Optimal correction of an indefinite estimated MA spectral density matrix

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Abstract

Consider a vector moving-average sequence of order \( n \), \( \text{MA}(n) \), and let \( \Phi(\omega) = \sum_{k=-n}^{n} R_k e^{-j\omega k} \) denote its spectral density matrix, where \( \{R_k\}_{k=-n}^{n} \) are the covariance matrices and \( \omega \) stands for the frequency variable. A nonparametric estimate \( \hat{\Phi}(\omega) = \sum_{k=-n}^{n} \hat{R}_k e^{-j\omega k} \) of \( \Phi(\omega) \) can easily become indefinite at some frequencies, and thus invalid, due to the estimation errors. In this paper, we provide a computationally efficient procedure that obtains the optimal (in a least-squares sense) valid approximation \( \hat{U}(\omega) \) to \( \hat{U}(\omega) \) in a polynomial time, by means of a semidefinite programming (SDP) algorithm.

Keywords: Vector moving-average; Spectral density matrix; Semidefinite programming

1. Introduction and the problem formulation

Let \( \{y(t)\}_{t=1,2,...} \) be a generic real-valued \( m \times 1 \)-vector \( \text{MA}(n) \) sequence generated by the equation:
\[
y(t) = C_0 e(t) + C_1 e(t-1) + \cdots + C_n e(t-n),
\]
where \( \{e(t)\} \) is an \( m \times 1 \)-vector white noise with mean zero and covariance matrix equal to \( I \), and \( \{C_k\}_{k=0}^{n} \) are \( m \times m \) matrices. The covariance matrices and the spectral density matrix of \( \{y(t)\} \) are given by, respectively,
\[
R_k \triangleq E[y(t)y^\top(t-k)] = R_{-k}^\top = \sum_{p=k}^{n} C_p C_p^\top \quad \text{for} \quad k = 0, 1, \ldots, n,
\]
and
\[
\Phi(\omega) \triangleq \sum_{k=-n}^{n} R_k e^{-j\omega k}
\]
\[
= [C_0 + C_1 e^{j\omega} + \cdots + C_n e^{-jn\omega}][C_0 + C_1 e^{-j\omega} + \cdots + C_n e^{jn\omega}]^\ast
\]
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\[
\begin{align*}
A^*(\omega) &= A^*(\omega) = \left[ I e^{-j\omega} I \cdots e^{-j\omega} I \right], \\
\end{align*}
\]

where \(( \cdot)^T\) denotes the transpose, \(( \cdot)^*\) denotes the conjugate transpose, and
\[
\begin{align*}
A^*(\omega) &= \left[ I e^{-j\omega} I \cdots e^{-j\omega} I \right]. \\
\end{align*}
\]

Let \(\{y(t)\}_{t=1}^N\) be the observed sequence, let \(\{\hat{R}_k\}_{k=-n}^n\) denote some nonparametric estimates of \(\{R_k\}_{k=-n}^n\) obtained from \(\{y(t)\}_{t=1}^N\), such as the sample covariance matrices
\[
\hat{R}_k = \frac{1}{N} \sum_{t=k+1}^N y(t)y^T(t-k) = \hat{R}_k^T, \quad k = 0, 1, \ldots, n, \\
\]
and let \(\Phi(\omega)\) be the following estimate of \(\Phi(\omega)\) obtained from \(\{\hat{R}_k\}_{k=-n}^n\):
\[
\hat{\Phi}(\omega) = \sum_{k=-n}^n \hat{R}_ke^{-j\omega k}.
\]

While \(\hat{\Phi}(\omega)\), as defined above, is easy to compute, it has the undesirable feature of not necessarily being positive semidefinite for all \(\omega \in [-\pi, \pi]\) (as required for a valid spectral density matrix). Among other things, this fact has negative consequences for MA parameter estimation. Indeed, if \(\Phi(\omega)\) is positive semidefinite at each \(\omega\), then we could obtain the estimates of the (minimum-phase) MA coefficient matrices by a matrix spectral factorization algorithm applied to \(\Phi(\omega)\) (see, e.g., Wilson, 1972; Vostrý, 1975; Ježek and Kučera, 1985; Anderson and Moore, 1979; Li, 2005). However, if \(\Phi(\omega)\) does not have the said property, then any spectral factorization algorithm applied to \(\Phi(\omega)\) will fail to provide estimates of \(\{C_k\}_{k=0}^n\) (as there is no MA(n) that has such a \(\Phi(\omega)\) as its spectral density matrix).

