Performances estimation for tensor CP decomposition with structured factors
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To cite this version:

HAL Id: hal-01072538
https://hal.archives-ouvertes.fr/hal-01072538v2
Submitted on 25 Aug 2015

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ABSTRACT

The Canonical Polyadic decomposition (CPD), also known as Candecomp/Parafac, is very useful in numerous scientific disciplines. Structured CPDs, i.e. with Toeplitz, circulant, or Hankel factor matrices, are often encountered in signal processing applications. As subsequently pointed out, specialized algorithms were recently proposed for estimating the deterministic parameters of structured CP decompositions. A closed-form expression of the Cramér-Rao bound (CRB) is derived, related to the problem of estimating CPD parameters, when the observed tensor is corrupted with an additive circular i.i.d. Gaussian noise. This CRB is provided for arbitrary tensor rank and sizes. Finally, the proposed CRB expression is used to assess the statistical efficiency of the existing algorithms by means of simulation results in the cases of third-order tensors having three circulant factors on one hand, and an Hankel factor on the other hand.

Index Terms— Multilinear Algebra, Tensor Decomposition, Performance Analysis, Cramér-Rao bound, Structured matrix

1. INTRODUCTION

An increasing number of signal processing applications deal with multidimensional data like polarimetric STAP [1], multidimensional harmonic retrieval [2, 3, 4] or tensor coding [5]. Multilinear algebra [6] provides a good framework to exploit these data [7, 2] by conserving the multidimensional structure of the information. Nevertheless, generalizing matrix-based algorithms to the multilinear algebra framework is not a trivial task. In particular, there exist several multilinear extensions of the Singular Value Decomposition (SVD), each enjoying only some properties of the matrix SVD.

The Canonical Polyadic decomposition (CPD), also sometimes referred to as Candecomp/Parafac and defined in Section 1.2, may be seen as one possible extension of the Singular Value Decomposition (SVD) to the multilinear case; see [8] and references therein. It decomposes a tensor into a sum of \( R \) rank-one tensors, which can also be written as matrix factors. In addition, unlike SVD, it is essentially unique under mild conditions. Therefore, it is naturally well suited for the analysis of data sets constituted by observations of a function of multiple discrete indices, as encountered in signal processing [9, 10, 11], data mining [12] and biomedical engineering [13]; see [8, 14] for other examples.

The factors entering the CPD are usually not assumed to be structured and all their elements have to be estimated. However, practical problems are encountered where the factor matrices have a structure [15, 16, 17] such as Toeplitz, circulant, Hankel or Vandermonde. In order to fill this gap, several algorithms have been proposed, including non iterative [16, 18] or iterative, e.g. exploiting a circulant structure [19].

It seems interesting to evaluate this kind of algorithms in the presence of Gaussian white noise by comparing them to their Cramér-Rao Bound [20]. The CPD Cramér-Rao bound has been derived for unstructured factor matrices [21], and for specific applications in antenna array processing [22]. Yet, the presence of structure in factor matrices not only reduces the number of indeterminacies, but also the number of parameters to estimate. The calculation of the CRB hence needs additional tools, and specific algorithms can be used for estimating the parameters.

In this paper, we derive the CRB for tensor CP decomposition with both structured (Hankel, Toeplitz and Toeplitz circulant) and unstructured factors. First, a model corresponding to this configuration is introduced. The identifiability conditions of this model are quoted. Two algorithms dedicated to the CP computation with structured factors are presented. Then, the CRB is derived, and especially a closed-form expression is proposed. Finally, some numerical simulations, which show the validity of our formula, are presented.

1.1. Notations

We assume the following notation throughout the paper: scalars are denoted by lowercase letters, e.g. \( \theta \), or \( a_{ij} \), vectors by lowercase boldface, e.g. \( \theta \) or \( a_{.j} \), matrices by boldface capitals, e.g. \( \mathbf{B} \) or \( \mathbf{A}^{(n)} \), and higher order arrays by calligraphic letters, e.g. \( \mathbf{X} \). We use the superscripts \( T \) for transposition, \( \dagger \) for pseudo-inverse, \( \boxtimes \) and \( \oslash \) denote the Kronecker and Khatri-Rao products, respectively, and \( \otimes \) stands for the (tensor) outer product. For our purpose, a tensor \( \mathbf{X} \) of order \( N \) will be assimilated to its array of coordinates, which is indexed by \( N \) indices. Its entries will be denoted by \( x_{i_1,\ldots,i_N} \).

