A NEW APPROACH TO SPECTRAL ESTIMATION: A TUNABLE HIGH-RESOLUTION SPECTRAL ESTIMATOR*

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ABSTRACT. Traditional maximum entropy spectral estimation determines a power spectrum from covariance estimates. Here we present a new approach to spectral estimation, which is based on the use of filter banks as a means of obtaining spectral interpolation data. Such data replaces standard covariance estimates. A computational procedure for obtaining suitable pole-zero (ARMA) models from such data is presented. The choice of the zeros (MA-part) of the model is completely arbitrary. By suitably choices of filter-bank poles and spectral zeros the estimator can be tuned to exhibit high resolution in targeted regions of the spectrum.

1. Introduction

In this paper we present a novel approach to spectral estimation, which relies on new results in analytic interpolation theory, developed in [10] and based on efforts by the authors over a number of years [2]–[10], [16]–[19].

The approach leads to a Tunable High REsolution Estimator (THREE), based on three elements, namely (i) a bank of filters, (ii) a theory for parameterizing the complete set of spectra which are consistent with the "filter measurements" and have bounded complexity, and (iii) computational procedures for constructing spectra from the set described in (ii).

The purpose of the bank of filters is to process, in parallel, the observation record in order to obtain estimates of the power spectrum at desired points. These points are related to the filter-bank poles and can be selected to give increased resolution over desired frequency bands. The theory in (ii) implies that a second set of tunable parameters are given by so-called spectral zeros which determine the Moving-Average (MA) part of solutions. The solutions turn out to be spectra of Auto-Regressive/Moving-Average (ARMA) filters of complexity at most equal to the dimension of the filter bank, and hence the method provides parametric spectral models.

The computational procedures in (iii) come in two forms: For the default setting when the spectral zeros are chosen equal to the filter-bank poles, a particularly simple algorithm, based on the so-called central solution of the classical interpolation theory, is available. For any other setting, a convex optimization problem needs to be solved. The theory for this was introduced

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in our companion paper [10], and for a similar problem in [9]. In this paper we consider only real processes. However, the framework is quite general and applies also to complex-valued stochastic processes [11].

Typically, the resulting spectra show significantly higher resolution as compared to traditional linear predictive filtering. Moreover, they appear to be more robust than linear predictive filtering due to the fact that we use statistical estimates of only zeroth, or first order, covariance lags as opposed to high order lags. Therefore THREE appears to be especially suitable for being applied to short observation records.

We demonstrate the applicability of the approach in identifying spectral lines and in estimating power spectra with steep variations. Such problems occur in many areas of signal processing and statistical prediction. In particular, in communications, radar, sonar and geophysical seismology, spectral analysis methods are needed which estimate or describe the signal as a sum of harmonics in additive noise [29, page 139]. The case when the noise is colored is considered especially challenging. Therefore, we illustrate the effectiveness of THREE filters for the problem of line-spectra estimation in colored noise and compare with periodogram and AR-based methods. We also demonstrate the effectiveness of THREE filters in estimating spectra with zeros and poles close to each other.

The structure of the paper is as follows. In Section 2 we introduce the bank of filters and discuss how the covariances of their outputs provide estimates of the power spectrum at the reflected pole positions. The variability of such statistical estimates and how they are affected by the position of the poles is briefly considered. Section 3 presents the basic elements of analytic interpolation that are relevant to the current problem. The classical results are reviewed first, and then our recent theory of analytic interpolation with degree constraint is explained in the context of spectral estimation. In Section 4 the computational procedure for the default setting when the spectral zeros coincide with the filter-bank poles is introduced, and the method is illustrated by estimation of spectral lines in colored noise. We present a simulation study comparing THREE with traditional AR filtering and with periodogram analysis. We also give an example indicating that spectral estimation of certain processes can be considerably improved if tuning of spectral zeros is used. This leads to Section 5, where the convex optimization approach is presented. This is based on a generalized concept of entropy and leads to state-space formulae for the bounded-complexity interpolants. The section is concluded by simulations illustrating the improved resolution of the THREE method in comparison with other methods.

To improve readability we defer mathematical proofs and certain technical details to the appendices.

2. Framework for spectral estimation

Let $\{y(t);\, t = \dots, -2, -1, 0, 1, 2, \dots\}$ be a scalar, real-valued, zero-mean, stationary (Gaussian) stochastic process, and consider the basic problem of estimating its power spectral density $\Phi(e^{i\theta})$, $\theta \in [-\pi, \pi]$, from a finite observation record

$$\{y_0, y_1, y_2, \dots, y_N\}. \tag{2.1}$$

Modern spectral estimation techniques typically rely on estimates of covariance lags

$$c_0, c_1, c_2, \dots, c_n, \qquad \text{where } c_k := \mathrm{E}\{y(t)y(t+k)\}. \tag{2.2}$$

Here $n << N$, and $\mathrm{E}\{\cdot\}$ denotes mathematical expectation. Typically, these estimates are obtained either by suitable averaging of products $y_t y_{t+k}$, or by estimating the partial autocorrelation coefficients first, using averaging schemes such as Burg's algorithm. In either case, the statistical reliability of such estimates decreases with the order k of the lag, due to the fact that averaging takes place over a shorter list of such cross products.

In this paper, the function

$$f(z) = \frac{1}{4\pi}\int_{-\pi}^{\pi} \Phi(e^{i\theta})\frac{z+e^{-i\theta}}{z-e^{-i\theta}}d\theta, \tag{2.3}$$

will play a key role. It is analytic in $|z|>1$ and has a positive real part there – such functions are called *positive real*. In fact, the spectral density can be written

$$\Phi(e^{i\theta}) = 2\mathrm{Re}\{f(e^{i\theta})\}, \tag{2.4}$$

and f admits a series representation

$$f(z) = \tfrac{1}{2}c_0 + c_1 z^{-1} + c_2 z^{-2} + c_3 z^{-3} + \dots \quad \text{for } |z|>1. \tag{2.5}$$

Equation (2.3) provides a bijective correspondence between positive-real functions f and functions Φ which are positive on the unit circle. We should note that in general Φ has to be interpreted as a distribution and, in such a case, (2.4) has to be understood as $\Phi(e^{i\theta}) = 2\lim_{r\searrow 1}\mathrm{Re}\{f(re^{i\theta})\}$ a.e., whereas "spectral lines" correspond to poles of $f(z)$ on the boundary $|z|=1$.

In this context, traditional spectral estimation techniques amount to estimating the real part of $f(z)$ from estimates of its value at ∞ and on the values of finitely many of its derivatives at ∞. By way of contrast, our approach is based on the observation that the values of $f(z)$ at points other than ∞ can be estimated directly from the data (2.1). The computation of such a positive real $f(z)$, and hence an estimate for $\Phi(e^{i\theta})$, is the subject of the theory discussed in Section 3.

We first describe how to estimate the value of $f(z)$ at any desired point in $|z|>1$ from the data (2.1).

2.1. Evaluation of f at a point. Consider a first-order stable linear filter with transfer function $G(z) = \frac{z}{z-p}$, where $|p|<1$, and let u be the stationary process obtained as the output of the filter when driven by y. Then

$$u(t) = pu(t-1) + y(t), \tag{2.6}$$

and hence we have

$$\begin{aligned}
\mathrm{E}\{u(t)^2\} &= \mathrm{E}\{(y(t)+py(t-1)+p^2y(t-2)+\dots)^2\} \\
&= c_0(1+p^2+p^4+\dots) \\
&\quad +2c_1p(1+p^2+p^4+\dots) \\
&\quad\quad +2c_2p^2(1+p^2+p^4+\dots)+\dots \\
&= \frac{2}{1-p^2}f(p^{-1}),
\end{aligned} \tag{2.7}$$

and consequently

$$f(p^{-1}) = \tfrac{1}{2}(1-p^2)\mathrm{E}\{u(t)^2\}. \tag{2.8}$$

This is an interpolation condition for f. It should be noted that, if p is a complex number, then u is a complex stochastic process. In this case, $E\{u(t)^2\}$ is not the traditional covariance. The actual covariance is

$$E\{u(t)\bar{u}(t)\} = \frac{f(p^{-1}) + f(\bar{p}^{-1})}{1 - |p|^2},$$

where bar denotes complex conjugation, but, since we want to preserve "phase information", we prefer to use (2.8). We should also mention that, in the complex case, the system with transfer function $G(z)$ is equivalent to a second-order real system, which is easy to derive.

2.2. Bank of filters. Next, given any choice of distinct real or complex numbers $p_0, p_1, \dots, p_n$ in the open unit disc and the corresponding transfer functions

$$G_k(z) = \frac{z}{z - p_k} \quad k = 0, 1, \dots, n, \tag{2.9}$$

consider the bank of filters depicted in Figure 1. In this parallel connection, each filter is first-order if complex arithmetic is used, and always when p is real. Otherwise, each complex pair $(p, \bar{p})$ corresponds to a second-order filter, as explained above. Then the values of the

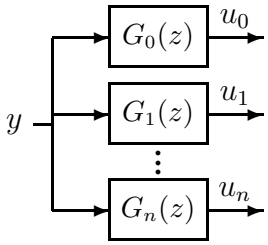

Figure 1: Bank of filters.

positive real function $f(z)$ at the points $\{p_0^{-1}, p_1^{-1}, \dots, p_n^{-1}\}$ can be expressed in terms of the covariances of the outputs $u_0, u_1, \dots, u_n$ of the filter bank as in (2.8). The idea is now to estimate these covariances from finite output data generated by the filter bank, thereby obtaining $n + 1$ interpolation conditions.

2.3. The Pick matrix. A central object in analytic interpolation theory is the so-called *Pick matrix*. This matrix arises naturally in the context of our filter bank as the covariance of the vector process $\mathbf{u}$ defined with the output processes $u_0, u_1, \dots, u_n$ as components. In fact,

$$P_n := \mathrm{E}\{\mathbf{u}(t)\bar{\mathbf{u}}(t)'\} = \begin{bmatrix} \frac{w_0+\bar{w}_0}{1-p_0\bar{p}_0} & \frac{w_0+\bar{w}_1}{1-p_0\bar{p}_1} & \cdots & \frac{w_0+\bar{w}_n}{1-p_0\bar{p}_n} \\ \frac{w_1+\bar{w}_0}{1-p_1\bar{p}_0} & \frac{w_0+\bar{w}_1}{1-p_1\bar{p}_1} & \cdots & \frac{w_0+\bar{w}_n}{1-p_1\bar{p}_n} \\ \vdots & \vdots & \ddots & \vdots \\ \frac{w_n+\bar{w}_0}{1-p_n\bar{p}_0} & \frac{w_n+\bar{w}_1}{1-p_n\bar{p}_1} & \cdots & \frac{w_n+\bar{w}_n}{1-p_n\bar{p}_n} \end{bmatrix}, \tag{2.10}$$

where

$$w_k = f(p_k^{-1}) \quad k = 0, 1, \dots n.$$

Thus, an alternative way to estimate $f(p_k^{-1})$ is through estimates of the Pick matrix P_n as a sample covariance of $\mathbf{u}(t)$.

In this paper we only consider distinct points $p_0, p_1, \ldots, p_n$. The general case will be presented elsewhere [11]. For example, the usual Toeplitz matrix

$$T_n = \begin{bmatrix} c_0 & c_1 & \dots & c_n \\ c_1 & c_0 & \dots & c_{n-1} \\ \vdots & \vdots & \ddots & \vdots \\ c_n & c_{n-1} & \dots & c_0 \end{bmatrix}, \tag{2.11}$$

formed from the partial covariance sequence (2.2) is the Pick matrix for the case in which $p_0 = p_1 = \cdots = p_n = 0$, in which case the filters in the bank are chosen as $G_k(z) = z^{-k}$ for $k = 0, 1, \ldots, n$. This is the case considered in usual AR modeling from covariance data.

