

THE FISHER INFORMATION MATRIX FOR TWO-DIMENSIONAL DATA SETS

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ABSTRACT

This paper shows how the Fisher information matrix of a given two-dimensional (2D) data set can be expressed using the matrices that determine the 2D system that generates the data set. For uniformly sampled data it is shown how the Fisher information matrix can be expressed through the solutions of Lyapunov equations. The novel techniques are demonstrated with an example arising from nuclear magnetic resonance spectroscopy.

1. INTRODUCTION

Data that can be considered to be generated by a two-dimensional (2D) linear continuous system appears in many areas of applications. For example, in nuclear magnetic resonance (NMR) spectroscopy it can be shown ([1]) that the data of a so-called 2D NMR experiment typically has the form

$$y(t_1, t_2) = C_1 e^{A_{11}t_1} A_{12} e^{A_{22}t_2} B_2, \quad t_1, t_2 \geq 0, \quad (1)$$

where $A_{11}, A_{12}, A_{22}, C_1, B_2$ are matrices of compatible sizes. The fundamental problem in NMR spectroscopy is that the system matrices are dependent on parameters (e.g. the resonant frequencies of the magnet spins) which need to be estimated through the experiment.

Estimation of parameters that determine dynamic data is a frequently encountered problem in many areas of applications. The question therefore naturally arises as to the accuracy with which these parameters can be estimated. The Cramer Rao lower bound (CRLB) gives a lower bound for the covariance of the parameter estimates of an unbiased estimation procedure for a given data set [2, 3]. The CRLB is in fact typically calculated as the inverse of a matrix called the Fisher information matrix. The relevance of this result is not only to evaluate a particular estimation procedure but can also give guidance for an appropriate design of an experiment to collect data (see e.g. [4]).

Various methods have been suggested for the computation of the CRLB for the parameter estimation problem of 2D undamped exponential signals with additive noise [5]. However, to our best knowledge, a closed form expression for the CRLB for the parameter estimation problem for 2D

damped exponential signals is not available in the literature. In [4] the Fisher information matrix was derived for a concrete problem arising in NMR spectroscopy. However the approach taken there uses the 'hand calculation' to derive the analytical expression, which is time-consuming and cumbersome. Recently, a systematic investigation of the CRLB or Fisher information matrix for the case of one-dimensional (1D) deterministic dynamic systems corrupted by measurement noise is presented in [6]. In this paper, we generalize the results of [6] to 2D data described by (1), using 2D system theoretic methods. This generalization is, however, not a straightforward extension of the results in [6] due to the significantly more intricate structure of 2D systems.

To derive a systematic approach to data sets described in (1) we consider a 2D complex single-input single-output continuous system with a separable denominator using Roesser's model (RM)

$$\begin{aligned} \begin{bmatrix} \frac{\partial}{\partial t_1} x_\theta^h(t_1, t_2) \\ \frac{\partial}{\partial t_2} x_\theta^v(t_1, t_2) \end{bmatrix} &= \begin{bmatrix} A_{11} & A_{12} \\ 0 & A_{22} \end{bmatrix} \begin{bmatrix} x_\theta^h(t_1, t_2) \\ x_\theta^v(t_1, t_2) \end{bmatrix} \\ &\quad + \begin{bmatrix} B_1 \\ B_2 \end{bmatrix} u(t_1, t_2), \\ y_\theta(t_1, t_2) &= \begin{bmatrix} C_1 & C_2 \end{bmatrix} \begin{bmatrix} x_\theta^h(t_1, t_2) \\ x_\theta^v(t_1, t_2) \end{bmatrix}, \end{aligned}$$

where $t_1 \geq 0, t_2 \geq 0, A_{11}, A_{12}, A_{22}, B_1, B_2, C_1$ and C_2 are complex matrices of appropriate dimensions depending on the unknown parameter vector $\Theta := [\theta_1 \ \theta_2 \ \dots \ \theta_K]^T$, $x_\theta^h(t_1, t_2)$, and $x_\theta^v(t_1, t_2)$ are horizontal and vertical state vectors respectively, $u(t_1, t_2)$ is the input, and $\frac{\partial}{\partial t_j}$ denotes partial derivative with respect to t_j ($j = 1, 2$). The boundary conditions are given by

$$x_\theta^h(0, t_2), \ x_\theta^v(t_1, 0), \quad t_1 \geq 0, \ t_2 \geq 0.$$

In the following lemma we characterize the input-output description of such a system. See [7] for a proof.