Let \(\lambda_1(\omega) \geq \lambda_2(\omega) \geq \cdots \geq \lambda_m(\omega)\) denote the eigenvalues of \(\Phi(\omega)\), for \(\omega \in [-\pi, \pi]\). However, such a possible idea of fixing an indefinite \(\hat{\Phi}(\omega)\) has at least three significant drawbacks: (i) it is computationally intensive since we have to compute a large number of eigen-decompositions; (ii) it cannot guarantee that \(\Phi(\omega)\) is positive semidefinite only at the frequencies for which the eigenvalues are computed; and, most important, (iii) the so-corrected spectral density matrix is not guaranteed to correspond to any MA(n) (or even to be rational, for that matter).

In this paper, we aim at fixing the potential indefiniteness problem of \(\hat{\Phi}(\omega)\) by means of an optimal (in a least-squares (LS) sense) correction which yields a corrected valid spectral density matrix that belongs to the MA(n) class. Mathematically, our goal is to solve the following constrained LS fitting problem:

\[
\begin{align*}
\min_{\{R_k\}_{k=-n}^n} & \quad \frac{1}{2\pi} \int_{-\pi}^{\pi} \| \hat{\Phi}(\omega) - \Phi(\omega) \|^2 d\omega \\
\text{s.t.} & \quad \Phi(\omega) \succeq 0 \quad \text{for } \omega \in [-\pi, \pi],
\end{align*}
\]

where \(\| \cdot \|_2^2\) denotes the Frobenius matrix norm, \(\hat{\Phi}(\omega)\) and \(\Phi(\omega)\) are, respectively, as defined in (8) and (4) above, and the notation \(\Phi(\omega) \succeq 0\) means that \(\Phi(\omega)\) is a positive semidefinite matrix.

At the first sight, the above problem appears to be a difficult one. Indeed, when viewed as an optimization over \(\{R_k\}_{k=-n}^n\), the loss function in (10) is quadratic in the unknowns but the constraints are nonlinear and infinitely many (therefore, when \(\{R_k\}_{k=-n}^n\) are the optimization variables, (10) is a semi-infinite optimization problem). Furthermore, if we view (10) as an optimization over \(\{C_k\}_{k=0}^n\) (with \(\{R_k\}_{k=-n}^n\) being obtained from \(\{C_k\}_{k=0}^n\) via (2)), then the constraints in (10) are automatically satisfied, but the loss is a quartic function of \(\{C_k\}_{k=0}^n\) that is not easily minimized. However, in spite of these apparent difficulties, (10) is a convex problem (as can be readily verified), a fact which suggests that there might be better ways to solve it.

In the next section, we exploit the convexity of (10) to reformulate it as a semidefinite program (SDP) that can be solved efficiently in polynomial time—see below for details. The solution to (10), presented in the
unlike the constraint so-called linear matrix inequality (LMI) that is easily handled by the current convex optimization packages, parsimonious parameterizations of block-Toeplitz matrix, following, is an extension to the vector case of the procedure proposed in Stoica et al. (2000) and Dumitrescu et al. (2001) to tackle the scalar \( m = 1 \) optimal correction problem.