2.4. Statistical considerations. This brings us to the statistical reasons for our new approach. In fact, for AR modeling from covariance estimates we need to estimate the Toeplitz matrix (2.11) from the data record (2.1). If this is done via

$$\hat{T}_n = \frac{1}{N-n} \sum_{t=n}^{N} \begin{bmatrix} y_t \\ y_{t-1} \\ \vdots \\ y_{t-n} \end{bmatrix} \begin{bmatrix} y_t & y_{t-1} & \dots & y_{t-n} \end{bmatrix},$$

where $\hat{}$ denotes "the sample estimate of", then a significant portion of the data has not been fully utilized in estimating lower order covariances due to the large time-lag of some of the filters. Moreover, $\hat{T}_n$ is not in general a Toeplitz matrix. If, instead, we use the covariance estimate

$$\hat{c}_k = \frac{1}{N-k} \sum_{t=k}^{N} y_t y_{t-k},$$

the corresponding Toeplitz matrix may not be positive definite, something that may be rectified by dividing by $N+1$ rather than $N-k$, by windowing or, by using Burg's algorithm. In any case, any of these methods suffers from the drawback that reliability of the estimate $\hat{c}_k$ of the covariance lag c_k decreases considerably as k grows, especially for relatively short time series [24].

By way of contrast, our method requires only estimating the zeroth covariance lag, or possibly the first covariance lag in the complex case. It is known that the sample variance of the covariance estimate

$$\hat{c}_0 := \frac{1}{N+1} \sum_{t=0}^{N} y_t^2$$

is given by

$$\operatorname{var}(\hat{c}_0) = \frac{2}{N+1} \sum_{k=-\infty}^{\infty} c_k^2.$$

(See [24, Section 48.1, Equation (48.6)].) But, using Parseval's theorem, this can be expressed in terms of the spectral density $\Phi(e^{i\theta})$ as follows:

$$\operatorname{var}(\hat{c}_0) = \frac{1}{\pi(N+1)} \int_{-\pi}^{\pi} |\Phi(e^{i\theta})|^2 d\theta.$$

Therefore, ignoring any transient effects and assuming that the output process u of a filter $G(z)$ driven by y is stationary, the sample variance of the estimate

$$\hat{c}_0(u) := \frac{1}{N+1}\sum_{t=0}^{N} u_t^2 \tag{2.12}$$

becomes

$$\mathrm{var}(\hat{c}_0(u)) = \frac{1}{\pi(N+1)}\int_{-\pi}^{\pi} |G(e^{i\theta})|^4 |\Phi(e^{i\theta})|^2 d\theta. \tag{2.13}$$

This quantifies the effect of the frequency response of $G(z) = \frac{z}{z-p}$, for real p, on the variance of statistical estimators for $f(p^{-1})$ when estimated by (2.12). In the simple case where $\Phi(e^{i\theta}) \equiv 1$,

$$\mathrm{var}(\hat{c}_0(u)) = \frac{2}{N+1}\frac{1+p^2}{(1-p^2)^3}.$$

In general, the shape of $|G(e^{i\theta})|$ and its relation to $|\Phi(e^{i\theta})|$ has a direct effect on $\mathrm{var}(\hat{c}_0(u))$. The analysis for complex p is similar. The general observation is that choosing the filter poles too close to the unit circle may produce larger errors. Such a strategy will also produce more accentuated transients and is therefore not without cost. We expect that detailed statistical analysis will point to suitable rules for dealing with the relevant trade-offs.

3. Interpolation theory for spectral estimation

In the following we assume that the filter-bank poles $p_0, p_1, \dots, p_n$ are distinct with $p_0 = 0$ and complex poles occurring in complex pairs. The condition $p_0 = 0$ implies that $G_0 \equiv 1$ so that the process y is itself one of the filter-bank outputs. Now, estimating the spectral density Φ from finite observation records of the outputs of the filter bank amounts to determining a positive real function f such that

$$f(p_k^{-1}) = w_k, \quad k = 0, 1, \dots, n, \tag{3.1}$$

where

$$w_k := \frac{1}{2}(1-p_k^2)\hat{c}_0(u_k), \quad k = 0, 1, \dots, n \tag{3.2}$$

with $\hat{c}_0(u_0), \hat{c}_0(u_1), \dots, \hat{c}_0(u_n)$ estimated as in (2.12). (Alternatively, if real arithmetic is required, statistical estimates consistent with the analysis in Section 2.3 could be used.) Then (2.4) provides us with an estimate of the spectral density of y. Since we want this estimate to be rational of minimal complexity, we also require that

$$\deg f \le n, \tag{3.3}$$

i.e., that f is a rational function of degree at most n.

3.1. Classical interpolation theory. For the moment, let us ignore the degree constraint (3.3). Then, given interpolation points $p_0, p_1, \dots, p_n$ inside the unit circle and values $w_0, w_1, \dots, w_n$ in the right half plane, the problem to determine all positive real functions f satisfying (3.1) is a classical analytic interpolation problem, the *Nevanlinna-Pick interpolation*, which has its roots in classical mathematics going back to the end of the 19th century, on approximate integration, quadrature formulae and the moment problem. The foundations of Nevanlinna-Pick interpolation were laid out by C. Carathéodory, I. Schur, R. Nevanlinna, G. Pick, G. Szegö in

the beginning of the 20th century; see, e.g., [20, 31]. The subject evolved into a rich topic in operator theory [28, 30, 15].

Nevanlinna-Pick theory states that a solution exists if and only if the so-called *Pick matrix*

$$P_n := \left[\frac{w_k + \bar{w}_\ell}{1 - p_k \bar{p}_\ell}\right]_{k,\ell=0}^{n} \tag{3.4}$$

is non-negative definite. In the case that P_n is positive semi-definite but singular, the solution is unique. In the case $P_n > 0$, the complete set of solutions is given by a linear fractional transformation, which is constructed from the interpolation data, acting on a "free" parameter which is only required to have certain analytic properties, e.g., to be a positive-real function. A detailed exposition can be found in [31].

A generalization of the problem known as the Carathéodory-Fejér problem, allows for the possibility that $f(z)$ is specified both in terms of values and derivatives up to some order at points outside the disc. Again, the solvability condition is expressed in terms of a suitable (generalized) Pick matrix and all solutions are parameterized by a linear fractional transformation. We refer the reader to the standard mathematics literature [31, 20, 28, 30] for details.

3.2. Interpolation with a degree constraint. This classical theory is very elegant, but the parameterization of all solutions to the interpolation problem includes functions which may have very high degree, or even be nonrational, and provides no means of characterizing those solutions which satisfy the degree constraint (3.3). One particular such solution, the so-called *central solution* to be described below, is obtained by a trivial choice of the free parameter, but a complete parameterization of all solutions satisfying (3.3) requires a new paradigm. In fact, the requirement that the degree of the interpolant f be at most n imposes (a highly nontrivial) nonlinear constraint on the class of solutions. The study of this constraint solution set has led to a rich theory, [2]–[10] and [16]–[19], which has lead to the following complete parameterization of all such solutions in terms of spectral zeros. We recall that a polynomial is called *stable* if all its root are located in the open unit disc $\{z \mid |z| < 1\}$.

Theorem 3.1. *Let $p_0, p_1, \ldots, p_n$ be a self-conjugate set of distinct points inside the unit circle and $w_0, w_1, \ldots, w_n$ a corresponding self-conjugate set of values in the right half plane with the property that the Pick matrix* (3.4) *is positive definite. Then, to any real stable polynomial*

$$\rho(z) = z^n + r_1 z^{n-1} + \cdots + r_{n-1} z + r_n$$

there corresponds a unique pair of real stable polynomials

$$\alpha(z) = a_0 z^n + a_1 z^{n-1} + \cdots + a_n \quad \textit{and} \quad \beta(z) = b_0 z^n + b_1 z^{n-1} + \cdots + b_n,$$

of degree n such that

$$\alpha(z)\beta(z^{-1}) + \beta(z)\alpha(z^{-1}) = \rho(z)\rho(z^{-1}) \tag{3.5}$$

and the rational function

$$f(z) := \frac{\alpha(z)}{\beta(z)} \tag{3.6}$$

is positive real and satisfies the interpolation condition

$$f(p_k^{-1}) = w_k \quad k = 0, 1, \ldots, n. \tag{3.7}$$

This theorem, here presented in a special form adapted to self-conjugate interpolation data, also holds in the more general case where the interpolation data are of the Carathéodory-Féjer type, i.e., include constraints on the derivative of $f(z)$, and was first formulated in the special (Carathèodory) case with a single multiple interpolation point at $z = \infty$, the so-called rational covariance extension problem. Existence was first proven in this context in [16, 18] and uniqueness, as well as well-posedness, in [5]; see [7, 8] for alternative proofs. Existence for the distinct point Pick-Nevaninna problem was proven in [17] and uniqueness in [19]. Theorem 3.1 is available in a somewhat more general form, allowing ρ to have roots on the circle [19].

However, all these proofs are nonconstructive and thus they do not provide a method of solution. A constructive proof based on convex optimization was presented in [9] for the Carathèodory case and in [10] for the Nevanlinna-Pick problem. This result, as well as an algorithm based on it, will be presented in Section 5.

The theorem extends to interpolation of matrix-valued functions (see [16] where existence of solutions were shown in the context of Carathèodory interpolation). An approach generalizing this result to the context of the commutant-lifting theory is the subject of [11].

Dividing (3.5) by $\alpha(z)\alpha(z^{-1})$ yields

$$f(z) + f(z^{-1}) = g(z)g(z^{-1}), \tag{3.8}$$

where

$$g(z) = \frac{\rho(z)}{\alpha(z)}, \tag{3.9}$$

i.e, (3.9) is the minimum-phase spectral factor of the spectral density (3.8). For this reason, we shall refer to the roots of ρ as the *spectral zeros* of f. In this notation, Theorem 3.1 states that to each self-conjugate set of n points $\sigma_1, \sigma_2, \dots, \sigma_n$ inside the unit circle there is a unique stable polynomial

$$\alpha(z) = a_0 z^n + a_1 z^{n-1} + \cdots + a_{n-1} z + a_n \tag{3.10}$$

so that the positive-real part f of

$$\frac{\rho(z)\rho(z^{-1})}{\alpha(z)\alpha(z^{-1})} \quad \text{with } \rho(z) = \prod_{k=1}^{n}(z - \sigma_k)$$

satisfies the interpolation conditions (3.1). Moreover, $\sigma_1, \sigma_2, \dots, \sigma_n$ are the spectral zeros of the interpolant f. Once both ρ and α are known, the stable polynomial

$$\beta(z) = b_0 z^n + b_1 z^{n-1} + \cdots + b_{n-1} z + b_n \tag{3.11}$$

is uniquely determined by (3.5). In fact, identifying coefficients of like powers in z, the coefficients of β are seen to satisfy the system of linear equations

$$\left(\begin{bmatrix} a_0 & \dots & a_{n-2} & a_{n-1} & a_n \\ a_1 & \dots & a_{n-1} & a_n & \\ a_2 & \dots & a_n & & \\ \vdots & \iddots & & & \\ a_n & & & & \end{bmatrix} + \begin{bmatrix} a_0 & a_1 & a_2 & \dots & a_n \\ & a_0 & a_1 & \dots & a_{n-1} \\ & & a_0 & \dots & a_{n-2} \\ & & & \ddots & \vdots \\ & & & & a_0 \end{bmatrix} \right) \begin{bmatrix} b_0 \\ b_1 \\ b_2 \\ \vdots \\ b_n \end{bmatrix} = \begin{bmatrix} 1 + r_1^2 + r_2^2 + \cdots + r_n^2 \\ r_1 + r_1 r_2 + r_{n-1} r_n \\ r_2 + r_1 r_3 + r_{n-2} r_n \\ \vdots \\ r_n \end{bmatrix}, \tag{3.12}$$

which has a unique solution for any stable polynomial $\alpha(z)$.