Lemma 1.1 *The output of the above 2D continuous separable-denominator system is given by*

$$y_\theta(t_1, t_2) = v_\theta(t_1, t_2) + q_\theta(t_1, t_2), \quad t_1 \geq 0, \ t_2 \geq 0.$$

Here $v_\theta(t_1, t_2)$ is the system response due to non-zero boundary conditions and $q_\theta(t_1, t_2)$ is the system response due to system input, which are given by

$$v_\theta(t_1, t_2) = C_1 e^{A_{11}t_1} x_\theta^h(0, t_2) + C_2 e^{A_{22}t_2} x_\theta^v(t_1, 0) + \int_0^{t_1} C_1 e^{A_{11}(t_1-\tau_1)} A_{12} e^{A_{22}t_2} x_\theta^v(\tau_1, 0) d\tau_1,$$

and

$$q_\theta(t_1, t_2) = \int_0^{t_1} C_1 e^{A_{11}(t_1-\tau_1)} B_1 u(\tau_1, t_2) d\tau_1 + \int_0^{t_2} C_2 e^{A_{22}(t_2-\tau_2)} B_2 u(t_1, \tau_2) d\tau_2 + \int_0^{t_1} \int_0^{t_2} C_1 e^{A_{11}(t_1-\tau_1)} A_{12} e^{A_{22}(t_2-\tau_2)} B_2 u(\tau_1, \tau_2) d\tau_1 d\tau_2.$$

Note that the data model that motivated our study in (1) can be seen to be the output of such a system if we set $u(t_1, t_2) = \delta(t_1, t_2)$, which is the 2D unit impulse function, $x_\theta^v(t_1, 0) = 0$, $x_\theta^h(0, t_2) = 0$, $B_1 = 0$ and $C_2 = 0$. For simplicity, the remainder of this paper is based on this assumption for the data model in (1).

Assume that we have acquired noise corrupted samples $s_\theta(n, m)$ ($n = 0, 1, \dots, N-1$; $m = 0, 1, \dots, M-1$) of the measured output of a 2D continuous separable-denominator system at various points (t_{1n}, t_{2m}) , i.e.

$$s_\theta(n, m) = y_\theta(t_{1n}, t_{2m}) + w(n, m),$$

where $y_\theta(t_{1n}, t_{2m})$ is the noise free data acquired at the sampling point (t_{1n}, t_{2m}) and $w(n, m)$ is the measurement noise component assumed to be complex Gaussian with zero mean. The real and imaginary parts of $w(n, m)$ are assumed to have variance $\sigma_{n,m}^2$, and to be independent/uncorrelated, i.e. $\text{var}(\text{Re}\{w(n, m)\}) = \text{var}(\text{Im}\{w(n, m)\}) = \sigma_{n,m}^2$ and $E(\text{Re}\{w(n, m)\}\text{Im}\{w(n, m)\}) = 0$.

By the Cramer Rao Lower bound, any unbiased estimate $\hat{\Theta}$ of Θ has a variance (provided certain regularity conditions hold) such that

$$\text{var}(\hat{\Theta}) \geq I^{-1}(\Theta),$$

where $\text{var}(\hat{\Theta}) \geq I^{-1}(\Theta)$ is interpreted as meaning that the matrix $(\text{var}(\hat{\Theta}) - I^{-1}(\Theta))$ is positive semidefinite [2]. Here $I(\Theta)$ is the Fisher information matrix given by

$$[I(\Theta)]_{st} = -E \left(\frac{\partial^2 \ln(p(S; \Theta))}{\partial \theta_s \partial \theta_t} \right), \quad 1 \leq s, t \leq K,$$

where Θ is the unknown $K \times 1$ parameter vector, S is the measured data set, $p(S; \Theta)$ is the probability density function of the measurements and $E(\cdot)$ is the expected value with respect to the underlying probability measure.

