Università degli Studi di Padova
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Constrained approximation of spectral densities and spectral estimation

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Summary

In this work, we consider the problem of finding, among the solutions of a generalized moment problem à la Byrnes/Georgiou/Lindquist, the best approximation to a given spectrum, with respect to different notions of distance. After an in-depth discussion of the moment problem in question, we first review the scalar spectrum approximation in the Kullback-Leibler metric. Then we pose and solve a similar problem with respect to the Hellinger distance. We show that the latter distance admits a nice extension to the case when multivariate spectra come into play, and we solve the resulting, generalized approximation problem. Finally, we present in detail a matricial version of the Newton algorithm designed to solve the corresponding dual problem, that eventually leads to an useful solution, and provide an application to multivariate spectrum estimation, testing it against well-known identification methods.

This work contains the result of three years of collaboration between my advisors Augusto Ferrante and Michele Pavon, and me. In essence, it is an assembly of four papers we have written together, namely [22], [21], [20], and [51], with minor corrections and improvements. Without their teaching, support, and continuous encouragement, I would have published nothing, and this thesis would consist of a few blank pages.
For the time spent together, to them goes my gratitude.

Also, we wish to thank Prof. Anders Lindquist and Prof. Tryphon Georgiou for an enduring, enlightening correspondence that helped us develop our results, and for their willingness to suggest and discuss these subjects during the time they were in Padova.

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Federico Ramponi

Chapter 1

A generalized moment problem

1.1 Introduction

1.1.1 Previous work of the Byrnes, Georgiou and Linquist school

ARMA identification methods usually lead to nonconvex optimization problems for which global convergence is not guaranteed, cf. e.g. [43, 55, 56, 17]. Although these algorithms are simple and perform effectively, as observed in [56, p.103], [42, Section 1], no theoretically satisfactory approach to ARMA parameter estimation appears to be available. Alternative, convex optimization approaches have been recently proposed by Byrnes, Georgiou, Lindquist and co-workers [6, 36] in the frame of a broad research effort on analytic interpolation with degree contraint, see [3, 5, 8, 9, 10, 11, 12, 7, 18, 28, 24, 25, 26, 27, 29, 30, 32, 33, 34, 35] and references therein. In particular, [7] describes a new setting for spectral estimation. The so-called *THREE* algorithm introduced there appears to allow for higher resolution in prescribed frequency bands and to be particularly suitable in case of short observation records. It effectively detects spectral lines and steep variations (see [47] for a recent biomedical application). An outline of this method is as follows. A given realization of a stochastic process (a finite collection of data $y_1 ... y_N$) is fed to a suitably structured bank of filters, and the steady-state covariance matrix of the resulting output is estimated by statistical methods. Only zeroth-order covariance lags of the output of the filters need to be estimated, ensuring statistical robustness of the method. Finding now an input process whose *rational* spectrum is compatible with the estimated covariance poses naturally a Nevanlinna-Pick interpolation problem with bounded degree. The solution of this interpolation problem is considered as a mean of estimating the spectrum. A particular case described in the paper is the *maximum differential entropy* spectrum estimate, which amounts to the so-called central solution in the Nevanlinna-Pick theory. More generally, the scheme allows for a non constant *a priori* estimate Ψ of the spectrum. The Byrnes-Georgiou-Lindquist school has shown how this and other important problems of control theory may be advantageously cast in the frame

of convex optimization. These problems admit a finite dimensional dual (multipliers are matrices!) that can be shown to be solvable. The latter result, due to Byrnes and Lindquist [12] (see also [20]) is, however, nontrivial since the optimization occurs on an open, unbounded set of Hermitian matrices. The numerical solution of the dual problem is also challenging [7, 18, 46], since the gradient of the dual functional tends to infinity at the boundary of the feasible set. Finally, reparametrization of the problem may lead to loss of global concavity, see the discussion in [34, Section VII].

This work adds to this effort in that we consider estimation of a multivariate spectral density in the spirit of THREE [7], but employing a different metric for the optimization part, namely the *Hellinger distance* as in [21]. In papers [10, 11], Byrnes, Gusev and Lindquist chose the Kullback-Leibler divergence as a frequency weighted entropy measure, thus introducing a broad generalization of Burg's maximum entropy method. More recently, this motivation was supported by the well-known connection with prediction error methods, see e.g. [57, 42]. In the multivariable case, a Kullback-Leibler pseudodistance may also be readily defined [30] inspired by the *von Neumann's relative entropy* [60, 59] of statistical quantum mechanics. The resulting spectrum approximation problem, however, leads to computable solutions of bounded McMillan degree only in the case when the prior spectral density is the identity matrix [30, 21] (maximum entropy solution). On the contrary, with a suitable extension of the scalar Hellinger distance introduced in [21], the Hellinger approximation generalizes nicely to the multivariable case for any prior estimate Ψ of the spectrum.

1.1.2 A generalized moment problem and the search for a solution

The method we propose to estimate a multivariate spectrum relies on the solution of a *constrained spectrum approximation* problem. Let us explain in simple words what this means.

Consider the following situation: a discrete-time, wide-sense stationary, m-dimensional random process y is fed to an asymptotically stable system with transfer function $G(z) = (zI - A)^{-1}B$. The asymptotic state covariance matrix of the system will be:

$$\Sigma = \int_{-\pi}^{\pi} G(\mathrm{e}^{\mathrm{j}\vartheta})\Phi(\mathrm{e}^{\mathrm{j}\vartheta})G^{\top}(\mathrm{e}^{-\mathrm{j}\vartheta})\frac{\mathrm{d}\vartheta}{2\pi} \tag{1.1}$$

where Φ is the spectrum of y. We consider the following *moment problem*:

Given G and Σ, find a spectral density Φ for which (1.1) holds.

Moment problems are generally considered as "inverse" problems (where the term "inverse" stems from the observation that the simple computation of Σ, given G and Φ, should be regarded as "direct"). Recall that a problem is said to be *well posed*, in the sense of Hadamard, if the following properties hold:

- a solution to the problem exists;

- such solution is unique;
- the solution depends continuously on the data.

Inverse problems such as the one we are considering (where "data" means the pair G, Σ) are typically *not* well posed. In particular, there may be no solution, and when a solution exists, usually there are infinitely many.

Thus, given (G, Σ), the question arises as whether there are solutions Φ to (1.1), and if this is the case, to find and eventually parameterize the family of such solutions. Being geared toward system-theoretic applications, we further ask whether *rational* solutions exist and, moreover, if the complexity of such solutions (their MacMillan degree) can be bounded *a priori*. A full answer to these questions has been given by Georgiou, Lindquist and their collaborators.

Let us change our point of view from a theoretical to a practical perspective. Suppose that we can *choose* $G(z) = (zI - A)^{-1}B$, with the only constraints of A being a stability matrix and (A, B) being reachable. Here $G(z)$ models a *bank of filters*. Now a realization of the system with transfer function $G(z)$ is "physically there", and we feed it with a *finite* chunk of the process y, say $\{y_1, ..., y_N\}$. Observing the states of the system, say $\{x_1, ..., x_N\}$, we then compute a Hermitian and positive definite *estimate* $\hat{\Sigma}$ of the asymptotic state covariance. Given G, our question is now how to exploit the estimated $\hat{\Sigma}$ to make inferences about the *true* spectrum Φ of y. That is, we want to provide an *estimate* of Φ, taking into account that the state variance we have obtained is $\hat{\Sigma}$. The issues are manifold:

1. The set of the Σ's for which a solution exists is, in general, a thin set. Therefore, if we set $\Sigma = \hat{\Sigma}$, (1.1) will be usually unfeasible. Thus, we need to find a second estimate $\bar{\Sigma}$, near to the first, that belongs to this set.

2. Having done so, the solutions Φ to problem (1.1) with $\Sigma = \bar{\Sigma}$ will however be infinitely many. Thus, in order to make inferences about Φ, we will have to choose *one* solution $\hat{\Phi}$, satisfying some optimality criterion, and elect it as an estimate of Φ.

3. Moreover, for practical purposes we require this particular solution to be rational and with bounded degree.

4. Finally, we may ask if tuning $G(z)$ we can somehow obtain better inferences about Φ.

This work is mainly devoted to the second issue, and precisely to a suitable choice of the optimality criterion.

One more or less obvious such choice is the maximum entropy principle. Adding milestones to a path that was pioneered by Burg, in [27] Georgiou has provided an explicit expression for the spectrum $\hat{\Phi}$ that exhibits *maximum entropy rate* among the solutions of (1.1), when they exist.

But, following [34], let us add another ingredient to the problem. Suppose that some information about Φ becomes available under the form of a *prior* spectrum Ψ. That is, suppose we are said that the spectrum Ψ is "near" to Φ, *for some notion of distance*. Now given G, Σ, and Ψ, we search the spectrum $\hat{\Phi}$, which is closest to Ψ, among the solutions of (1.1). In the following we choose *this* as the optimality criterion, and we call the search for such a solution a *spectrum approximation* problem, subject to the *constraint* (1.1).

The paper [34] poses and solves a variational problem in this very spirit. It deals with the case when y is a scalar process, and employs the minimization of the Kullback-Leibler pseudo-distance from Ψ to Φ as the optimality criterion. This approach has relevant advantages, namely that it leads to a simple, rational expression for the optimal solution, and with bounded degree. Moreover, it admits Georgiou's maximum entropy solution as a particular case ($\Psi \equiv 1$, when y is scalar). But it has a major drawback: For any notion of multivariable extension of the Kullback-Leibler pseudo-distance that can be regarded as "natural", the analysis that is proposed there seems impossible to be carried through. That is, this approach cannot be employed in the multivariate case.

The main contribution of this work, which in essence is a rewriting of papers [21] and [51], is a multivariable extension of another metric, namely the Hellinger distance, in which the variational analysis can be carried through, and is relatively simple. The spectrum $\hat{\Phi}$ which is closest to Ψ with respect to this distance is again rational, and with bounded degree.

1.1.3 Structure of the work

The rest of Chapter 1 contains a more precise statement of the moment problem in question, and some properties of the vector space of the matrices Σ for which it admits solutions.

Chapter 2 presents a review of spectrum approximation in the Kullback-Leibler pseudo-distance, and an explanation of *why* is difficult to extend it to the multivariable case.

Chapter 3 introduces the Hellinger distance, and presents the variational analysis that leads to the minimizing spectrum both in the scalar and in the multivariable case. In either setting, however, the optimal spectrum depends on the Lagrange parameter Λ. To meet the constraint (1.1) and come to a true solution, one must pursue the solution of the *dual problem*, which is now finite-dimensional.

Chapter 4 contains a detailed description of a matricial version of the Newton algorithm suited to solve the dual problem.

Finally, Chapter 5 presents an application to multivariable spectrum estimation, tests it through simulation, and deals in some measure with the first and fourth issues of the previous section, namely the choice of a suitable estimate of Σ and the tuning of $G(z)$.

1.2 A generalized moment problem

We consider the following basic set-up patterned after [27, 34, 30]. Let $\mathcal{S}_+^{m\times m}(\mathbb{T})$ be the family of bounded, coercive, $\mathbb{C}^{m\times m}$-valued spectral density functions on the unit circle. Thus, a measurable, bounded matrix valued function Φ belongs to $\mathcal{S}_+^{m\times m}(\mathbb{T})$ if it satisfies the following properties:

- the values of Φ are $m \times m$, Hermitian, non negative definite matrices;
- there exists a positive constant c_Φ such that $\Phi(e^{i\vartheta}) - c_\Phi I$ is positive definite a.e. on $\mathbb{T}$.

Notice that $\Phi \in \mathcal{S}_+^{m\times m}(\mathbb{T})$ if and only if $\Phi^{-1} \in \mathcal{S}_+^{m\times m}(\mathbb{T})$. Let $\Psi \in \mathcal{S}_+^{m\times m}(\mathbb{T})$ represent an *a priori* estimate of the spectrum of an underlying zero-mean, wide-sense stationary m-dimensional stochastic process $\{y(n), n \in \mathbb{T}\}$. We consider a rational transfer function

$$G(z) = (zI - A)^{-1}B, \qquad A \in \mathbb{C}^{n\times n}, B \in \mathbb{C}^{n\times m}, \tag{1.2}$$

where A is a stability matrix, B is full column rank, and (A, B) is a reachable pair. Suppose moreover that we *know* the asymptotic state covariance $\Sigma > 0$ of the system with transfer function G and input the unknown process y. In other words, we suppose we know the covariance of the n- dimensional stationary process $\{x_k; k \in \mathbb{T}\}$ satisfying

$$x_{k+1} = Ax_k + By_k, \quad k \in \mathbb{T}. \tag{1.3}$$

In general, Ψ is not consistent with Σ, and it is necessary to find Φ in $\mathcal{S}_+^{m\times m}(\mathbb{T})$ that is closest to Ψ in a suitable sense among spectra consistent with Σ, namely satisfying

$$\int G\Phi G^* = \Sigma, \tag{1.4}$$

where star denotes transposition plus conjugation. Here, and throughout the work, integration takes place on $[-\pi, \pi]$ with respect to the normalized Lebesgue measure $d\vartheta/2\pi$, i.e.:

$$\int f := \int_{-\pi}^{\pi} f(\mathrm{e}^{\mathrm{j}\vartheta}) \, \frac{\mathrm{d}\vartheta}{2\pi}$$

The question of existence of $\Phi \in \mathcal{S}_+^{m\times m}(\mathbb{T})$ satisfying (1.4) and, when existence is granted, the parametrization of all solutions to (1.4), may be viewed as a generalized moment problem.

Here, "generalized" stands for the fact that the *classical* moment problem, where we search $\Phi \in \mathcal{S}_+^{1\times 1}(\mathbb{T})$ under constraints on its moments $\int \Phi$, $\int \mathrm{e}^{\mathrm{j}\vartheta}\Phi$, $\int \mathrm{e}^{2\mathrm{j}\vartheta}\Phi$, ..., is a particular case of this. More precisely, in the case $m = 1$, take $G(z)$ with k-th component $G_k(z) = z^{k-n-1}$. Take moreover

$$A = \begin{bmatrix} 0 & 1 & 0 & \dots & 0 \\ 0 & 0 & 1 & \dots & 0 \\ \vdots & \vdots & & \ddots & \vdots \\ 0 & 0 & 0 & \dots & 1 \\ 0 & 0 & 0 & \dots & 0 \end{bmatrix}, \quad B = \begin{bmatrix} 0 \\ 0 \\ \vdots \\ 0 \\ 1 \end{bmatrix},$$
$$\Sigma = \begin{bmatrix} c_0 & c_1 & c_2 & \dots & c_{n-1} \\ \bar{c}_1 & c_0 & c_1 & \ddots & c_{n-2} \\ \bar{c}_2 & \ddots & \ddots & \ddots & \ddots \\ \vdots & \ddots & \ddots & \ddots & \ddots \\ \bar{c}_{n-1} & \bar{c}_{n-2} & \ddots & \ddots & c_0 \end{bmatrix}, \tag{1.5}$$

where $c_k := E\{y(n)\bar{y}(n+k)\}$. This is the *covariance extension problem*, where the information available on the process y is the finite sequence of covariance lags $c_0, c_1, \dots, c_{n-1}$. It is known that the set of densities consistent with the data is nonempty if $\Sigma \geq 0$ and contains infinitely many elements if $\Sigma > 0$ (see for instance [37]).

As another example, again in the case $m = 1$, take $G_k(z) = \frac{1}{z-p_k}$, or

$$A = \begin{bmatrix} p_1 & 0 & 0 & \dots & 0 \\ 0 & p_2 & 0 & \dots & 0 \\ \vdots & \vdots & & \ddots & \vdots \\ 0 & 0 & 0 & \dots & 0 \\ 0 & 0 & 0 & \dots & p_n \end{bmatrix}, \quad B = \begin{bmatrix} 1 \\ 1 \\ \vdots \\ 1 \\ 1 \end{bmatrix} \tag{1.6}$$

where the p_i's lie inside the unit circle, and let Σ be the Pick matrix with elements

$$\Sigma_{i,j} = \frac{w_i + \bar{w}_j}{1 - p_i \bar{p}_j}$$

where

$$w_k = \frac{1}{4\pi} \int_{-\pi}^{\pi} \frac{e^{-i\theta} + p_k}{e^{-i\theta} - p_k} \Phi(e^{i\theta}) d\theta, \quad k = 1, 2, \dots, n.$$

In this case the problem is a *Nevanlinna-Pick interpolation problem.* Solutions exist if and only if $\Sigma \geq 0$, and the solution is unique if and only if Σ is singular.

1.2.1 Existence of solutions

Existence of $\Phi \in \mathcal{S}_+^{m\times m}(\mathbb{T})$ satisfying constraint (1.4) is a nontrivial issue. It was shown in [28] that such family is nonempty if and only if there exists $H \in \mathbb{C}^{m\times n}$ such that

$$\Sigma - A\Sigma A^* = BH + H^*B^*, \tag{1.7}$$

or, equivalently, the following rank condition holds:

$$\operatorname{rank}\begin{pmatrix} \Sigma - A\Sigma A^* & B \\ B^* & 0 \end{pmatrix} = 2m. \tag{1.8}$$

Remark 1.2.1 *Since we develop our theory under the assumption that $\Sigma > 0$, without loss of generality we can always assume $\Sigma = I$. Indeed, if $\Sigma \neq I$, it suffices to replace G with $G' := \Sigma^{-1/2}G$ and (A, B) with $(A' = \Sigma^{-1/2}A\Sigma^{1/2}, B' = \Sigma^{-1/2}B)$. Thus, throughout the rest of the work, (1.4) will read*

$$\int G\Phi G^* = I. \tag{1.9}$$

We wish to give an alternative formulation of the existence result (1.7). Let $\Pi_B = B(B^*B)^{-1}B^*$ denote the orthogonal projection onto Range B.

Proposition 1.2.2 *A necessary and sufficient condition for the existence of spectra in $\mathcal{S}_+^{m\times m}(\mathbb{T})$ satisfying (1.9) is that the following relation holds*

$$(I - \Pi_B)\,(I - AA^*)\,(I - \Pi_B) = 0. \tag{1.10}$$

When (1.10) is satisfied, there exists $\Phi \in \mathcal{S}_+^{m\times m}(\mathbb{T})$ satisfying (1.9) of McMillan degree less than or equal to $2n$.

