\mathrm{m},\omega_\mathrm{m},\varphi_\mathrm{m}\}$ is a FID signal in this contribution.

Unfortunately, contrary to achievements in this field, final presentation of parameters is sometimes less understandable and in the case of statistical analysis it makes it difficult to orientate in the final set of parameters. This is caused by several reasons.

The main reason is the IC ( Initial Condition )specification in case of nonlinear processing. For linear techniques usually the number of FIDs is required. Most often number of real FIDs composing signal NMR is unknown before estimation, so IC is formulated for estimation of higher count of components. As a result, redundant FIDs mix with real FIDs and make them difficult to suppress. In the case of statistical parameter results, each quantified realization can have a specific mixture of real and redundant FIDs. So, in other words, an output parameter vector can be any variance of real and redundant FIDs and in another realization the same order may not be preserved.

This contribution solves this problem by forcing its own order defined by power contribution of individual FIDs to signal NMR. For this purpose the discussed FIDs are reconstructed from the estimated parameters. Some experimets showing that power sorting may not be sufficient, so two level sorting is applied. The second sorting level is based on the additional criteria such as amplitude, angular frequency, damping or initial phase of individual FIDs. Most promising is sorting using amplitude, because of the lowest variance defined by Cramer – Rao lower bounds (CRBs) [3]. But another second level criteria can be applied, especially in cases of nonsimilarity of other parameters. Amplitude sorting is important at noisy signal NMR estimations which contains parametrically similar FIDs, because due to presence of noise variation of estimated parameters is observable. This variation is defined CRBs and can cause swap order of closely related FIDs. Second amplitude sorting criteria significantly reduce this phenomena. Sorting by amplitude at the second stage is recommended, because the variation of estimated amplitudes is the lowest from other estimated parameters, its variance is defined by CRBs.

## 2 POWER SORTING CRITERIA

Output parameters are sorted from the most significant to negligible in power contribution sense. Assume an output parameter vector from each estimation having a form:

$$\bar{x}_n = \left(\alpha_{n1} \ldots \alpha_{nM}, A_{n1} \ldots A_{nM}, \omega_{n1} \ldots \omega_{nM}, \varphi_{n1} \ldots \varphi_{nM}\right) \quad (2)$$

where $n$ denotes index of realization. $M$ means number of estimated FIDs, this number corresponds with number of components stated in IC in case of nonlinear algorithm. It is

obvious that estimated $M$ components contain both real components and redundant components:

$$M_{est} = M_{real} + M_{red} \tag{3}$$

For purposes of the proposed solution it is convenient to split each output parametric vector (2) to parametric matrixes, which have the form:

$$Y_\alpha = \begin{pmatrix} \alpha_{11} & \cdots & \alpha_{1Mest} \\ \vdots & \ddots & \vdots \\ \alpha_{N1} & \cdots & \alpha_{NMest} \end{pmatrix} \qquad Y_A = \begin{pmatrix} A_{11} & \cdots & A_{1Mest} \\ \vdots & \ddots & \vdots \\ A_{N1} & \cdots & A_{NMest} \end{pmatrix}$$
$$Y_\omega = \begin{pmatrix} \omega_{11} & \cdots & \omega_{1Mest} \\ \vdots & \ddots & \vdots \\ \omega_{N1} & \cdots & \omega_{NMest} \end{pmatrix} \qquad Y_\varphi = \begin{pmatrix} \varphi_{11} & \cdots & \varphi_{1M} \\ \vdots & \ddots & \vdots \\ \varphi_{N1} & \cdots & \varphi_{NMest} \end{pmatrix} \tag{4}$$

where rows of each matrix $\boldsymbol{Y}$ are representing individual estimations of particular realizations, the number of realizations is equal to $N$. Columns represent unsorted parameters of estimated FIDs. The number of columns means number of estimated FIDs specified in initial condition. $\boldsymbol{Y}_\alpha$ denotes matrix of damping parameters, $\boldsymbol{Y}_A$ is matrix of amplitudes, $\boldsymbol{Y}_\omega$ stands for matrix of angular frequencies and $\boldsymbol{Y}_\varphi$ denotes matrix of initial phases.

From parametric matrixes is generated a power matrix $\boldsymbol{P}$ as a basis for power sorting criteria. The matrix is given by formula:

$$P_{n,m} = \sum_{k=0}^{N-1} (A_{n,m} \exp(\alpha_{n,m}.k.T) \cos(\omega_{n,m}.k.T + \varphi_{n,m}))^2 \tag{5}$$

For computed power matrix the sorting procedure for each row is applied. Elements are ordered from most significant to negligible. In case of an implementation in Matlab environment it is proper to use the "sort" function. From each row sorting operation an index vector is provided. It is a link from an old element position to a new element position, and in general it has a form:

$${}_{Psort} I_n = per(1,2 \ldots M_{est}) \tag{6}$$

where per stands for permutation of an old elements positions in the power matrix. From index vectors it is possible to order parametric matrixes:

$$\begin{aligned} {}_{Psort}Y_\alpha(n,m) &= Y_\alpha(n, I(n,m)) \\ {}_{Psort}Y_A(n,m) &= Y_A(n, I(n,m)) \\ {}_{Psort}Y_\omega(n,m) &= Y_\omega(n, I(n,m)) \\ {}_{Psort}Y_\varphi(n,m) &= Y_\varphi(n, I(n,m)) \end{aligned} \tag{7}$$

As a result we have parametric matrixes sorted by power of individual FIDs. Now it is up to be determined, which elements are real and which redundant – it is determined by the noise level threshold.

