

Gaussian Graphical Models For Proper Quaternion Distributions

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Abstract—In this paper we extend Gaussian graphical models to proper quaternion Gaussian distributions. The properness assumption reduces the number of unknowns by a factor of four and allow for improved accuracy. We begin by showing that the unconstrained proper quaternion maximum likelihood problem is convex and has a closed form solution that resembles the classical sample covariance. Then, we proceed and add convex sparsity constraints to the inverse covariance matrix and minimize them using convex optimization toolboxes. Finally, we show that in the special case of chordal graphs, the estimates follow a simple closed form which aggregates the unconstrained solutions in each of the cliques. We demonstrate the performance of our suggested estimators on both synthetic and real data.

Index Terms—Quaternions, covariance estimation, graphical models, chordal graphs

I. INTRODUCTION

Covariance estimation is a fundamental problem in the field of statistical signal processing, and many algorithms for detection and estimation rely on accurate solutions to this problem [1], [2]. When the number of samples is larger than the matrix dimension, the Gaussian maximum likelihood (ML) coincides with the sample covariance estimator and the problem can be easily solved. However, in many modern applications this assumption does not hold and we are faced with high dimensional parameter estimation from a small number of samples. The standard approach to such scenarios is to reduce the degrees of freedom by imposing low order models. Gaussian graphical models reduce the number of unknowns by assuming sparsity on the inverse covariance matrix. Proper models reduce the degrees of freedom by imposing symmetry constraints. In this paper, these two types of structures are combined into proper quaternion Gaussian graphical models.

The main idea of graphical models is to represent a multivariate probability distribution over a set of random variables, exploiting its underlying structure stemming from conditional independence properties. A Markov network is a graph whose vertices represent random variables and whose edges represent conditional statistical independence. Two variables are statistically independent given the rest if there is no edge between their vertices. In case of a Gaussian distribution this is equivalent to a sparse inverse covariance matrix. The maximum likelihood estimation of the inverse covariance with known sparsity constraints is convex, whereas the problem of learning the sparsity pattern can be solved via convex L_1 norm structure learning [3]. When the graphical model is chordal

(also known as decomposable), the minimization has a closed form solution which aggregates the local estimates in each of the cliques of the graph [4]–[7].

Quaternions are a four element generalization of complex numbers and allow for convenient and effective statistical modeling of multichannel signals. The need to better model such signals stems from several technological developments that require handling of four element signals. One such example is a radar with two polarizations. Recent work on quaternion signal processing with includes [8], [9].

In this paper, we combine Gaussian graphical models with the proper quaternion structure. First, we show that the proper quaternion Gaussian assumption reduces the number of unknowns in the covariance estimation problem by four. We then prove that for proper quaternion Gaussian random variables, the problem of sparse inverse covariance estimation is convex and can be solved using off-the-shelf optimization packages. In addition, in the important case of chordal graphs, the minimization has a simple closed form solution that aggregates the unconstrained proper solution on each of the cliques. As a byproduct, we prove that the strong product of a chordal graph with a graph represented by a square matrix of ones is chordal. This paper is the short version of [10], where all further details and proofs can be found.

II. PROPERNESS

We begin with a brief overview of the concept of properness. A zero mean complex random vector is called proper if its probability distribution is invariant to rotations. Similarly, a zero mean quaternion random vector is called proper if its probability distribution is invariant to a specific type of rotation. Quaternion variables are an extension of complex numbers to hyper-complex numbers with 4 elements. A quaternion matrix has one real part and three imaginary parts:

$$\mathbf{Z} = \mathbf{A} + i\mathbf{B} + j\mathbf{C} + k\mathbf{D}. \quad (1)$$

Multiplication by a unit norm quaternion is equivalent to a rotation. A general quaternion rotation requires both a left and a right multiplication

$$\mathbf{z}' = e^{\nu_1 \theta_1} \mathbf{z} e^{\nu_2 \theta_2} \quad (2)$$

with some pure imaginary unit quaternions ν_1 and ν_2 and some angles θ_1 and θ_2 . A standard definition of quaternion properness involves only the right rotation and assumes $\nu_1 = \theta_1 = 0$ (See [11], [12] for more details on this definition and its

complementary left rotation). Thus, in this paper, a quaternion is proper if the second order statistics of \mathbf{z} equals the second order statistics of $\mathbf{z}e^{\nu\theta}$ for all possible angles and for all pure unit quaternions ν , i.e.