Proof. Necessity: Suppose there exists y m-dimensional, wide-sense stationary with spectral density $\Phi \in \mathcal{S}_+^{m\times m}(\mathbb{T})$ satisfying (1.9). Let x be defined by (1.3). Taking covariances on both sides of (1.3), we get

$$I = AA^* + AE\{x_k y_k^*\}B^* + BE\{y_k x_k^*\}A^* + BE\{y_k y_k^*\}B^*.$$

Now taking AA^* to the left-hand side of the equation, and pre- and post-multiplying each side by $(I - \Pi_B)$, we obtain (1.10).
Sufficiency: We adapt the argument in [27, p.1814]. For a given purely non deterministic m-dimensional process y with spectrum Φ, define the process w as the output of the linear stable system

$$\begin{aligned} x_{k+1} &= Ax_k + By_k, \\ w_k &= (B^*B)^{-1}B^*x_{k+1} \end{aligned} \tag{1.11}$$

Inverting the system (1.11), we get

$$\begin{aligned} x_{k+1} &= (I - \Pi_B)Ax_k + Bw_k, \\ y_k &= -(B^*B)^{-1}B^*Ax_k + w_k. \end{aligned} \tag{1.12}$$

Write (1.10) as a Lyapunov identity

$$I = (I - \Pi_B)\,AA^*\,(I - \Pi_B) + \Pi_B. \tag{1.13}$$

Since (A, B) is controllable, so is the pair $\big((I - \Pi_B)A, B(B^*B)^{-1/2}\big)$. It now follows from (1.13) that $(I - \Pi_B)A$ has all eigenvalues in the open unit disc $\mathbb{D}$. Thus, system (1.12) is stable, $(B^*B)^{-1}B^*G(z)$ is minimum phase and the processes y and w are causally equivalent. It follows that if we choose w to be a white noise sequence with intensity $E\{w_k w_k^*\} = (B^*B)^{-1}$ and y to be defined by (1.12) then:

1. (1.12) is the innovation representation of y;
2. the state covariance of the steady-state Kalman filter (1.12) satisfies the Lyapunov equation (1.13) and is therefore the identity;
3. the spectral density of y is given by

$$\Phi_y = W(z)(B^*B)^{-1}W(z)^*, \tag{1.14}$$

where

$$W(z) = I - (B^*B)^{-1}B^*A\,(zI - (I - \Pi_B)A)^{-1}\,B,$$

is the transfer function of (1.12).

We conclude that if we feed G in (1.11) with such a process y, the filter state x will have the required covariance, namely the identity matrix, and (1.9) will be satisfied. Moreover, Φ_y is rational of McMillan degree at most $2n$ and it belongs to $\mathcal{S}_+^{m\times m}(\mathbb{T})$ since its values and the values of Φ_y^{-1} on $\mathbb{T}$ are positive definite matrices. ■

The geometric condition (1.10) seems more amenable to generalization than (1.8). The spectrum (1.14) has been shown in [27, Section III] to be the maximum entropy spectrum among those satisfying (1.9). This is there accomplished in a clever way, by relating the constrained maximum entropy problem to a special one-step-ahead prediction problem.

1.3 Feasibility and the operator Γ

In this section, we discuss in depth the feasibility of (1.4). We adopt the following notation for the vector space of all the $n \times n$ Hermitian matrices:

$$\mathcal{H}(n) := \{M \in \mathbb{C}^{n\times n} : M = M^*\}. \tag{1.15}$$

Let $\mathcal{C}(\mathbb{T}; \mathcal{H}(m))$ be the space of $\mathcal{H}(m)$-valued continuous functions defined on the unit circle, and let the operator $\Gamma : \mathcal{C}(\mathbb{T}; \mathcal{H}(m)) \to \mathcal{H}(n)$ be defined as follows:

$$\Gamma(\Phi) := \int G\Phi G^* \tag{1.16}$$

We are interested in the *range* of the operator Γ which, having to deal with Hermitian matrices, we consider as a vector space over the reals.

Proposition 1.3.1 *The following facts hold:*

1. *Let $\Sigma = \Sigma^* > 0$. The following are equivalent:*
   - *There exists $H \in \mathbb{C}^{m\times n}$ such that identity (1.7) holds.*
   - *There exists $\Phi \in \mathcal{S}_+^{m\times m}(\mathbb{T})$ such that $\int G\Phi G^* = \Sigma$.*
   - *There exists $\Phi \in \mathcal{C}(\mathbb{T}; \mathcal{H}(m))$, $\Phi > 0$ such that $\Gamma(\Phi) = \Sigma$.*
2. *Let $\Sigma = \Sigma^*$ (not necessarily positive definite). There exists $H \in \mathbb{C}^{m\times n}$ such that identity (1.7) holds if and only if $\Sigma \in \operatorname{Range}\Gamma$.*
3. *$X \in \operatorname{Range}\Gamma^\perp$ if and only if $G^*(\mathrm{e}^{\mathrm{j}\vartheta})XG(\mathrm{e}^{\mathrm{j}\vartheta}) = 0\ \forall \vartheta \in [0, 2\pi]$.*

Proof. As stated above, it was proved in [28] that there exists $H \in \mathbb{C}^{m\times n}$ such that identity (1.7) holds with Hermitian and positive definite Σ if and only if $\Sigma = \int G\Phi G^*$ for some $\Phi \in \mathcal{S}_+^{m\times m}(\mathbb{T})$, $\Phi > 0$. The proof of Fact 1 is straightforward once we note that the "if" part of the proof of Proposition 1.2.2 is *constructive*, and exhibits a *continuous* spectrum. Hence, the fact that there exists a spectrum Φ such that $\Sigma = \int G\Phi G^*$ is equivalent to there exists a *continuous* spectrum such that the same holds.

As for the second assertion, let $\Sigma \in \operatorname{Range}\Gamma$. Then there exists $\Phi \in \mathcal{C}(\mathbb{T}; \mathcal{H}(m))$ such that

$$\begin{aligned}\Sigma &= \int G\Phi G^* = \int G(\Phi_+ - \Phi_-)G^* \\ &= \int G\Phi_+ G^* - \int G\Phi_- G^* = \Sigma_+ - \Sigma_-\end{aligned}$$

where Φ_+ and Φ_- are two spectra such that $\Phi_+ - \Phi_- = \Phi$ (they can be chosen to be bounded away from zero) and where Σ_+ and Σ_- are symmetric positive definite. Hence Σ is a difference of *positive* matrices for which (1.7) holds. This establishes (1.7) for Σ itself. Vice versa, suppose that (1.7) holds for an Hermitian Σ. Let Σ_α be the unique solution of the following Lyapunov equation:

$$\Sigma_\alpha - A\Sigma_\alpha A^* = B\,(\alpha B^*) + (\alpha B^*)^*\, B^* = 2\alpha BB^*$$

where $\alpha \in \mathbb{R}$. Then Σ_α depends linearly upon α, i.e. $\Sigma_\alpha = \alpha\Sigma_1$, where $\Sigma_1 > 0$ since (A, B) is reachable. Thus, there exists an α such that $\Sigma_\alpha > 0$ and $\Sigma_\alpha > \Sigma$. Let $\Sigma_- = \Sigma_\alpha - \Sigma$. Then $\Sigma_- > 0$, and since (1.7) holds for Σ and Σ_α, it also holds for Σ_-. Then assertion 1 implies that there exist $\Phi_\alpha > 0$ and $\Phi_2 > 0$ in $\mathcal{C}(\mathbb{T}; \mathcal{H}(m))$ such that $\Sigma_\alpha = \int G\Phi_\alpha G^*$ and $\Sigma_- = \int G\Phi_2 G^*$, hence $\Sigma = \int G(\Phi_\alpha - \Phi_2)G^*$ and assertion 2 follows.

The third assertion is a simple geometrical fact: If $X \in \operatorname{Range}\Gamma^\perp$, then for any $\Phi \in \mathcal{C}(\mathbb{T}; \mathcal{H}(m))$

$$0 = \left\langle X, \int G\Phi G^* \right\rangle = \operatorname{tr} X \int G\Phi G^* = \operatorname{tr} \int (G^* X G)\Phi$$

and the conclusion follows. ∎

Remark 1.3.2 *The underlying statement in Proposition 1.3.1, Facts 1 and 2, is that if we defined* Γ *over the vector space of finite linear combinations of functions in* $\mathcal{S}_+^{m\times m}(\mathbb{T})$*, its range would remain the same. Let us restate this in another way. Let* $\overline{\Gamma}$ *be an extension of* Γ *to* $\operatorname{span}\mathcal{S}_+^{m\times m}$*, defined exactly as in (1.16). Given a spectrum* $\Phi \in \operatorname{span}\mathcal{S}_+^{m\times m}$ *(recall that this implies that* Φ *is bounded), there exists a uniformly bounded sequence of continuous functions* $\{\Phi_c^n\} \subset \mathcal{C}(\mathbb{T};\mathcal{H}(m))$ *that converges to* Φ *in the* L^1 *topology. Then there exists a subsequence* $\{\Phi_c^{n_i}\}$ *that converges to* Φ *pointwise, and by dominated convergence it holds* $\lim_{i\to\infty}||\overline{\Gamma}(\Phi_c^{n_i}) - \overline{\Gamma}(\Phi)|| = 0$*. Thus, any* $\Sigma \in \operatorname{Range}\bar{\Gamma}$ *is a limit point of* $\overline{\Gamma}(\mathcal{C}(\mathbb{T};\mathcal{H}(m))) \equiv \operatorname{Range}\Gamma$*. But* $\operatorname{Range}\Gamma$*, being finite dimensional, hence* closed*, already contains all its limit points.*

Remark 1.3.3 *Proposition 1.3.1 shows that* $\operatorname{Range}\Gamma$ *is the set of all the Hermitian matrices* Σ *for which there exists* H *such that (1.7) holds. This fact will be useful in numerical computations. Indeed,* $\operatorname{Range}\Gamma$ *is obviously finite-dimensional, and if* $\{H_1, ..., H_N\}$ *is a base of* $\mathbb{C}^{m\times n}$*, then the corresponding solutions* $\{\Sigma_1, ..., \Sigma_N\}$ *of (1.7),* considered as a discrete-time Lyapunov equation in the unknown Σ*, generate* $\operatorname{Range}\Gamma$*. Note that* $\{\Sigma_1, ..., \Sigma_N\}$ *are not necessarily linearly independent.*

Chapter 2

Approximation in the Kullback-Leibler distance

2.1 Scalar spectrum approximation

In [34], the Kullback-Leibler measure of distance for spectra in $\mathcal{S}_+(\mathbb{T}) := \mathcal{S}_+^{1\times 1}(\mathbb{T})$ was introduced:

$$\mathbb{D}(\Psi\|\Phi) = \int \Psi \log\left(\frac{\Psi}{\Phi}\right).$$

As is well known, this pseudo-distance originates in hypothesis testing, where it represents the mean information for observation for discrimination of an underlying probability density from another [41]. It also plays a central role in information theory, identification, stochastic processes, etc., see e.g. [39, 16, 15, 23, 2, 13, 59, 50] and references therein. It is also known in these fields as *divergence*, *relative entropy*, *information distance*. etc. If

$$\int \Phi = \int \Psi,$$

we have $\mathbb{D}(\Psi\|\Phi) \geq 0$. The choice of $\mathbb{D}(\Psi\|\Phi)$ as a distance measure, even for spectra that have different zeroth moment, is discussed in [34, Section III]. It is observed there that the constraint (1.4) often fixes the zeroth Fourier coefficient of feasible spectra (this happens for sure when A is singular). In that case, rescaling Ψ, we are guaranteed that the index is nonnegative and equal to zero if and only if the two spectra are equal. T. Georgiou has kindly informed us that even when A is nonsingular, under a rather mild assumption, it is possible to modify the index so that all Φ satisfying the constraint have the same zeroth moment. In any case, the method entails a rescaling of the *a priori* density Ψ, so that the optimization problem amounts to approximating the "shape" of the *a priori* spectrum. This is of course sensible to pursue in several engineering applications such as speech processing.

We mention that, in the same spirit, Georgiou has very recently investigated other distances for power spectra, [32, 33]. Motivated by classical prediction theory, where

the optimal one step ahead predictor does not depend on the L^1 norm of the spectrum, he seeks natural distances between *rays* of spectral densities. Considering the degradation of performance when an optimal predictor for one stochastic process is employed to predict a different stochastic process, he is naturally led to introduce a certain metric on rays.

Note that minimizing $\Phi \to \mathbb{D}(\Psi\|\Phi)$ rather than $\Phi \to \mathbb{D}(\Phi\|\Psi)$ is unusual with respect to the statistics-probability-information theory world. Besides leading to a more tractable form of the optimal solution, however, it also includes as special case ($\Psi \equiv 1$) maximization of entropy [27]. In [34], the following problem is considered:

Problem 2.1.1 *Given $\Psi \in \mathcal{S}_+(\mathbb{T})$, find $\hat{\Phi}$ that solves*

$$\begin{aligned} &\text{minimize} \quad \mathbb{D}(\Psi\|\Phi) \\ &\text{over} \quad \left\{ \Phi \in \mathcal{S}_+(\mathbb{T}) \mid \int G\Phi G^* = I \right\}. \end{aligned} \tag{2.1}$$

Remark 2.1.2 *In the context of the covariance extension problem (1.5), the minimizers in Problem 2.1.1, when Ψ ranges over positive trigonometric polynomials of degree n, are precisely the coercive spectra consistent with the first n covariance lags and of degree at most $2n$, [10, 11, 24, 25]. This illustrates the role of the "*a priori *parameter" Ψ in obtaining a description of all solution to the moment problem of prescribed complexity.*

2.1.1 Optimality conditions

Consider Problem 2.1.1. With minor notational differences, the variational analysis in [34] is outlined as follows (see also [49]). Let

$$\mathcal{L}^{KL} := \{\Lambda \in \mathcal{H}(n) \mid G^*\Lambda G > 0, \forall e^{i\vartheta} \in \mathbb{T}\}. \tag{2.2}$$

For $\Lambda \in \mathcal{L}^{KL}$, consider the *Lagrangian function*

$$\begin{aligned} L(\Phi, \Lambda) &= \mathbb{D}(\Psi\|\Phi) + \left\langle \Lambda, \int G\Phi G^* - I \right\rangle \\ &= \mathbb{D}(\Psi\|\Phi) + \operatorname{tr}\left(\Lambda\left(\int G\Phi G^* - I\right)\right) \\ &= \mathbb{D}(\Psi\|\Phi) + \int G^*\Lambda G\Phi - \operatorname{tr}(\Lambda) \end{aligned} \tag{2.3}$$

Consider the *unconstrained* minimization of the strictly convex functional $L(\Phi, \Lambda)$:

$$\text{minimize}\{L(\Phi, \Lambda) \mid \Phi \in \mathcal{S}_+(\mathbb{T})\} \tag{2.4}$$

This is a convex optimization problem. The variational analysis yields the following result.

Theorem 2.1.3 *The unique solution $\hat{\Phi}$ to problem (2.4) is given by*

$$\hat{\Phi} = \frac{\Psi}{G^*\Lambda G}. \tag{2.5}$$

Moreover, suppose $\hat{\Lambda} \in \mathcal{L}^{KL}$ is such that

$$\int G \, \frac{\Psi}{G^*\hat{\Lambda}G} \, G^* = I. \tag{2.6}$$

Then $\hat{\Phi}$ given by

$$\hat{\Phi} = \frac{\Psi}{G^*\hat{\Lambda}G} \tag{2.7}$$

is the unique solution of the approximation Problem (2.1.1).

Thus, the original Problem 2.1.1 is now reduced to finding $\hat{\Lambda} \in \mathcal{L}^{KL}$ satisfying (2.6). This is accomplished via duality theory. Consider the dual functional

$$\Lambda \mapsto \inf\{L(\Phi, \Lambda) \mid \Phi \in \mathcal{S}_+(\mathbb{T})\}.$$

For $\Lambda \in \mathcal{L}^{KL}$, the dual functional takes the form

$$\Lambda \mapsto L\left(\frac{\Psi}{G^*\Lambda G}, \Lambda\right) = \int \Psi \log G^*\Lambda G - \operatorname{tr}(\Lambda) + \int \Psi. \tag{2.8}$$

Consider now the maximization of the dual functional (2.8) over $\mathcal{L}^{KL}$. Let, as in [34],

$$J_\Psi(\Lambda) := -\int \Psi \log G^*\Lambda G + \operatorname{tr}(\Lambda) \tag{2.9}$$

The dual problem is then equivalent to

$$\text{minimize} \quad \{J_\Psi(\Lambda) \mid \Lambda \in \mathcal{L}^{KL}\}. \tag{2.10}$$

The dual problem is also a convex optimization problem. In [34], Λ is further restricted to belong to the range of the operator Γ defined in section 1.3 (equation (1.16)). The problem then becomes

$$\text{minimize} \quad \{J_\Psi(\Lambda) \mid \Lambda \in \mathcal{L}^{KL}_\Gamma\} \tag{2.11}$$

where

$$\mathcal{L}^{KL}_\Gamma := \mathcal{L}^{KL} \cap \operatorname{Range}\Gamma. \tag{2.12}$$

The reason for this is that, in the Lagrangian (2.3), the term $\int G\Phi G^*$ between brackets belongs to $\operatorname{Range}\Gamma$ by construction, while I belongs to $\operatorname{Range}\Gamma$ *by the feasibility assumption*. Then it is natural, though not strictly necessary, to restrict also Λ to $\operatorname{Range}\Gamma$, thus excluding any component belonging to $\operatorname{Range}\Gamma^\perp$. It should be clear from fact 3 in Proposition 1.3.1 that any such component would not play any role in the Lagrangian.

The functional J_Ψ is shown in [34] to be strictly convex on the restricted domain $\mathcal{L}^{KL}_\Gamma$. It is also shown in [12] that J_Ψ has a unique minimum point in $\mathcal{L}^{KL}_\Gamma$. This result implies that, under the feasibility assumption, there exists a (unique) $\hat{\Lambda}$ in $\mathcal{L}^{KL}_\Gamma$ satisfying (2.6). Such a $\hat{\Lambda}$ then provides the optimal solution of the primal problem (2.1.1) via (2.7).

2.2 An existence theorem

In [34] the existence of a minimum of J_Ψ on $\mathcal{L}_\Gamma^{KL}$ is established resorting to a profound homeomorphism result for continuous maps between open, connected sets of the same dimension. In this section we want to show a different proof, based on less abstract results.