With the above background, the next section discusses the derivation of the Fisher information matrix for the 2D data set given by (1). For the special but important case of uniformly sampled data we show in Section 3 that the computation of the Fisher information matrix can be reduced to

the computation of solutions to certain Lyapunov equations. Proofs can be found in [7]. An NMR example is given in Section 4.

We denote by $\text{diag}(M_1, M_2, \dots, M_r)$ the block diagonal matrix whose diagonal block entries are M_1, M_2, \dots, M_r , and all other block entries are zero matrices.

2. FISHER INFORMATION MATRIX

With the Gaussian noise model discussed in Section 1 the probability density function is given by

$$p(S; \Theta) = \prod_{n=0}^{N-1} \prod_{m=0}^{M-1} \frac{1}{\sqrt{2\pi\sigma_{n,m}^2}} \cdot e^{-\frac{1}{2\sigma_{n,m}^2} [\text{Re}\{s_\theta(n, m)\} - \text{Re}\{y_\theta(t_{1n}, t_{2m})\}]^2} \cdot e^{-\frac{1}{2\sigma_{n,m}^2} [\text{Im}\{s_\theta(n, m)\} - \text{Im}\{y_\theta(t_{1n}, t_{2m})\}]^2}.$$

In the following lemma we are going to collect some basic results on the Fisher information matrix adapted to the particular data model that we consider (see e.g. [2]).

Lemma 2.1 1.) For $1 \leq s, t \leq K$

$$[I(\Theta)]_{st} = -E \left(\frac{\partial^2 \ln(p(S; \Theta))}{\partial \theta_s \partial \theta_t} \right) = \sum_{n=0}^{N-1} \sum_{m=0}^{M-1} \frac{1}{\sigma_{n,m}^2} \cdot \text{Re} \left\{ \frac{\partial y_\theta(t_{1n}, t_{2m})}{\partial \theta_s} \frac{\partial y_\theta^*(t_{1n}, t_{2m})}{\partial \theta_t} \right\},$$

where $(\cdot)^*$ denotes complex conjugate.

2.) Let

$$D_{y_\theta(t_{1n}, t_{2m})} := \begin{bmatrix} \frac{\partial y_\theta(t_{1n}, t_{2m})}{\partial \theta_1} \\ \frac{\partial y_\theta(t_{1n}, t_{2m})}{\partial \theta_2} \\ \vdots \\ \frac{\partial y_\theta(t_{1n}, t_{2m})}{\partial \theta_K} \end{bmatrix}.$$

Then

$$I(\Theta) = \sum_{n=0}^{N-1} \sum_{m=0}^{M-1} \frac{1}{\sigma_{n,m}^2} \text{Re} \left\{ D_{y_\theta(t_{1n}, t_{2m})} D_{y_\theta(t_{1n}, t_{2m})}^H \right\},$$

where $(\cdot)^H$ denotes complex conjugate transpose.

In order to calculate the Fisher information matrix it is necessary to compute the derivative $\frac{\partial y_\theta(t_{1n}, t_{2m})}{\partial \theta_s}$ of the output with respect to the element θ_s of the parameter vector Θ , $s = 1, \dots, K$.

Lemma 2.2 For the 2D continuous separable-denominator system with impulse input $u(t_1, t_2) = \delta(t_1, t_2)$, and $B_1 = 0$, $C_2 = 0$, $x_\theta^v(t_1, 0) = 0$, $x_\theta^h(0, t_2) = 0$,

$$\frac{\partial y_\theta(t_1, t_2)}{\partial \theta_s} = \partial_s C_1 e^{\partial_s A_{11} t_1} \partial_s A_{12} e^{\partial_s A_{22} t_2} \partial_s B_2.$$