3.3. Application to the problem of spectral estimation. As suggested earlier, passing data (2.1) through a bank of filters with a pole setting $p_0, p_1, \ldots, p_n$ and estimating the covariance of the output variables, gives a set of parameters $w_1, w_2, \ldots, w_n$ via (3.2). In the ergodic limit, the corresponding Pick matrix P_n, defined by (3.4), will be given by (2.10) and hence must be positive definite as required, e.g. in Theorem 3.1. The THREE method relies on the preceding interpolation theory and identifies transfer functions g, as in (3.9), such that $|g(e^{i\theta})|^2$ are approximations of the power spectrum $\Phi(e^{i\theta})$ of y. Thus, a process $\{\hat{y}(t)\}_{t\in\mathbb{Z}}$, obtained by passing (normalized) white noise $\{\nu(t)\}_{t\in\mathbb{Z}}$ through the modeling filter

$$\text{white noise} \xrightarrow{\nu} \boxed{g(z)} \xrightarrow{\hat{y}}$$

and letting it come to a statistical steady state, will generate a statistical approximant of y. The relevant ARMA model is given by the difference equation

$$a_0\hat{y}(t) + a_1\hat{y}(t-1) + \cdots + a_n\hat{y}(t-n) = \nu(t) + r_1\nu(t-1) + \cdots + r_n\nu(t-n). \tag{3.13}$$

Consequently, we shall refer to $r_1, r_2, \ldots, r_n$ as the *MA parameters* and to $a_0, a_1, \ldots, a_n$ as the *AR parameters* of the *THREE filter* (3.13). The complete set of MA and AR parameters will be called the *THREE filter parameters*. In this context, Theorem 3.1 states that to any choice of MA parameters (such that $\rho(z)$ is a stable polynomial) there corresponds a unique choice of AR parameters (with $\alpha(z)$ likewise stable) so that the positive-real part of the spectral density satisfies the interpolation conditions (3.1). Hence the MA parameters can be chosen arbitrarily. It is interesting to note that the analogous statement for the AR parameters is false. In other words, an arbitrary choice of AR parameters may not have a matching selection of MA parameters so that together they meet the required constraints.

Theorem 3.1, is an existence result. The computational problem at hand amounts to the following: given a choice of MA parameters (with $\rho(z)$ stable as usual), find the corresponding set of AR parameters and hence the unique pair (α, β) of stable polynomials satisfying (3.5), (3.6) and (3.7). In conclusion, there are two sets of design parameters:

(i) the filter-bank parameters $p_1, p_2, \ldots, p_n$, $p_0 = 0$ being fixed, which we represent as the roots of a polynomial

$$\tau(z) := \prod_{k=1}^{n}(z - p_k) = z^n + \tau_1 z^{n-1} + \cdots + \tau_{n-1}z + \tau_n, \tag{3.14}$$

and

(ii) the MA parameters $r_1, r_2, \ldots, r_n$, or, alternatively, the spectral zeros $\sigma_1, \sigma_2, \ldots, \sigma_n$, which are the roots of

$$\rho(z) := \prod_{k=1}^{n}(z - \sigma_k) = z^n + r_1 z^{n-1} + \cdots + r_{n-1}z + r_n. \tag{3.15}$$

The power of THREE filtering stems from the flexibility in the above choices. In particular, if reliable approximation of $\Phi(e^{i\theta})$ is required over some specified part of the spectrum $\theta \in \mathcal{S} \subset [-\pi, \pi]$, this can be accomplished by placing the filter-bank poles $p_0, p_1, \ldots, p_n$ near the corresponding arc $\{e^{i\theta} \mid \theta \in \mathcal{S}\}$. However, it should be noted that the filter-bank poles must not be selected too close to the circle, because then, statistical estimates of the output covariances become less reliable as explained in Section 2. We should also mention another related caveat: if the observation record is too short, the Pick matrix may fail to be positive. In this case we

must either collect more data, select a different set of filter-bank poles (e.g., select a new set closer to the origin, or simply a subset of the existing one), or add a small positive bias to the estimated values $w_0, w_1, \dots, w_n$ (e.g., add to each a constant λ larger than the absolute value of the minimal negative eigenvalue of $P_n E_n^{-1}$, where $E_n = [2/(1 - p_j \bar{p}_k)]_{j,k=0}^n$).

There is a special default setting of the spectral zeros, namely $\sigma_k = p_k$ for $k = 1, 2, \dots, n$, i.e., setting

$$\rho(z) \equiv \tau(z), \tag{3.16}$$

for which the problem of computing $\alpha(z)$ requires solving only linear equations. This relates to the so-called *central solution*, in classical interpolation theory and is discussed in Section 4. The general case, which is capable of higher resolution, requires a proper choice of spectral zeros and then the solution of a convex optimization problem. This will be discussed in Section 5. It is interesting to remark that, even if AR-modeling is required, which fixes $\rho(z) = z^n$, the solution claimed by Theorem 3.1 and the THREE method cannot be obtained with the Levinson algorithm – the Levinson algorithm is only applicable when the covariance lags $c_0, c_1, \dots, c_n$ of y are available.

4. The central solver for the default filter

In this section we consider the special case that the MA parameters are set to the default values, $r_k = \tau_k$ for $k = 1, 2, \dots, n$, i.e., $\rho = \tau$. Determining the AR parameters is then considerably simplified, since this choice corresponds to the central solution, mentioned above. As it turns out, the central solution is precisely the positive real function maximizing the entropy gain

$$\frac{1}{2\pi} \int_{-\pi}^{\pi} \log(f(e^{i\theta}) + f(e^{-i\theta})) d\theta, \tag{4.1}$$

subject to the constraints (3.1). In Section 5 we shall see that this optimization problem can be generalized to yield interpolants for any other choice of MA parameters.

4.1. The algorithm. Next, we explain the steps of the algorithm for the central solution, deferring technical details to Appendix A.

Consider the subset of interpolation conditions (3.1) for $k = 1, 2, \dots, n$, excluding $f(p_0^{-1}) = w_0$. Any positive-real function satisfying these n conditions is given by a linear fraction transformation

$$f(z) = \frac{M_1(z)\varphi(z) + M_2(z)}{M_3(z)\varphi(z) + M_4(z)}, \tag{4.2}$$

where φ is a positive real function, and

$$M(z) = \begin{bmatrix} M_1(z) & M_2(z) \\ M_3(z) & M_4(z) \end{bmatrix} \tag{4.3}$$

is the (J-unitary) rational matrix function (4.13) which depends on the interpolation data. The proof is deferred to Appendix A, while the construction of the $M(z)$ is described in this section. The particular choice

$$f(z) = \frac{M_1(z)\mu + M_2(z)}{M_3(z)\mu + M_4(z)} \tag{4.4}$$

with $\varphi(z)$ constant and equal to

$$\mu = \frac{w_0 M_4(\infty) - M_2(\infty)}{M_1(\infty) - w_0 M_3(\infty)}, \tag{4.5}$$

turns out to satisfy the omitted interpolation condition $f(p_0^{-1}) = w_0$. In fact, this choice turns out to be the solution to our original problem, i.e. $f(z)$ has the required degree and the default values of the MA parameters. Moreover, this is the unique solution which maximizes the entropy gain (4.1). The proof of this last fact is given in Appendix A.

It is well-known that solutions to interpolation problems can be represented by linear fractional transformations. Hence, one may wonder why we decompose our problem into two steps – first omitting one condition, and then trying to satisfy it by a suitable choice of the free parameter φ. The reason is that a formula (4.2) for the complete set of interpolation conditions (including the condition at $k = 0$) requires finding an appropriate free parameter φ *of degree one* in order to satisfy the degree constraint (3.3), which is slightly more complicated.

We now explain how to construct the matrix function $M(z)$ in (4.3). Consider the set of analytic functions F, mapping the right half-plane into the unit disc, which satisfy the interpolation conditions

$$F(s_k) = v_k \quad k = 1, 2, \ldots, n, \tag{4.6}$$

where

$$s_k = \frac{1 - p_k}{1 + p_k} \quad \text{and} \quad v_k = \frac{1 - w_k}{1 + w_k} \quad k = 1, 2, \ldots, n. \tag{4.7}$$

It is well-known and easy to prove that the all-pass filter (i.e., Blaschke product)

$$B(s) = \prod_{k=1}^{n} \frac{s - s_k}{s + s_k}$$

has a state-space representation

$$B(s) = c(sI - A)^{-1} P^{-1} c' + 1,$$

where the symmetric positive definite matrix P is the solution of the Lyapunov equation

$$A'P + PA = c'c. \tag{4.8}$$

Here the matrix A is unstable, in the sense that it has all its eigenvalues in the right half-plane. In fact, its characteristic polynomial is

$$\hat{\tau}(s) := \prod_{k=1}^{n} (s - s_k) = s^n + \hat{\tau}_1 s^{n-1} + \cdots + \hat{\tau}_{n-1} s + \hat{\tau}_n,$$

and hence we may choose A and c in the observer canonical form

$$\begin{aligned} A &= \begin{bmatrix} -\hat{\tau}_1 & -\hat{\tau}_2 & \ldots & -\hat{\tau}_{n-1} & -\hat{\tau}_n \\ 1 & 0 & \ldots & 0 & 0 \\ 0 & 1 & \ldots & 0 & 0 \\ \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & \ldots & 1 & 0 \end{bmatrix}, \\ c &= \begin{bmatrix} 0 & 0 & \ldots & 0 & 1 \end{bmatrix} \end{aligned} \tag{4.9}$$

Note that $\hat{\tau}(s)$ is the polynomial obtained from $\tau(z)$, defined by (3.14), under the linear fractional transformation $s = \frac{z-1}{z+1}$.

Next, we determine the coefficients $\pi_1, \pi_2, \dots, \pi_n$ so that the rational function

$$V(s) = \frac{\pi_1 s^{n-1} + \pi_2 s^{n-2} + \cdots + \pi_n}{\hat{\tau}(s)}$$

satisfies the interpolation (4.6). This is done by solving the Vandermonde system

$$\begin{bmatrix} s_1^{n-1} & \dots & s_1 & 1 \\ s_2^{n-1} & \dots & s_2 & 1 \\ \vdots & \vdots & \vdots & \vdots \\ s_n^{n-1} & \dots & s_n & 1 \end{bmatrix} \begin{bmatrix} \pi_1 \\ \pi_2 \\ \vdots \\ \pi_n \end{bmatrix} = \begin{bmatrix} \hat{\tau}(s_1)v_1 \\ \hat{\tau}(s_2)v_2 \\ \vdots \\ \hat{\tau}(s_n)v_n \end{bmatrix}.$$

Clearly, $V(s)$ has a realization

$$V(s) = c(sI - A)^{-1}b,$$

where A and c are given by (4.9) and b can be determined from $\pi_1, \pi_2, \dots, \pi_n$ by standard methods.