$$\mathbf{z}e^{\nu\theta} \sim \mathbf{z} \quad (3)$$

It is convenient to represent the quaternion in (1) using three real-valued notations, see e.g. [13]:

$$\tilde{\mathbf{z}} = \begin{bmatrix} \mathbf{A} \\ \mathbf{B} \\ \mathbf{C} \\ \mathbf{D} \end{bmatrix} \quad \bar{\mathbf{z}} = \begin{bmatrix} \mathbf{A} & -\mathbf{B} & -\mathbf{C} & -\mathbf{D} \\ \mathbf{B} & \mathbf{A} & -\mathbf{D} & \mathbf{C} \\ \mathbf{C} & \mathbf{D} & \mathbf{A} & -\mathbf{B} \\ \mathbf{D} & -\mathbf{C} & \mathbf{B} & \mathbf{A} \end{bmatrix} \quad (4)$$

$$\hat{\mathbf{z}} = \begin{bmatrix} \mathbf{A} & -\mathbf{B} & -\mathbf{C} & -\mathbf{D} \\ \mathbf{B} & \mathbf{A} & \mathbf{D} & -\mathbf{C} \\ \mathbf{C} & -\mathbf{D} & \mathbf{A} & \mathbf{B} \\ \mathbf{D} & \mathbf{C} & -\mathbf{B} & \mathbf{A} \end{bmatrix}. \quad (5)$$

Hereinafter, we use the tilde, the overline and the hat operators to denote these three representations. Using these operators, a right quaternion rotation can be written as

$$\mathbf{z}' = \mathbf{z}e^{\nu\theta} \Leftrightarrow \tilde{\mathbf{z}}' = \mathbf{R}_{\nu\theta}\tilde{\mathbf{z}} \quad (6)$$

where $\mathbf{R}_{\nu\theta}$ is defined as $\mathbf{R}_{\nu\theta} = \widehat{e^{\nu\theta}} \otimes \mathbf{I}_p$. This leads to the following definition of properness: A covariance matrix \mathbf{C} is proper if $\mathbf{C} \in \mathbb{Q}_p$ where

$$\mathbb{Q}_p = \{\mathbf{C} \in \mathbb{R}_{++}^{4p \times 4p} : \mathbf{C} = \mathbf{R}_{\nu\theta}\mathbf{C}\mathbf{R}_{\nu\theta}^T \forall \nu : \|\nu\| = 1, \theta\}. \quad (7)$$

Note that this definition shows that quaternion properness is similar to the case of group symmetry as defined in [14]. This observation is actually the motivation for the current paper. Our first result is a simple equivalent condition for properness which involves only a finite number of constraints.

Lemma 1. An equivalent definition of \mathbb{Q}_p in (7) is

$$\mathbb{Q}_p = \{\mathbf{C} \in \mathbb{R}_{++}^{4p \times 4p} : \exists \mathbf{A}, \mathbf{B}, \mathbf{C}, \mathbf{D} : \mathbf{C} \text{ satisfies (9); } \mathbf{A} = \mathbf{A}^T; \mathbf{B} = -\mathbf{B}^T; \mathbf{C} = -\mathbf{C}^T; \mathbf{D} = -\mathbf{D}^T\} \quad (8)$$

where

$$\mathbf{C} = \begin{bmatrix} \mathbf{A} & -\mathbf{B} & -\mathbf{C} & -\mathbf{D} \\ \mathbf{B} & \mathbf{A} & -\mathbf{D} & \mathbf{C} \\ \mathbf{C} & \mathbf{D} & \mathbf{A} & -\mathbf{B} \\ \mathbf{D} & -\mathbf{C} & \mathbf{B} & \mathbf{A} \end{bmatrix} \quad (9)$$

In addition, since \mathbf{C} is positive definite then \mathbf{C}^{-1} is also positive definite and $\mathbf{C} \in \mathbb{Q}_p$ iff $\mathbf{C}^{-1} \in \mathbb{Q}_p$.