Here

$$\begin{aligned}\partial_s A_{11} &:= \begin{bmatrix} A_{11} & 0 \\ \frac{\partial A_{11}}{\partial \theta_s} & A_{11} \end{bmatrix}, \quad \partial_s A_{12} := \begin{bmatrix} A_{12} & 0 \\ \frac{\partial A_{12}}{\partial \theta_s} & A_{12} \end{bmatrix}, \\ \partial_s A_{22} &:= \begin{bmatrix} A_{22} & 0 \\ \frac{\partial A_{22}}{\partial \theta_s} & A_{22} \end{bmatrix}, \quad \partial_s B_2 := \begin{bmatrix} B_2 \\ \frac{\partial B_2}{\partial \theta_s} \end{bmatrix}, \\ \partial_s C_1 &:= \begin{bmatrix} \frac{\partial C_1}{\partial \theta_s} & C_1 \end{bmatrix}.\end{aligned}$$

In the following theorem we summarize the previous results and state the general expression for the Fisher information matrix for the data set corresponding to the output of the 2D continuous separable-denominator system.

Theorem 2.1 Consider the augmented derivative system given by

$$\begin{aligned}D_{A_{11}} &:= \text{diag}(\partial_1 A_{11}, \partial_2 A_{11}, \dots, \partial_K A_{11}), \\ D_{A_{12}} &:= \text{diag}(\partial_1 A_{12}, \partial_2 A_{12}, \dots, \partial_K A_{12}), \\ D_{A_{22}} &:= \text{diag}(\partial_1 A_{22}, \partial_2 A_{22}, \dots, \partial_K A_{22}), \\ D_{B_2} &:= \begin{bmatrix} \partial_1 B_2 \\ \partial_2 B_2 \\ \vdots \\ \partial_K B_2 \end{bmatrix}, \\ D_{C_1} &:= \text{diag}(\partial_1 C_1, \partial_2 C_1, \dots, \partial_K C_1).\end{aligned}$$

Assume that the 2D system is the same as that in Lemma 2.2. We have

$$D_{y_\theta(t_1, t_2)} = D_{C_1} e^{D_{A_{11}} t_1} D_{A_{12}} e^{D_{A_{22}} t_2} D_{B_2}.$$

For the 2D data set sampled at (t_{1n}, t_{2m}) ($n = 0, 1, \dots, N-1; m = 0, 1, \dots, M-1$) with noise variance $\sigma_{n,m}^2 =: \sigma^2$, the Fisher information matrix is given by

$$I(\Theta) = \frac{1}{\sigma^2} \sum_{n=0}^{N-1} \sum_{m=0}^{M-1} \text{Re} \left\{ D_{y_\theta(t_{1n}, t_{2m})} D_{y_\theta(t_{1n}, t_{2m})}^H \right\}. \quad (2)$$

3. FISHER INFORMATION MATRIX FOR UNIFORMLY SAMPLED 2D DATA

Although Theorem 2.1 in the previous section is valid for both uniform and nonuniform sampling schemes, it is computationally rather inefficient to directly compute the 2D summations in (2), particularly in the case when the number of samples is large. In this section, we develop an efficient method for calculating the Fisher information matrix for 2D data generated by uniformly sampling the output of the 2D continuous separable-denominator system in Lemma 2.2. To this end, it is assumed that all the eigenvalues of $e^{A_{11}T_1}$ and $e^{A_{22}T_2}$ are in the open unit disk or equivalently the eigenvalues of A_{11} and A_{22} are in the open half

plane, where T_1 and T_2 are the sampling intervals for the variables t_1 and t_2 respectively. Theorem 2.1 can then be simplified significantly with the Lyapunov approach. For convenience of exposition, we denote $A_{d1} := e^{D_{A_{11}}T_1}$ and $A_{d2} := e^{D_{A_{22}}T_2}$.