1.2. CP decomposition

Let \( \mathbf{X} \) be a tensor of order \( N \). Its Canonical Polyadic (CP) decomposition is defined by:

\[
\mathbf{X} = \sum_{r=1}^{R} a_r^{(1)} \otimes a_r^{(2)} \otimes \ldots \otimes a_r^{(N)} \tag{1}
\]

where \( a_r^{(n)} \) is the \( r \)th column of \( \mathbf{A}^{(n)} \in \mathbb{R}^{I_n \times R} \). The minimal value of \( R \) such that \( \mathbf{X} \) can be written as in (1) is called the rank of \( \mathbf{X} \). The CP decomposition may be seen as one possible extension of the Singular Value Decomposition (SVD) of matrices; see [8] and references therein.
2. ANALYTICAL OXCRB FOR CP MODEL WITH UNSTRUCTURED FACTORS

2.1. Alternative expression for the CP decomposition with (un)structured factors

We consider a third-order tensor $\mathbf{Y} \in \mathbb{R}^{I \times J \times K}$, following model (1) up to an additional noise tensor $\mathbf{N}$ with circular i.i.d. Gaussian entries of variance $\sigma^2$:

$$\mathbf{y} = \mathbf{X} + \mathbf{N}. \quad (2)$$

The factor matrices of $\mathbf{X}$ are denoted $A^{(n)} = [a^{(n)}_1, \ldots, a^{(n)}_N] \in \mathbb{R}^{I_n \times R}$, $1 \leq n \leq N = 3$. The aim of this section is to derive the CRB of this model when some factors are structured. Throughout the rest of the paper, the equivalent vector model will be considered:

$$\mathbf{y} = \text{vec} (\mathbf{y}) = \text{vec} (\mathbf{X}) + \text{vec}(\mathbf{N}) = \mathbf{x}(\theta) + \mathbf{n}, \quad (3)$$

where $\mathbf{x}(\theta) = \sum_{r=1}^{R} a^{(1)}_r \otimes a^{(2)}_r \otimes a^{(3)}_r$. A model corresponding to this case is proposed in the following proposition.

**Lemma 2.1** Let $\mathbf{X} \in \mathbb{R}^{I_1 \times I_2 \times I_3}$ be a third-order tensor, and $\mathbf{x} = \text{vec}(\mathbf{X})$. The matrices $A^{(1)}$, $A^{(2)}$ and $A^{(3)}$ are assumed to be unknown and some of them may be structured (Hankel, Toeplitz or Toeplitz circulant). Also denote by $\theta$ the vector containing the parameters of interest, which can be written as:

$$\theta^T = \left[ \theta_1^T, \theta_2^T, \theta_3^T \right], \quad (4)$$

with $\theta_n \in \mathbb{R}^{I_n}$, where $U_n$ is the number of free parameters describing matrix $A^{(n)}$ (which depends on the structure of the matrix, see Table 1). Because the matrices we consider (unstructured, Hankel, Toeplitz, or Toeplitz circulant) form a linear space, it is always possible to write each column $a^{(n)}$ of $A^{(n)}$, as follows:

$$a^{(n)} = S^{(n)} \theta_n, \quad (5)$$

where $S^{(n)} \in \mathbb{R}^{I_n \times U_n}$ depends on the structure of $A^{(n)}$ (see Table 1).

Then it is possible to rewrite $\mathbf{x}(\theta)$ as follows:

$$\mathbf{x}(\theta) = \left( \sum_{r=1}^{R} S^{(1)}_r \otimes S^{(2)}_r \otimes S^{(3)}_r \right) \left[ \theta_1 \otimes \theta_2 \otimes \theta_3 \right].$$

Note that the above Lemma means that any CP model can be rewritten as a linear model with respect to $f(\theta)$. This compact expression allows to considerably simplify the derivation of the presented MSE lower bound.