It turns out that all interpolants F satisfying (4.6) are given by

$$F(s) = \frac{L_1(s)Y(s) + L_2(s)}{L_3(s)Y(s) + L_4(s)}, \tag{4.10}$$

for some function Y which is analytic and bounded by one in the right half-plane, where

$$L(s) := \begin{bmatrix} L_1(s) & L_2(s) \\ L_3(s) & L_4(s) \end{bmatrix} = \begin{bmatrix} c \\ -b'P \end{bmatrix} (sI - A)^{-1} \begin{bmatrix} P^{-1}Nc' & -N'b \end{bmatrix} + I. \tag{4.11}$$

Here $N = (I - PQ)^{-1}$, where Q is the symmetric positive definite solution of the Lyapunov equation

$$(A - P^{-1}c'c)Q + Q(A - P^{-1}c'c) = bb'. \tag{4.12}$$

The matrix $I - PQ$ is invertible precisely when solutions do exist.

Returning to our original interpolation problem, the matrix function (4.3) needed in the representation (4.4) is given by

$$M(z) = \frac{1}{\sqrt{2}} \begin{bmatrix} -1 & 1 \\ 1 & 1 \end{bmatrix} L(\frac{z-1}{z+1}). \tag{4.13}$$

Since $\hat{\tau}$ corresponds to τ under the transformation $s = \frac{z-1}{z+1}$, $\tau(z)M(z)$ is a matrix polynomial, and consequently the central interpolant (4.4) is given by

$$f(z) = \frac{\hat{\beta}(z)}{\hat{\alpha}(z)},$$

where $\hat{\alpha}(z)$ and $\hat{\beta}(z)$ are the polynomials

$$\begin{aligned} \hat{\alpha}(z) &:= \hat{\alpha}_0 z^n + \hat{\alpha}_1 z^{n-1} + \cdots + \hat{\alpha}_n = \tau(z)[M_3(z)\mu + M_4(z)], \\ \hat{\beta}(z) &:= \hat{\beta}_0 z^n + \hat{\beta}_1 z^{n-1} + \cdots + \hat{\beta}_n = \tau(z)[M_1(z)\mu + M_2(z)]. \end{aligned}$$

However, to obtain the $\alpha(z)$ which matches the MA parameters $r = \tau$, and hence the THREE-filter parameters, $\hat{\alpha}(z)$ needs to be normalized by setting

$$\alpha(z) = \frac{1 + \tau_1^2 + \cdots + \tau_n^2}{2(\hat{\alpha}_0\hat{\beta}_0 + \hat{\alpha}_1\hat{\beta}_1 + \hat{\alpha}_n\hat{\beta}_n)}\hat{\alpha}(z).$$

4.2. Simulation studies. In this section we demonstrate the performance of THREE filters in the default setting of the central solution, and compare with traditional spectral estimation techniques.

Example 1. We begin by estimating spectral lines in colored noise – a problem which is regarded as challenging [27, pages 285–286]. Consider the following signal y comprised of two superimposed sinusoids in colored noise:

$$\begin{aligned} y(t) &= 0.5\sin(\omega_1 t + \phi_1) + 0.5\sin(\omega_2 t + \phi_2) + z(t) \quad t = 0, 1, 2, \ldots, \\ z(t) &= 0.8z(t-1) + 0.5\nu(t) + 0.25\nu(t-1) \end{aligned}$$

with ϕ_1, ϕ_2 and $\nu(t)$ independent normal random variables with zero mean and unit variance. The objective is to estimate the power spectrum in the vicinity of the spectral lines. In particular, it is desirable to be able to resolve the two distinct spectral peaks. Two cases are investigated, which differ in the separation of the spectral lines. In Case A we take the spectral lines at frequencies $\omega_1 = 0.42$ and $\omega_2 = 0.53$, and in Case B at frequencies $\omega_1 = 0.45$ and $\omega_2 = 0.47$.

The model is used to generate five sets of 300 data points in separate runs. This is done in order to investigate the statistical variability of the estimates and the robustness of the estimation methods. Three different spectral estimation methods are compared: (i) periodograms, computed with state-of-the-art windowing technology, as implemented in the Identification Matlab Toolbox command `etfe`, with smoothing parameter `M` set to `60`; (ii) Levinson/AR filtering of order 12, based on covariance lags; and (iii) THREE filter design of order 12 with the filter-bank poles chosen at

$$(0, .85, -.85, \rho e^{.42i}, \rho e^{.44i}, \rho e^{.46i}, \rho e^{.48i}, \rho e^{.50i}),$$

where $\rho = 0.9$ in Case A and $\rho = 0.93$ in Case B, and the MA parameters set at the default setting corresponding to the central solution in both cases. The choice of ρ was dictated by an *ad hoc* rule of thumb that the time constant of the system is of the order 1/10 of the length of the data record, whereas the phases of some of the poles were selected in the part of the spectrum where high resolution is desired. In Case B, the separation of the sinusoids is smaller than the theoretically possible distance that can be resolved by the periodogram using a 300 point record under ideal noise conditions, not satisfied here [29, page 33]. In fact, with white noise and large S/N ratio, this minimum separation between the lines is $\frac{2\pi}{300} \sim .021$. To achieve a better resolution (at the expense of some increased variability) the complex filter-bank poles were chosen slightly closer to the circle in Case B.

The results are depicted in Figure 2. The subplots in the first column correspond to Case A and those in the second column to Case B. From top to bottom, we display the results using methods (i) through (iii). In Case A, the estimated spectra from five separate data sets are superimposed, shown together with a smooth curve representing the true power spectrum of the colored noise and two vertical lines at the position of the spectral lines. For clarity, in Case B we only show the outcome of one run.

The periodogram does reasonably well in Case A but fails in Case B. In both cases, the Levinson/AR method fails to identify the peaks. It is apparent that only the THREE filter is capable of resolving the two sinusoids in both cases, clearly delineating their position by the presence of two peaks. In comparing (i) and (iii), it should be further noted that (i) is nonparametric, and hence the estimates are not as easily coded for transmission to a remote receiver as the case is for (iii).

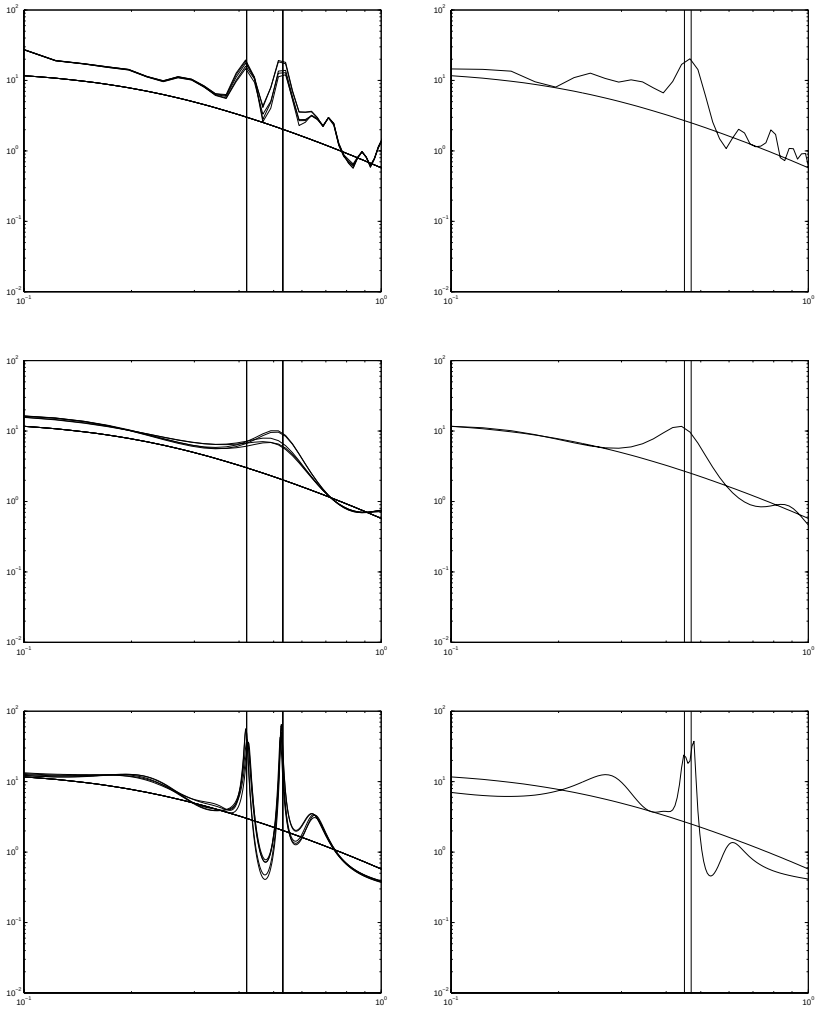

Figure 2: Spectral estimates of two sinosoids in colored noise.

Example 2. We consider the effectiveness of THREE-based filtering in a case where the power spectrum has sharp transitions. More specifically, we consider data generated by passing white noise through a filter with the transfer function

$$T_\theta(z) = \frac{(z - .9e^{i\pi/3.2})(z - .9e^{-i\pi/3.2})}{(z - .9e^{i\theta})(z - .9e^{-i\theta})(z - .3e^{i\pi/3.5})(z - .3e^{-i\pi/3.5})}. \tag{4.14}$$

We consider three cases, where θ takes values $\pi/2.9$, $\pi/3$ and $\pi/3.1$. In each case, the spectrum of the output has sharp transitions due to the fact that poles and zeros are close to each other.

In Figure 3 we show the results of numerical simulation, where we compare (a) periodogram-based spectral estimates (`etfe(y,50)` in Matlab), with (b) Levinson/AR modeling of order four,

and (c) THREE-based modeling of order four with default setting corresponding to the central solution and a *fixed* selection of filter-bank poles set at $0, .8e^{\pm .8i}, .8e^{\pm 1.3i}$. In order to avoid the effects of variability in the estimates we choose a long record of 2000 data samples. Although, with such long data record, higher order models would be possible and hence more appropriate, the issue here is to compare performance for fixed order models.

The first column in Figure 3 corresponds to the choice $\theta = \pi/2.9$, the second to $\theta = \pi/3$, and the third to $\theta = \pi/3.1$, whereas each row corresponds to a different methods: The first row corresponds to (a), the second row to (b), the third row to (c) as explained above. In each of these figures, for easy comparison, the true power spectrum of the process has been superimposed, drawn by a dashed curve.