The threshold is derived from the power of noise contained in processed signal NMR – most often we have a separate noise channel. The noise level threshold is compared with power matrix and produces a column index Mreal enables real and valid FIDs to second level

amplitude sorting. The Mreal threshold is given by the formula:

$$M_{real} = ({}_{sort}P_{n,m} > \sum_{k=1}^{K} \mu.e_k^2)\Big|_{m\max} \tag{8}$$

where $\boldsymbol{P}$ denotes sorted power matrix, $\boldsymbol{e}$ denotes individual noise realization samples, $K$ means number of samples. μ stands for real value constant including margin for the lowest significant acceptable valid FID, based on experimental results.

## 3 SECOND LEVEL SORTING CRITERIAS

Parametric matrixes from the first level power sorting (7) are now splitted vertically by column index $M_{\text{real}}$, their left sides are processed in additional criteria sorting procedure.

Second level sorting procedure has the same flow as described in the power sorting, but the reference power matrix is replaced by an amplitude parametric (in case additional amplitude criteria) matrix and the whole process is applied on the real parameters only. In other words the sorting order and creating new swapping index vectors is derived from matrix ${}_{\text{Psort}}\boldsymbol{Y}_{\text{A}}(n,m)$ with dimension $\{N,M_{\text{real}}\}$.

Final parameters are presented as a composite of power – amplitude (phase, damping, frequency) sorted parametric matrixes appended by redundant parameters matrixes for convenience (for residual estimation). Most convenient power – amplitude sorting approach is called PA sort and was presented previously in AMIS engineering forum [4].

## 4 OBSERVATIONS, RESULTS

Using proposed sorting approach is usefull only in cases of unsorted parameters, in another cases it is useless. For example, shuffle of parametric order is observed at output parameters produced by AMARES, LPSVD, VARPRO implementations in profesional biomedical software package called jMRUI (Java Magnetics Resonance User Interface). Output parameters are shuffled in case of multiexponential input signals. They are at the same frequency, zero frequency, which is confusing for original implemented sorting procedure in jMRUI. So for these multiexponencial parameters it is a quite good reason to apply this.

An example of multiexponential output parameters has been choosen for demonstration. Input parameters was obtained from jMRUI v.1.3. First, four noisy realizations of signal NMR containing two exponential FIDs was processed by nonlinear parameter estimation AMARES algorithm. Output of AMARES from each realization is parametric vector xn. Each parametric vector serves as an input for sorting procedure. Each new realization generize a new parametric vector, from them it is easy to create parametric matrixes stated in (4). Tab. 1 shows PA sort application on signal NMR containing two parametrically similar FIDs with an eye to noise level in the signal. Estimations are achieved from four realizations of discussed signal, noise level is set to 10% from the lowest amplitude of FIDs and has the uniform distribution. Signal has 512 samples with a sampling interval 10ms. Because before estimation exact number of estimated components is not known, IC is specified for four FIDs. After estimation redundant parameters are shuffling with real parameters. Redundant components can have some of the parameters close to real components in general, compensated by rest of the parameters to its contribution to be negligible as is shown in some redundant estimations.

| Original parameters | | 1.FID | 2.FID | 3.FID | 4.FID |
|---|---|---|---|---|---|
| Amplitudes | | 10 | 15 | - | - |
| Dampings | | -0,9 | -2,8 | - | - |
| Estimation of parameters using nonlinear processing, 4 noisy realizations | | | | | |
| Amplitudes | Realization | γ.FID | δ.FID | ε.FID | ζ.FID |
| | 1. | 15,30 | 0,03 | 10,25 | 0,11 |
| | 2. | 8,21 | 0,27 | 13,21 | 16,76 |
| | 3. | 15,17 | 10,25 | 0,04 | 0,00 |
| | 4. | 10,03 | 0,17 | 14,40 | 0,05 |
| Dampings | Realization | γ.FID | δ.FID | ε.FID | ζ.FID |
| | 1. | -2,8115 | 0 | -0,9050 | -0,2635 |
| | 2. | -0,8391 | -2,6265 | -62,6266 | -2,4854 |
| | 3. | -2,7817 | -0,9137 | 0 | 0 |
| | 4. | -0,9008 | -1,4018 | -2,7930 | -0,0861 |
| PA sort of estimated parameters | | | | | |
| Amplitudes | Realization | 1.FID | 2.FID | 3.FID | 4.FID |
| | 1. | 10,25 | 15,30 | 0,11 | 0,03 |
| | 2. | 8,21 | 16,76 | 0,27 | 13,21 |
| | 3. | 10,25 | 15,17 | 0,04 | 0,00 |
| | 4. | 10,03 | 14,40 | 0,05 | 0,17 |
| Dampings | Realization | 1.FID | 2.FID | 3.FID | 4.FID |
| | 1. | -0,9050 | -2,8115 | -0,2635 | 0 |
| | 2. | -0,8391 | -2,4854 | -2,6265 | -62,6266 |
| | 3. | -0,9137 | -2,7817 | 0 | 0 |
| | 4. | -0,9008 | -2,7930 | -0,0861 | -1,4018 |

**Tab. 1:** *Example of sorted results*

## 5 CONCLUSION

Proposed sorting solution is intended as a postprocessing method for cases of shuffled parameters produced from signal fitting algorithms. Significance of the method is rising in statistical signal processing. Method is not bounded necessarily on biomedical signal processing.

The essential part of the paper was previously introduced in AMIS Engineering forum 2005 conference held in Oudenaarde (Belgium) / Pocatello (USA).

## REFERENCES


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