Let us consider the closure of $\mathcal{L}^{KL}$, given by

$$\overline{\mathcal{L}^{KL}} = \{\Lambda = \Lambda^* \in \mathbb{C}^{n\times n} : \ G^*\Lambda G \geq 0, \forall e^{i\vartheta} \in \mathbb{T}\},$$

and the closure of $\mathcal{L}_\Gamma^{KL}$, given by

$$\overline{\mathcal{L}_\Gamma^{KL}} = \overline{\mathcal{L}^{KL}} \cap \operatorname{Range}\Gamma \tag{2.13}$$

On the convex set $\overline{\mathcal{L}_\Gamma^{KL}}$, we define the sequence of functions

$$J_\Psi{}^n(\Lambda) := \operatorname{tr}(\Lambda) - \int \Psi \log\left(G^*\Lambda G + \frac{1}{n}\right). \tag{2.14}$$

Lemma 2.2.1 *The pointwise limit $J_\Psi{}^\infty(\Lambda) = \lim_n J_\Psi{}^n(\Lambda)$ exists and defines a lower semicontinuous, convex function on $\overline{\mathcal{L}_\Gamma^{KL}}$ with values in the extended reals.*

Proof. For each n, $J_\Psi{}^n$ is a continuous, convex function on the closed convex set $\overline{\mathcal{L}_\Gamma^{KL}}$. Hence $\operatorname{epi}(J_\Psi{}^n)$, the epigraph of $J_\Psi{}^n$, is a closed, convex subset of $\mathbb{C}^{n\times n} \times \mathbb{R}$. Moreover, for $\Lambda \in \overline{\mathcal{L}_\Gamma^{KL}}$, $J_\Psi{}^n(\Lambda) < J_\Psi{}^{n+1}(\Lambda)$. Hence, $J_\Psi{}^\infty$ is well defined and in fact $J_\Psi{}^\infty(\Lambda) = \sup_n J_\Psi{}^n(\Lambda)$. It follows that $\operatorname{epi}(J_\Psi{}^\infty) = \cap_n \operatorname{epi}(J_\Psi{}^n)$ is also closed and convex. We conclude that $J_\Psi{}^\infty$ is lower semicontinuous and convex on $\overline{\mathcal{L}_\Gamma^{KL}}$. ∎

Lemma 2.2.2 *Assume that the feasibility condition (1.7) holds. Then,*

1. *$J_\Psi{}^\infty$ is bounded below on $\overline{\mathcal{L}_\Gamma^{KL}}$;*
2. *$J_\Psi{}^\infty(\Lambda) = J_\Psi(\Lambda)$ on $\mathcal{L}_\Gamma^{KL}$;*
3. *$J_\Psi{}^\infty(\Lambda)$ is finite on all of $\overline{\mathcal{L}_\Gamma^{KL}} \setminus \{0\}$.*

Proof. By (1.7), there exists $\Phi_1 \in \mathcal{S}_+(\mathbb{T})$ satisfying (1.9), namely $\int G\Phi_1 G^* = I$. Hence, $\operatorname{tr}(\Lambda)$ can be written as $\operatorname{tr}(\Lambda \int G\Phi_1 G^*) = \int G^*\Lambda G\Phi_1$, and we get

$$\begin{aligned} J_\Psi{}^n(\Lambda) &= \int \left[G^*\Lambda G\Phi_1 - \Psi \log\left(G^*\Lambda G + \frac{1}{n}\right)\right] \\ &= \int \Phi_1 \left[G^*\Lambda G - \frac{\Psi}{\Phi_1}\log\left(G^*\Lambda G + \frac{1}{n}\right)\right]. \end{aligned}$$

Since the function $x - \beta \log(x + \frac{1}{n})$ with $\beta > 0$ attains its minimum at $x = \beta - \frac{1}{n}$, we get

$$J_\Psi{}^n(\Lambda) = \int \Phi_1 \left[G^*\Lambda G - \frac{\Psi}{\Phi_1} \log\left(G^*\Lambda G + \frac{1}{n} \right) \right] \geq \int \psi - \frac{1}{n} \int \Phi_1 - \mathbb{D}(\Psi||\Phi_1).$$

We conclude that $J_\Psi{}^\infty \geq \int \psi - \mathbb{D}(\Psi||\Phi_1)$ on all of $\overline{\mathcal{L}_\Gamma^{KL}}$. To establish 2, notice that, by Beppo Levi's theorem,

$$J_\Psi{}^\infty(\Lambda) := \mathrm{tr}(\Lambda) - \int \lim_{n\to\infty} \Psi \log\left(G^*\Lambda G + \frac{1}{n} \right), \quad \Lambda \in \overline{\mathcal{L}_\Gamma^{KL}}. \tag{2.15}$$

To prove 3, observe that for $0 \neq \Lambda \in \partial\mathcal{L}_\Gamma^{KL}$, the boundary of $\mathcal{L}_\Gamma^{KL}$, $G^*\bar{\Lambda}G$ is a nonzero rational spectral density so that $\log G^*\bar{\Lambda}G$ is integrable over $\mathbb{T}$ [52, pag. 64]. Since Ψ is bounded, also $\Psi \log G^*\bar{\Lambda}G$ is integrable. ∎

In view of these lemmata, we extend $J_\Psi(\Lambda)$ to all of $\overline{\mathcal{L}_\Gamma^{KL}}$ by setting $J_\Psi(\Lambda) := J_\Psi{}^\infty(\Lambda)$ on $\partial\mathcal{L}_\Gamma^{KL}$. Notice that, by (2.15), J_Ψ is finite and given by (2.9) on $\overline{\mathcal{L}_\Gamma^{KL}} \setminus \{0\}$, and it is $+\infty$ in $\Lambda = 0$.

Lemma 2.2.3 *Assume that the feasibility condition (1.7) holds. Then*

$$\lim_{\|\Lambda\|\to+\infty} J_\Psi(\Lambda) = +\infty. \tag{2.16}$$

Proof. Recall that by (1.7), there exists $\Phi_1 \in \mathcal{S}_+(\mathbb{T})$ satisfying (1.9), and, consequently, $\mathrm{tr}(\Lambda) = \int G^*\Lambda G\Phi_1 > 0, \forall \Lambda \in \mathcal{L}_+$. Suppose Λ_k is a sequence of matrices in $\mathcal{L}_\Gamma^{KL}$ such that $\lim_{k\to\infty} ||\Lambda_k|| = +\infty$. Define the normalized sequence $\Lambda_k^0 := \frac{\Lambda_k}{||\Lambda_k||}$ (of course, we can assume $\Lambda_k \neq 0, \forall k$). Since $\mathrm{tr}\,\Lambda_k^0 > 0$,

$$\eta := \liminf_{k\to+\infty} \mathrm{tr}\,\Lambda_k^0 \geq 0.$$

Consider a sub-sequence such that the limit of its trace is η. This subsequence contains a convergent sub-subsequence $\{\Lambda_{k_m}^0\}$ since Λ_k^0 belongs to the surface of the unit ball, which is compact. Let $\Lambda_\infty := \lim_{m\to\infty} \Lambda_{k_m}^0$. Since $G^*\Lambda_n^0 G > 0$ on $\mathbb{T}$, $G^*\Lambda_\infty G \geq 0$ on $\mathbb{T}$. Moreover, $\Lambda_\infty \in \mathrm{Range}\,\Gamma$, since $\mathrm{Range}\,\Gamma$ is finite-dimensional, and hence closed. This implies that $G^*\Lambda_\infty G$ cannot be identically zero. In fact, if so, $\Lambda_\infty \in \mathcal{L}_\Gamma^{KL} = \mathrm{Range}\,\Gamma^\perp$. Then $\Lambda_\infty \in \mathrm{Range}\,\Gamma \cap \mathrm{Range}\,\Gamma^\perp = \{0\}$, which is a contradiction since $\|\Lambda_\infty\| = 1$. Thus

$$\eta = \lim_{n\to\infty} \mathrm{tr}\,\Lambda_n^0 = \mathrm{tr}\,\Lambda_\infty = \int G^*\Lambda_\infty G\Phi_1 > 0 \tag{2.17}$$

Hence, there exists a K such that $\mathrm{tr}\,\Lambda_k^0 > \eta/2$ for all $k \geq K$. Finally, since $G^*\Lambda_k^0 G \leq$

G^*G, we obtain:

$$\begin{aligned}
\liminf_{k\to\infty} J_\Psi(\Lambda_k) &= \liminf_{k\to\infty} ||\Lambda_k|| \operatorname{tr} \Lambda_k^0 - \int \Psi \log ||\Lambda_k|| G^* \Lambda_k^0 G \\
&= \liminf_{k\to\infty} ||\Lambda_k|| \operatorname{tr} \Lambda_k^0 - (\int \Psi) \log ||\Lambda_k|| - \int \Psi \log G^* \Lambda_k^0 G \\
&\geq \liminf_{k\to\infty} ||\Lambda_k|| \operatorname{tr} \Lambda_k^0 - (\int \Psi) \log ||\Lambda_k|| - \int \Psi \log G^* G \\
&\geq \liminf_{k\to\infty} ||\Lambda_k|| \frac{\eta}{2} - (\int \Psi) \log ||\Lambda_k|| - \int \Psi \log G^* G \\
&= \liminf_{k\to\infty} \frac{\eta}{2} \left(||\Lambda_k|| - \frac{\int \Psi}{\eta/2} \log ||\Lambda_k|| \right) - \int \Psi \log G^* G \\
&= +\infty.
\end{aligned}$$

■

Theorem 2.2.4 *Assume that the feasibility condition (1.7) is satisfied. Then the problem of minimizing the functional $J_\Psi(\Lambda) = \operatorname{tr} \Lambda - \int \Psi \log G^* \Lambda G$ over $\mathcal{L}_\Gamma^{KL}$ admits a unique solution $\hat{\Lambda} \in \mathcal{L}_\Gamma^{KL}$.*

Proof. In view of Lemma 2.2.1, Lemma 2.2.2 and Lemma 2.2.3, the functional J_Ψ is inf-compact on the closed set $\overline{\mathcal{L}_\Gamma^{KL}}$, and therefore it admits a minimum point $\hat{\Lambda}$ there. We show next that $\hat{\Lambda} \in \mathcal{L}_\Gamma^{KL}$. Of course, $\hat{\Lambda}$ is not the zero matrix since $J_\Psi(0) = +\infty$. Let $0 \neq \overline{\Lambda} \in \partial \mathcal{L}_\Gamma^{KL}$. By Lemma 2.2.2, $J_\Psi(\overline{\Lambda})$ is finite. Observe that, by (1.7), $I \in \mathcal{L}_\Gamma^{KL}$. By convexity of $\overline{\mathcal{L}_\Gamma^{KL}}$, it then follows that $\overline{\Lambda} + \epsilon(I - \overline{\Lambda}) \in \overline{\mathcal{L}_\Gamma^{KL}}, \forall \epsilon \in [0, 1]$. We compute the one-sided directional derivative or hemidifferential

$$\begin{aligned}
J'_{\Psi_+}(\overline{\Lambda}; I - \overline{\Lambda}) &:= \lim_{\epsilon \searrow 0} \left[\frac{J_\Psi(\overline{\Lambda} + \epsilon(I - \overline{\Lambda})) - J_\Psi(\overline{\Lambda})}{\epsilon} \right] \\
&= \operatorname{tr}(I - \overline{\Lambda}) + \int \Psi - \int \frac{G^* G \Psi}{G^* \overline{\Lambda} G} = -\infty.
\end{aligned} \tag{2.18}$$

Hence, $\overline{\Lambda}$ cannot be a minimum point. We conclude that $\hat{\Lambda} \in \mathcal{L}_\Gamma^{KL}$. ■

2.3 The Pavon-Ferrante algorithm

In general, the optimal solution of the dual problem needs to be computed numerically. This is a delicate problem because of the unboundeness of the gradient of J_Ψ at the boundary of $\mathcal{L}^{KL}$, see (2.18). The approaches proposed in [34] and references therein involve some preliminary reparametrization of $\mathcal{L}^{KL}$, which may imply loss of global convexity.

In [49], a different matricial iterative method was proposed that appears to be very fast and numerically robust. This method does not restrict the search of $\hat{\Lambda}$ to

$\mathcal{L}_\Gamma^{KL}$ and indeed it normally converges to a $\hat{\Lambda} \notin \text{Range}\,\Gamma$. We show below that this method may be viewed as a modified *gradient descent method* with fixed step size. This method is described as follows.
Let

$$\mathcal{M} := \{M \in \mathcal{L}^{KL} \mid 0 \leq M \leq I,\ \text{tr}[M] = 1\}, \tag{2.19}$$
$$\mathcal{M}_+ := \{M \in \mathcal{M} \mid M > 0\}. \tag{2.20}$$

For $M \in \mathcal{M}$, define the map Θ by

$$\Theta(M) := \int M^{1/2} G \left[\frac{\Psi}{G^* M G}\right] G^* M^{1/2}. \tag{2.21}$$

Theorem 2.3.1 [49]. *The map Θ maps $\mathcal{M}$ into $\mathcal{M}$ and $\mathcal{M}_+$ into $\mathcal{M}_+$.*

Consider the following iterative algorithm.
Algorithm. Let $M_0 = \frac{1}{n} I$. Note that $M_0 \in \mathcal{M}_+$. Define the sequence $\{M_k\}_{k=0}^{\infty}$ by

$$M_{k+1} := \Theta(M_k). \tag{2.22}$$

Notice that, by Theorem 2.3.1, $M_k \in \mathcal{M}_+$ for all k. Moreover, since $M_k \in \mathcal{M}, \forall k$, the sequence is bounded. Hence it has at least one accumulation (limit) point in the closure $\bar{\mathcal{M}}$ of $\mathcal{M}$.

Theorem 2.3.2 *Suppose that the sequence $\{M_k\}_{k=0}^{\infty}$ has a limit $\hat{M} \in \mathcal{M}_+$. Then $\hat{M} \in \mathcal{L}^{KL}$ and satisfies (2.6), and therefore provides the optimal solution of the approximation problem via (2.7).*

Notice that even when the sequence generated by (2.22) converges to a singular matrix $\hat{M} \in \mathcal{M}$, it is still possible, though not guaranteed, that such a matrix solves the original problem. We next show that the algorithm may be viewed as a modified gradient descent method. To this aim, rewrite (2.22) as

$$M_{k+1} = M_k + M_k^{1/2} \left[\int \frac{G \Psi G^*}{G^* M_k G} - I\right] M_k^{1/2}. \tag{2.23}$$

Proposition 2.3.3 *Define*

$$\Delta M_k := M_k^{1/2} \left[\int \frac{G \Psi G^*}{G^* M_k G} - I\right] M_k^{1/2}, \tag{2.24}$$

so that (2.23) reads $M_{k+1} = M_k + \Delta M_k$. Then, ΔM_k is a descent direction *at M_k for J_Ψ.*

Proof. Let

$$\nabla J_\Psi(M_k) = I - \int \frac{G\Psi G^*}{G^* M_k G}$$

denote the "gradient" of J_Ψ at M_k. Then,

$$\langle \nabla J_\Psi(M_k), \Delta M_k \rangle = \operatorname{tr}\left(\nabla J_\Psi(M_k)\Delta M_k\right) = -\operatorname{tr}\left(M_k^{1/4}\nabla J_\Psi(M_k)M_k^{1/4}\right)^2.$$

By Theorem2.3.1, $M_k > 0$, for all k. It follows that $\operatorname{tr}\left(\nabla J_\Psi(M_k)\Delta M_k\right) < 0$, unless $\nabla J_\Psi(M_k) = 0$ in which case M_k is a fixed point of the iteration which solves the dual problem by Theorem(2.3.2). ■

One could implement the matricial iteration as

$$M_{k+1} = M_k + \alpha_k \Delta M_k, \tag{2.25}$$

where $0 < \alpha_k \leq 1$ is determined through backstepping, see e.g. [4]. Our extensive simulation (see e.g. [49]), however, shows that convergence in fact occur with $\alpha_k \equiv 1$. Indeed, the algorithm appears to perform numerically very well. In fact, at each step the integral (2.21) may be computed very precisely and efficiently via a spectral factorization technique that only requires to solve an algebraic Riccati equation and a Lyapunov equation, both of dimension n. We have performed an extensive number of simulations where the sequence generated by (2.22) never failed to converge. In a very small number of cases, we have observed convergence toward a singular matrix which, however, satisfied (2.6), and therefore provided the optimal solution of the approximation problem.

2.4 Difficulties in extending to the multivariate case

In this section, we state and derive some results on multivariable spectrum approximation where a "natural" generalization of the scalar Kullback-Leibler is employed. We also point out the difficulties involved in this approach which bring to a sudden stop the variational analysis.

Multivariable Kullback-Leibler approximation has been investigated in [27, 30], whereas [3] deals with the multivariate Nevanlinna-Pick problem. In statistical quantum mechanics, the state of an n-level system is represented by a *density matrix* ρ, namely a Hermitian, positive-semidefinite matrix in $\mathbb{C}^{n\times n}$ with unit trace [54]. The convex set of density matrices has as extreme points the one dimensional projections. The latter can be identified with the *pure states* of the system $|\psi\rangle$, where ψ is a unit vector in $\mathbb{C}^n$, via $\rho = \langle\psi, \cdot\rangle\psi$. Quantum analogues of entropy-like functionals have been considered since the early days of quantum mechanics [60]. Recently, renewed interest has originated in Quantum Information applications [48]. The quantum relative entropy between two density matrices is defined by:

$$\mathbb{D}(\rho||\sigma) := \operatorname{tr}(\rho(\log\rho - \log\sigma)). \tag{2.26}$$

Klein's inequality yields that $\mathbb{D}(\rho||\sigma) \geq 0$, and $\mathbb{D}(\rho||\sigma) = 0$ if and only if $\rho = \sigma$. Moreover, as in the classical case, the quantum relative entropy is jointly convex in its arguments. We are then led to the following definition: Given Φ and Ψ in $\mathcal{S}_+^{m\times m}(\mathbb{T})$, the relative entropy $\mathbb{D}(\Psi||\Phi)$ is given by

$$\mathbb{D}(\Psi||\Phi) = \int \operatorname{tr}\left(\Psi(\log\Psi - \log\Phi)\right). \tag{2.27}$$

First of all, we need to worry about nonnegativity of $\mathbb{D}(\Psi||\Phi)$ and whether it is zero iff $\Psi = \Phi$.

Proposition 2.4.1 Let $\Phi, \Psi \in \mathcal{S}_+^{m\times m}(\mathbb{T})$. Define $\Psi_1 = \Psi/\operatorname{tr}\Psi$ and $\Phi_1 = \Phi/\operatorname{tr}\Phi$. Then

$$\mathbb{D}(\Psi||\Phi) = \mathbb{D}(\operatorname{tr}\Psi||\operatorname{tr}\Phi) + \int (\operatorname{tr}\Psi)\operatorname{tr}\left(\Psi_1(\log\Psi_1 - \log\Phi_1)\right). \tag{2.28}$$

It follows that when $\int \operatorname{tr}\Psi = \int \operatorname{tr}\Phi$, then $\mathbb{D}(\Psi||\Phi) \geq 0$. Moreover, $\mathbb{D}(\Psi||\Phi) = 0$ if and only if the two spectra coincide.