III. PROPER QUATERNION COVARIANCE ESTIMATION

In this section, we consider covariance estimation under properness constraints. The problem is to find the estimate that maximizes the likelihood of n independent and identically distributed realizations of a length $4p$ Gaussian random vector, denoted by $\tilde{\mathbf{z}}_1, \dots, \tilde{\mathbf{z}}_n$. The likelihood is given by

$$l(\mathbf{C}_{\tilde{\mathbf{z}}\tilde{\mathbf{z}}}) = \sum_{i=1}^n \tilde{\mathbf{z}}_i^T \mathbf{C}_{\tilde{\mathbf{z}}\tilde{\mathbf{z}}}^{-1} \tilde{\mathbf{z}}_i - n \log \det [\mathbf{C}_{\tilde{\mathbf{z}}\tilde{\mathbf{z}}}^{-1}]. \quad (10)$$

The following result provides closed form solutions to this optimization problem with and without proper constraints.

Theorem 1. Let $\tilde{\mathbf{z}} \in \mathbb{R}^{4p}$ be a Gaussian random vector with zero mean and a covariance $\mathbf{C}_{\tilde{\mathbf{z}}\tilde{\mathbf{z}}} \in \mathbb{Q}_p$, $\tilde{\mathbf{z}}$ the real representation vector of a quaternion $\mathbf{z} \in \mathbb{H}^p$. Consider the Gaussian ML problem

$$\min_{\mathbf{C}_{\tilde{\mathbf{z}}\tilde{\mathbf{z}}}} l(\mathbf{C}_{\tilde{\mathbf{z}}\tilde{\mathbf{z}}}). \quad (11)$$

If $n > 4p$ the solution exists with probability one and is

$$\mathbf{S} \triangleq \frac{1}{n} \sum_{i=1}^n \tilde{\mathbf{z}}_i \tilde{\mathbf{z}}_i^T, \quad (12)$$

otherwise the solution is unbounded. Next, consider the problem with an additional proper quaternion constraint

$$\begin{aligned} \min_{\mathbf{C}_{\tilde{\mathbf{z}}\tilde{\mathbf{z}}}} & l(\mathbf{C}_{\tilde{\mathbf{z}}\tilde{\mathbf{z}}}) \\ \text{s.t.} & \mathbf{C}_{\tilde{\mathbf{z}}\tilde{\mathbf{z}}} \in \mathbb{Q}_p \end{aligned} \quad (13)$$

If $n > p$ the solution to this problem exists with probability one and is

$$\mathbf{S}_h \triangleq \frac{1}{4n} \sum_{i=1}^n \bar{\mathbf{z}}_i \bar{\mathbf{z}}_i^T, \quad (14)$$

where $\bar{\mathbf{z}}_i \in \mathbb{R}^{4p \times 4}$ is the real matrix representation of \mathbf{z}_i . Otherwise the solution is unbounded.

In an attempt to further improve our estimation by taking into account additional prior knowledge, we move on to formulate quaternion Gaussian graphical models.

IV. PROPER QUATERNION GRAPHICAL MODELS

A modern approach to large scale covariance estimation modifies the optimization in order to exploit additional prior knowledge. In particular, Gaussian graphical models allow for additional sparsity constraints. The sparsity pattern is conveniently modeled via graphs. Let $G(V, E)$ be a graph with vertices $V = \{v_1, \dots, v_p\}$ and an edge set E . We say that a real valued p -variate Gaussian random vector \mathbf{x} follows $G(V, E)$ if \mathbf{x}_i and \mathbf{x}_j are conditionally independent given the rest of the elements in \mathbf{x} for all non-adjacent vertices in the graph. Using simple algebra this leads to $[\mathbf{K}]_{i,j} = 0 \quad \forall (i, j) \notin E$, where $\mathbf{K} = \mathbf{C}^{-1} \in \mathbb{R}^{p \times p}$ is the inverse covariance matrix.

Moving on to extend this to the quaternion case, let $\tilde{\mathbf{z}} \in \mathbb{R}^{4p}$ be the real representation of a proper quaternion Gaussian random vector with n observations $\tilde{\mathbf{z}}_1, \dots, \tilde{\mathbf{z}}_n \in \mathbb{R}^{4p}$. Let $\mathbf{C}_{\tilde{\mathbf{z}}\tilde{\mathbf{z}}}$ be the covariance matrix of $\tilde{\mathbf{z}}$, and let $G(V, E)$ be the associated graphical models with $4p$ nodes. From Lemma 1 we know that $\mathbf{K}_{\tilde{\mathbf{z}}\tilde{\mathbf{z}}} \in \mathbb{Q}_p$ leading to the following ML inverse covariance estimation problem

$$\begin{aligned} \min_{\mathbf{K}_{\tilde{\mathbf{z}}\tilde{\mathbf{z}}}} & l(\mathbf{K}^{-1}) \\ \text{s.t.} & \mathbf{K}_{\tilde{\mathbf{z}}\tilde{\mathbf{z}}} \in \mathbb{Q}_p \\ & [\mathbf{K}_{\tilde{\mathbf{z}}\tilde{\mathbf{z}}}]_{i,j} = 0 \quad \forall (i, j) \notin E. \end{aligned} \quad (15)$$

Using the characterization of \mathbb{Q}_p in Lemma 1, this is a convex minimization with a finite number of linear constraints. As such, it can be easily solved using existing convex optimization toolboxes, e.g., CVX [15], [16].