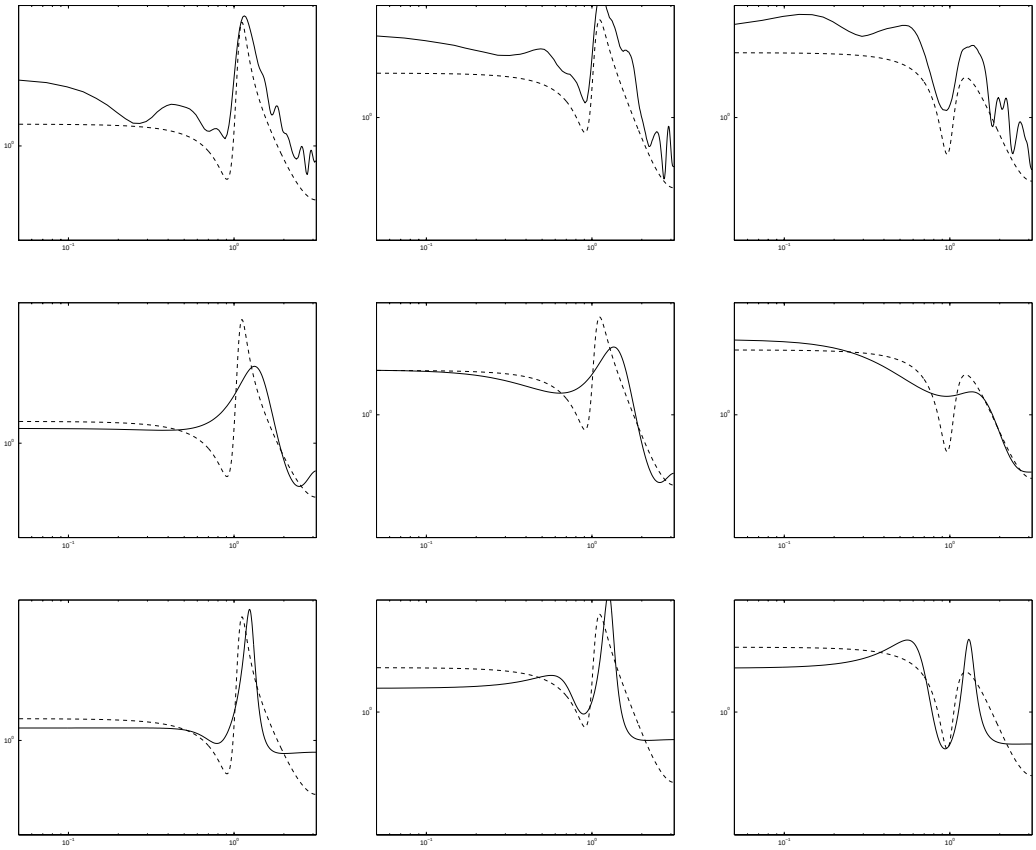

Figure 3: Estimates of sharp spectral transitions.

We see that the THREE filter does considerably better than the other two methods. However, its performance can be improved further by allowing a choice of spectral zeros away from the default setting. This requires the theory developed in the next section. Hence, Example 2 is considered again in Section 5 (Figure 4) with appropriate zero settings.

5. Generalized entropy and convex optimization

In this section we describe how an arbitrary solution of the Nevanlinna-Pick interpolation problem with degree constraints, as described in Theorem 3.1, can be obtained from a convex optimization problem, and we summarize the steps of a numerical algorithm based on this optimization problem. The basic theory has been developed in [10], while Appendix B in the present

paper complements and extends certain of the key constructions in [10].

5.1. Entropy functionals and convex optimization. Given the polynomial $\tau(z)$, defined by (3.14), let $\mathcal{K}$ be the $(n+1)$-dimensional vector space of all proper, real, rational functions

$$q(z) = \frac{\pi(z)}{\tau(z)} \tag{5.1}$$

with denominator $\tau(z)$, where

$$\pi(z) = \pi_0 z^n + \pi_1 z^{n-1} + \cdots + \pi_n$$

for some real numbers $\pi_0, \pi_1, \dots, \pi_n$, and let $\mathcal{S}_+$ be the convex set of rational functions with the properties

$$Q(z) := q(z) + q(z^{-1}) \quad \text{for some } q \in \mathcal{K}, \tag{5.2}$$

$$Q(e^{i\theta}) > 0 \quad \text{for } \theta \in [-\pi, \pi]. \tag{5.3}$$

Moreover, for each real function f, we define f^* by $f^*(z) := f(z^{-1})$.

It turns out to be useful to represent the positive-real function f to be estimated, as a quotient between two functions in $\mathcal{K}$, rather than a quotient between two polynomials, as before. In fact, the polynomials $\alpha(z)$ and $\beta(z)$ in Theorem 3.1 can be replaced by

$$a(z) = \frac{\alpha(z)}{\tau(z)} \quad \text{and} \quad b(z) = \frac{\beta(z)}{\tau(z)}. \tag{5.4}$$

Then (3.5) becomes

$$a(z)b(z^{-1}) + b(z)a(z^{-1}) = \Psi(z), \tag{5.5}$$

where

$$\Psi(z) = \frac{\rho(z)\rho(z^{-1})}{\tau(z)\tau(z^{-1})} \tag{5.6}$$

belongs to $\mathcal{S}_+$. In the central solution, $\Psi(z) \equiv 1$.

Now, for any $\Psi \in \mathcal{S}_+$, define the functional

$$\mathbb{I}_\Psi(f) = \frac{1}{2\pi} \int_{-\pi}^{\pi} \log[f(e^{i\theta}) + f(e^{-i\theta})]\Psi(e^{i\theta}) d\theta, \tag{5.7}$$

on the space of positive real functions f. This functional is a generalization of the entropy gain (4.1). In fact, (4.1) is precisely $\mathbb{I}_1(f)$.

The generalized entropy gain plays a key role in our theory. In fact, in [10, Theorem 4.1] we have the following result.

Theorem 5.1. *Given any $\Psi \in \mathcal{S}_+$ there exists a unique solution to the constrained optimization problem*

$$\max\{\mathbb{I}_\Psi(f) \mid f \text{ is positive real}, \quad f(p_k^{-1}) = w_k \text{ for } k = 0, 1, \dots, n\}. \tag{5.8}$$

This solution is of the form

$$f(z) = \frac{b(z)}{a(z)}, \quad a, b \in \mathcal{K}, \tag{5.9}$$

where

$$a(z)b^*(z) + b(z)a^*(z) = \Psi(z). \tag{5.10}$$

Conversely, if f is a positive-real function which satisfies the interpolation conditions as well as (5.9) *and* (5.10)*, then it is the unique solution to* (5.8)*.*

Note that (5.9) is equivalent to requiring that f is of degree at most n. The choice $\Psi = 1$ yields the central solution of the Nevanlinna-Pick theory which is also known as the "maximum entropy" solution. All other interpolants of degree $\leq n$ can be obtained by choosing the corresponding Ψ and solving the generalized entropy maximization problem given above. However, this optimization problem is infinite-dimensional and therefore not easy to solve. As it turns out, it has a dual with finitely many variables, and next we shall turn to this problem.

To this end, let $w(z)$ be any real function which is analytic on and outside the unit circle and satisfies the interpolation conditions

$$w(p_k) = w_k, \quad k = 0, 1, \dots, n.$$

Then, define for each function $Q \in \mathcal{S}_+$ the functional

$$\mathbb{J}_\Psi(Q) := \frac{1}{2\pi} \int_{-\pi}^{\pi} \{Q(e^{i\theta})[w(e^{i\theta}) + w(e^{-i\theta})] - \log Q(e^{i\theta})\Psi(e^{i\theta})\}\theta. \tag{5.11}$$

It will be shown in Appendix B that this functional does not depend on the particular choice of $w(z)$ but only on its values in the interpolation points. In fact, it is a quadratic form whose coefficients are the entries of the Pick matrix (3.4). We could choose the unique such function in $\mathcal{K}$, which is easily determined by solving a linear system of equations (Appendix B). Note that w is not positive real in general, and therefore cannot be used as an interpolant.

Using duality theory, the maximization problem of Theorem 5.1 can be seen to be equivalent to the following convex optimization problem; see [10, Theorem 4.5].

Theorem 5.2. *For each $\Psi \in \mathcal{S}_+$, the convex optimization problem*

$$\min\{\mathbb{J}_\Psi(Q) \mid Q \in \mathcal{S}_+\} \tag{5.12}$$

has a unique solution. Moreover, to this minimizing Q, there corresponds a unique positive real function f satisfying the interpolation conditions

$$f(p_k^{-1}) = w_k, \quad k = 0, 1, \dots, n \tag{5.13}$$

where $p_0^{-1} := \infty$, and

$$\frac{\Psi(z)}{Q(z)} = f(z) + f^*(z). \tag{5.14}$$

The function $f(z)$ is precisely the maximizing function (5.9) *in Theorem* 5.1*, where $a(z)$ is the minimum-phase spectral factor of*

$$a(z)a^*(z) = Q(z), \tag{5.15}$$

and $b(z)$ the unique solution of (5.10)*, given Ψ and a. Conversely, any positive real function satisfying* (5.13)*,* (5.9) *and* (5.10) *is obtained in this way.*

The proofs of Theorem 5.1 and Theorem 5.2, which are very nontrivial, are given in [10]. Since $\mathbb{J}_\Psi$ is a strictly convex function on a convex set $\mathcal{S}_+$, the minimization problem of Theorem 5.2 is a convex optimization problem. Therefore, if there is a minimum in the open set $\mathcal{S}_+$, this minimum is unique and occurs at a stationary point, i.e., at a point where the gradient is zero. It is proved in [10] that this is indeed the case. It is then quite straight-forward to show that

the optimal Q defines a unique interpolant f with the required properties. Since this is quite instructive, we give an alternative proof of this, tailored to our present exposure in Appendix B. Elements from this derivation will also be needed to derive the gradient and Hessian of $\mathbb{J}_\Psi$ needed in solving the convex optimization problem.

An advantage of the proof of Theorem 5.2 is that it is constructive and therefore yields an algorithm for computing an arbitrary interpolant of degree at most n. Since Q is determined by $n+1$ variables via (5.2), it is a finite-dimensional optimization problem. What these $n+1$ variables should be depends on what basis we choose for $\mathcal{K}$. Any function $q \in \mathcal{K}$ has a state-space representation

$$q(z) = c(zI - A)^{-1}b + d, \tag{5.16}$$

where

$$\left[\begin{array}{c|c} A & b \\ \hline c & d \end{array}\right] = \left[\begin{array}{ccccc|c} -\tau_1 & -\tau_2 & \dots & -\tau_{n-1} & -\tau_n & h_n \\ 1 & 0 & \dots & 0 & 0 & h_{n-1} \\ 0 & 1 & \dots & 0 & 0 & h_{n-2} \\ \vdots & \vdots & \ddots & \vdots & \vdots & \vdots \\ 0 & 0 & \dots & 1 & 0 & h_1 \\ \hline 0 & 0 & \dots & 0 & 1 & h_0 \end{array}\right] \tag{5.17}$$

with $\tau_1, \tau_2, \dots, \tau_n$ given by(3.14). The coordinates

$$\begin{bmatrix} b \\ d \end{bmatrix} := h = \begin{bmatrix} h_n \\ \vdots \\ h_1 \\ h_0 \end{bmatrix} \tag{5.18}$$

of this representation are the $n+1$ first Markov parameters in the series expansion

$$q(z) = h_0 + h_1 z^{-1} + h_2 z^{-2} + \dots,$$

and therefore they will be referred to as the *Markov coordinates* of $\mathcal{K}$. We shall write $q(z) \sim (b, d)$ to denote this correspondence.

Thus, to formulate an algorithm, we express the functional (5.11) via (5.16) in terms of its Markov coordinates to obtain

$$J(h) = \mathbb{J}_\Psi(q + q^*), \tag{5.19}$$

which is a function $\mathbb{R}^{n+1} \to \mathbb{R}$. To each $q \in \mathcal{K}$ satisfying (5.2) and (5.3), there corresponds a positive real function f, obtained from $Q := q + q^*$ via (5.14). The idea is now to minimize $J(h)$ over the region where

$$q(e^{i\theta}) + q(e^{-i\theta}) > 0, \quad \text{for } -\pi \le \theta \le \pi. \tag{5.20}$$

This is done recursively by Newton's method, upholding condition (5.5), or, equivalently, condition(3.5), while successively trying to satisfy the interpolation condition (5.13) by reducing the interpolation errors

$$e_k = w_k - f(p_k^{-1}), \quad k = 0, 1, \dots, n. \tag{5.21}$$

In order to obtain an expression for the gradient, define the $n \times n$ Vandermonde matrix

$$V = \begin{bmatrix} z_1^{n-1} & z_1^{n-2} & \dots & 1 \\ z_2^{n-1} & z_2^{n-2} & \dots & 1 \\ \vdots & \vdots & \ddots & \vdots \\ z_n^{n-1} & z_n^{n-2} & \dots & 1 \end{bmatrix}, \tag{5.22}$$

where $z_k := p_k^{-1}$ for $k = 1, 2, \dots, n$. Since the points $z_0, z_1, \dots, z_n$ are distinct, this matrix is nonsingular.