2.2. Identifiability

Even when the CP decomposition is unique, in the sense that there is a unique $R$-plet of rank-1 tensors satisfying (1), there generally exist infinitely many ways of writing a rank-1 tensor as an outer product of vectors. In fact, there generally exist $\sum_{n=1}^{N} I_n - 1$ scaling indeterminacies, each represented by a $R \times R$ diagonal matrix. It turns out that these indeterminacies can be partly fixed by the structure of factor matrices. For instance, since the structures we are interested in are not preserved by post-multiplication by invertible matrices, one can impose one entry in each factor matrix $A^{(n)}$ to be equal to one [18]. And because of the structure, this fixes other entries as well.

If $P_n$ denotes the number of known elements in $A^{(n)}$, the vector of unknown parameters is now denoted $\hat{\theta} \in \mathbb{R}^{U_1+U_2+U_3}$, where $U_1 = U_2 = P_2$ and $U_3 = P_3$. It can be related to the vector $\theta$, which contains all model parameters thanks to a selection matrix $B \in \mathbb{R}^{(U_1+U_2+U_3) \times (U_1+U_2+U_3)}$:

$$\hat{\theta} = B \theta. \quad (6)$$

Local identifiability of the parameter $\hat{\theta}$ is ensured if the Jacobian of the corresponding log-likelihood is full rank, or equivalently, if the Fisher information matrix is invertible. In this respect, Cramér-Rao bounds indicate how far we are from the identifiability limit.

**Remark.** Since the order in which rank-1 terms are added in (1) does not matter, the columns of factor matrices $A^{(n)}$ can be affected by a common permutation. This indeterminacy is not part of the model identifiability. On the other hand, it must be taken into account in computer experiments to access performances.

2.3. CP computation with structured factor matrices

2.3.1. Non iterative algorithm

In this section, we briefly describe how to compute the CP decomposition in a non iterative manner when one factor matrix, say $A^{(3)}$, is structured, and when $R$ is not too large, the upper bound being given by [18]:

$$I_3 R \geq R^2 + U_3 - 1.$$ 

By unfolding tensor $\mathbf{X}$ properly into $I_1 \times I_2 I_3$ matrix $\mathbf{X}_3$, we have the well known relation $\mathbf{X}_3 = A^{(3)} (A^{(2)} \otimes A^{(1)})^T$. On the other hand, relating this to its SVD $\mathbf{X}_3 = \Sigma \mathbf{V}^H$ leads to two equations, in which matrix $\mathbf{N}$ is unknown invertible:

$$N^{-1} \Sigma \mathbf{V}^H = (A^{(2)} \otimes A^{(1)})^T \text{ and } \mathbf{UN} = A^{(3)}. \quad (7)$$

The point is that the second equation can be solved for both $\mathbf{N}$ and $A^{(5)}$ if matrix $A^{(3)}$ is structured. In fact, since $A^{(3)}$ is linearly structured, it can be written as $A^{(3)} = E_1 + \sum_{r=2}^{R} y_r E_r$, where $\{E_1\}^{U_3}_{i=1}$ is a given basis. Then, it suffices to solve the linear system of $I_3 R$ equations in $R^2 + U_3 - 1$ unknowns:

$$\mathbf{M} \left[ \begin{array}{c} \text{vec}(\mathbf{N}) \\ \mathbf{y}_r \end{array} \right] = -\text{vec}(\mathbf{E}_1),$$

where $\mathbf{M} = [-I_R \otimes \mathbf{U}, \text{vec}(E_2), \ldots, \text{vec}(E_{U_3})]$, and $\mathbf{y}_r$ denotes the vector of dimension $U_3 - 1$ whose entries are $y_{r}$. Once $\mathbf{N}$ and $\mathbf{y}_r$ have been obtained, the first equation allows to compute matrices $A^{(1)}$ and $A^{(2)}$ via $R$ successive rank-1 matrix approximations. To

| Table 1. Characteristics of the matrix $A^{(3)}$ for several structures. |
|---------------------------------|------------------|
| $U_n$ | $S^{(3)}$ |
| Unstructured | $I_n \times I_n (r-1)$ | $I_n \otimes I_n (r-1)$ |
| Hankel | $I_n + R - 1$ | $0_{I_n \times (r-1)}$ with $\Psi_n = [I_n \otimes I_n (n-1)]$ |
| Toeplitz | $I_n + R - 1$ | $[I_n \otimes I_n (n-1)]$ where $A_{n1}$ is the $I_n \times I_n$ matrix with ones on its anti-diagonal and zeros elsewhere. |
| Circulant | $I_n - 1$ | $I_{n-1} \times I_{n-1}$ |