In some applications, it is more reasonable to assume that $\mathbf{K}_{\tilde{\mathbf{z}}\tilde{\mathbf{z}}}$ is sparse but the pattern is unknown. In this case, we can jointly detect the structure and estimate $\mathbf{K}_{\tilde{\mathbf{z}}\tilde{\mathbf{z}}}$ using sparsity enforcing penalties, e.g., the L_1 norm:

$$\begin{aligned} \min_{\mathbf{K}_{\tilde{\mathbf{z}}\tilde{\mathbf{z}}}} \quad & l(\mathbf{K}^{-1}) + \lambda \|\mathbf{K}_{\tilde{\mathbf{z}}\tilde{\mathbf{z}}}\|_1 \\ \text{s.t.} \quad & \mathbf{K}_{\tilde{\mathbf{z}}\tilde{\mathbf{z}}} \in \mathbb{Q}_p \\ & [\mathbf{K}_{\tilde{\mathbf{z}}\tilde{\mathbf{z}}}]_{i,j} = 0 \quad \forall (i,j) \notin E. \end{aligned} \quad (16)$$

V. PROPER QUATERNION CHORDAL MODELS

In this section we discuss the important case of chordal graphs. We will show that in this case the proper quaternion ML problem in (15) satisfies a closed form solution and does not require the use of optimization packages.

A graph is chordal (also known as decomposable) if it can be represented using a junction tree. A clique is a maximal subset of vertices that are fully connected and is denoted by C . A junction tree T is a tree whose vertices are usually referred to as nodes. Each node contains a subset of the graph vertices that form a clique (see [17]). We use the term separator to refer to the minimal separator between two sets, see [18, page 6].

To appreciate chordal graphical models, it is instructive to recall the standard chordal solutions for real-valued (non-quaternion) distributions. Consider the unconstrained optimization problem in (15), excluding the constraint $\mathbf{K}_{\tilde{\mathbf{z}}\tilde{\mathbf{z}}} \in \mathbb{Q}_p$ where E is the edge set of a chordal graph with cliques C_i and separators S_i . Its solution is [4, Proposition 5.9]

$$\mathbf{K}_{\tilde{\mathbf{z}}\tilde{\mathbf{z}}} = \sum_{k=1}^K \left[(\mathbf{S}_{C_k, C_k})^{-1} \right]^0 - \sum_{k=2}^K \left[(\mathbf{S}_{S_k, S_k})^{-1} \right]^0 \quad (17)$$

where \mathbf{S} is defined in (12), and the zero fill-in operator $[\cdot]^0$ outputs a matrix of the same dimension as $\mathbf{K}_{\tilde{\mathbf{z}}\tilde{\mathbf{z}}}$ where the argument occupies the appropriate sub-block and the rest of the matrix has zero valued elements. Note how (17) simply aggregates the inverse local sample covariances and then subtracts their intersections.

The rest of this section is devoted to finding a similar solution to proper quaternion chordal models. More specifically, we assume the following structure. Due to Lemma 1, the proper inverse covariance is parameterized via \mathbf{A} , \mathbf{B} , \mathbf{C} and \mathbf{D} . We will assume that these matrices have the same chordal sparsity pattern. This pattern is defined via a $\mathbf{G} \in \mathbb{R}^{p \times p}$ adjacency matrix. The augmented matrix $\mathbf{G}^a \in \mathbb{R}^{4p \times 4p}$ is defined as

$$\mathbf{G}^a = \mathbf{G} \otimes \mathbf{I}_4 \quad (18)$$

where \mathbf{I}_4 is a 4×4 identity matrix and \otimes denotes the Kronecker product. Suppose v_i is the i_{th} vertex in \mathbf{G} . \mathbf{G}^a contains four times more vertices. In what follows we denote by $v_{1i}, v_{2i}, v_{3i}, v_{4i}$ the copies of v_i in \mathbf{G}^a . The advantage of this specific form of augmented matrix lies in the following result.