Proposition 5.3. *Let* (5.18) *be a point in* $\mathbb{R}^{n+1}$ *such that* (5.16) *satisfies* (5.20)*, let* $e_0, e_1, \dots, e_n$ *be the corresponding interpolation errors* (5.21)*, and set*

$$L_m = \begin{bmatrix} & & & 1 \\ & & 1 & \tau_1 \\ & \iddots & \iddots & \vdots \\ 1 & \tau_1 & \dots & \tau_m \end{bmatrix} \quad \textit{and} \quad v = \begin{bmatrix} (e_1 - e_0)\tau(p_1^{-1}) \\ (e_2 - e_0)\tau(p_2^{-1}) \\ \vdots \\ (e_n - e_0)\tau(p_n^{-1}) \end{bmatrix}. \tag{5.23}$$

Then the gradient of (5.19) *at* h *is given by*

$$\nabla J(h) = 2 \begin{bmatrix} P L_{n-1}^{-1} V^{-1} v \\ 2e_0 \end{bmatrix}, \tag{5.24}$$

where P *is the solution to the Lyapunov equation*

$$P = A'PA + c'c, \tag{5.25}$$

where A *and* c *are given by* (5.17)*.*

The proof of this proposition is given in Appendix B. Note that, since A is a stable matrix and (c, A) is an observable pair, P is positive definite. Hence the gradient is zero if and only if the interpolation errors $e_0, e_1, \dots, e_n$ are all zero, in harmony with Theorem 5.2.

To apply Newton's method we also need the Hessian. To this end, we need some notation. Given an arbitrary real polynomial

$$\gamma(z) = g_0 z^m + g_1 z^{m-1} + \cdots + g_m, \tag{5.26}$$

define first the $(n+1) \times (m+1)$ matrix

$$M(\gamma) := \begin{bmatrix} g_0 & g_1 & \dots & g_n & g_{n+1} & \dots & g_m & & \\ & g_0 & g_1 & \dots & g_n & g_{n+1} & \dots & g_m & \\ & & \ddots & \ddots & & \ddots & \ddots & & \ddots \\ & & & g_0 & g_1 & \dots & g_n & g_{n+1} & \dots & g_m \end{bmatrix}. \tag{5.27}$$

Secondly, for any (5.26), determine $\lambda_0, \lambda_1, \dots, \lambda_m$ such that

$$\gamma(z)(\lambda_0 z^m + \lambda_1 z^{m-1} + \cdots + \lambda_m) = z^{2m} + \pi(z),$$

where $\pi(z)$ is a polynomial of at most degree $m-1$. This yields $m+1$ linear equation for the $m+1$ unknowns $\lambda_0, \lambda_1, \dots, \lambda_m$, in terms of which we define the $(m+1)\times(m+1)$ matrix

$$N(\gamma) = \begin{bmatrix} \lambda_m & \dots & \lambda_1 & \lambda_0 \\ \lambda_{m-1} & \dots & \lambda_0 & \\ \vdots & \iddots & & \\ \lambda_0 & & & \end{bmatrix}. \tag{5.28}$$

Finally, for an arbitrary stable polynomial (5.26), let $A(\gamma)$ be the companion matrix with characteristic polynomial γ, formed analogously to A in (5.17) replacing $\tau(z)$ by $\gamma(z)$, and let $P(\gamma)$ be the unique $m\times m$-matrix solution of the Lyapunov equation

$$P(\gamma) = A(\gamma)'P(\gamma)A(\gamma) + c(\gamma)'c(\gamma),$$

where $c(\gamma)$ is the m row vector $(0,0,\dots,0,1)$.

Then, we have the following proposition for the $(n+1)\times(n+1)$ Hessian matrix

$$H = \left[\frac{\partial^2\varphi}{\partial h_k \partial h_\ell}\right]_{k,\ell=0}^{n}. \tag{5.29}$$

The proof will be given in Appendix B.

Proposition 5.4. *Given $\Psi(z)$, where the polynomials $\rho(z)$ and $\tau(z)$ are given by* (3.15) *and* (3.14)*, respectively, let* (5.18) *be a point in $\mathbb{R}^{n+1}$ such that* (5.16) *satisfies* (5.20)*, and let $\alpha(z)$ be the unique stable polynomial satisfying*

$$\frac{\alpha(z)\alpha(z^{-1})}{\tau(z)\tau(z^{-1})} = q(z) + q^*(z). \tag{5.30}$$

Then the Hessian (5.29) *of* (5.19) *at h is given by*

$$H = 2H_1 + H_2 + H_2', \tag{5.31}$$

where

$$H_1 = L_n M(\rho) N(\alpha^2) \begin{bmatrix} P(\alpha^2) & 0 \\ 0 & 1 \end{bmatrix} N(\alpha^2) M(\rho)' L_n \tag{5.32}$$

$$H_2 = L_n M(\tau_*\rho) N(\alpha^2\tau) \begin{bmatrix} P(\alpha^2\tau) & 0 \\ 0 & 1 \end{bmatrix} N(\alpha^2\tau) M(\tau\rho)' \tilde{L}_n. \tag{5.33}$$

Here L_n is given by (5.23)*, $\tilde{L}_n$ is the corresponding matrix obtained by reversing the order of the rows in* (5.23)*, and $\tau_*(z) := z^n\tau(z^{-1})$.*

5.2. The algorithm for the tunable filter. We now outline the steps of the algorithm provided by Theorem 5.2 using Newton's method in Markov coordinates.

0. Given an initial a, compute $q \in \mathcal{K}$, satisfying $aa^* = q + q^*$.
1. Compute $b \in \mathcal{K}$ such that $a^*b + b^*a = \Psi$, and form $f = b/a$.
2. Check the interpolation error. Stop if it is sufficiently small.
3. Determine the search direction $d = H^{-1}\nabla J$.
4. Update q, and compute a minimum-phase $a \in \mathcal{K}$ such that $aa^* = q + q^*$. Then return to Step 1.

To initiate the algorithm, one needs to choose an initial value for $a(z)$, or, equivalently, for $\alpha(z)$, to be recursively updated. The tuning is done by selecting the polynomials $\tau(z)$ and $\rho(z)$, given by (3.14) and (3.15), respectively.

Given the initial $\alpha(z)$, solve (5.30) for $q(z)$. This can be done in several ways. One is to solve

$$\tau(z)\sigma(z^{-1}) + \sigma(z)\tau(z^{-1}) = \alpha(z)\alpha(z^{-1}) \tag{5.34}$$

for $\sigma(z)$ to obtain

$$q(z) = \frac{\sigma(z)}{\tau(z)}. \tag{5.35}$$

Identifying coefficients of like powers in z this amounts to solving a regular linear system of $n+1$ equations in $n+1$ variables, of the same type as (3.12). Then determining the initial point in Markov coordinates (5.18) is standard and can be done by premultiplying the vector of coefficients of $\sigma(z)$ by L_n, given by (5.23).

The algorithm now proceeds in four steps:

Step 1. In this step we compute f. Given the current α-polynomial (3.10), solve (3.5) for the β-polynomial (3.11). This is equivalent to solving the linear system (3.12). Next, form the corresponding positive real function f, defined by (3.6), and compute the interpolation errors $e_0, e_1, \ldots, e_n$, defined by (5.21).

Step 2. In this step we test whether our iterate is sufficiently close to be a minimizing solution. The algorithm is terminated if the errors $e_0, e_1, \ldots, e_n$ are sufficiently small, e.g., when $\sum_0^n (e_k)^2$ is less than a prespecified tolerance. Otherwise, continue.

Step 3. In this step the search direction of the optimization algorithm is determined. Given the interpolation errors $e_0, e_1, \ldots, e_n$, determine the gradient ∇J from Proposition 5.3, and, given the current $\alpha(z)$, compute the Hessian H as in Proposition 5.4. Then, the search direction, corresponding to one Newton step, is given by

$$d = H^{-1}\nabla J. \tag{5.36}$$

Let d_{previous} denote the search direction d obtained in the previous iteration. If this is the first iteration, initialize by setting $d_{\text{previous}} = 0$.

Step 4. In this step the solution is being updated, to yield a new

$$q(z) = c(zI - A)^{-1}g + h_0, \quad g = \begin{bmatrix} h_n \\ \vdots \\ h_1 \end{bmatrix},$$

with Markov parameters

$$h_{\text{new}} = h - \lambda d, \tag{5.37}$$

where λ should be chosen so that the new $q(z)$ satisfies the positivity condition (5.20). We may also use a variant of Wolfe's test [26] for accelerating the line search. If, for some constant κ, $\|d\| < \kappa\|d_{\text{previous}}\|$, increase the value of a parameter λ. Otherwise, retain the previous value of λ.

Then, $a \in \mathcal{K}$ is obtained by spectral factorization. More precisely, given $q(z)$ we solve

$$a(z)a(z^{-1}) = q(z) + q(z^{-1})$$

for the minimum-phase solution $a(z)$, in terms of which $\alpha(z) = \tau(z)a(z)$. This is standard and is done by solving the algebraic Riccati equation

$$P - APA' - (g - APc')(2h_0 - cPc')^{-1}(g - APc')' = 0,$$

for the stabilizing solution. This yields

$$a(z) = c(zI - A)^{-1}(g - APc')/\sqrt{2h_0 - cPc'} + \sqrt{2h_0 - cPc'}.$$

This factorization can be performed if and only if $q(z)$ satisfies condition (5.20). If this condition fails, this is determined in the factorization procedure, In this case, the value of λ is scaled down, and (5.37) is used to compute a new value for h_{new} and then of $q(z)$ successively until condition (5.20) is met.

Alternatively, an updated value for a can be obtained by determining the polynomial (3.10) with all roots less than one in absolute value, satisfying (5.34) with $\sigma(z)$ being the updated numerator polynomial of $q(z)$, as shown in (5.35). This is a standard polynomial factorization problem.

Finally, set $h := h_{\text{new}}$ and return to Step 1.

Example 2 (continued). To illustrate the advantages of the tunable THREE filter, we now reprocess the data in Example 2 using nontrivial spectral zeros. In general, the spectral zeros can be selected in the vicinity of the unit circle at approximately the frequencies where the spectrum has less energy. This selection can be guided by an initial estimate using periodogram.

In the present example, we select spectral zeros at $0, -.8, .8e^{\pm i\pi/3.3}$ while keeping the same filter-bank poles as before. We use the same setting when processing each data set, i.e., the ones corresponding the parameter $\theta = 2.9, 3.0$ and 3.1. Comparing with the results in Figure 3, it is evident that the performance is much improved and fairly robust with respect to changes in θ.

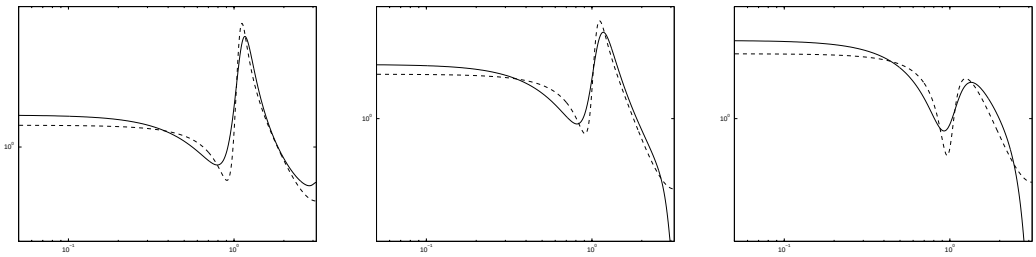

Figure 4: THREE spectral estimates with nondefault spectral-zero setting.