Proof.

$$\begin{aligned}
\mathbb{D}(\Psi||\Phi) &= \operatorname{tr}\int \Psi\left(\log\Psi - \log\Phi\right) \\
&= \operatorname{tr}\int \operatorname{tr}(\Psi)\Psi_1\left(\log\operatorname{tr}(\Psi)\Psi_1 - \log\operatorname{tr}(\Phi)\Phi_1\right) \\
&= \operatorname{tr}\int \operatorname{tr}(\Psi)\Psi_1\left((\log\operatorname{tr}(\Psi))I + \log\Psi_1\right. \\
&\quad \left. - (\log\operatorname{tr}(\Phi))I - \log\Phi_1\right) \\
&= \operatorname{tr}\int \operatorname{tr}(\Psi)\Psi_1\left(\log\Psi_1 - \log\Phi_1\right) \\
&\quad + \operatorname{tr}\int \operatorname{tr}(\Psi)\Psi_1\left((\log\operatorname{tr}(\Psi)) - (\log\operatorname{tr}(\Phi))\right)I \\
&= \int \operatorname{tr}(\Psi)\operatorname{tr}\left(\Psi_1\left(\log\Psi_1 - \log\Phi_1\right)\right) \\
&\quad + \int \operatorname{tr}(\Psi_1)\operatorname{tr}\Psi\log\frac{\operatorname{tr}\Psi}{\operatorname{tr}\Phi} \\
&= \int \operatorname{tr}(\Psi)\operatorname{tr}\left(\Psi_1\left(\log\Psi_1 - \log\Phi_1\right)\right) \\
&\quad + \mathbb{D}(\operatorname{tr}\Psi||\operatorname{tr}\Phi).
\end{aligned}$$

Since $\operatorname{tr}\Psi_1(e^{i\vartheta}) = \operatorname{tr}\Phi_1(e^{i\vartheta}) = 1, \forall\vartheta \in [-\pi,\pi]$, it follows from Klein's inequality that

$$\operatorname{tr}\Psi_1(e^{i\vartheta})\left(\log\Psi_1(e^{i\vartheta}) - \log\Phi_1(e^{i\vartheta})\right) \geq 0, \quad \forall\vartheta.$$

The latter implies that

$$\int (\operatorname{tr}\Psi)\operatorname{tr}\left(\Psi_1\left(\log\Psi_1 - \log\Phi_1\right)\right) \geq 0.$$

When $\int \operatorname{tr} \Psi = \int \operatorname{tr} \Phi$, we also have $\mathbb{D}(\operatorname{tr} \Psi || \operatorname{tr} \Phi) \geq 0$. Thus, when $\int \operatorname{tr} \Psi = \int \operatorname{tr} \Phi$, $\mathbb{D}(\Psi||\Phi)$ is the sum of two nonnegative terms and the conclusion follows. ■

Consider again Problem 2.1.1.

Problem 2.4.2 *For* $\Psi \in \mathcal{S}_+^{m\times m}(\mathbb{T})$

$$\text{minimize} \quad \mathbb{D}(\Psi\|\Phi) \tag{2.29}$$

$$\text{over} \quad \left\{ \Phi \in \mathcal{S}_+^{m\times m}(\mathbb{T}) \mid \int G\Phi G^* = I \right\}, \tag{2.30}$$

where $\mathbb{D}(\Psi\|\Phi)$ is defined by (2.27). As in the scalar case, an *a posteriori* rescaling of the prior density is in general necessary. In the light of Proposition 2.4.1, if $\hat{\Phi}$ is the solution of (2.4.2), the new prior is

$$\hat{\Psi} = \frac{\int \operatorname{tr} \hat{\Phi}}{\int \operatorname{tr} \Psi} \Psi.$$

For $\Lambda \in \mathbb{C}^{n\times n}$ Hermitian such that $G^*\Lambda G$ is positive definite on all of $\mathbb{T}$, define again the *Lagrangian*

$$\begin{aligned} L(\Phi, \Lambda) &= \mathbb{D}(\Psi\|\Phi) + \operatorname{tr}\left(\Lambda\left(\int G\Phi G^* - I\right)\right) \\ &= \mathbb{D}(\Psi\|\Phi) + \operatorname{tr} \int G^*\Lambda G\Phi - \operatorname{tr}(\Lambda). \end{aligned} \tag{2.31}$$

The following step, entailing the *unconstrained* minimization of the strictly convex functional $L(\Phi, \Lambda)$ on $\Psi \in \mathcal{S}_+^{m\times m}(\mathbb{T})$, is a stumbling block. The optimality condition reads [30, Section IV]

$$\int_0^\infty (\hat{\Phi}_{KL} + \tau I)^{-1} \Psi (\hat{\Phi}_{KL} + \tau I)^{-1} d\tau = G^*\Lambda G. \tag{2.32}$$

In general, an explicit expression for $\hat{\Phi}_{KL}$ in terms of Ψ and Λ cannot be obtained, and the variational analysis ends here. We mention that the minimization with respect to the first argument of the relative entropy can instead be carried out explicitly, leading to a solution of the exponential form

$$\Phi^o = c \exp(\log \Psi - G^*\Lambda G),$$

see [30, Section IV]. Homotopy like methods are described in [30] to find Λ, when it exists, such that Φ^o satisfies the constraint.

These difficulties in solving the approximation problem in the multivariable case, with respect to the Kullback-Leibler metric, motivated the search for other distances between spectra that could be regarded as "natural", and in which the variational analysis could be carried through. This lead us to the Hellinger distance, which is described in the next chapter.

Chapter 3

Approximation in the Hellinger distance

3.1 The Hellinger distance

The Hellinger distance between two probability densities p and q, defined over a set $X \subset \mathbb{R}$, is defined as follows:

$$d_H(p,q) := \sqrt{\int_X \left(\sqrt{p(x)} - \sqrt{q(x)}\right)^2 dx}$$

Let us apply the same concept to spectral density functions. Given $\Phi \geq 0$ and $\Psi \geq 0$ in $L^1(\mathbb{T})$, we define the *Hellinger distance* between them by

$$d_H(\Phi,\Psi) := \left[\int_{-\pi}^{\pi} \left(\sqrt{\Phi(e^{i\theta})} - \sqrt{\Psi(e^{i\theta})}\right)^2 \frac{d\theta}{2\pi}\right]^{1/2}.$$

The following properties hold:

Proposition 3.1.1 *d_H is a* bona fide *distance.*

Proof. Since Φ and Ψ belong to $L^1(\mathbb{T})$, $\sqrt{\Phi}$ and $\sqrt{\Psi}$ belong to $L^2(\mathbb{T})$, and $d_H(\Phi,\Psi)$ is nothing more than the L^2 distance between $\sqrt{\Phi}$ and $\sqrt{\Psi}$. Thus:

- $d_H(\Phi,\Psi) \geq 0$,
- $d_H(\Phi,\Psi) = 0$ if and only if $\Phi = \Psi$ a.e., because the square root is injective,
- the symmetry is obvious, and
- $d_H(\Phi,\Psi) = ||\sqrt{\Phi} - \sqrt{\Psi}||_2 \leq ||\sqrt{\Phi} - \sqrt{\Omega}||_2 + ||\sqrt{\Omega} - \sqrt{\Psi}||_2 = d_H(\Phi,\Omega) + d_H(\Omega,\Psi)$ for any Φ, Ψ, Ω, which proves the triangular inequality.

■

Proposition 3.1.2 *Consider* $\Phi, \Psi \in \mathcal{S}_+(\mathbb{T})$. *Then*

1. $d_H(\Phi, \Psi) \leq \sqrt{\|\Phi\|_1 + \|\Psi\|_1}$;
2. $d_H(\Phi, \Psi)^2 \leq \|\Phi - \Psi\|_1$;
3. $\|\Phi - \Psi\|_1 \leq \left(\sqrt{\|\Phi\|_1} + \sqrt{\|\Psi\|_1}\right) d_H(\Phi, \Psi)$.

Proof. Observe that

$$\begin{aligned}\int_{-\pi}^{\pi} \left(\sqrt{\Phi} - \sqrt{\Psi}\right)^2 \frac{d\theta}{2\pi} &= \int_{-\pi}^{\pi} \left(\Phi + \Psi - 2\sqrt{\Phi\Psi}\right) \frac{d\theta}{2\pi} \\ &\leq \int_{-\pi}^{\pi} (\Phi + \Psi) \frac{d\theta}{2\pi}\end{aligned}$$

which proves 1). Also

$$\begin{aligned}\int_{-\pi}^{\pi} |\Phi - \Psi| \frac{d\theta}{2\pi} &= \int_{-\pi}^{\pi} |\sqrt{\Phi} - \sqrt{\Psi}||\sqrt{\Phi} + \sqrt{\Psi}| \frac{d\theta}{2\pi} \\ &\geq \int_{-\pi}^{\pi} |\sqrt{\Phi} - \sqrt{\Psi}||\sqrt{\Phi} - \sqrt{\Psi}| \frac{d\theta}{2\pi}\end{aligned}$$

which proves 2). Finally

$$\begin{aligned}\int_{-\pi}^{\pi} |\Phi - \Psi| \frac{d\theta}{2\pi} &= \int_{-\pi}^{\pi} |\sqrt{\Phi} - \sqrt{\Psi}||\sqrt{\Phi} + \sqrt{\Psi}| \frac{d\theta}{2\pi} \\ &\leq d_H(\Phi, \Psi) \left[\int_{-\pi}^{\pi} \left(\Phi + \Psi + 2\sqrt{\Phi\Psi}\right) \frac{d\theta}{2\pi}\right]^{1/2} \\ &\leq d_H(\Phi, \Psi) \left[\int_{-\pi}^{\pi} (\Phi + \Psi) \frac{d\theta}{2\pi} + 2\sqrt{\int \Phi \int \Psi}\right]^{1/2} \\ &= \left(\sqrt{\|\Phi\|_1} + \sqrt{\|\Psi\|_1}\right) d_H(\Phi, \Psi),\end{aligned}$$

where we have used the Cauchy-Schwarz inequality twice. This establishes 3). ∎

Remark 3.1.3 *On a finite-dimensional statistical manifold, endowed with the Fisher information as the metric tensor, both the Hellinger distance and the Kullback-Leibler pseudo-distance can be viewed as instances of the broader concept of* α-divergences *between two points, which arise from the so-called Amari connections. In particular, the* 0*-divergence, which indeed is the Hellinger distance, arises from the Levi-Civita connection. See [1, p. 66 and following].*

3.2 Scalar approximation

As was said before, the choice of the Hellinger distance was motivated by the fact that it generalizes nicely to the case when Φ and Ψ are multivariate spectra. More precisely, the scalar distance, the scalar variational analysis, the result of such analysis, and the existence proof for the optimum of the *dual* problem, will all be particular cases of their multivariable counterparts.

Nevertheless, in order to bridge between the scalar Kullback-Leibler and the multivariable Hellinger theories, let us show how to compute the solution to the problem of finding the scalar spectrum Φ that is closest to the scalar Ψ with respect to the classical Hellinger distance we have just introduced.

3.2.1 Variational analysis

The fast-paced variational analysis that follows will omit some details, results and proofs which will be given when we will consider the multivariable case. The reader will notice many similarities with the Kullback-Leibler analysis that was shown in Chapter 2.

Problem 3.2.1 *Let $\Psi \in \mathcal{S}_+(\mathbb{T})$, and suppose that the feasibility condition (1.7) holds (i.e. $I \in \operatorname{Range}\Gamma$). Find $\hat{\Phi}$ that solves*

$$\begin{aligned} &\text{minimize} \quad d_H^2(\Phi, \Psi) \\ &\text{over} \quad \left\{ \Phi \in \mathcal{S}_+(\mathbb{T}) \;\middle|\; \int G\Phi G^* = I \right\}, \end{aligned} \tag{3.1}$$

Define

$$\mathcal{L}^H := \{\Lambda \in \mathcal{H}(n) \mid 1 + G^*\Lambda G > 0 \; \forall e^{i\theta} \in \mathbb{T}\}.$$

For $\Lambda \in \mathcal{L}^H$, consider the *Lagrangian function*

$$\begin{aligned} L(\Phi, \Lambda) &= d_H^2(\Phi, \Psi) + \left\langle \Lambda, \int G\Phi G^* - I \right\rangle \\ &= d_H^2(\Phi, \Psi) + \operatorname{tr}\left(\Lambda\left(\int G\Phi G^* - I\right)\right) \\ &= d_H^2(\Phi, \Psi) + \int G^*\Lambda G\Phi - \operatorname{tr}\Lambda. \end{aligned} \tag{3.2}$$

Next, consider the *unconstrained* minimization of $L(\Phi, \Lambda)$.

$$\text{minimize}\{L(\Phi, \Lambda) \mid \Phi \in \mathcal{S}_+(\mathbb{T})\} \tag{3.3}$$

Remark 3.2.2 *First of all, observe that $\mathcal{S}_+(\mathbb{T})$ is an open, convex set. Second, notice that, for each Λ, the functional*

$$\Phi \mapsto L(\Phi, \Lambda)$$

is strictly convex. Thus, (3.3) is a convex optimization problem. Finally, observe that $L(\Phi, \Lambda)$ Gâteaux is differentiable at Φ in any direction $\delta\Phi \in L^1(\mathbb{T})$.

It then follows from a basic result of convex optimization that $\hat{\Phi} \in \mathcal{S}_+(\mathbb{T})$ solves problem (3.3) if and only if it satisfies the condition

$$\delta L(\hat{\Phi}, \Lambda; \delta\Phi) = 0, \quad \forall \delta\Phi \in C(\mathbb{T}). \tag{3.4}$$

Here, $\delta L(\hat{\Phi}, \Lambda; \delta\Phi)$, the first variation of L at $\hat{\Phi}$ in direction $\delta\Phi$, is defined by

$$\delta L(\hat{\Phi}, \Lambda; \delta\Phi) = \lim_{\epsilon \to 0} \frac{1}{\epsilon} \left[L(\hat{\Phi} + \epsilon\delta\Phi, \Lambda) - L(\hat{\Phi}, \Lambda) \right].$$

Proposition 3.2.3 *The unique solution $\hat{\Phi}$ to problem (3.3) is given by*

$$\hat{\Phi} = \frac{\Psi}{(1 + G^*\Lambda G)^2}. \tag{3.5}$$

Proof. For $\Phi \in \mathcal{S}_+(\mathbb{T})$, we get

$$\delta L(\Phi, \Lambda; \delta\Phi) = \int \left(1 - \Psi^{1/2}\Phi^{-1/2} + G^*\Lambda G\right) \delta\Phi.$$

By (3.4), $\hat{\Phi} \in \mathcal{S}_+(\mathbb{T})$ solves (3.3) if and only if

$$\int \left(1 - \Psi^{1/2}\Phi^{-1/2} + G^*\Lambda G\right) \delta\Phi = 0, \quad \forall \delta\Phi \in L^1(\mathbb{T}). \tag{3.6}$$

We get

$$\hat{\Phi}^{1/2} = \frac{\Psi^{1/2}}{1 + G^*\Lambda G}, \tag{3.7}$$

from which (3.5) follows. ∎

In the spirit of Lagrange, we get the following elementary, albeit fundamental, result .

Theorem 3.2.4 *Suppose $\hat{\Lambda} \in \mathcal{L}^H$ is such that*

$$\int G \, \frac{\Psi}{(1 + G^*\hat{\Lambda}G)^2} \, G^* = I. \tag{3.8}$$

Then $\hat{\Phi}$ given by

$$\hat{\Phi} = \frac{\Psi}{(1 + G^*\hat{\Lambda}G)^2} \tag{3.9}$$

is the unique solution of the approximation problem (3.2.1).

Proof. Let $\Phi \in \mathcal{S}_+(\mathbb{T})$ satisfy the constraint

$$\int G\Phi G^* = I. \tag{3.10}$$

By Proposition (3.2.3), and by the strict convexity of the functional $L(\cdot, \hat{\Lambda})$, we get

$$d_H^2(\Phi, \Psi) = L(\Phi, \hat{\Lambda}) > L(\hat{\Phi}, \hat{\Lambda}) = d_H^2(\hat{\Phi}, \Psi).$$

By (3.8), $\hat{\Phi}$ in (3.9) satisfies the constraint (3.10). Hence it is optimal for the original constrained problem. ∎

Thus, the original problem (3.2.1) is now reduced to finding $\hat{\Lambda} \in \mathcal{L}^H$ satisfying (3.8). This is accomplished via duality theory.

3.2.2 The dual problem

In view of Proposition 3.2.3, for $\Lambda \in \mathcal{L}^H$, the dual functional takes the form

$$\Lambda \mapsto L\left(\frac{\Psi}{(1+G^*\Lambda G)^2}, \Lambda\right) = \int \frac{\Psi G^*\Lambda G}{1+G^*\Lambda G} - \mathrm{tr}(\Lambda). \tag{3.11}$$

We consider the maximization of (3.11) over $\mathcal{L}^H$. Let

$$J_\Psi(\Lambda) := \mathrm{tr}\,\Lambda - \int \frac{\Psi G^*\Lambda G}{1+G^*\Lambda G}$$

The dual problem is then equivalent to

$$\text{minimize} \quad \{J_\Psi(\Lambda) \mid \Lambda \in \mathcal{L}^H\}. \tag{3.12}$$

Remark 3.2.5 *Notice that $\mathcal{L}^H$ is convex. Moreover, $J_\Psi(\Lambda)$ is convex on $\mathcal{L}^H$, but, in general,* not strictly convex.

J_Ψ is indeed strictly convex when restricted to $\mathrm{Range}\,\Gamma$. *This can be established along the lines of [34, Section V], and will be shown in detail in the treatment of the multivariable case. Observe that $\mathcal{L}^H$ is an open subset of $\mathcal{H}(n)$ and J_Ψ is Gâteaux differentiable in any direction $\delta\Lambda \in \mathcal{H}(n)$.*

Hence, $\hat{\Lambda} \in \mathcal{L}$ solves (3.12) if and only if, for all $\delta\Lambda \in \mathcal{H}$, we have

$$\delta J_\psi(\hat{\Lambda}; \delta\Lambda) = \mathrm{tr}\left[\left(I - \int \frac{G\Psi G^*}{(1+G^*\hat{\Lambda}G)^2}\right)\delta\Lambda\right] = 0. \tag{3.13}$$

Arguing as in the minimization of the Lagrangian, we get the following result.

Proposition 3.2.6 *$\hat{\Lambda} \in \mathcal{L}$ solves (3.12) if and only if it satisfies (3.8).*

Remark 3.2.7 Existence *of a minimum of Jpsi on $\mathcal{L}^H$ may be established along the lines of [34], or in a similar fashion to Section 2.2. Such a $\hat{\Lambda}$ then provides the optimal solution of the primal problem (3.2.1).*

As for the Kullback-Leibler case, a closed form solution of the dual problem may be obtained only in certain specific cases. In general, one needs to resort to an iterative scheme.