$\otimes$ means the Kronecker product.
see this, let $F = (N^{-1} SVH^T)^T$. Matrix $F$ is now known, and $\mathbf{F} = \mathbf{A}^{(2)} \odot \mathbf{A}^{(1)}$. This means that if we unfold each column $f_i$ of $F$, we should have a rank-one matrix:

$$\text{Unvec}(f) = a_{\mathbf{n}^{(2)}} a_{\mathbf{n}^{(1)}}^T$$

In other words, the $R$ columns of matrices $\mathbf{A}^{(1)}$ and $\mathbf{A}^{(2)}$ can be obtained by $R$ successive rank-one matrix approximations. The algorithm hence terminates within a finite number of steps.

### 2.3.2. Iterative CALS Algorithm

Now, when all factor matrices are structured, the previous algorithm cannot be executed, and we must resort to an iterative procedure. Let us consider circulant matrix factors $\mathbf{A}^{(n)} \in \mathbb{R}^{I_n \times R}$ defined as

$$\mathbf{A}^{(n)} = \begin{bmatrix} \theta_n & \Pi_n \theta_n & \cdots & \Pi_n^{R-1} \theta_n \end{bmatrix},$$

where $n \in \mathbb{R}^{I_n}$ is its generating vector, $\Pi_n$ is the $I_n \times I_n$ permutation matrix defined in the last row of Table 1, and $S^{(n)} = \Pi_n^{-1}$. A circulant-constrained ALS (CALS) algorithm was derived in [19] by considering a particular basis $\{E^{(n)}_k\}_{k=1}^{I_n}$ for the subspace of circulant $I_n \times R$ matrices, with the canonical basis vector $e^{(n)}_k$ of $\mathbb{R}^{I_n}$ as generating vector of $E^{(n)}_k$. Defining $E^{(n)} = \text{vec}(E^{(n)}_1) \cdots \text{vec}(E^{(n)}_{I_n}) \in \mathbb{R}^{I_n \times I_n}$, the CALS algorithm is summarized below.

**Inputs:** $X \in \mathbb{R}^{I_1 \times I_2 \times I_3}$, rank $R$ and initial generating vectors $\theta^{(0)}_1, \theta^{(0)}_2, \theta^{(0)}_3$.

**Outputs:** Circulant $I_n \times R$ complex matrix factors $\mathbf{A}^{(1)}, \mathbf{A}^{(2)}, \mathbf{A}^{(3)}$.

Recursion until convergence:

$$\theta^{(i)}_1 = \frac{1}{R} E^{(1)}^T (I_{R} \otimes X_1) \text{vec}\left(\left[\mathbf{A}^{(3)}_{k=1} \odot \mathbf{A}^{(2)}_{k=1} \right]^{T}\right)$$

$$\theta^{(i)}_2 = \frac{1}{R} E^{(2)}^T (I_{R} \otimes X_2) \text{vec}\left(\left[\mathbf{A}^{(3)}_{k=1} \odot \mathbf{A}^{(1)}_{k=1} \right]^{T}\right)$$

$$\theta^{(i)}_3 = \frac{1}{R} E^{(3)}^T (I_{R} \otimes X_3) \text{vec}\left(\left[\mathbf{A}^{(2)}_{k=1} \odot \mathbf{A}^{(1)}_{k=1} \right]^{T}\right)$$

where $X_i, i \in \{1, 2, 3\}$, denotes the mode-$i$ matrix unfolding of $X$, and the estimate $\mathbf{A}^{(n)}_i$ of $\mathbf{A}^{(n)}$ at iteration $i$ is formed in replacing $\theta_n$ by $\theta^{(i)}_n$ in (7).