6. Conclusions

In this paper we have introduced a new approach to spectral estimation, which is based on the use of filter banks as a means of obtaining spectral interpolation data, and which produces an ARMA model with arbitrary MA-part. An essential property of this Tunable High REsolution Estimator (THREE) is that its performance can be enhanced for specific applications by tuning two sets of tunable parameters, the filter-bank poles and the spectral zeros. In particular, improved resolution can be achieved in designated parts of the spectrum. More specifically, we

have demonstrated that selection of the filter-bank poles in the vicinity of any arc of the unit circle results in improved reproduction of the power spectrum in the corresponding frequency band, as compared to, e.g., traditional AR filtering. Placing them too close to the unit circle will, however, increase the statistical variability, so there is a trade-off between resolution and variability of the estimates. The other set of tunable parameters, the spectral zeros, may be placed anywhere in the unit circle. Choosing them in the default setting, namely equal to the filter-bank poles, leads to a simpler solution, namely the classical central solution, for which we give an efficient algorithm. However we demonstrate that even higher resolution can be achieved by choosing the spectral zeros appropriately, away from the filter-bank poles, close to the unit circle for frequencies where notches in the spectrum are expected. Practical rules for selection of such parameters, in absence of prior information about the process, need to be worked out. In cases where spectral zeros of the nominal power spectrum are known *a priori* or can be estimated from longer data records, these same zeros can be enforced to coincide with the spectral zeros of the estimates of the power spectrum, without unduly increasing the complexity of the filters. For arbitrary tuning we need to solve a convex optimization problem, which amounts to maximizing a generalized entropy gain. A Newton-type algorithm for this problem has been presented.

Appendix A. An algorithm for the central interpolant

The parameterization of all solutions to the classical Nevanlinna-Pick problem (without degree constraints) takes the form of a linear fractional transformation (LFT) on a free parameter function which is typically normalized to be contractive [31]. The computation of the LFT elements amounts to solving linear equations, which can be done either recursively, e.g., by the Schur algorithm [31], or by reducing them to a pair of Lyapunov equations [14].

In [14] an LFT is derived for the Nehari problem, and the corresponding formula can be easily modified to the following Nevanlinna-Pick problem: Given a set

$$\{(s_k, v_k) \mid k = 1, 2, \dots, n, \text{ with } \mathrm{Re}(s_k) > 0 \text{ and } |v_k| < 1\},$$

determine all functions F which satisfy the interpolation conditions (4.6) and are analytic with modulus less than one in $\mathrm{Re}(s) > 0$. In fact, the interpolation formulas (4.10) and (4.11) follow directly from analogous formulas for the Nehari problem given in [14, page 125] by the following steps, using the notation of Section 4:

(a) Show that the symbol $B(-s)V(s)$ appearing in the Nehari problem is given by

$$B(-s)V(s) = c(sI - A_0)^{-1}b$$

where $A_0 := A - P^{-1}c'c$, and

(b) multiply the numerator coefficients of the LFT for the Nehari problem, given in [14, page 125], by $B(-s)$ to obtain the coefficients of the LFT for the Nevanlinna-Pick problem.

In this context, it is important to note that $L(s)$ is J-unitary in the sense that

$$L(-s)' \begin{bmatrix} -1 & 0 \\ 0 & 1 \end{bmatrix} L(s) = \begin{bmatrix} -1 & 0 \\ 0 & 1 \end{bmatrix}. \tag{A.1}$$

Applying the transformations $s = \frac{z-1}{z+1}$ and $v = \frac{1-w}{1+w}$ to the domain and range, respectively, the interpolation formulas (4.10) and (4.11) are transformed into (4.2) and (4.13), respectively.

Also condition (A.1) transforms into the condition that $M(z)$ is J-unitary in the sense that

$$M(z^{-1})' \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix} M(z) = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}. \tag{A.2}$$

However, the functions defined by (4.2) satisfy the interpolation conditions (3.1) only for $k = 1, 2, \dots, n$. In order to include $k = 0$, we must have $f(\infty) = w_0$, and hence we must impose the extra condition that

$$w_0 = \frac{M_1(\infty)\varphi(\infty) + M_2(\infty)}{M_3(\infty)\varphi(\infty) + M_4(\infty)},$$

or, equivalently, that

$$\varphi(\infty) = \mu, \tag{A.3}$$

where μ is given by (4.5) and is less than one in modulus. Thus, all interpolants satisfying the complete set of interpolation conditions (3.1) are still given by (4.2) with the additional constraint that φ is contractive and satisfies (A.3).

It remains to prove that the choice $\varphi(z) \equiv \mu$ is in fact the one which maximizes the entropy gain $\mathbb{I}_1(f) := \langle \log(f + f^*), 1 \rangle$. To this end, let

$$\begin{bmatrix} b(z) \\ a(z) \end{bmatrix} = M(z) \begin{bmatrix} \varphi(z) \\ 1 \end{bmatrix} \tag{A.4}$$

where $\varphi(z)$ is contractive and satisfies (A.3). Clearly, $f(z) = b(z)/a(z)$ is a solution to the interpolation problem for the complete set of data, and all solutions are generated this way. Then,

$$\begin{aligned} \mathbb{I}_1(f) &= \langle \log(a^*b + b^*a), 1 \rangle - \langle \log(a^*a), 1 \rangle \\ &= \langle \log(1 - \varphi^*\varphi), 1 \rangle - \langle \log(a^*a), 1 \rangle \end{aligned} \tag{A.5}$$

where the last equality follows from (A.4) and (A.2). Since $a(z)$ is outer, i.e., analytic and invertible outside the unit disc, we have that

$$\frac{1}{2\pi} \int_0^{2\pi} \log \left| a(e^{i\theta}) \right| d\theta = \log |a(\infty)|, \tag{A.6}$$

by Szegö's theorem [22, pp. 19 and 125]. On the other hand, all contractive φ which satisfy (A.3) with $|\mu| < 1$ are parameterized by

$$\varphi(z) = \frac{\mu + z^{-1}\psi(z)}{1 + \mu z^{-1}\psi(z)}$$

with ψ an arbitrary function which is contractive outside the disc. Hence,

$$1 - \varphi(z)^*\varphi(z) = \frac{(1 - \mu^2)(1 - \psi(z)^*\psi(z))}{|1 + \mu z^{-1}\psi(z)|^2}. \tag{A.7}$$

Again, $1 + \gamma z^{-1}\psi(z)$ is outer, and hence Szegö's theorem applies to give that

$$\langle \log \left| 1 + \gamma z^{-1}\psi \right|, 1 \rangle = 0. \tag{A.8}$$

Then, inserting (A.7) into (A.5) and using (A.8) and (A.6), we obtain

$$\mathbb{I}_1(f) = \langle \log(1 - \psi^*\psi), 1 \rangle + \langle \log(1 - \mu^2), 1 \rangle - 2 \log |M_3(\infty)\mu + M_4(\infty)|,$$

where, in the last term we have also used the fact, derived from (A.4), that $a(\infty) = M_3(\infty)\mu + M_4(\infty)$. Clearly, this expression attains it maximum value

$$\mathbb{I}_1(f_c) = \log \frac{1-\mu^2}{|M_3(\infty)\mu + M_4(\infty)|^2}$$

precisely for $\psi(z) \equiv 0$, i.e., for $\varphi \equiv \mu$, as claimed, and hence the central solution is given by (4.4).

Appendix B. Properties of the functional $\mathbb{J}_\Psi$

Denote by L_2 the space of functions which are square-integrable on the unit circle. This is a Hilbert space with inner product

$$\langle f, g\rangle = \frac{1}{2\pi}\int_{-\pi}^{\pi} f(e^{i\theta})g^*(e^{i\theta})d\theta,$$

where $g^*(z) := \bar{g}(z^{-1})$. Next, let H_2 be the Hardy space of all functions which are analytic *outside* the unit circle and have square-integrable limits on the boundary

$$\lim_{r\to+1}\frac{1}{2\pi}\int_{-\pi}^{\pi}|f(re^{i\theta})|^2 d\theta < \infty.$$

As usual, H_2 is identified with the subspace of L_2 with vanishing positive Fourier coefficients.

Given the real polynomial (3.14), consider the all-pass function

$$B(z) := z^{-1}\frac{1+\tau_1 z + \cdots + \tau_{n-1}z^{n-1} + \tau_n z^n}{z^n + \tau_1 z^{n-1} + \cdots + \tau_{n-1}z + \tau_n} = z^{n-1}\frac{\tau^*(z)}{\tau(z)}. \tag{B.1}$$

Such an all-pass function is called a (finite) Blaschke product. Next, introduce the coinvariant subspace

$$H(B) := H_2 \ominus BH_2,$$

i.e., the orthogonal complement of the invariant subspace $BH_2 \subset H_2$ in H_2. The subspace $H(B)$ consists of precisely all rational functions (5.1) where $\pi(z)$ is allowed to have complex coefficients, and therefore $\mathcal{K}$, introduced in Section 5, is the subspace of all real rational functions in $H(B)$.

The filter-bank transfer functions

$$G_k(z) = \frac{z}{z-p_k}, \quad k = 0, 1, \ldots, n, \tag{B.2}$$

are Cauchy kernels in the sense that, for any function $f \in H_2$,

$$\langle G_k, f\rangle = \bar{f}(p_k^{-1}) \tag{B.3}$$

$$\langle G_k, f^*\rangle = f(\infty). \tag{B.4}$$

In particular, if f is real, $\bar{f}(p_k^{-1}) = f(p_k^{-1})$. It is easy to see that (B.2) form a basis for $H(B)$. Hence, if $a \in H(B)$, then

$$a(z) = \sum_{k=0}^{n}\gamma_k G_k(z) \tag{B.5}$$

for some complex $\gamma_0, \gamma_1, \ldots, \gamma_n$. If $a \in \mathcal{K}$, $\gamma_\ell = \bar{\gamma}_k$ whenever $p_\ell = \bar{p}_k$.

In this notation, the functional (5.11) of Theorem 5.2 can now be written

$$\mathbb{J}_\Psi(Q) = \langle Q, w + w^*\rangle - \langle \log Q, \Psi\rangle, \tag{B.6}$$

where, in view of (5.15), the first term may be written

$$\langle a, (w + w^*)a\rangle = \langle a, wa\rangle + \overline{\langle a, wa\rangle}.$$

But, using the representation (B.5) for a and (B.3), we have

$$\langle a, wa\rangle = \sum_{k=0}^{n}\sum_{k=0}^{n} \bar{\gamma}_k\gamma_j w_k \bar{G}_j(p_k).$$

Therefore, the first term in (B.6) becomes

$$\langle Q, w + w^*\rangle = \gamma^* P_n \gamma, \quad \gamma := (\gamma_0, \gamma_1, \dots, \gamma_n)', \tag{B.7}$$

where P_n is the Pick matrix (3.4). Clearly this quadratic form depends only on w via its values at the interpolation points, precisely as claimed in Section 5.

To any $Q \in \mathcal{S}_+$ there is a unique positive real function f satisfying (5.14). In fact, the left member of (5.14) is positive on the unit circle, and hence it can be split into a sum of an analytic function $f(z)$ and its conjugate $f^*(z)$. Clearly f is positive real.