2. The solution

It follows from (5) that the spectral density matrix of any MA(n) can be written as

\[
\Phi(\omega) = \Lambda^*(\omega)X\Lambda(\omega),
\]

for a certain \((m(n + 1) \times m(n + 1))\) positive semidefinite matrix \( X \). Interestingly, (11) with an arbitrary matrix \( X \geq 0 \) is an MA(n) spectral density matrix. To see this, let \( S \) be a square root of \( X \), that is \( X = SS^T \),

and consider the following block partition of \( S \)

\[
S = \begin{bmatrix}
S_{00} & S_{01} & \cdots & S_{0n} \\
S_{10} & S_{11} & \cdots & S_{1n} \\
\vdots & \vdots & \ddots & \vdots \\
S_{n0} & S_{n1} & \cdots & S_{nn}
\end{bmatrix},
\]

(13)

where \( \{S_{jk}\} \) are \( m \times m \) matrices. Using this notation we can rewrite (11) with an arbitrary \( X \geq 0 \) as follows:

\[
\Phi(\omega) = \Lambda^*(\omega)SS^T\Lambda(\omega)
= \sum_{k=0}^{n} [S_{0k} + S_{1k}e^{-j\omega} + \cdots + S_{nk}e^{-jnk\omega}][S_{0k} + S_{1k}e^{-j\omega} + \cdots + S_{nk}e^{-jnk\omega}]^T.
\]

(14)

Each term of the above sum is the spectral density matrix of an MA(n), and therefore so is the sum.

The conclusion of the previous discussion is that we can parameterize the class of MA(n) spectral density matrices \( \Phi(\omega) \) via the \((m(n + 1) \times m(n + 1))\) matrix \( X \geq 0 \) as in (11). This parameterization has the advantage that \( \Phi(\omega) \) is a linear function of the elements of \( X \), and that the constraint on \( X \), namely \( X \geq 0 \), is a so-called linear matrix inequality (LMI) that is easily handled by the current convex optimization packages, such as SDP (see, e.g., Boyd and Vandenberghe, 2004; Sturm, 1999). In comparison with this, the more parsimonious parameterizations of \( \Phi(\omega) \) via \( \{R_k\} \) and \( \{C_k\} \) have the significant drawbacks indicated in the previous section. In particular, while \( \Phi(\omega) \) is also a linear function of \( \{R_k\} \) (as it is of \( X \)), the constraint imposed on \( \{R_k\} \) by the requirement that \( \Phi(\omega) \geq 0 \) for all \( \omega \in [-\pi, \pi] \) is a rather complicated one, unlike the constraint \( X \geq 0 \). In this context, we should note that the positive semidefiniteness of the symmetric block-Toeplitz matrix,

\[
\text{Toeplitz}(R_0, R_1, \ldots, R_n) \triangleq \begin{bmatrix}
R_0 & R_1^T & \cdots & R_n^T \\
R_1 & R_0 & \cdots & R_{n-1}^T \\
\vdots & \vdots & \ddots & \vdots \\
R_n & R_{n-1} & \cdots & R_0
\end{bmatrix},
\]

(15)

is only necessary, not sufficient, for \( \Phi(\omega) \geq 0 \), \( \forall \omega \) (in effect, the sample covariance matrices \( \{R_k\} \) are such that \( \text{Toeplitz}(R_0, R_1, \ldots, R_n) \geq 0 \), yet \( \Phi(\omega) \) can be indefinite at some \( \omega \)'s).

Inserting (11) into the LS fitting criterion (10), we obtain:

\[
\frac{1}{2\pi} \int_{-\pi}^{\pi} \|\hat{\Phi}(\omega) - \Lambda^*(\omega)X\Lambda(\omega)\|^2 d\omega
= \text{const.} - \frac{1}{\pi} \int_{-\pi}^{\pi} \text{tr}[^{\ast}\Phi(\omega)\Lambda^*(\omega)X\Lambda(\omega)] d\omega + \frac{1}{2\pi} \int_{-\pi}^{\pi} \text{tr}[\Lambda^*(\omega)X\Lambda(\omega)\Lambda^*(\omega)X\Lambda(\omega)] d\omega,
\]