3.3 A naïve multivariable generalization

Recall that, for a positive semidefinite Hermitian matrix M, the *square root* $M^{1/2}$ of M is the unique Hermitian matrix whose square is M. If V is a unitary matrix that diagonalizes M so that $M = V^*\,\mathrm{diag}(\alpha_1^2, \ldots, \alpha_m^2)V$, then simply $M^{1/2} =$

$V^* \operatorname{diag}(\alpha_1, \ldots, \alpha_m) V$. Motivated by the analogy with the Kullback-Leibler case, and by the scalar case, we define the Hellinger distance for Φ and Ψ in $\mathcal{S}_+^{m\times m}(\mathbb{T})$ to be

$$d_H^2(\Phi, \Psi) := \int_{-\pi}^{\pi} \operatorname{tr}\left[\Phi^{1/2}(e^{i\vartheta}) - \Psi^{1/2}(e^{i\vartheta})\right]^2 \frac{d\vartheta}{2\pi}. \tag{3.14}$$

Notice that (3.14) appears also as the natural generalization of the Hellinger distance for density operators of statistical quantum physics introduced in [44]. Consider again the strictly convex Problem 3.2.1:

$$\text{minimize} \quad d_H^2(\Phi, \Psi) \tag{3.15}$$

$$\text{over} \quad \left\{\Phi \in \mathcal{S}_+^{m\times m}(\mathbb{T}) \mid \int G\Phi G^* = I\right\}, \tag{3.16}$$

where $d_H^2(\Phi, \Psi)$ is now given by (3.14). Define $\mathcal{L}^H$ by

$$\mathcal{L}^H := \{\Lambda \in \mathcal{H}(n) \mid I + G^*\Lambda G > 0 \text{ a.e.on} \mathbb{T}\}. \tag{3.17}$$

For $\Lambda \in \mathcal{L}^H$, consider the *Lagrangian*

$$L(\Phi, \Lambda) = d_H^2(\Phi, \Psi) + \operatorname{tr}\left(\Lambda\left(\int G\Phi G^* - I\right)\right).$$

The unconstrained minimization of the strictly convex functional L over $\Phi \in \mathcal{S}_+^{m\times m}(\mathbb{T})$, however, leads to an optimality condition (expressing the unique optimum $\hat{\Phi}_H$ in terms of Ψ and Λ) that does not appear to be useful.

To obtain such optimality condition, we first need an expression for the directional derivative of the matrix square root. More precisely, given $P = P^* > 0$ let $S(P) := P^{1/2}$ and $\delta P = \delta P^*$: We want to compute

$$\delta S(P, \delta P) := \lim_{\varepsilon \to 0} \frac{(P + \varepsilon \delta P)^{1/2} - P^{1/2}}{\varepsilon}$$

Employing the chain rule, it is easy to see that

$$\delta S(P, \delta P) P^{1/2} + P^{1/2} \delta S(P, \delta P) = \delta P$$

so that

$$\delta S(P, \delta P) = \int_0^\infty \exp(-P^{1/2}t) \delta P \exp(-P^{1/2}t) \mathrm{d}t. \tag{3.18}$$

Taking (3.18) into account, we get the optimality condition

$$\int_0^\infty \left[\exp(-\hat{\Phi}_H^{1/2}t)\left(\hat{\Phi}_H^{1/2} - \Psi^{1/2}\right)\exp(-\hat{\Phi}_H^{1/2}t)\right] dt + \frac{1}{2} G^*\Lambda G = 0. \tag{3.19}$$

The integral in (3.19) is the unique solution of the Lyapunov equation

$$\hat{\Phi}^{1/2} X + X \hat{\Phi}^{1/2} = \hat{\Phi}^{1/2} - \Psi^{1/2}. \tag{3.20}$$

Equations (3.19)-(3.20) now yield

$$-\frac{1}{2}\hat{\Phi}^{1/2}(G^*\Lambda G) - \frac{1}{2}(G^*\Lambda G)\hat{\Phi}^{1/2} = \hat{\Phi}^{1/2} - \Psi^{1/2},$$

which in turn gives

$$\hat{\Phi}^{1/2}\,(I + G^*\Lambda G) + (I + G^*\Lambda G)\,\hat{\Phi}^{1/2} = 2\Psi^{1/2}. \tag{3.21}$$

Since $I + G^*\Lambda G > 0$ almost everywhere on $\mathbb{T}$, we finally get

$$\hat{\Phi}^{1/2} = 2\int_0^\infty \exp\left[-(I + G^*\Lambda G)t\right]\Psi^{1/2}\exp\left[-(I + G^*\Lambda G)t\right]dt. \tag{3.22}$$

The maximization of the *dual functional* $\Lambda \mapsto L(\hat{\Phi}, \Lambda)$, however, appears quite problematic.

3.4 Hellinger distance and spectral factorization

This section and the following one are the core of the whole work. We show in this section that it is possible to define a sensible Hellinger distance for matricial functions that leads to a full unraveling of the complexity of the optimization problem. This will be accomplished by connecting this problem to a most classical topic at the hearth of systems and control theory, namely the *spectral factorization problem*.
Let F be a measurable function defined on the unit circle $\mathbb{T}$ and taking values in $\mathbb{C}^{m\times p}$. Then F belongs to the Hilbert space $L_2^{m\times p}$ if it satisfies $\int \mathrm{tr}(FF^*) < \infty$. For F, G in $L_2^{m\times p}$, the scalar product is defined by

$$\langle F, G\rangle_2 = \int \mathrm{tr}(FG^*),$$

so that $\|F\|_2^2 = \int \mathrm{tr}(FF^*)$. Let $\Phi \in \mathcal{S}_+^{m\times m}(\mathbb{T})$. Then a measurable $\mathbb{C}^{m\times p}$-valued function W is called a spectral factor of Φ if it satisfies

$$W(e^{i\vartheta})W(e^{i\vartheta})^* = \Phi(e^{i\vartheta}), \quad \text{a.e. on } \mathbb{T}.$$

Notice that necessarily $p \geq m$ and $W(e^{i\vartheta})$ is a.e. full row rank. Moreover, W is bounded on $\mathbb{T}$, and therefore it belongs to $L_2^{m\times p}$. When $p = m$, W^{-1} is also bounded and, consequently, $W^{-1} \in L_2^{m\times m}$. Any $\Phi \in \mathcal{S}_+^{m\times m}(\mathbb{T})$ satisfies the Szegö condition

$$\int_{-\pi}^{\pi} \log\det\Phi(e^{i\vartheta})\frac{d\vartheta}{2\pi} > -\infty,$$

and admits therefore spectral factors W in $H_2^{m\times m}$, namely the Hardy space of functions in $L_2^{m\times m}$ that possess an analytic extension in $|z| > 1$, see e.g. [52, 38].

Let W_1 and W_2 be spectral factors of the same $\Phi \in \mathcal{S}_+^{m\times m}(\mathbb{T})$ with W_1 square. Then trivially $U := W_1^{-1}W_2$ is a $m \times p$ *all-pass* function, i.e

$$U(e^{i\vartheta})U(e^{i\vartheta})^* = I, \quad \forall e^{i\vartheta} \in \mathbb{T}.$$

For $\Phi, \Psi \in \mathcal{S}_+^{m\times m}(\mathbb{T})$, consider the following function

$$\begin{aligned} D_H(\Phi,\Psi) = \inf \big\{ \|W_\Psi - W_\Phi\|_2 :\ & W_\Psi, W_\Phi \in L_2^{m\times m}, \\ & W_\Psi W_\Psi^* = \Psi,\ W_\Phi W_\Phi^* = \Phi \big\}. \end{aligned} \tag{3.23}$$

Theorem 3.4.1 The following facts hold true:

1. For any square spectral factor $\bar{W}_\Psi$ of Ψ, we have:

$$\begin{aligned} D_H(\Phi,\Psi) = \inf \big\{ \|\bar{W}_\Psi - W_\Phi\|_2 :\ & W_\Phi \in L_2^{m\times m}, \\ & W_\Phi W_\Phi^* = \Phi \big\}. \end{aligned} \tag{3.24}$$

2. The infimum in the above equation is a minimum: Indeed the unique spectral factor of Φ minimizing (3.24) is given by

$$\hat{W}_\Phi := \Phi^{1/2}\left(\Phi^{1/2}\Psi\Phi^{1/2}\right)^{-1/2}\Phi^{1/2}\bar{W}_\Psi.$$

3. D_H is a *bona fide* distance function.

4. D_H coincides with the Hellinger distance in the scalar case.

Proof.
1) First of all, observe that, once fixed the spectral factor $\bar{W}_\Psi$, any square spectral factor W_Ψ of Ψ can be written as $W_\Psi = \bar{W}_\Psi U$, where U is a $m \times m$ all-pass. Hence,

$$\begin{aligned} &\int \mathrm{tr}(W_\Psi - W_\Phi)(W_\Psi - W_\Phi)^* d\vartheta \\ &= \int \mathrm{tr}(\bar{W}_\Psi - W_\Phi U^*)(\bar{W}_\Psi - W_\Phi U^*)^* d\vartheta. \end{aligned}$$

Observe, moreover, that $W_\Phi U^*$ is a square spectral factor of Φ, so that (3.24) holds.
2) To show that the infimum in (3.24) is a minimum, notice that (3.24) may be rewritten in the form

$$\begin{aligned} D_H(\Phi,\Psi)^2 = \inf\Big\{ \int \mathrm{tr}(\bar{W}_\Psi - \Phi^{1/2}V)(\bar{W}_\Psi - \Phi^{1/2}V)^* d\vartheta :\ \\ V \in L_\infty^{m\times m},\ \ VV^* = I \Big\}. \end{aligned} \tag{3.25}$$

We shall solve this problem by unconstrained minimization of the Lagrangian

$$L = \int \mathrm{tr}[(\bar{W}_\Psi - \Phi^{1/2}V)(\bar{W}_\Psi - \Phi^{1/2}V)^* + \Delta(VV^* - I)],$$

where $\Delta = \Delta^* > 0$. The first variation of the Lagrangian (at V in direction $\delta V \in L_\infty^{m\times m}$) is

$$\delta L(V;\delta V) = \int \mathrm{tr}[(\Delta V - \Phi^{1/2} W_\Psi)\delta V^* + \delta V(\Delta V - \Phi^{1/2} W_\Psi)^*]$$

The second variation of the Lagrangian is

$$\delta^2 L(V;\delta V) = 2\int \mathrm{tr}[\Phi^{1/2}\delta V \delta V^* \Phi^{1/2} + \Delta^{1/2}\delta V \delta V^* \Delta^{1/2}].$$

Hence, L is strictly convex and therefore V is a minimizer of the unconstrained minimization problem if and only if:

$$\delta L(V;\delta V) = 0, \qquad \forall\ \delta V. \tag{3.26}$$

Condition (3.26) is clearly equivalent to $\Delta V - \Phi^{1/2} W_\Psi = 0$ or to

$$V = \Delta^{-1}\Phi^{1/2} W_\Psi.$$

Thus, if there exists $\Delta = \Delta^* > 0$ such that

$$VV^* = \Delta^{-1}\Phi^{1/2}\Psi\Phi^{1/2}\Delta^{-1} = I,$$

then V minimizes (3.25). Such a Δ is readily seen to be given by

$$\Delta = [\Phi^{1/2}\Psi\Phi^{1/2}]^{1/2}.$$

In conclusion, the infimum in (3.24) is a minimum and

$$\hat{W}_\Phi = \Phi^{1/2}\hat{V} = \Phi^{1/2}[\Phi^{1/2}\Psi\Phi^{1/2}]^{-1/2}\Phi^{1/2}\bar{W}_\Psi$$

is the unique minimizer.

3) The distance properties of D_H are easy to check: (i) Symmetry is an immediate consequence of the definition of D_H. (ii) It is clear that $D_H(\Phi,\Phi) = 0$. Conversely, if $D_H(\Phi,\Psi) = 0$, then Φ and Ψ share a.e. a common spectral factor and are, therefore, a.e. the same spectral density. (iii) The triangular inequality is inherited by the definition of D_H as the infimum of the L_2 distance among spectral factors. Thus, given Φ, Ψ and Υ and chosen an arbitrary square spectral factor W_Υ of Υ, we have

$$\begin{aligned} D_H(\Phi,\Psi) &= \inf_{W_\Phi, W_\Psi} \|W_\Phi - W_\Psi\|_2 \\ &\le \inf_{W_\Phi, W_\Psi} [\|W_\Phi - W_\Upsilon\|_2 + \|W_\Psi - W_\Upsilon\|_2] \\ &= \inf_{W_\Phi} \|W_\Phi - W_\Upsilon\|_2 + \inf_{W_\Psi} \|W_\Psi - W_\Upsilon\|_2 \\ &= D_H(\Phi,\Upsilon) + D_H(\Psi,\Upsilon) \end{aligned}$$

where the last equality is a consequence of point 1).

4) By choosing $\bar{W}_\Psi = \Psi^{1/2}$, it is immediate to check that in the scalar case ($m = 1$) $\hat{V} \equiv 1$ and hence D_H coincides with the Hellinger distance d_H. ■

3.5 D_H-optimal multivariable spectrum approximation

Theorem 3.4.1 shows that D_H is a natural extension to the multivariable case of the Hellinger distance. The corresponding multivariable version of Problem 3.2.1 is the following:

Problem 3.5.1 *Given $\Psi \in \mathcal{S}_+^{m\times m}(\mathbb{T})$, find $\hat{\Phi} \in \mathcal{S}_+^{m\times m}(\mathbb{T})$ that solves*

$$\text{minimize } {D_H}^2(\Phi, \Psi) \tag{3.27}$$

$$\text{subject to } \int G\Phi G^* = I. \tag{3.28}$$

It is in this form that the optimization problem is amenable to the variational analysis even in multivariable version. Let

$$\mathcal{L}^H := \{\Lambda \in \mathcal{H}(n) \mid I + G^*\Lambda G > 0 \ \forall e^{i\vartheta} \in \mathbb{T}\}, \tag{3.29}$$

and

$$\mathcal{L}_\Gamma^H := \mathcal{L}^H \cap \operatorname{Range}\Gamma \tag{3.30}$$

The following is our main result.

Theorem 3.5.2 Assume condition (1.8) (or, equivalently, condition (1.10)) is satisfied. Then there exists a unique $\hat{\Lambda} \in \mathcal{L}_\Gamma^H$ such that

$$\int G(I + G^*\hat{\Lambda}G)^{-1}\Psi(I + G^*\hat{\Lambda}G)^{-1}G^* = I. \tag{3.31}$$

The unique solution of the constrained approximation Problem 3.5.1 is then given by

$$\hat{\Phi}_H := (I + G^*\hat{\Lambda}G)^{-1}\Psi(I + G^*\hat{\Lambda}G)^{-1}. \tag{3.32}$$

Remark 3.5.3 *Let $\Psi_0 \in \mathcal{S}_+(\mathbb{T})$ and suppose $\Psi = \Psi_0 I$ has the form of a scalar matrix. Then, a simple calculation shows that (3.32) and (3.22) give the same form for the optimal solution $\hat{\Phi}$.*

We break the proof of Theorem 3.5.2 into three parts: First, by unconstrained minimization of the Lagrangian function, we obtain an expression for a spectral factor of the optimal Φ depending on the Lagrange multiplier matrix Λ (Lemma 3.5.5). Second, we establish some regularity properties of the functional J_Ψ, in particular its strict convexity (Theorem 3.5.8). Third, we establish existence of a unique $\Lambda \in \mathcal{L}_\Gamma^H$ satisfying (3.31) (Theorem3.5.10).

We begin by recalling a few basic definitions and facts from multivariate analysis. A function $f : S \subset \mathbb{R}^N \to \mathbb{R}^M$ is (*Fréchet*) differentiable on the open set S if for all $x \in S$ there exists a linear map $L_x : \mathbb{R}^N \to \mathbb{R}^M$ such that

$$\lim_{h\to 0} \frac{||f(x+h) - f(x) - L_x(h)||}{||h||} = 0.$$

A function f is said to be $C^0(S)$ if it is continuous on S. Also, f is said to be $C^1(S)$ if it is differentiable at each $x \in S$ and if the operator Df defined by

$$Df(x) := L_x$$

is $C^0(S)$. Now the derivative $Df : S \to L(\mathbb{R}^N, \mathbb{R}^M) \simeq \mathbb{R}^{MN}$ is itself a function between finite-dimensional spaces. If Df is $C^1(S)$, then f is said to be $C^2(S)$. Proceeding in this way, the C^k-differentiability of f can be defined. Finally, f is said to be of class $C^\infty(S)$ if it is $C^k(S)$ for all $k \in \mathbb{N}$. A standard result in analysis states that $f \in C^1(S)$ if and only if the partial derivatives $\frac{\partial f_m}{\partial x_n}$ (where f_m is the m-th component of f) exist and are continuous on S (see for instance [53, Theorem 9.21]). It follows that $f \in C^k(S)$ if and only if f has in S continuous partial derivatives of any order up to k, that is:

$$\frac{\partial^h f_m}{\partial x_{n_1} \cdots \partial x_{n_h}} \in C^0(S)$$

for all m, n_i, h s.t. $1 \leq m \leq M$, $1 \leq n_i \leq N$, and $0 \leq h \leq k$.

Remark 3.5.4 *In the following, we will deal with* functionals*, such as the Lagrangian and (the opposite of) the dual functional $J_\Psi : \mathcal{L}_\Gamma^H \to \mathbb{R}$. In particular, with respect to J_Ψ the role of the above partial derivatives is played by the directional (or* Gâteaux*) derivatives,*

$$\delta^h J_\Psi(\Lambda; \bar{\delta\Lambda}_{n_1}, ..., \bar{\delta\Lambda}_{n_h})$$

where $1 \leq n_i \leq d$ and $\{\bar{\delta\Lambda}_1, ..., \bar{\delta\Lambda}_d\}$ is a fixed orthonormal base of $\operatorname{Range}\Gamma$. A fortiori*, if we show that J_Ψ has on $\mathcal{L}_\Gamma^H$* continuous *directional derivatives of any order up to k, taken in* whatever *directions $\{\delta\Lambda_1, ..., \delta\Lambda_k\} \subset \operatorname{Range}\Gamma$, then we can say that $J_\Psi \in C^k(\mathcal{L}_\Gamma^H)$.*

Finally, a standard result in the theory of convex functions states that if a function $f : S \subset \mathbb{R}^N \to \mathbb{R}$ is $C^2(S)$ (where S is open), then f is *strictly convex* on S if and only if its Hessian H_x is positive definite at each $x \in S$.