Theorem 3.1 Consider the data model of Theorem 2.1 and assume that the signal is uniformly sampled with sampling intervals T_1 for the variable t_1 and T_2 for t_2 , i.e., at $t_{1n} = nT_1, n = 0, 1, \dots, N-1; t_{2m} = mT_2, m = 0, 1, \dots, M-1$. Moreover, assume that all the eigenvalues of A_{11} and A_{22} are in the open left half plane. Then the Fisher information matrix is given by

$$I(\Theta) = \frac{1}{\sigma^2} \text{Re} \{ D_{C_1} P_1 D_{C_1}^H \},$$

where P_1 is solved as follows. Obtain P_2 as the unique solution to the following Lyapunov equation

$$A_{d2} P_2 A_{d2}^H - P_2 = -D_{B_2} D_{B_2}^H + A_{d2}^M D_{B_2} D_{B_2}^H (A_{d2}^M)^H,$$

and then get P_1 as the unique solution to the following Lyapunov equation

$$A_{d1} P_1 A_{d1}^H - P_1 = -D_{A_{12}} P_2 D_{A_{12}}^H + A_{d1}^N D_{A_{12}} P_2 D_{A_{12}}^H (A_{d1}^N)^H.$$

In the case that there are an infinite number of equidistant samples in either of the variable t_1 , t_2 or both, Theorem 3.1 can be simplified to the following two corollaries.

Corollary 3.1 Assume that the 2D system is the same as that in Theorem 3.1, except that there are an infinite number of equidistance samples in the t_1 variable, i.e. $t_{1n} = nT_1, n = 0, 1, \dots, \infty$. Then the Fisher information matrix is given by

$$I(\Theta) = \frac{1}{\sigma^2} \text{Re} \{ D_{C_1} P_1 D_{C_1}^H \},$$

where P_1 is solved as follows. Obtain P_2 as the unique solution to the following Lyapunov equation

$$A_{d2} P_2 A_{d2}^H - P_2 = -D_{B_2} D_{B_2}^H + A_{d2}^M D_{B_2} D_{B_2}^H (A_{d2}^M)^H,$$

and then get P_1 as the unique solution to the following Lyapunov equation

$$A_{d1} P_1 A_{d1}^H - P_1 = -D_{A_{12}} P_2 D_{A_{12}}^H.$$

Corollary 3.2 Assume that the 2D system is the same as that in Theorem 3.1, except that an infinite number of equidistant samples are acquired in both the t_1 and t_2 variables, i.e., $t_{1n} = nT_1, n = 0, 1, \dots, \infty; t_{2m} = mT_2, m = 0, 1, \dots, \infty$. Then the Fisher information matrix is given by

$$I(\Theta) = \frac{1}{\sigma^2} \text{Re} \{ D_{C_1} P_1 D_{C_1}^H \},$$

where P_1 can be solved as follows. First obtain P_2 as the unique solution to the Lyapunov equation

$$A_{d2}P_2A_{d2}^H - P_2 = -D_{B2}D_{B2}^H,$$

then get P_1 as the unique solution to the Lyapunov equation

$$A_{d1}P_1A_{d1}^H - P_1 = -D_{A12}P_2D_{A12}^H.$$

4. EXAMPLE

Consider the simulated 2D NMR data having the form

$$y_\theta(t_1, t_2) = \sum_{k=1}^2 \sum_{l=1}^2 c_{kl} e^{(r_{1k} + i\omega_{1k})t_1 + (r_{2l} + i\omega_{2l})t_2 + i\phi_{kl}}$$

where the parameter vector is given by

$$\Theta = [c_{11}, c_{12}, c_{21}, c_{22}, r_{11}, r_{12}, r_{21}, r_{22}, \omega_{11}, \omega_{12}, \omega_{21}, \omega_{22}, \phi_{11}, \phi_{12}, \phi_{21}, \phi_{22}]^T.$$

The above simulated 2D NMR data can be considered as the output of a 2D continuous separable-denominator system with a state-space realization given by

$$\begin{aligned} A_{11} &= \begin{bmatrix} r_{11} + i\omega_{11} & 0 \\ 0 & r_{12} + i\omega_{12} \end{bmatrix}, \quad C_1 = \begin{bmatrix} 1 & 1 \end{bmatrix}, \\ A_{12} &= \begin{bmatrix} c_{11}e^{i\phi_{11}} & c_{12}e^{i\phi_{12}} \\ c_{21}e^{i\phi_{21}} & c_{22}e^{i\phi_{22}} \end{bmatrix}, \quad C_2 = 0, \\ A_{22} &= \begin{bmatrix} r_{21} + i\omega_{21} & 0 \\ 0 & r_{22} + i\omega_{22} \end{bmatrix}, \quad B_1 = 0, \quad B_2 = \begin{bmatrix} 1 \\ 1 \end{bmatrix} \end{aligned}$$