Theorem 2. *If the graph induced by some matrix $\mathbf{G} \in \mathbb{R}^{p \times p}$ is chordal with cliques C_k and separators S_k , $k = 1, \dots, K$, then the graph induced by a matrix $\mathbf{G}^a = \mathbf{G} \otimes \mathbf{I}_N$, where \mathbf{I}_N is an $N \times N$ matrix of ones is also chordal with cliques C_k^a and separators S_k^a . If a vertex $v_i \in C_k$ or $v_i \in S_k$ in graph \mathbf{G} , then $v_{1i}, v_{2i}, \dots, v_{Ni} \in C_k$ or $v_{1i}, v_{2i}, \dots, v_{Ni} \in S_k$ in graph \mathbf{G}^a .*

With the power of Theorem 2, we obtain a closed form solution to the proper and chordal ML optimization problem.

Theorem 3. *Let $\tilde{\mathbf{z}} \in \mathbb{R}^{4p}$ be a Gaussian random vector with inverse covariance $\mathbf{K}_{\tilde{\mathbf{z}}\tilde{\mathbf{z}}} \in \mathbb{Q}_p$. The unconstrained chordal solution to*

$$\begin{aligned} \min_{\mathbf{K}_{\tilde{\mathbf{z}}\tilde{\mathbf{z}}}} \quad & l(\mathbf{K}_{\tilde{\mathbf{z}}\tilde{\mathbf{z}}}^{-1}) \\ \text{s.t.} \quad & [\mathbf{K}_{\tilde{\mathbf{z}}\tilde{\mathbf{z}}}]_{i,j} = 0 \quad \forall (i,j) \notin E^a, \end{aligned} \quad (19)$$

where E^a is the edge set of the graph induced by \mathbf{G}^a . When the graph induced by \mathbf{G} is chordal the solution is

$$\mathbf{K}_{\tilde{\mathbf{z}}\tilde{\mathbf{z}}} = \sum_{k=1}^K \left[(\mathbf{S}_{C_k^a, C_k^a})^{-1} \right]^0 - \sum_{k=2}^K \left[(\mathbf{S}_{S_k^a, S_k^a})^{-1} \right]^0 \quad (20)$$

where $\mathbf{S}_{(\cdot)_k^a, (\cdot)_k^a}$ is the sample covariance over clique C_k^a or the separator S_k^a in the graph induced by \mathbf{G}^a using $\tilde{\mathbf{z}}_i$. The solution exists for $n > 4 \max |C_k|$ with probability one and is unbounded otherwise, where C_k are the cliques in the graph induced by \mathbf{G} .

The constrained chordal solution to

$$\begin{aligned} \min_{\mathbf{K}_{\tilde{\mathbf{z}}\tilde{\mathbf{z}}}} \quad & l(\mathbf{K}_{\tilde{\mathbf{z}}\tilde{\mathbf{z}}}^{-1}) \\ \text{s.t.} \quad & [\mathbf{K}_{\tilde{\mathbf{z}}\tilde{\mathbf{z}}}]_{i,j} = 0 \quad \forall (i,j) \notin E^a \\ & \mathbf{K}_{\tilde{\mathbf{z}}\tilde{\mathbf{z}}} \in \mathbb{Q}_p \end{aligned} \quad (21)$$

is

$$\begin{aligned} \mathbf{K}_{\tilde{\mathbf{z}}\tilde{\mathbf{z}}} = \quad & \sum_{k=1}^K \left[(\mathbf{S}_{h, C_k^a})^{-1} \right]^0 \\ & - \sum_{k=2}^K \left[(\mathbf{S}_{h, S_k^a})^{-1} \right]^0 \end{aligned} \quad (22)$$

where \mathbf{S}_h is defined in (14), is the quaternion sample covariance defined in (14). Therefore $\mathbf{S}_{h, (\cdot)_k^a, (\cdot)_k^a}$ is the sample covariance over clique C_k^a or the separator S_k^a in the graph induced by \mathbf{G}^a , as defined in Theorem 2, using $\tilde{\mathbf{z}}_i$. The solution exists for $n > \max |C_k|$ with probability one and is unbounded otherwise, here C_k are the cliques in the graph induced by \mathbf{G} .