For $\Lambda \in \mathcal{L}^H$, W_Ψ a spectral factor of Ψ, and $W, W^{-1} \in L_\infty^{m\times m}(\mathbb{T})$, form the Lagrangian function:

$$\begin{aligned} L(W, \Lambda) = \operatorname{tr} &\int (W - W_\Psi)(W - W_\Psi)^* \\ &+ \operatorname{tr}\Lambda \left(\int GWW^*G^* - I \right). \end{aligned} \tag{3.33}$$

Consider the unconstrained minimization problem:

$$\min_W \left\{ L(W, \Lambda) \mid W, W^{-1} \in L_\infty^{m\times m}(\mathbb{T}) \right\} \tag{3.34}$$

Lemma 3.5.5 *The unique solution to problem (3.34) is given by*

$$\hat{W} = (I + G^*\Lambda G)^{-1} W_\Psi. \tag{3.35}$$

Proof. The first variation (or *directional derivative*) of the Lagrangian in an arbitrary direction $\delta W_1 \in L_\infty^{m\times m}(\mathbb{T})$ is:

$$\begin{aligned} \delta L(W, \Lambda; \delta W_1) &= \operatorname{tr} \int \left[\delta W_1 \left(W - W_\Psi\right)^* + \left(W - W_\Psi\right) \delta W_1^* \right. \\ &\quad + \left. \Lambda \left(G \delta W_1 W^* G^* + G W \delta W_1^* G^*\right)\right] \\ &= \operatorname{tr} \int \left(W - W_\Psi + G^*\Lambda G W\right) \delta W_1^* \\ &\quad + \left(\operatorname{tr} \int \left(W - W_\Psi + G^*\Lambda G W\right) \delta W_1^*\right)^* \end{aligned} \tag{3.36}$$

As W varies in a bounded subset of $L_\infty^{m\times m}(\mathbb{T})$, $\delta L(W, \Lambda; \delta W_1)$ is a bounded quantity. As a function of W, $\delta L(W, \Lambda; \delta W_1)$ is therefore the sum of a constant term $(-\operatorname{tr} \int \delta W_1 W_\Psi^* + W_\Psi \delta W_1^*)$ and of a bounded linear functional. Hence, in the variable W it is a *continuous* functional. By taking into account the cyclic property of the trace operator, the second variation of the Lagrangian in an arbitrary direction $\delta W_2 \in L_\infty^{m\times m}(\mathbb{T})$ is easily seen to be given by

$$\delta^2 L(W, \Lambda; \delta W_1, \delta W_2) = \operatorname{tr} \int \delta W_1^* \left(I + G^*\Lambda G\right) \delta W_2 + \operatorname{tr} \int \delta W_2^* \left(I + G^*\Lambda G\right) \delta W_1 \tag{3.37}$$

This second variation does not depend on W, hence it is trivially continuous as a function of W. In particular, the second variation taken two times in the same direction δW is:

$$\delta^2 L(W, \Lambda; \delta W) = 2 \operatorname{tr} \int \delta W^* \left(I + G^*\Lambda G\right) \delta W \tag{3.38}$$

which is clearly positive for any $\Lambda \in \mathcal{L}^H$ and $\delta W \neq 0$. Resuming, on any finite-dimensional subspace of $L_\infty^{m\times m}(\mathbb{T})$, both $\delta L(W, \Lambda; \delta W_1)$ (the "gradient" of L) and $\delta^2 L(W, \Lambda; \delta W_1, \delta W_2)$ (the "Hessian" of L) are continuous in the variable W, and the second is a positive definite bilinear form. Hence L is strictly convex with respect to W on any finite-dimensional subspace of $L_\infty^{m\times m}(\mathbb{T})$, and therefore on $L_\infty^{m\times m}(\mathbb{T})$ itself, which implies that any minimum is unique. Finally, the set $\mathcal{L}^H$ is open and convex. To find the minimum point of L, we impose $\delta L(W, \Lambda; \delta W) = 0$ in each direction δW. This yields (3.35). ∎

We now consider the question of existence of a matrix $\hat{\Lambda} \in \mathcal{L}^H$ satisfying (3.31). To this end, we introduce the dual functional

$$\begin{aligned} L(\hat{W}, \Lambda) &= \operatorname{tr} \int \left((I + G^*\Lambda G)^{-1} W_\Psi - W_\Psi\right) \times \\ &\quad \times \left((I + G^*\Lambda G)^{-1} W_\Psi - W_\Psi\right)^* \\ &\quad + \operatorname{tr} \left[\Lambda \left(\int G(I + G^*\Lambda G)^{-1} W_\Psi \times \right.\right. \\ &\quad \left.\left. \times\ W_\Psi^* (I + G^*\Lambda G)^{-1} G^* - I\right)\right] \\ &= \operatorname{tr} \int \Psi - (I + G^*\Lambda G)^{-1}\Psi - \operatorname{tr}\Lambda, \qquad \Lambda \in \mathcal{L}^H. \end{aligned} \tag{3.39}$$

Instead of maximizing (3.39), we consider the equivalent problem of minimizing the functional:

$$\begin{aligned} J_\Psi(\Lambda) &:= -L(\hat{W}, \Lambda) + \operatorname{tr} \int \Psi \\ &= \operatorname{tr} \int (I + G^*\Lambda G)^{-1}\Psi + \operatorname{tr}\Lambda, \qquad \Lambda \in \mathcal{L}^H. \end{aligned} \tag{3.40}$$

In order to establish the fundamental properties of J_Ψ, we need two other lemmas.

Lemma 3.5.6 *Let $H \in \mathcal{H}(n)$ and m be its minimum eigenvalue. The map $H \mapsto m$ is continuous.*

Proof. See Appendix A, Lemma A.0.1. ■

Lemma 3.5.7 *Define $Q_\Lambda(z) = I + G^*(z)\Lambda G(z)$. Consider a sequence $\Lambda_n \in \mathcal{L}_\Gamma^H$ converging to $\Lambda \in \mathcal{L}_\Gamma^H$. Then $Q_{\Lambda_n}^{-1}$ are well defined and continuous on $\mathbb{T}$ and converge* uniformly *to Q_Λ^{-1} on $\mathbb{T}$.*

Proof. Observe that, for $\Lambda \in \mathcal{L}_\Gamma^H$, Q_Λ is a positive definite, continuous matrix function on $\mathbb{T}$. By Lemma 3.5.6, there exists a continuous function $m_\Lambda(\mathrm{e}^{\mathrm{j}\vartheta}) > 0$ such that $Q_\Lambda(\mathrm{e}^{\mathrm{j}\vartheta}) \geq m_\Lambda(\mathrm{e}^{\mathrm{j}\vartheta})I$ for each ϑ. Hence, $Q_\Lambda(\mathrm{e}^{\mathrm{j}\vartheta}) \geq m_\Lambda I, \forall\vartheta$, where $m_\Lambda := \min_\vartheta m_\Lambda(\mathrm{e}^{\mathrm{j}\vartheta}) > 0$. Let $\delta\Lambda \in B(0,\varepsilon)$, the *closed* ball of radius ε centered in 0. Now,

$$||G^*(\mathrm{e}^{\mathrm{j}\vartheta})\delta\Lambda G(\mathrm{e}^{\mathrm{j}\vartheta})|| \leq ||\delta\Lambda|| M_G \leq \varepsilon M_G$$

where

$$M_G = \max_\vartheta ||G^*(\mathrm{e}^{\mathrm{j}\vartheta})||\ ||G(\mathrm{e}^{\mathrm{j}\vartheta})||.$$

Thus, if we choose $\varepsilon < m_\Lambda/M_G$, then $||G^*(\mathrm{e}^{\mathrm{j}\vartheta})\delta\Lambda G(\mathrm{e}^{\mathrm{j}\vartheta})|| < m_\Lambda$. Hence, $I + G^*(\Lambda + \delta\Lambda)G$ describes, as $(\delta\Lambda, \vartheta)$ varies in $B(0,\varepsilon) \times [-\pi, \pi]$, a compact set that does not

contain any singular matrix. Now recall that the matrix inversion operator is continuous at any nonsingular matrix. Hence, $Q^{-1}_{\Lambda+\delta\Lambda}(\mathrm{e}^{\mathrm{j}\vartheta})$ admits a uniform bound $M(\Lambda,\epsilon)$ on $B(0,\varepsilon)\times[-\pi,\pi]$. Since $\Lambda_n\to\Lambda$, for n sufficiently large, $(\Lambda_n-\Lambda)\in B(0,\varepsilon)$. Then

$$\begin{aligned}\sup_{\vartheta}\|Q^{-1}_{\Lambda_n}-Q^{-1}_{\Lambda}\| &= \sup_{\vartheta}\|Q^{-1}_{\Lambda_n}\left[G^*(\Lambda-\Lambda_n)G\right]Q^{-1}_{\Lambda}\|\\ &\le M^2\sup_{\vartheta}\|G^*(\Lambda-\Lambda_n)G\|\\ &\le M^2\varepsilon M_G.\end{aligned}$$

This implies that $Q^{-1}_{\Lambda_n}\to Q^{-1}_{\Lambda}$ uniformly on $\mathbb{T}$. ■

Theorem 3.5.8 *Consider $J_\Psi:\mathcal{L}^H_\Gamma\subset\operatorname{Range}\Gamma\to\mathbb{R}$. Then*

1. *$J_\Psi\in C^\infty(\mathcal{L}^H_\Gamma)$.*
2. *J_Ψ is strictly convex on $\mathcal{L}^H_\Gamma$.*

Proof.

Let $\mathcal{I}:A\mapsto A^{-1}$ be the matrix inversion operator. Making use of

$$\delta\mathcal{I}(A;\delta A)=-A^{-1}\delta AA^{-1}, \tag{3.41}$$

the first variation of $J_\Psi(\Lambda)$ in an arbitrary direction $\delta\Lambda_1$ is found to be:

$$\begin{aligned}\delta J_\Psi(\Lambda;\delta\Lambda_1) &= -\operatorname{tr}\int Q^{-1}_\Lambda G^*\delta\Lambda_1 GQ^{-1}_\Lambda\Psi+\operatorname{tr}\delta\Lambda_1\\ &= \left\langle I-\int GQ^{-1}_\Lambda\Psi Q^{-1}_\Lambda G^*,\quad \delta\Lambda_1\right\rangle\end{aligned} \tag{3.42}$$

The linear functional $\nabla J_{\Psi,\Lambda}(\cdot):=\delta J_\Psi(\Lambda;\cdot)$ defined by (3.42) is the *gradient* of J_Ψ at Λ. To prove that $J_\Psi\in C^1(\mathcal{L}^H_\Gamma)$ we must show that, for any fixed $\delta\Lambda_1$, $\delta J_\Psi(\Lambda;\delta\Lambda_1)$ is continuous in the variable Λ (it follows that $\nabla J_{\Psi,\Lambda}(\cdot)$ is also continuous in Λ). Consider a sequence $M_n\in\operatorname{Range}\Gamma$ converging to 0. By Lemma 3.5.7, $Q^{-1}_{\Lambda+M_n}$ converge uniformly to Q^{-1}_Λ. Recall that Ψ is bounded. Applying elementwise the bounded convergence theorem, we get

$$\lim_{n\to+\infty}\int Q^{-1}_{\Lambda+M_n}G^*\delta\Lambda_1GQ^{-1}_{\Lambda+M_n}\Psi=\int Q^{-1}_\Lambda G^*\delta\Lambda_1GQ^{-1}_\Lambda\Psi$$

Hence, for all $\delta\Lambda_1\in\operatorname{Range}\Gamma$, $\delta J_\Psi(\Lambda;\delta\Lambda_1)$ is continuous, i.e. $J_\Psi\in C^1(\mathcal{L}^H_\Gamma)$. The second variation of J_Ψ, say in direction $\delta\Lambda_2$, is easily obtained applying (3.41) and the chain rule to (3.42):

$$\begin{aligned}&\delta^2J_\Psi(\Lambda;\delta\Lambda_1,\delta\Lambda_2)\\ &=\operatorname{tr}\int W^*_\Psi Q^{-1}_\Lambda G^*\delta\Lambda_2GQ^{-1}_\Lambda G^*\delta\Lambda_1GQ^{-1}_\Lambda W_\Psi\\ &+\operatorname{tr}\int W^*_\Psi Q^{-1}_\Lambda G^*\delta\Lambda_1GQ^{-1}_\Lambda G^*\delta\Lambda_2GQ^{-1}_\Lambda W_\Psi\end{aligned} \tag{3.43}$$

The bilinear form $H_\Lambda(\cdot,\cdot) := \delta^2 J_\Psi(\Lambda;\cdot,\cdot)$ is the *Hessian* of J_Ψ at Λ. Again, continuity of $\delta^2 J_\Psi(\Lambda;\delta\Lambda_1,\delta\Lambda_2)$ can be established by the previous argument in view of Lemma 3.5.7. Similarly, it can be shown that J_Ψ has continuous directional derivatives of any order. Thus $J_\Psi \in C^k(\mathcal{L}_\Gamma^H)$ for any k, and the first assertion follows. Finally, we show that J_Ψ is *strictly* convex on $\mathcal{L}_\Gamma^H$. A standard result in the theory of convex functions states that if a function $f : S \subset \mathbb{R}^N \to \mathbb{R}$ is $C^2(S)$ (where S is open), then f is *strictly convex* on S if and only if its Hessian H_x is positive definite at each $x \in S$. Consider $H_\Lambda(\delta\Lambda,\delta\Lambda) = \delta^2 J_\Psi(\Lambda;\delta\Lambda,\delta\Lambda)$ for $\delta\Lambda \in \operatorname{Range}\Gamma \setminus \{0\}$. Since the integrand in (3.43) is positive semidefinite, it follows that $H_\Lambda(\delta\Lambda,\delta\Lambda) \geq 0$. In view of Point 3 in Proposition 1.3.1, the integrand is not identically zero and $H_\Lambda(\delta\Lambda,\delta\Lambda) > 0$. It follows that J_Ψ is strictly convex. ■

As an immediate consequence of the above theorem, we have the following corollary.

Corollary 3.5.9 The dual problem

$$\text{Find } \Lambda \in \mathcal{L}_\Gamma^H \text{ minizing } J_\Psi(\Lambda) \tag{3.44}$$

admits at most one solution. Moreover, (3.31) is necessary and sufficient for $\hat{\Lambda}$ to solve the dual problem (3.44).

We now tackle the existence issue for the dual problem. Although this is a finite-dimensional, convex optimization problem, the existence question is quite delicate since the set $\mathcal{L}_\Gamma^H$ is *open* and *unbounded*. The proof of the following theorem is partially inspired by the proof of the corresponding result for the scalar, Kullback-Leibler case in [12, Section 2].

Theorem 3.5.10 *If Problem 3.5.1 is feasible, i.e. (1.8) (or, equivalently, condition (1.10)) is satisfied, then the dual functional (3.40) has a unique minimum point in* $\mathcal{L}_\Gamma^H$.

Proof. In view of Corollary 3.5.9, we only need to show that J_Ψ takes a minimum value on $\mathcal{L}_\Gamma^H$. First, we observe that J_Ψ is continuous on its domain. Second, we show that J_Ψ is bounded below on $\mathcal{L}_\Gamma^H$. Indeed, by feasibility, there exists a $\bar{\Phi} \in \mathcal{S}_+^{m\times m}(\mathbb{T})$ such that $\int G\bar{\Phi}G^* = I$. Hence, for all $M \in \mathbb{C}^{n\times n}$, $\int G\bar{\Phi}G^*M = M$, which implies

$$\operatorname{tr} M = \operatorname{tr} \int \bar{\Phi}^{1/2} G^* M G \bar{\Phi}^{1/2}. \tag{3.45}$$

Recalling that, for $\Lambda \in \mathcal{L}_\Gamma^H$, $I + G^*(e^{i\vartheta})\Lambda G(e^{i\vartheta})$ is positive definite for all $\vartheta \in [0, 2\pi)$, and using the monotonicity property of the trace, we get

$$\operatorname{tr}\Lambda = \operatorname{tr} \int \bar{\Phi}^{1/2} G^* \Lambda G \bar{\Phi}^{1/2} > -\operatorname{tr} \int \bar{\Phi}, \quad \forall \Lambda \in \mathcal{L}_\Gamma^H. \tag{3.46}$$

Define $\bar{f} := -\operatorname{tr}\int\bar{\Phi} < 0$. We get

$$\begin{aligned} J_\Psi(\Lambda) &:= \operatorname{tr}\int (I + G^*\Lambda G)^{-1}\Psi + \operatorname{tr}\Lambda \\ &= \operatorname{tr}\int \Psi^{1/2}(I + G^*\Lambda G)^{-1}\Psi^{1/2} + \operatorname{tr}\Lambda \\ &> \bar{f}, \qquad \forall\Lambda \in \mathcal{L}_\Gamma^H, \end{aligned} \tag{3.47}$$

where we have used $\operatorname{tr}\int \Psi^{1/2}(I + G^*\Lambda G)^{-1}\Psi^{1/2} > 0$. on $\mathcal{L}_\Gamma^H$.

Finally, we show that J_Ψ is *inf-compact* i.e. the sub-level sets $J_\Psi^{-1}(-\infty, r]$ are compact. This implies existence of a minimum point. Indeed, observing that $J_\Psi(0) = \operatorname{tr}\int\Psi$, we can then restrict the search for a minimum point to the compact set $J_\Psi^{-1}(-\infty, \operatorname{tr}\int\Psi]$. Existence for the latter problem then follows from a version of Weierstrass Theorem since an inf-compact function has closed level sets and is therefore lower semicontinuous [40, p.56]. To prove inf-compactness of J_Ψ, we proceed to show that:

1. $$\lim_{\Lambda\to\partial\mathcal{L}_\Gamma^H} J_\Psi(\Lambda) = +\infty,$$

   where $\partial\mathcal{L}_\Gamma^H$ denotes the boundary of $\mathcal{L}_\Gamma^H$;

2. $$\lim_{\|\Lambda\|\to\infty} J_\Psi(\Lambda) = +\infty.$$

To prove property 1), notice that $\partial\mathcal{L}_\Gamma^H$ is the set of Λ in $\operatorname{Range}\Gamma$ for which: (i) $I + G^*\Lambda G$ is positive semidefinite on $\mathbb{T}$ and (ii) $\exists\bar{\vartheta}$ s.t. $I + G^*(e^{i\bar{\vartheta}})\Lambda G(e^{i\bar{\vartheta}})$ is singular. Thus, for $\Lambda \to \partial\mathcal{L}_\Gamma^H$, all the eigenvalues of $[I + G^*\Lambda G]^{-1}$ are positive on $\mathbb{T}$ and, at least one of them, has a pole tending to the unit circle ($[I + G^*\Lambda G]$ and $[I + G^*\Lambda G]^{-1}$ are *rational* matrix functions!). Since Ψ is fixed and coercive, then also $\Psi^{1/2}[I + G^*\Lambda G]^{-1}\Psi^{1/2}$ has all eigenvalues positive on $\mathbb{T}$ and, at least one of them with a pole tending to the unit circle as $\Lambda \to \partial\mathcal{L}_\Gamma^H$. Rewrite now J_Ψ, as in (3.47), in the form $J_\Psi = \operatorname{tr}\int\Psi^{1/2}(I + G^*\Lambda G)^{-1}\Psi^{1/2} + \operatorname{tr}\Lambda$. Since $\operatorname{tr}\Lambda$ is bounded below in view of (3.46), we get the conclusion.