(16)
where \( \text{tr}(\cdot) \) denotes the trace of a matrix. To rewrite the above loss in a more compact form, as a function of the elements of \( X \), first we note that:

\[
\frac{1}{2\pi} \int_{-\pi}^{\pi} A(\omega) \Phi(\omega) A^*(\omega) d\omega \\
= \left[ \frac{1}{2\pi} \int_{-\pi}^{\pi} \Phi(\omega) e^{i(k-p)d} d\omega \right]_{k,p=0}^n = [\hat{R}_{k-p}]_{k,p=0}^n \\
= \text{Toeplitz}(\hat{R}_0, \hat{R}_1, \ldots, \hat{R}_n).
\]

(17)

Let \( x \) be the \( m(n+1)(m(n+1)+1)/2 \times 1 \) vector made from the (distinct) elements of \( X \) that lie in the upper-triangular part of this matrix (including the diagonal). Then it follows from (17) that the second term in (16) can be written as

\[
-2 \text{tr}\left\{ \left[ \frac{1}{2\pi} \int_{-\pi}^{\pi} A(\omega) \Phi(\omega) A^*(\omega) d\omega \right] X \right\} = -2\hat{f}^T \text{vec}(X) = -2\hat{f}^T Jx,
\]

(18)

where \( \text{vec}(\cdot) \) denotes the vector obtained by stacking the columns of a matrix on top of each other,

\[
\hat{r} = \text{vec[Toeplitz}(\hat{R}_0, \hat{R}_1, \ldots, \hat{R}_n)\]

and \( J \) is the duplication matrix (e.g., Harville, 1997) that satisfies

\[
\text{vec}(X) = Jx.
\]

(20)

To express also the third term in (16) as a simple function of \( x \), we make use of some properties of the \( \text{vec} \) operator to write:

\[
\text{tr}[A^*(\omega)XA(\omega)A^*(\omega)X]\]

\[
= \text{tr}[A(\omega)A^*(\omega)XA(\omega)X] \\
= \text{vec}^T [X(A(\omega)A^*(\omega))] \text{vec}[A(\omega)A^*(\omega)X] \\
= [(A(\omega)A^*(\omega) \otimes I) \text{vec}(X)]^T [I \otimes (A(\omega)A^*(\omega))] \text{vec}(X)] \\
= x^T J^T [(A(\omega)A^*(\omega))^T \otimes (A(\omega)A^*(\omega))] Jx,
\]

(21)

where \( \otimes \) denotes the Kronecker matrix product. It follows from the above equation that the third term of the LS loss in (16) is given by

\[
x^T J^T \Omega Jx,
\]

(22)

where

\[
\Omega = \frac{1}{2\pi} \int_{-\pi}^{\pi} [A(\omega)A^*(\omega)]^T \otimes [A(\omega)A^*(\omega)] d\omega.
\]

(23)

To evaluate \( \Omega \) we note that the \( (km+s,pm+l) \) element of the matrix \( A(\omega)A^*(\omega) \), for \( k,p = 0,1,\ldots,n \) and \( s,l = 1,2,\ldots,m \), is equal to:

\[
e^{ikp\omega}\delta_{s,l} = \begin{cases} 
1 & \text{if } s=l, \\
0 & \text{else}.
\end{cases}
\]

(24)

Therefore, the \( (km+s,pm+l) \) block (of size \( m(n+1) \times m(n+1) \)) of \( \Omega \) is given by

\[
\frac{1}{2\pi} \int_{-\pi}^{\pi} e^{ikp\omega} A(\omega)A^*(\omega) \delta_{s,l} d\omega.
\]

(25)

The \( (\alpha,\beta) \) block (of size \( m \times m \), for \( \alpha,\beta = 0,1,\ldots,n \), of the latter matrix is readily derived:

\[
\frac{1}{2\pi} \int_{-\pi}^{\pi} e^{ikp\omega} e^{i(\alpha-p)\omega}\delta_{s,l} d\omega = \delta_{s,l}\delta_{k-p,\alpha-\beta} I.
\]