### 2.4. Closed-form expression of the CRB

In this section, we derive the deterministic CRB for the vectorized model given in (3) for the parameters of interest given in (4). We follow the ideas introduced in [23]. Let $C(\theta)$ be the CRB matrix, the global Mean Square Error of any (locally) unbiased estimator $\hat{\theta}(y)$, admits the following lower bound [20]:

$$\text{E} \left[ \| \theta - \hat{\theta}(y) \|^2 \right] \geq \text{Tr}(C(\theta)) = \sum_{n=1}^{3} \sum_{k=1}^{U_n} \text{CRB}(\theta_n(k))$$

where $\text{CRB}(\theta_n(k))$ is given by the diagonal terms of matrix $C(\theta)$. Using the assumptions on the noise probability density function (pdf) and Lemma 2.1, the observation vector pdf is also Gaussian according to $y \sim N(\Phi f(\theta), \sigma^2 I)$. According to the Slepian-Bangs formula (see [24], equation B.3.3), the CRB matrix can be given with respect to the Jacobian of $\mathbf{x}(\theta) = \Phi f(\theta)$ according to

$$C(\theta) = \sigma^2 \left( J(\theta)^T J(\theta) \right)^{-1}$$

where

$$J(\theta) = [J_1(\theta) \ J_2(\theta) \ J_3(\theta)]$$

with $J_n(\theta)$ contains the derivative of $\mathbf{x}(\theta)$ with respect to $\theta_n(k)$. More precisely, we obtain

$$J_1(\theta) = \Phi(I_{I_1} \otimes \theta_2 \otimes \theta_3),$$

$$J_2(\theta) = \Phi(\theta_1 \otimes I_{U_2} \otimes \theta_3),$$

$$J_3(\theta) = \Phi(\theta_1 \otimes \theta_2 \otimes I_{U_3}).$$

To provide against a singular CRB matrix [25], we have to take into account the indeterminacy conditions introduced in section 2.2. In the next Lemma, we present some relation of the Jacobian with respect to selection and permutation matrices.

**Lemma 2.2** Let $\hat{\theta} = \begin{bmatrix} \hat{\theta}_1^T \hat{\theta}_2^T \hat{\theta}_3^T \end{bmatrix}^T$ be the vector of unknown model parameters, $B$ the associated selection matrix and $\Pi_k^{(n)} \in \mathbb{R}^{(U_1+U_2+U_3) \times (U_1+U_2+U_3)}$ the permutation matrix which moves the $k^{th}$ element of $\theta_n$, such as $\Pi_k^{(n)} \hat{\theta} = [\hat{\theta}_n(k) \hat{\theta}_n(1) \ldots \hat{\theta}_n(k-1) \hat{\theta}_n(k+1) \ldots \hat{\theta}_n(U_n)] \hat{\theta}_n^{(k)} \hat{\theta}_n^{(k)}^{T}$ with $1 \leq n \neq n' \neq n'' \leq 3$.

The relation between the Jacobian considered for vector $\Pi_k^{(n)} \hat{\theta}$ and $\theta$ is given by

$$J \left( \Pi_k^{(n)} B \theta \right) = J \left( \hat{\theta} \right) \Pi_k^{(n)^T}$$

where $J \left( \hat{\theta} \right) = J(\theta)B^T$.

**Proof.** The proof is straightforward. It is clear that $B$ and $\Pi_k^{(n)}$ will remove and permute the columns of $J$ similarly to the elements of $\theta$.

**Proposition 2.1** The closed-form expression of the lower bound on the global MSE is given by

$$\text{E} \left[ \| \hat{\theta} - \theta(y) \|^2 \right] \geq \sum_{n=1}^{3} \sum_{k=1}^{U_n} \text{CRB}(\theta_n(k))$$

where the CRB for the $k^{th}$ element of vector $\theta_n$ is given by

$$\text{CRB}(\theta_n(k)) = \frac{\sigma^2}{\text{vec}(P^T_{\mathbf{G}_{k,n}^{(1)}} \mathbf{G}_{k,n}^{(1)} \mathbf{G}_{k,n}^{(1)})},$$

where $\mathbf{P}_{\mathbf{G}_{k,n}^{(1)}}^{(1)} = \mathbf{I}_{U_1 U_2 U_3} - \mathbf{G}_{k,n}^{(1)} \mathbf{G}_{k,n}^{(1)}$ with

$$J \left( \Pi_k^{(n)} B \theta \right) = \left[ \mathbf{G}_{k,n} \mathbf{G}_{k,n} \right]$$

the partitioned Jacobian matrix.