Point 2) is more delicate. Let $\Lambda_k \in \mathcal{L}_\Gamma^H$ be a sequence such that $\lim_{k\to\infty}\|\Lambda_k\| = \infty$. Let $\Lambda_k^0 := \frac{\Lambda_k}{\|\Lambda_k\|}$. It is easy to see that if $\Lambda \in \mathcal{L}_\Gamma^H$, then $\alpha\Lambda \in \mathcal{L}_\Gamma^H$ for all $\alpha \in [0, 1]$. Hence, for sufficiently large k, we have $\Lambda_k^0 \in \mathcal{L}_\Gamma^H$.

Let $\eta = \liminf \operatorname{tr}\Lambda_k^0$. We want to show that η is strictly positive. We first observe that $\eta \geq 0$. In fact, $\operatorname{tr}\Lambda_k^0 = \frac{1}{\|\Lambda_k\|}\operatorname{tr}\Lambda_k > \frac{1}{\|\Lambda_k\|}\bar{f} \to 0$, where we have used (3.46).

Consider a sub-sequence of Λ_k^0 such that the limit of its trace is η. Since this sub-sequence remains on the surface of the unit ball $\partial\mathcal{B} := \{\Lambda = \Lambda^* : \|\Lambda\| = 1\}$, which is compact, it has a sub-sub-sequence converging in $\partial\mathcal{B}$. Let $\Lambda_{k_i}^0$ be such a sub-sub-sequence, and let $\Lambda^\infty \in \partial\mathcal{B}$ be its limit. Clearly,

$$\lim_{i\to\infty}\operatorname{tr}\Lambda_{k_i}^0 = \operatorname{tr}\Lambda^\infty = \eta. \tag{3.48}$$

We now prove that $\Lambda^\infty \in \mathcal{L}_\Gamma^H$. To this aim, notice that Λ^∞ is the limit of a sequence in the finite dimensional linear space Range Γ and hence it belongs to the same space Range Γ. It remains to show that $(I + G^*\Lambda^\infty G)$ is positive definite on $\mathbb{T}$. Indeed, since (the unnormalized sub-sequence) Λ_{k_i} belongs to $\mathcal{L}_\Gamma^H$, we have that $(I + G^*\Lambda_{k_i}G)$ is positive definite on $\mathbb{T}$ so that $(\frac{1}{\|\Lambda_{k_i}\|}I + G^*\Lambda_{k_i}^0 G)$ is also positive definite on $\mathbb{T}$ for each i. Taking the limit for $i \to \infty$, we get that $G^*\Lambda^\infty G$ is positive semi-definite on $\mathbb{T}$ so that $(I + G^*\Lambda^\infty G)$ is strictly positive definite on $\mathbb{T}$. This proves that $\Lambda^\infty \in \mathcal{L}_\Gamma^H$. The latter, together with (3.45) yields

$$\operatorname{tr}\Lambda^\infty = \operatorname{tr}\int \bar{\Phi}^{1/2} G^*\Lambda^\infty G \bar{\Phi}^{1/2}. \tag{3.49}$$

As seen before, $G^*\Lambda^\infty G$ is positive semi-definite on $\mathbb{T}$. Moreover, $G^*\Lambda^\infty G$ is not identically zero since $\Lambda^\infty \in$ Range Γ, and $\Lambda^\infty \neq 0$ (it is not the zero matrix) since $\Lambda^\infty \in \partial\mathcal{B}$. We conclude, in view of (3.48) and (3.49), that $\eta = \operatorname{tr}\Lambda^\infty > 0$.

Finally, we have

$$J_\Psi(\Lambda_k) = \operatorname{tr}\int \Psi^{1/2}(I + G^*\Lambda_k G)^{-1}\Psi^{1/2} + \operatorname{tr}\Lambda_k \geq \|\Lambda_k\| \operatorname{tr}\Lambda_k^0. \tag{3.50}$$

Since $\|\Lambda_k\| \to \infty$ and $\liminf \operatorname{tr}\Lambda_k^0 > 0$, we get

$$\lim_{k\to\infty} J_\Psi(\Lambda_k) = +\infty. \tag{3.51}$$

■

Let $\hat{\Lambda} \in \mathcal{L}_\Gamma^H$ be the unique solution of the dual problem whose existence has just been proven in Theorem 3.5.10. We show below that it also provides via (3.32) the unique solution to the primal problem 3.5.1.

Proof of Theorem 3.5.2: Let W_Ψ be any spectral factor of Ψ. Let $\hat{W} = (I + G^*\Lambda G)^{-1}W_\Psi$ as in (3.35). Let W, belonging to$L_\infty^{m\times m}(\mathbb{T})$ together with its inverse, satisfy the constraint

$$\int GWW^*G^* = I. \tag{3.52}$$

By Lemma (3.5.5), and by the strict convexity of the functional $L(\cdot, \hat{\Lambda})$, we get

$$\|\hat{W} - W_\Psi\|_2^2 = L(\hat{W}, \hat{\Lambda}) < L(W, \hat{\Lambda}) = \|W - W_\Psi\|_2^2.$$

Thus, $\hat{W}$ minimizes the L_2 distance to W_Ψ among W belonging to $L_\infty^{m\times m}(\mathbb{T})$ together with their inverse and satisfying constraint (3.52). Theorem 3.4.1 now shows that $\hat{\Phi}_H = \hat{W}\hat{W}^*$ (coinciding with $\hat{\Phi}_H$ in (3.32)), is the unique solution to the multivariate approximation Problem 3.5.1. ■

Remark 3.5.11 *Consider the important* covariance extension *problem when, as it is often the case, the process y is real-valued. Then A and B are real matrices and* Ψ *is a real spectral density, i.e.* $\Psi(z)$ *is real (and symmetric) for all* $z \in \mathbb{T}$. *In this case,* $\hat{\Lambda}$ *is a real symmetric matrix.*

Chapter 4

A matricial Newton algorithm

4.1 The Newton algorithm

The Newton algorithm is an iterative procedure for the search of roots of a function or the *minimization* of a functional. With respect to the latter objective, it can be formulated as follows. Let $f : S \to \mathbb{R}$ be a functional defined over $S \subset \mathbb{R}^n$. In order to find an estimate $\hat{x}$ of a minimum point x^* of f,

1. Make an initial guess x_0, possibly near the minimum point.

2. At each iteration, compute the Newton step

$$\Delta x_i = -H_{x_i}^{-1} \nabla f_{x_i} \tag{4.1}$$

   where H_{x_i} is the Hessian of f at x_i and ∇f_{x_i} is the gradient of f at x_i (understood as a column vector).

3. Set $t_i^0 = 1$, and let $t_i^{k+1} = t_i^k/2$ until both of the following conditions hold:

$$x_i + t_i^k \Delta x_i \in S \tag{4.2}$$

$$f(x_i + t_i^k \Delta x_i) < f(x_i) + \alpha t_i^k \nabla f_{x_i}^\top \Delta x_i \tag{4.3}$$

   where α is a real constant, $0 < \alpha < 1/2$.

4. Set $x_{i+1} = x_i + t_i^k \Delta x_i$.

5. Repeat steps 2, 3 and 4 until $|\nabla f_{x_i}| < \varepsilon$, where ε is a (small) tolerance threshold, then set $\hat{x} = x_i$.

In its "pure" form, the iteration of the Newton algorithm only consists in step 2, which is indeed its essential part. Step 3 is the so-called *backtracking* procedure. For small t, if f is sufficiently regular, we have $f(x_i + t\Delta x_i) \simeq f(x_i) + t\nabla f_{x_i}^\top \Delta x_i$. Since $\nabla f_{x_i}^\top \Delta x_i = -\nabla f_{x_i}^\top H_{x_i}^{-1} \nabla f_{x_i} < 0$, condition (4.3) *must* hold for small t, hence step 3

must terminate at some iteration. Since $\nabla f_{x_i}^{\top} \Delta x_i < 0$, (4.3) implies $f(x_i + t_i^k \Delta x_i) < f(x_i)$. That is, $\{f(x_i)\}$ is a strictly decreasing sequence.

In essence, the "pure" Newton algorithm works *very* well when the starting point happens to be near the minimum and the function f is there effectively approximated by a quadratic form, but it can suffer from numerical problems when this is not the case. The backtracking line search is a remedy to this drawback; moreover it can be shown that, under certain regularity assuptions on f, *which hold in our case* (see Section 4.3), after a finite number of iterations step 3 always selects the multiplier $t = 1$, that is, the full step. During the latter stage, the convergence to the minimizing solution is *quadratic*, meaning that there exists a constant C such that $||x_{i+1} - x^*|| \leq C||x_i - x^*||^2$. This rate of convergence makes the Newton algorithm often preferable over other minimization methods (see [4]).

4.2 Hellinger distance minimization with the Newton Algorithm

We must minimize the functional $J_\Psi(\Lambda)$ over the set $\mathcal{L}_\Gamma^H$. As initial condition, we can safely choose 0. Hence, set

$$\Lambda_0 = 0. \tag{4.4}$$

It turns out that, although the problem is finite-dimensional, the *inversion of the Hessian* is more demanding than inverting a matrix. In order to compute the Newton step $\Delta\Lambda_i$, we must solve at Λ_i the following linear equation:

$$H_{\Lambda_i}(\Delta\Lambda_i, \cdot) = -\nabla J_{\Psi,\Lambda_i}(\cdot) \tag{4.5}$$

where, once fixed Λ_i, $\nabla J_{\Psi,\Lambda_i}(\cdot)$ and $H_{\Lambda_i}(\cdot,\cdot)$ must be understood as a linear and a bilinear form, defined by (3.42) and (3.43) respectively. Comparing with the above definitions, (4.5) reduces to:

$$\begin{aligned} &\int GQ_{\Lambda_i}^{-1} \left[(G^*(\Delta\Lambda_i) G Q_{\Lambda_i}^{-1} \Psi) + (G^*(\Delta\Lambda_i) G Q_{\Lambda_i}^{-1} \Psi)^* \right] Q_{\Lambda_i}^{-1} G^* \\ &= \int GQ_{\Lambda_i}^{-1} \Psi Q_{\Lambda_i}^{-1} G^* - I \end{aligned} \tag{4.6}$$

In principle, equation (4.6) is not difficult to solve. We suggest the following procedure:

- At the beginning of the procedure, take a base $\{H_1, ..., H_k, ..., H_N\}$ of $\mathbb{C}^{m\times n}$. [1] Then compute the solutions $\{\Sigma_1, ..., \Sigma_k, ..., \Sigma_N\}$ of the following discrete-time Lyapunov equations:

$$\Sigma_k - A\Sigma_k A^* = BH_k + H_k^* B^*$$

[1] Actually, it suffices to take the $\{H_k\}$ to be a base of $\mathbb{C}^{m\times n} \ominus \operatorname{Ker} R$, where the map R is defined by

$$R : H \mapsto BH + H^* B^*.$$

As shown before, these solutions generate Range Γ.

- To compute $\Delta\Lambda_i$ at each step,

  1. Compute the integral
  $$Y = \int GQ_{\Lambda_i}^{-1}\Psi Q_{\Lambda_i}^{-1}G^* - I \tag{4.7}$$
  2. For each Σ_k in the precomputed generators, compute the following integral:
  $$\begin{aligned} Y_k = \int GQ_{\Lambda_i}^{-1} \big[&(G^*\Sigma_k G Q_{\Lambda_i}^{-1}\Psi) \\ &+(G^*\Sigma_k G Q_{\Lambda_i}^{-1}\Psi)^*\big] Q_{\Lambda_i}^{-1}G^* \end{aligned} \tag{4.8}$$
  3. Solve, by means of linear algebraic methods (the Moore-Penrose pseudoinverse), the equation
  $$\sum_k \alpha_k Y_k = Y \tag{4.9}$$
  4. By linearity, the solution to (4.6) is
  $$\Delta\Lambda_i = \sum_k \alpha_k \Sigma_k. \tag{4.10}$$

It is clear that the real difficulty here is the computation of the integrals (4.7) and (4.8). This task requires extensive use of the following results of linear stochastic systems theory.

Lemma 4.2.1 *Let A be a stability matrix and $W(z) = C(zI-A)^{-1}B+D$ a minimal realization of a spectral factor of $\Phi(z)$. Let Π be the unique solution to the Lyapunov equation*
$$\Pi = A\Pi A^* + BB^* \tag{4.11}$$
Then the following hold:

1. $\int_{-\pi}^{\pi} \Phi(\mathrm{e}^{\mathrm{j}\vartheta})\frac{\mathrm{d}\vartheta}{2\pi} = C\Pi C^* + DD^*$.
2. $Z(z) = C(zI-A)^{-1}(A\Pi C^* + BD^*) + \frac{1}{2}(C\Pi C^* + DD^*)$ *is a realization of the* causal part *of $\Phi(z)$; that is, $Z(z)$ is analytic outside the unit circle and $\Phi(z) = Z(z) + Z^*(z)$.*

Lemma 4.2.2 *Let $Z(z) = C(zI-A)^{-1}G + \frac{1}{2}\Sigma$ be a minimal realization of the causal part of a spectrum $\Phi(z)$. Let P_- be the stabilizing solution of the following Algebraic Riccati Equation (ARE):*
$$P = APA^* + (G - APC^*)(\Sigma - CPC^*)^{-1}(G^* - CPA^*) \tag{4.12}$$
Let moreover $D = (\Sigma - CP_-C^*)^{1/2}$ and $B = (G - AP_-C^*)D^{-1}$. Then $W(z) = C(zI-A)^{-1}B + D$ is the minimum phase *spectral factor of $\Phi(z)$; that is, $W(z)$ is stable and with stable causal inverse, and $\Phi(z) = W(z)W^*(z)$.*

Lemma 4.2.3 *Let $F(z) = C(zI - A)^{-1}B + D$ be a square transfer function, where D is invertible. Then*

$$F^{-1}(z) = -D^{-1}C\left(zI - (A - BD^{-1}C)\right)^{-1}BD^{-1} + D^{-1} \tag{4.13}$$

is a realization of its inverse.

Lemma 4.2.4 *For all matrices $P = P^* \in \mathbb{C}^{n\times n}$ the following identity holds:*

$$\begin{aligned}&\begin{bmatrix} B^*(z^{-1}I - A^*)^{-1} & I \end{bmatrix}\begin{bmatrix} A^*PA - P & A^*PB \\ B^*PA & B^*PB \end{bmatrix}\times \\ &\times\begin{bmatrix} (zI - A)^{-1}B \\ I \end{bmatrix} = 0\end{aligned} \tag{4.14}$$

Lemma 4.2.5 *Let A be a stability matrix and $H(z) = C(zI-A)^{-1}B+D$ be a minimal realization. Let P be the solution of the Lyapunov equation*

$$P = A^*PA + C^*C. \tag{4.15}$$

Let $\begin{bmatrix} K \\ J \end{bmatrix}$ be an ortho-normal basis of $\ker\begin{bmatrix} A^*P^{1/2} & C^* \end{bmatrix}$ *i.e.*

$$\begin{bmatrix} A^*P^{1/2} & C^* \end{bmatrix}\begin{bmatrix} K \\ J \end{bmatrix} = 0, \qquad \begin{bmatrix} K^* & J^* \end{bmatrix}\begin{bmatrix} K \\ J \end{bmatrix} = I. \tag{4.16}$$

Let $G := P^{-1/2}K$ and

$$H_1(z) := (D^*C + B^*PA)(zI - A)^{-1}G + B^*PG + D^*J. \tag{4.17}$$

Then, $H^*(z)H(z) = H_1(z)H_1^*(z)$.

Lemmas 4.2.1, 4.2.2 and 4.2.3 are standard results (see for example [19]). The proof of Lemma 4.2.4 can be found in [14, Appendix A]. The proof of Lemma 4.2.5 can be found in Appendix A, Lemma A.0.2.

Remark 4.2.6 *Lemma 4.2.5 not only gives us a tool to compute a left factor from a right factor of a given spectrum. It also works in the opposite direction. Indeed, let $W(z) = C(zI - A)^{-1}B + D$ be a minimal realization, and let $\zeta = z^{-1}$. Then*

$$\begin{aligned}&\Phi(z) = W(z)W^*(z)\\ &= (C(zI - A)^{-1}B + D)(B^\top(z^{-1}I - A^\top)^{-1}C^\top + D^\top)\\ &= (B^\top(\zeta^{-1}I - A^\top)^{-1}C^\top + D^\top)^\top(B^\top(\zeta I - A^\top)^{-1}C^\top + D^\top)\\ &= (B^\top(\zeta I - A^\top)^{-1}C^\top + D^\top)^*(B^\top(\zeta I - A^\top)^{-1}C^\top + D^\top)\\ &:= H^*(\zeta)H(\zeta)\end{aligned}$$

Applying Lemma 4.2.5 we can find an $H_1(\zeta) = H(\zeta I - F)^{-1}G + K$ *such that* $H^*(\zeta)H(\zeta) = H_1(\zeta)H_1^*(\zeta)$. *Now turning back to* z:

$$\begin{aligned}
&H_1(\zeta)H_1^*(\zeta) \\
&= (H(\zeta I - F)^{-1}G + K)(G^\top(\zeta^{-1}I - F^\top)^{-1}H^\top + K^\top) \\
&= (G^\top(z^{-1}I - F^\top)^{-1}H^\top + K^\top)^\top(G^\top(zI - F^\top)^{-1}H^\top + K^\top) \\
&= (G^\top(zI - F^\top)^{-1}H^\top + K^\top)^*(G^\top(zI - F^\top)^{-1}H^\top + K^\top) \\
&= W_1^*(z)W_1(z) = \Phi(z)
\end{aligned}$$

4.2.1 Factorization of $Q_\Lambda^{-1}(z)$

The first problem to solve is to obtain a spectral factor of $Q_\Lambda^{-1}(z)$, where $Q_\Lambda(z) = (I + G^*(z)\Lambda G(z))$. To this end, note that

$$\begin{aligned}
Q_\Lambda(z) = &\begin{bmatrix} B^*(z^{-1}I - A^*)^{-1} & I \end{bmatrix} \begin{bmatrix} \Lambda & 0 \\ 0 & I \end{bmatrix} \times \\
&\times \begin{bmatrix} (zI - A)^{-1}B \\ I \end{bmatrix}
\end{aligned} \tag{4.18}$$

Applying lemma 4.2.4, we can rewrite (4.18) as

$$\begin{aligned}
Q_\Lambda(z) = &\begin{bmatrix} B^*(z^{-1}I - A^*)^{-1} & I \end{bmatrix} \times \\
&\times \begin{bmatrix} A^*PA - P + \Lambda & A^*PB \\ B^*PA & B^*PB + I \end{bmatrix} \times \\
&\times \begin{bmatrix} (zI - A)^{-1}B \\ I \end{bmatrix}
\end{aligned} \tag{4.19}$$