where the input and initial conditions are given by

$$u(t_1, t_2) = \delta(t_1, t_2), \quad x_\theta^h(0, t_2) = 0, \quad x_\theta^v(t_1, 0) = 0.$$

we fix the values of the parameter vector Θ as

$$[0.15, 0.22, 0.12, 0.13, -0.1, -0.35, -0.15, -0.45, 1.445, 2.136, 2.702, 0.88, 0.683, 1.366, 2.4167, 0.982]^T.$$

To apply the methods in Section 3, the first step is the calculation of the derivative system determined by D_{A11} , D_{A12} , D_{A22} , D_{C1} and D_{B2} in Theorem 2.1. Detailed calculation is omitted here but can be found in [7]. Next, we obtain the CRLB for the simulated NMR data with additive Gaussian noise using the method of [4] and the new methods proposed in this paper. From Table 1, it can be seen that the values in columns 1 and 2 are indeed very close (the differences are caused by numerical errors only), while there are some small differences between the values in column 1 and column 3 (or 4). In fact, it is easy to see that Corollary 3.1 gives expressions for the Fisher information matrix associated with the asymptotic CRLB for an infinite number of samples for t_1 while Corollary 3.2 gives expressions for the Fisher information matrix associated with the asymptotic CRLB for an

infinite number of samples for both t_1 and t_2 , as verified by this example. The significance is that the new methods are computationally much more efficient than the method of [4]. For this example as well as many other simulations we have conducted, the computational time using the method of [4] is at least 100 times more than that using the new methods for the same PC under the same conditions.

Table 1. CRLB for Different Methods with $T_1 = 0.015$, $T_2 = 1.54$, $N = 2048$, $M = 16$

Θ	Method of [4]	Theorem 3.1	Corollary 3.1	Corollary 3.2
c_{11}	5.1551e-005	5.1559e-005	5.0550e-005	4.9898e-005
c_{12}	7.9816e-005	7.9828e-005	7.7776e-005	7.7365e-005
c_{21}	1.1731e-004	1.1733e-004	1.1645e-004	1.1609e-004
c_{22}	2.0245e-004	2.0249e-004	1.9971e-004	1.9956e-004
r_{11}	1.1433e-005	1.1435e-005	1.0231e-005	1.0228e-005
r_{12}	1.1673e-003	1.1674e-003	1.1568e-003	1.1563e-003
r_{21}	7.4231e-005	7.4236e-005	7.4050e-005	7.0916e-005
r_{22}	4.3089e-004	4.3088e-004	4.3022e-004	4.2877e-004
ω_{11}	1.1433e-005	1.1435e-005	1.0231e-005	1.0228e-005
ω_{12}	1.1673e-003	1.1674e-003	1.1568e-003	1.1563e-003
ω_{21}	7.4231e-005	7.4236e-005	7.4050e-005	7.0916e-005
ω_{22}	4.3089e-004	4.3088e-004	4.3022e-004	4.2877e-004
ϕ_{11}	2.2911e-003	2.2915e-003	2.2466e-003	2.2177e-003
ϕ_{12}	1.6490e-003	1.6493e-003	1.6069e-003	1.5984e-003
ϕ_{21}	8.1469e-003	8.1479e-003	8.0871e-003	8.0618e-003
ϕ_{22}	1.1979e-002	1.1981e-002	1.1817e-002	1.1808e-002

5. CONCLUSIONS

In this paper, we have developed an explicit expression for the calculation of the Cramer Rao lower bound for a class of 2D signals which are samples of outputs of 2D continuous separable-denominator systems. For the special but important case of uniform sampling, the Lyapunov approach is exploited which has speeded up considerably for the calculation of the Fisher information matrix. We believe that the presented results will have a significant impact on applications dealing with a large number of data samples and a large number of parameters to be estimated.

6. REFERENCES

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