VI. SIMULATIONS

In this section, we present numerical results testing the suggested quaternion estimators on a real world dataset. We used the McMaster IPIX radar data available online [19]. This radar is a fully coherent X-band radar that was used to measure sea clutter data. We used data from the file 19980227_213016_antstep.cdf in the Grimsby database which was collected on the shore of Lake Ontario. The file contains two complex valued matrices X_{vv} and X_{hh} of dimensions 60000×28 , representing the vertical and horizontal polarizations respectively. The 60000 rows are different time slots and the 28 columns belong to different points in space. We

used the 14th column as the cell under test and used columns 10 – 13 and 15 – 18 for estimating the clutter's unknown covariance. At each experiment, we used a different group of length 6 adjacent rows. To compute detection rates, we artificially added normalized random targets with independent, zero mean and unit variance normal random variables. We then tried to detect these targets using a whitened matched filter approach:

$$\tilde{\mathbf{z}}^T \hat{\mathbf{C}}^{-1} \tilde{\mathbf{t}} \geq \gamma \quad (23)$$

where $\tilde{\mathbf{z}}$ is the measured vector, $\hat{\mathbf{C}}$ is the estimated covariance as described below, $\tilde{\mathbf{t}}$ is the known target and γ is the detection threshold. We tested five covariance estimators:

- I: no whitening.
- S: the sample covariance in (12).
- Q: the proper sample covariance in (14).
- BS: the banded estimator in (20).
- BQ: the banded proper estimator in (22).

Note that a banded structure corresponds to a time-varying autoregressive model which seems appropriate for modeling the clutter's time series [5]. This is a simple chordal model and we used the efficient closed form solutions. The bandwidth for the banded estimators (also known as the order of the autoregressive model) was chosen through a standard leave-one-out cross validation procedure. We repeated the experiment over 1000 different time slots, and report the average results in the ROC curve depicted in Fig. 1. It is easy to see that S has the worst performance. Clearly, it has too many unknowns and does not succeed in approximating the clutter's true covariance, to the point the I which means no whitening at all shows better results. The BS estimator considerably decreases the number of unknowns and provides improved performance. But this estimator does not exploit the (presumed) proper quaternion structure. The best results are obtained by the proper estimators with an advantage to BQ which enjoys the advantages of both worlds: graphical models and quaternions.

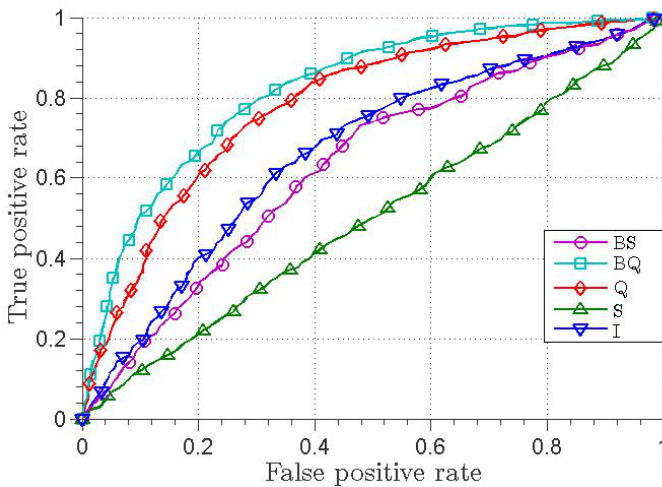


Fig. 1. ROC curve for IPIX data with covariance estimation of dimension 6 using 8 observations from neighboring cells and a target of length 6.

VII. CONCLUSIONS

In this paper, we have extended Gaussian graphical model to proper quaternion Gaussian distributions. We considered proper quaternion maximum likelihood estimators in different scenarios: unconstrained, known sparsity, known chordal sparsity and unknown sparsity. The proposed estimators allow for a physically motivated reduction of unknown parameters, e.g., in a properly polarized time varying autoregressive model. Thus, they achieve high accuracy using a very small number of observations. The estimators were assessed on real radar data and demonstrated improved performance compared to the standard approaches.

ACKNOWLEDGEMENTS

The authors would like to thank Guy Kindler and Ilya Soloveyichik for fruitful discussions, and Maria Greco and Simon Haykin for the databases. This work was supported in part by an ISF grant 786/11. Part of this work was conducted within the Labex CIMI during visits of A. Wiesel at the university of Toulouse.

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