(26)

Consequently, the elements of \( \Omega \) are either 0 or 1 and they can be easily obtained with the above formula.
Making use of the results in (18) and (22) of the previous calculations, we can rewrite the constrained LS fitting problem under discussion (see (16)) as follows:

$$\begin{align*}
\min_{x} & \quad x^T \Gamma x - 2 \gamma^T x \\
\text{s.t.} & \quad X(x) \succeq 0,
\end{align*}$$

(27)

where we have emphasized via notation the (linear) dependence of $X$ on $x$, and where

$$\Gamma = J^T \Omega J, \quad \gamma = J^T \bar{r}.$$  

(28)

Let $F$ be a square-root of $\Gamma$, i.e.,

$$\Gamma = FF^T.$$  

(29)

Then we can rewrite (27) as

$$\begin{align*}
\min_{\rho,x} & \quad \rho \\
\text{s.t.} & \quad X(x) \succeq 0, \quad \begin{bmatrix} \rho + 2 \gamma^T x & x^T F \\ F^T x & I \end{bmatrix} \succeq 0.
\end{align*}$$

(30)

The above problem has precisely the form of a SDP, and thus it can be solved efficiently by means of readily available interior-point algorithms (see, e.g., Boyd and Vandenberghe, 2004; Sturm, 1999). Specifically, it can be shown that a typical interior-point algorithm, when applied to (30), requires $O(m^6 n^6)$ floating-point operations (flops) per iteration; furthermore, the number of iterations required by such an algorithm to achieve practical convergence is usually quite small and nearly independent of $m$ and $n$. It follows that the reformulation of the original constrained LS fitting problem in (10) as the SDP in (30) makes it possible to compute the solution in a polynomial number of flops of the order $O(m^6 n^6)$.

**Remark.** The SDP in (30) can be rewritten in a different (dual) form that can be solved in $O(m^6 n^4)$ flops. For $m = 1$, this has been done in Dumitrescu et al. (2001) and Stoica and Moses (2005). However, doing so for $m > 1$, while quite possible, would result in a complication of the notation, and we chose to omit any discussion on the dual form of (30).

Once the solution $X$ to the SDP in (30) has been computed, we can obtain $\Phi(\omega)$ directly as $A^*(\omega)XA(\omega)$. Alternatively, we can compute $\{R_k\}_{k=-n}^n$ from $X$ and then obtain $\Phi(\omega)$ as $\sum_{k=-n}^n R_k e^{-j \omega k}$. The second way of obtaining $\Phi(\omega)$ is usually more efficient computationally; it is also more useful than the first way when we want to estimate the MA coefficient matrices $\{C_k\}_{k=0}^n$, in addition to the estimation of $\Phi(\omega)$—as already mentioned, this can be done by inputting $\{R_k\}_{k=-n}^n$ to a matrix spectral factorization algorithm, such as those in Wilson (1972), Vostrý (1975), or Li (2005). We should note, however, that $\{C_k\}_{k=0}^n$ can also be obtained from $X$ directly, by using a different type of spectral factorization based on state-space realizations (see, e.g., Anderson and Moore, 1979).

Given the indicated usefulness of $\{R_k\}_{k=-n}^n$, and to conclude this section, we explain how to obtain the covariance matrices from $X$. Using the following block partition of $X$:

$$X = [X_{kp}]_{k,p=0}^n,$$

(31)

with $X_{kp}$ being an $m \times m$ matrix, in $\Phi(\omega) = A^*(\omega)XA(\omega)$, we have that:

$$\begin{align*}
\Phi(\omega) & = \sum_{k=0}^n \sum_{p=0}^n X_{kp} e^{-j(k-p)\omega} \\
& = \sum_{k=0}^n \sum_{s=k-n}^k X_{k,k-s} e^{-j s \omega} \\
& = \sum_{s=-n}^n \left( \sum_{k=0}^n X_{k,k-s} \right) e^{-j s \omega},
\end{align*}$$