**Proof.** The crux of the proof relies on the use of the permutation matrix $\Pi_k^{(n)}$. First note that using the invariance of the trace operator to any permutations, the trace of $C(\hat{\theta})$ is equal to the trace of the
permutated matrix $\Pi_k^{(n)^T} C(\tilde{\theta}) \Pi_k^{(n)}$. Now, using expression (9) for vector $\tilde{\theta}$, we have

$$
\Pi_k^{(n)^T} C(\tilde{\theta}) \Pi_k^{(n)} = \sigma^2 \Pi_k^{(n)^T} \left( J(\tilde{\theta})^T J(\tilde{\theta}) \right)^{-1} \Pi_k^{(n)} \tag{18}
$$

$$
= \sigma^2 \left( J(\tilde{\theta}) \Pi_k^{(n)^T} \right)^T \left( J(\tilde{\theta}) \Pi_k^{(n)} \right)^{-1} \tag{19}
$$

$$
= \sigma^2 \left( J \left( \Pi_k^{(n)^T} B\theta \right)^T J \left( \Pi_k^{(n)} B\theta \right) \right)^{-1} \tag{20}
$$

$$
= C(\Pi_k^{(n)^T} B\theta) \tag{21}
$$

where to obtain equality $(a)$ we use Lemma 2.2. Finally, using the partition of the Jacobian (see (17)) in expression (20), we obtain

$$
\text{CRB}(\tilde{\theta}_n(k)) = \left[ C(\Pi_k^{(n)^T} B\theta) \right]_{11} \tag{22}
$$

$$
= \sigma^2 \left[ \frac{\| g_{k,n} \|^2}{G_{g,k,n}^T G_{g,k,n}} \right]_{11} \tag{23}
$$

So, the CRB for $\tilde{\theta}_n(k)$ given in (16) is obtained by using the inverse of the block-matrix (23) with respect to its $(1, 1)$-th element. Using (18)-(23), we conclude that

$$
\text{Tr} \left( C(\tilde{\theta}) \right) = \text{Tr} \left( C(\Pi_k^{(n)^T} B\theta) \right) = \sum_{i=1}^{3} \sum_{k=1}^{R} \text{CRB}(\tilde{\theta}_n(k)). \tag{24}
$$

3. NUMERICAL SIMULATIONS

In order to illustrate our theoretical results, we compute the CRB for two cases: (i) three factors are Toeplitz circulant and (ii) one factor is Hankel and two factors are unstructured. More precisely, for the two cases the CRB is compared to the associated global MSE given by the algorithms presented in Section 2.3. The global MSE are computed thanks to Monte-Carlo simulations with $N_{rea} = 1000$ realizations for several values of $\sigma^2$.

3.1. Three Toeplitz circulant matrices

In this case, the three matrices $A^{(1)}$, $A^{(2)}$ and $A^{(3)}$ are Toeplitz circulant. All the dimensions are equal to 5. In order to ensure identifiability, the following parameters are assumed to be known: $\theta_1(1) = \theta_2(1) = 1$. The results are presented in Figure 1, and show the validity of our formula since the CRB and the MSE match perfectly for low noise variance. For the lowest values, there is a gap, which is normal since the CRB is only valid for low noise variance.

3.2. One Hankel matrix and two unstructured matrices

In this case, the matrix $A^{(3)}$ is Hankel structured and the matrices $A^{(1)}$ and $A^{(2)}$ have no structure. The parameters are: $I_3 = 10$, $I_2 = 11$, $I_1 = 12$ and $R = 3$. In order to ensure identifiability, the first element of $\theta_3$ is assumed to be known and equal to $\theta_3(1) = 1$ (that is, the main anti diagonal of the Hankel matrix is formed of ones), and all elements of the first line of $A^{(1)}$ are equal to one, without restricting the generality. The results are presented in Figure 2. They show the validity of our formula since the CRB and the MSE match perfectly for high values of $\sigma^2$.

4. CONCLUSION

In this paper, we derived a closed-form CRB expression for the estimation of structured (Hankel, Toeplitz or Toeplitz circulant) or unstructured factors involved in the CP decomposition of arbitrary rank and sizes. The derived bound is useful as a touchstone against which the efficiency of the iterative and non-iterative algorithms dedicated to the estimation of structured factors in the CP model. This work has set the basis for several developments. A more general model, taking into account random amplitudes in the CP decomposition would allow to derive an Hybrid CRB and to consider other applications like parameter estimation of Wiener-Hammerstein models from their associated Volterra kernels [19] and blind channel identification using output cumulant tensors [10].
5. REFERENCES