Next, we prove that, if $Q \in \mathcal{S}_+$ is optimal for the problem to minimize $\mathbb{J}_\Psi$, then the function f defined by (5.14) is an interpolant. For this, and for later analysis, we need the directional derivative

$$\delta\mathbb{J}_\Psi(Q;\delta Q) = \lim_{\epsilon\to 0} \frac{\mathbb{J}_\Psi(Q + \epsilon\delta Q) - \mathbb{J}_\Psi(Q)}{\epsilon},$$

where δQ is a symmetric pseudo-polynomial such that $Q + \epsilon\delta Q \in \mathcal{S}_+$ for sufficiently small $\epsilon > 0$. Performing the differentiation, we have

$$\delta\mathbb{J}_\Psi(Q;\delta Q) = \langle \delta Q, w + w^* - \frac{\Psi}{Q}\rangle, \tag{B.8}$$

which, in view of (5.14), yields

$$\delta\mathbb{J}_\Psi(Q;\delta Q) = \langle \delta Q, w + w^*\rangle - \langle \delta Q, f + f^*\rangle. \tag{B.9}$$

Now, suppose Q is the unique minimizing function. Then, $\delta\mathbb{J}_\Psi(Q;\delta Q) = 0$ for all directions $\delta Q := \delta q + \delta q^*$ for which $\delta q \in \mathcal{K}$. Concequently,

$$\delta\mathbb{J}_\Psi(Q;\delta Q) = 2\langle \delta q, w - f\rangle + 2\langle \delta q^*, w - f\rangle = 2\langle \delta q + \delta q(\infty), w - f\rangle = 0$$

for all $\delta q \in \mathcal{K}$, and therefore $w - f \perp \mathcal{K}$, i.e., $f = w + Bg$ for all H_2, which, in turn, yields the interpolation conditions (5.13).

Next, to derive an expression for the gradient of $\mathbb{J}_\Psi$, we shall need the following lemma.

Lemma B.1. *Let g_1 and g_2 be stable, real, rational functions with realizations*

$$\left[\begin{array}{c|c} A & b_1 \\ \hline c & d_1 \end{array}\right] \quad \textit{and} \quad \left[\begin{array}{c|c} A & b_2 \\ \hline c & d_2 \end{array}\right].$$

Then

$$\langle g_1, g_2\rangle = b_1' P b_2 + d_1 d_2 \tag{B.10}$$

$$\langle g_1, g_2^*\rangle = d_1 d_2, \tag{B.11}$$

where P is the unique solution of the Lyapunov equation

$$P = A'PA + c'c,$$

i.e., the observability gramian.

Proof. First note that $\langle z^k, z^\ell \rangle = 0$ for $k \neq \ell$. Therefore, since

$$g(z) := c(zI - A)^{-1}b + d = d + cbz^{-1} + cAbz^{-2} + \dots \quad \text{for } z \geq 1,$$

and $g^*(z) = g(z^{-1})$, (B.11) follows directly by orthogonality. For the same reason,

$$\langle g_1, g_2 \rangle = \langle g_1 - d_1, g_2 - d_2 \rangle + d_1 d_2.$$

But

$$\langle g_1 - d_1, g_2 - d_2 \rangle = \frac{1}{2\pi} \int_{-\pi}^{\pi} b_1'(e^{-i\theta}I - A')^{-1}c'c(e^{i\theta}I - A)^{-1}b_2 d\theta = b_1' P b_2,$$

and hence (B.10) follows. □

We are now in the position to verify the expressions (5.24) and (5.29) for the gradient and Hessian of $\mathbb{J}_\Psi$, respectively.

Proof of Proposition 5.3. The interpolation errors (5.21) can be written

$$e_k = \varphi(z_k) := w_k - f(z_k), \quad k = 0, 1, \dots, n,$$

where $z_k := p_k^{-1}$ and φ is defined as

$$\varphi(z) = w(z) - f(z).$$

Now, let $\hat{\varphi}$ be the orthogonal projection of φ onto $\mathcal{K}$. Since $\hat{\varphi}(z) = \varphi(z) + B(z)g(z)$ for some $g \in H_2$, we have

$$\hat{\varphi}(z_k) = \varphi(z_k) \quad k = 0, 1, \dots, n.$$

Therefore the column vector y of coefficients of the numerator polynomial

$$\hat{\varphi}(z) := e_0 + \frac{y(z)}{\tau(z)}, \quad \text{where } y(z) = y_1 z^{n-1} + y_2 z^{n-2} + \dots + y_n$$

is the unique solution of the Vandermonde system $Vy = v$, where V and v are given by (5.22) and (5.23), respectively. Then, it is easy to check that $\hat{\varphi}$ has the realization

$$\left[\begin{array}{c|c} A & x \\ \hline c & e_0 \end{array}\right], \quad x = L_{n-1}^{-1} V^{-1} v,$$

where L_{n-1} is given by (5.23).

Let $\delta q(z) \in \mathcal{K}$, and consider the directional derivative at $Q \in \mathcal{S}_+$ in the direction $\delta Q := \delta q + \delta q^*$. From (B.9) we see that

$$\delta \mathbb{J}_\Psi(Q; \delta Q) = \langle \delta q + \delta q^*, \varphi + \varphi^* \rangle = 2\langle \delta q, \varphi \rangle + 2\langle \delta q, \varphi^* \rangle = 2\langle \delta q, \hat{\varphi} \rangle + 2e_0 \langle \delta q, 1 \rangle.$$

Consequently, it follows directly from Lemma B.1 that

$$\delta \mathbb{J}_\Psi(Q; \delta Q) = 2 \begin{bmatrix} Px \\ 2e_0 \end{bmatrix}' \begin{bmatrix} b_\delta \\ d_\delta \end{bmatrix},$$

where (b_δ, d_δ) are the Markov parameters of δq, and P is the solution of the Lyapunov equation (5.25). But, by definition,

$$\delta \mathbb{J}_\Psi(Q; \delta Q) = \nabla J(h)' \begin{bmatrix} b_\delta \\ d_\delta \end{bmatrix},$$

which establishes the expression (5.24) for the gradient ∇J, as claimed. □

Proof of Proposition 5.3. To compute the Hessian, we determine

$$\delta^2\mathbb{J}_\Psi(Q;\delta Q) := \lim_{\epsilon\to 0}\frac{\delta\mathbb{J}_\Psi(Q+\epsilon\delta Q)-\delta\mathbb{J}_\Psi(Q)}{\epsilon} = \langle \delta Q^2, \frac{\Psi}{Q^2}\rangle.$$

Then, the Hessian is the symmetric $(n+1)\times(n+1)$ matrix H such that

$$h'Hh = \langle \delta Q^2, \frac{\Psi}{Q^2}\rangle,$$

where $h := \begin{bmatrix} b_\delta \\ d_\delta \end{bmatrix}$ is the (reversed) vector of Markov parameters of δq. Now, replacing δQ by $\delta q + \delta q^*$, we obtain

$$\begin{aligned}\langle \delta Q^2, \frac{\Psi}{Q^2}\rangle &= 2\langle \delta q\delta q^*, \frac{\Psi}{Q^2}\rangle + 2\langle \delta q^2, \frac{\Psi}{Q^2}\rangle \\ &= 2\langle \frac{\pi\rho}{\alpha^2}, \frac{\pi\rho}{\alpha^2}\rangle + 2\langle \frac{\pi\tau_*\rho}{\alpha^2\tau}, \frac{\pi_*\tau\rho}{\alpha^2\tau}\rangle, \end{aligned} \tag{B.12}$$

where

$$\pi(z) = \pi_0 z^n + \pi_1 z^{n-1} + \cdots + \pi_n := \tau(z)\delta q(z)$$

is the numerator polynomial of δq, which can be determined via the system of linear equations

$$\pi := \begin{bmatrix} \pi_0 \\ \pi_1 \\ \vdots \\ \pi_n \end{bmatrix} = L(\tau)h, \quad \text{where } L(\tau) := \begin{bmatrix} & & & 1 \\ & & 1 & \tau_1 \\ & \iddots & \iddots & \vdots \\ 1 & \tau_1 & \dots & \tau_n \end{bmatrix},$$

and π_*, τ_* denote the reverse polynomials $\pi_n z^n + \cdots + \pi_0$ and $\tau_n z^n + \cdots + 1$, respectively. A simple computation then yields

$$h = N(\tau)\pi,$$

where $N(\tau)$ is given by (5.28). We shall use Lemma B.1 to compute these expressions. Note that we have refrained from canceling the common factor τ in the first position of the second term of (B.12). This is in order to obtain the same denominator in the two positions of the inner product, leading to a Lyapunov equation instead of a somewhat smaller, but computationally more demanding, Sylvester equation.

To determine the first term in (B.12), we need a state space representation

$$\frac{\pi(z)\rho(z)}{\alpha(z)^2} = (\hat{c}(zI-\hat{A})^{-1},1)\hat{h}$$

on the canonical form (5.17), where $\hat{A}$ is the companion matrix of $\alpha(z)^2$ and $\hat{c}$ is the $2n$-vector $(0,0,\dots,0,1)$. The coefficient vector η of the numerator polynomial

$$\pi(z)\rho(z) = \eta_0 z^{2n} + \eta_1 z^{2n-1} + \cdots + \eta_{2n}$$

can be computed as $\eta = M(\rho)\pi$, where $M(\rho)$ is given by (5.27), and consequently

$$\hat{h} = L(\alpha^2)^{-1}M(\rho)'L(\tau)h.$$

Lemma B.1 then implies that

$$\langle \frac{\pi\rho}{\alpha^2}, \frac{\pi\rho}{\alpha^2}\rangle = h'L(\tau)M(\rho)N(\alpha^2)\begin{bmatrix} P(\alpha^2) & 0 \\ 0 & 1 \end{bmatrix}N(\alpha^2)M(\rho)'L(\tau)h, \tag{B.13}$$

where $P(\alpha^2)$ is defined as in the theorem.

To determine the second term in (B.12), we need a state space realization

$$\begin{bmatrix} \frac{\pi(z)\tau_*(z)\rho(z)}{\alpha(z)^2\tau(z)} & \frac{\pi_*(z)\tau(z)\rho(z)}{\alpha(z)^2\tau(z)} \end{bmatrix} = \begin{bmatrix} \tilde{c}(zI-\tilde{A})^{-1} & 1 \end{bmatrix} \begin{bmatrix} \tilde{h} & \tilde{k} \end{bmatrix},$$

where $\tilde{A}$ is the companion matrix of $\alpha(z)^2\tau(z)$ and $\tilde{c}$ is the $3n$-vector $(0,0,\dots,0,1)$. In the same way as above, we obtain,

$$\tilde{h} = L(\alpha^2\tau)^{-1}M(\tau_*\rho)'L(\tau)h, \qquad \tilde{k} = L(\alpha^2\tau)^{-1}M(\tau\rho)'\tilde{L}(\tau)h,$$

where the matrix $\tilde{L}(\tau)$ is obtained by reversing the order of the rows in $L(\tau)$and where $M(\cdot)$ is given by (5.27). Consequently, Lemma B.1 yields

$$\langle \frac{\pi\tau_*\rho}{\alpha^2\tau}, \frac{\pi_*\tau\rho}{\alpha^2\tau} \rangle = h'L(\tau)M(\tau_*\rho)N(\alpha^2\tau) \begin{bmatrix} P(\alpha^2\tau) & 0 \\ 0 & 1 \end{bmatrix} N(\alpha^2\tau)M(\tau\rho)'\tilde{L}(\tau)h. \tag{B.14}$$

From (B.12), (B.13) and (B.14) the Hessian is then obtained as (5.31), where we have adjusted for the fact that H_2 is not symmetric. □

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