(32)
where, to derive the last equality, we set $X_{kp} = 0$ for $p \notin [0, n]$. Comparing (4) and (32), we obtain the following expressions for $\{R_s\}$ as functions of $X$:

$$R_s = \sum_{k=s}^{n} X_{k,k-s} = R_s^T, \quad s = 0, 1, \ldots, n. \tag{33}$$

3. Numerical example

Consider an MA sequence, as in (1), with $m = 5, n = 2$, and the following (randomly generated) coefficient matrices:

$$C_0 = I,$$

$$C_1 = \begin{bmatrix}
-0.12 & 0.07 & -0.12 & -0.37 & 0.09 \\
-0.05 & -0.12 & -0.27 & -0.13 & 0.18 \\
-0.43 & 0.01 & -0.04 & -0.17 & -0.08 \\
-0.06 & -0.18 & -0.21 & -0.16 & 0.07 \\
-0.24 & 0.00 & -0.10 & -0.35 & 0.13
\end{bmatrix}, \tag{34}$$

and

$$C_2 = \begin{bmatrix}
0.11 & -0.18 & -0.23 & -0.19 & -0.14 \\
-0.07 & -0.09 & -0.35 & -0.31 & 0.00 \\
0.31 & -0.2 & 0.24 & -0.44 & 0.11 \\
-0.25 & -0.17 & 0.08 & 0.15 & -0.15 \\
0.09 & -0.03 & -0.08 & -0.22 & 0.05
\end{bmatrix}. \tag{35}$$

The minimum eigenvalue, $\lambda_m(\omega)$, of $\Phi(\omega)$ associated with this MA(2) is nearly zero at a number of frequencies, which suggests that there exists a high potential risk of $\Phi(\omega)$ becoming indefinite at and around these frequencies. Fig. 1, obtained by means of 1000 Monte-Carlo simulation runs, confirms the expected high risk. When $N$ varies from 5000 to 100, the estimated probability of the occurrence of an indefinite $\Phi(\omega)$ increases from 0.01 to 0.8.

![Fig. 1. The probability of the occurrence of an indefinite $\Phi(\omega)$.](image-url)
For a typical case in which $\hat{\Phi}(\omega)$ was indefinite, Fig. 2 shows $\lambda_m(\omega)$ along with the minimum eigenvalues of $\hat{\Phi}(\omega)$, $\hat{\lambda}_m(\omega)$, and of the corrected spectral density matrix, $\lambda_{\text{corr}}(\omega)$, as functions of $\omega$, for $N = 100$ and 1000. Finally, Fig. 3 shows the relative differences between $\Phi(\omega)$ and $\Phi_{\text{corr}}(\omega)$, namely,

$$\frac{\|\Phi(\omega) - \Phi_{\text{corr}}(\omega)\|^2}{\|\Phi(\omega)\|^2} \quad \text{for } \omega \in [-\pi, \pi].$$

which correspond to the two cases in Fig. 2. We see from these figures that, as expected, $\Phi_{\text{corr}}(\omega) \geq 0$, $\forall \omega \in [-\pi, \pi]$, and that $\Phi_{\text{corr}}(\omega)$ is close to $\Phi(\omega)$, particularly so in the frequency intervals where $\Phi(\omega) \geq 0$.

![Fig. 2](image1.png)

Fig. 2. The minimum eigenvalues of $\Phi(\omega)$, $\hat{\Phi}(\omega)$ and $\Phi_{\text{corr}}(\omega)$, versus $\omega$, when (a) $N = 100$; and (b) $N = 1000$.

![Fig. 3](image2.png)

Fig. 3. Relative differences between $\Phi_{\text{corr}}(\omega)$ and $\hat{\Phi}(\omega)$, for $N = 100$ and 1000.
References

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