Now, the following linear matrix inequality:

$$\begin{aligned}
&\begin{bmatrix} A^*PA - P + \Lambda & A^*PB \\ B^*PA & B^*PB + I \end{bmatrix} \\
&= \begin{bmatrix} M^* \\ N^* \end{bmatrix} \begin{bmatrix} M & N \end{bmatrix} \geq 0
\end{aligned} \tag{4.20}$$

is solvable for $P = P^* > 0$ if and only if such is the following ARE:

$$P = A^*PA - A^*PB(B^*PB + I)^{-1}B^*PA + \Lambda \tag{4.21}$$

The stabilizing solution P of (4.21) gives a realization for the square, minimum phase *co-analytic* spectral factor of $Q(z)$. We have:

$$\begin{aligned} N &= N^* = (B^*PB + I)^{1/2} \\ M &= (B^*PB + I)^{-1/2} B^*PA \\ \Delta_\Lambda(z) &= \begin{bmatrix} M & N \end{bmatrix} \begin{bmatrix} (zI - A)^{-1}B \\ I \end{bmatrix} \\ &= (B^*PB + I)^{-1/2} B^*PA(zI - A)^{-1}B \\ &\quad + (B^*PB + I)^{1/2} \\ Q_\Lambda(z) &= {\Delta_\Lambda}^*(z)\Delta_\Lambda(z) \end{aligned} \tag{4.22}$$

and finally $Q_\Lambda^{-1}(z) = {\Delta_\Lambda}^{-1}(z){\Delta_\Lambda}^{-*}(z)$ where, by means of lemma 4.2.3,

$$\begin{aligned} {\Delta_\Lambda}^{-1}(z) &= -(B^*PB + I)^{-1}B^*PA(zI - \Gamma)^{-1}B\times \\ &\quad \times (B^*PB + I)^{-1/2} + (B^*PB + I)^{-1/2} \\ \Gamma &= A - B(B^*PB + I)^{-1}B^*PA \end{aligned} \tag{4.23}$$

4.2.2 Computation of the integrals in (4.7) and (4.8)

By virtue of Lemma 4.2.5 and Remark 4.2.6, we can switch from a *right* factorization of a spectrum ($\Phi = H^*H$) to a *left* factorization ($\Phi = WW^*$), and vice versa. We will now show that both (4.7) and (4.8) can be reduced to integrals of the form

$$\int G(z){\Delta_\Lambda}^{-1}(z)\Phi(z){\Delta_\Lambda}^{-*}(z)G^*(z) \tag{4.24}$$

where $\Phi(z)$ is a spectrum. Indeed, let $\Phi_\Psi(z) = {\Delta_\Lambda}^{-*}(z)\Psi(z){\Delta_\Lambda}^{-1}(z)$. Then

$$\begin{aligned} &\int G(z)Q_\Lambda^{-1}(z)\Psi(z)Q_\Lambda^{-1}(z)G^*(z) \\ &= \int G(z){\Delta_\Lambda}^{-1}(z)\left({\Delta_\Lambda}^{-*}(z)\Psi(z){\Delta_\Lambda}^{-1}(z)\right){\Delta_\Lambda}^{-*}(z)G^*(z) \end{aligned} \tag{4.25}$$

which has the form (4.24) with $\Phi = \Phi_\Psi$. Applying Lemma 4.2.5 we obtain a (left) spectral factor of $\Phi_\Psi(z)$:

$$\begin{aligned} \Phi_\Psi(z) &= {\Delta_\Lambda}^{-*}(z)(W_\Psi(z)W_\Psi^*(z)){\Delta_\Lambda}^{-1}(z) \\ &= {\Delta_\Lambda}^{-*}(z)(H_\Psi^*(z)H_\Psi(z)){\Delta_\Lambda}^{-1}(z) \\ &= (H_\Psi(z){\Delta_\Lambda}^{-1}(z))^*(H_\Psi(z){\Delta_\Lambda}^{-1}(z)) \\ &= W_1(z)W_1^*(z) \end{aligned} \tag{4.26}$$

Finally, (4.25) can be computed obtaining a realization of $G(z){\Delta_\Lambda}^{-1}(z)W_1(z)$ and applying Lemma 4.2.1. Now, let $\Phi_\Sigma(z) = {\Delta_\Lambda}^{-*}(z)G^*(z)\Sigma G(z){\Delta_\Lambda}^{-1}(z)$, where Σ is

one of the precomputed generators of Range Γ. Then

$$\begin{aligned}
&\int GQ_\Lambda^{-1}\left[(G^*\Sigma GQ_\Lambda^{-1}\Psi)+(G^*\Sigma GQ_\Lambda^{-1}\Psi)^*\right]Q_\Lambda^{-1}G^*\\
&=\int G{\Delta_\Lambda}^{-1}{\Delta_\Lambda}^{-*}\left[(G^*\Sigma G{\Delta_\Lambda}^{-1}{\Delta_\Lambda}^{-*}\Psi)\right.\\
&\qquad\left.+(\Psi{\Delta_\Lambda}^{-1}{\Delta_\Lambda}^{-*}G^*\Sigma G)\right]{\Delta_\Lambda}^{-1}{\Delta_\Lambda}^{-*}G^*\\
&=\int G{\Delta_\Lambda}^{-1}\left[({\Delta_\Lambda}^{-*}G^*\Sigma G{\Delta_\Lambda}^{-1}{\Delta_\Lambda}^{-*}\Psi{\Delta_\Lambda}^{-1})\right.\\
&\qquad\left.+({\Delta_\Lambda}^{-*}\Psi{\Delta_\Lambda}^{-1}{\Delta_\Lambda}^{-*}G^*\Sigma G{\Delta_\Lambda}^{-1})\right]{\Delta_\Lambda}^{-*}G^*\\
&=\int G{\Delta_\Lambda}^{-1}\left[\Phi_\Sigma\Phi_\Psi+\Phi_\Psi\Phi_\Sigma\right]{\Delta_\Lambda}^{-*}G^*\\
&=\int G{\Delta_\Lambda}^{-1}\left[(\Phi_\Sigma+\Phi_\Psi)(\Phi_\Sigma+\Phi_\Psi)\right.\\
&\qquad\left.-\Phi_\Psi\Phi_\Psi-\Phi_\Sigma\Phi_\Sigma\right]{\Delta_\Lambda}^{-*}G^*\\
&=\int G{\Delta_\Lambda}^{-1}\left[(\Phi_\Sigma+\Phi_\Psi)(\Phi_\Sigma+\Phi_\Psi)\right]{\Delta_\Lambda}^{-*}G^*\\
&-\int G{\Delta_\Lambda}^{-1}\left[\Phi_\Psi\Phi_\Psi\right]{\Delta_\Lambda}^{-*}G^*-\int G{\Delta_\Lambda}^{-1}\left[\Phi_\Sigma\Phi_\Sigma\right]{\Delta_\Lambda}^{-*}G^*
\end{aligned}\tag{4.27}$$

which is a difference of integrals of the form (4.24). To compute (4.27), we must obtain (left) spectral factors of $\Phi_\Psi{\Phi_\Psi}^*$, $\Phi_\Sigma\Phi_\Sigma^*$ and $(\Phi_\Sigma+\Phi_\Psi)(\Phi_\Sigma+\Phi_\Psi)^*$. Suppose, first, that $\Sigma>0$. For the first spectrum we have

$$\begin{aligned}
\Phi_\Psi{\Phi_\Psi}^* &= W_1(W_1^*W_1)W_1^*=W_1(H_1H_1^*)W_1^*\\
&=(W_1H_1)(W_1H_1)^*
\end{aligned}\tag{4.28}$$

For the second, we have

$$\begin{aligned}
\Phi_\Sigma &= ({\Delta_\Lambda}^{-*}G^*\Sigma^{1/2})(\Sigma^{1/2}G{\Delta_\Lambda}^{-1})=H_\Sigma^*H_\Sigma=W_\Sigma W_\Sigma^*\\
\Phi_\Sigma\Phi_\Sigma^* &= W_\Sigma(W_\Sigma^*W_\Sigma)W_\Sigma^*=W_\Sigma(K_\Sigma K_\Sigma^*)W_\Sigma^*\\
&=(W_\Sigma K_\Sigma)(W_\Sigma K_\Sigma)^*
\end{aligned}\tag{4.29}$$

And for the third:

$$\begin{aligned}
&(\Phi_\Sigma+\Phi_\Psi)(\Phi_\Sigma+\Phi_\Psi)^*\\
&=(Z_\Sigma+Z_\Sigma^*+Z_1+Z_1^*)(Z_\Sigma+Z_\Sigma^*+Z_1+Z_1^*)^*\\
&=((Z_\Sigma+Z_1)+(Z_\Sigma+Z_1)^*)((Z_\Sigma+Z_1)+(Z_\Sigma+Z_1)^*)^*\\
&=(Z_{1\Sigma}+Z_{1\Sigma}^*)(Z_{1\Sigma}+Z_{1\Sigma}^*)^*\\
&=W_{1\Sigma}(W_{1\Sigma}^*W_{1\Sigma})W_{1\Sigma}^*\\
&=W_{1\Sigma}(H_{1\Sigma}H_{1\Sigma}^*)W_{1\Sigma}^*\\
&=(W_{1\Sigma}H_{1\Sigma})(W_{1\Sigma}H_{1\Sigma})^*
\end{aligned}\tag{4.30}$$

where Z_1 is the causal part of Φ_Ψ, $Z_{1\Sigma} = Z_1 + Z_\Sigma$, $W_{1\Sigma}$ is a left factor of the spectrum $Z_{1\Sigma} + Z_{1\Sigma}^*$, $H_{1\Sigma}$ is a left factor of the spectrum $W_{1\Sigma}^* W_{1\Sigma}$, and where we used Lemma 4.2.1 to obtain the causal part of Φ_Σ and Φ_Ψ from their spectral factors, and Lemma 4.2.2 to obtain the minimum phase spectral factor of the sum $\Phi_\Sigma + \Phi_\Psi$ from its causal part. Thus, if $\Sigma > 0$, we really have all the tools to compute integral (4.27).

Now, Σ is *not* necessarily positive definite, but if $-\lambda < 0$ is the minimum between the eigenvalues of all the generators Σ_k, then $\Sigma + (\lambda+1)I$ *is* positive definite. Thus, in the general case, by linearity (4.27) can be reduced to:

$$\begin{aligned}
&\int G{\Delta_\Lambda}^{-1} \left[\Phi_\Sigma \Phi_\Psi + \Phi_\Psi \Phi_\Sigma\right] {\Delta_\Lambda}^{-*} G^* \\
&= \int G{\Delta_\Lambda}^{-1} \left[\Phi_{\Sigma+(\lambda+1)I-(\lambda+1)I}\ \Phi_\Psi \right. \\
&\qquad\qquad \left. +\ \Phi_\Psi\ \Phi_{\Sigma+(\lambda+1)I-(\lambda+1)I}\right] {\Delta_\Lambda}^{-*} G^* \qquad (4.31)\\
&= \int G{\Delta_\Lambda}^{-1} \left[\Phi_{\Sigma+(\lambda+1)I}\ \Phi_\Psi + \Phi_\Psi\ \Phi_{\Sigma+(\lambda+1)I}\right] {\Delta_\Lambda}^{-*} G^* \\
&- (\lambda+1) \int G{\Delta_\Lambda}^{-1} \left[\Phi_I\ \Phi_\Psi + \Phi_\Psi\ \Phi_I\right] {\Delta_\Lambda}^{-*} G^*
\end{aligned}$$

which is a difference of integrals with the same structure of (4.27), and that are computable with the above tools (obviously $\int G{\Delta_\Lambda}^{-1} \left[\Phi_I\ \Phi_\Psi + \Phi_\Psi\ \Phi_I\right] {\Delta_\Lambda}^{-*} G^*$ needs to be computed only once). This enables us to solve equation (4.5).

4.2.3 Computations in the backtracking step

The backtracking stage involves similar, though easier, computations. We must check the following conditions:

$$\Lambda_i + t_i^k \Delta\Lambda_i \in \mathcal{L}_\Gamma^H \qquad (4.32)$$

$$J_\Psi(\Lambda_i + t_i^k \Delta\Lambda_i) < J_\Psi(\Lambda_i) + \alpha t_i^k \nabla J_{\Psi\Lambda_i} \Delta\Lambda_i \qquad (4.33)$$

Checking (4.32) is really a matter of checking whether we can factorize $I + G^*(\Lambda_i + t_i^k \Delta\Lambda_i)G$. Thus t_i^k must be halved until the ARE (4.21) is solvable having $\Lambda = \Lambda_i + t_i^k \Delta\Lambda_i$.

Finally, to check (4.33), we need to compute J_Ψ. This can be done in a way similar

to the above computations:

$$\begin{aligned} J_\Psi(\Lambda) &= \operatorname{tr} \int (I + G^*\Lambda G)^{-1}\Psi + \operatorname{tr}\Lambda \\ &= \operatorname{tr} \int {\Delta_\Lambda}^{-1}{\Delta_\Lambda}^{-*} W_\Psi W_\Psi^* + \operatorname{tr}\Lambda \\ &= \operatorname{tr} \int {\Delta_\Lambda}^{-*}(W_\Psi W_\Psi^*){\Delta_\Lambda}^{-1} + \operatorname{tr}\Lambda \\ &= \operatorname{tr} \int {\Delta_\Lambda}^{-*}(H_\Psi^* H_\Psi){\Delta_\Lambda}^{-1} + \operatorname{tr}\Lambda \\ &= \operatorname{tr} \int (H_\Psi {\Delta_\Lambda}^{-1})^*(H_\Psi {\Delta_\Lambda}^{-1}) + \operatorname{tr}\Lambda \\ &= \operatorname{tr} \int WW^* + \operatorname{tr}\Lambda \end{aligned} \tag{4.34}$$

4.3 Proof of global convergence

Given that the minimum of J_Ψ exists *and is unique*, we investigate global convergence of our Newton algorithm. First, we recall the following

Definition: a function $f(x)$ twice differentiable in a set S is said to be *strongly convex* in S if there exists a constant $m > 0$ such that $H(x) \geq mI$ for $x \in S$, where $H(x)$ is the Hessian of f at x.

We restrict our analysis to a sublevel set of J_Ψ. Let $\Lambda_0 = 0$. The set

$$S := \left\{\Lambda \in \mathcal{L}_\Gamma^H : J_\Psi(\Lambda) \leq J_\Psi(\Lambda_0) = \operatorname{tr}\textstyle\int \Psi\right\} \tag{4.35}$$

is *compact* (as it was shown in [21, Section VII]). Because of the backtracking in the algorithm, the sequence $J_\Psi(\Lambda_0), J_\Psi(\Lambda_1), ...$ is decreasing. Thus $\Lambda_n \in S$, $\forall n \geq 0$. We now wish to apply a theorem in [4, 9.5.3, p. 488] on convergence of the Newton algorithm with backtraking for strongly convex functions on $\mathbb{R}^n$. This theorem ensures linear decrease for a finite number of steps, and quadratic convergence to the minimum after the linear stage, thus establishing *global* convergence of the Newton algorithm with backtracking. We proceed to establish first *strong convexity* of J_Ψ on S. To do that, we employ the following result.

Lemma 4.3.1 *Let $f(x)$ be defined over an open convex subset D of a finite-dimensional linear space V. Assume that f is twice continuously differentiable and strictly convex on D. Then f is* strongly *convex on any compact set $S \subset D$.*

Proof.

First, recall that since f is twice continuously differentiable and strictly convex, its Hessian H_x is an Hermitian positive-definite matrix at each point x. By Lemma 3.5.6, the mapping from H to its minimum (real) eigenvalue is continuous. It follows

that the mapping from x to the minimum eigenvalue of the Hessian of f at x is also continuous, being a composition of continuous functions. Hence the latter admits a minimum m in the compact set S by Weierstrass' theorem. Thus m is the minimum of the eigenvalues of all the Hessians computed in S, and m cannot be zero, since otherwise there would be an x with H_x singular, and this cannot happen since f is strictly convex. Hence $H_x \geq mI \ \forall x \in S$, i.e. f is strongly convex on S. ■

Remark 4.3.2 *By an argument similar to that of Lemma 3.5.6, it can be shown that for a twice continuously differentiable function which is strictly convex on D, there exists $M > 0$ such that $H_x \leq MI$ for all $x \in S$. Moreover, strong convexity on a* closed *set S implies boundedness of the latter. Thus, strong convexity and boundedness of the Hessian are intertwined, and both are* essential *in the proof of Theorem 4.3.3 (see [4]).*

Theorem 4.3.3 *The following facts hold true:*

1. *J_Ψ is twice* continuously *differentiable on S;*
2. *J_Ψ is strongly convex on S;*
3. *the Hessian of J_Ψ is Lipschitz-continuous over S;*
4. *the sequence $\{\Lambda_i; i \geq 0\}$ generated by the Newton algorithm of Section 4.2 (4.4)-(4.33) converges to the unique minimum point of J_Ψ in $\mathcal{L}_\Gamma^H$.*

Proof.

Property 1 is a trivial consequence of Theorem 3.5.8. To prove 2, remember that J_Ψ is strictly convex on $\mathcal{L}_\Gamma^H$, hence also on S, and apply Lemma 4.3.1. As for property 3, what it really says is that the following operator:

$$\mathcal{H} : \Lambda \mapsto H_\Lambda(\cdot, \cdot)$$

is Lipschitz continuous on S. Theorem 3.5.8 implies that $J_\Psi \in C^3(\mathcal{L}_\Gamma^H)$ or, which is the same, that $\mathcal{H} \in C^1(\mathcal{L}_\Gamma^H)$. The continuous differentiability of $\mathcal{H}$ implies its Lipschitz continuity over an arbitrary compact subset of $\mathcal{L}_\Gamma^H$, hence also over the sublevel set S, and property 3 follows. Finally, to prove 4, notice that all the hypotheses of [4, 9.5.3, p. 488] are satisfied. Namely, the function to be minimized J_Ψ is strongly convex on the compact set S, and its Hessian is Lipschitz-continuous over S. It remains to observe that J_Ψ is defined over a subset of the linear space $\operatorname{Range}\Gamma$ which has *finite dimension* d over $\mathbb{R}$ (recall that $\operatorname{Range}\Gamma$ is spanned by a finite set of matrices. See Proposition 1.3.1 and Remark 1.3.3, where $d \leq N$). Thus, once we choose a base in $\operatorname{Range}\Gamma$, to every $\Lambda \in \mathcal{L}_\Gamma^H$ there corresponds a vector in $\mathbb{R}^d$, to every positive definite bilinear form over $\operatorname{Range}\Gamma$ there corresponds a positive definite matrix in $\mathbb{R}^{d\times d}$, and to every compact set in $\mathcal{L}_\Gamma^H$ there corresponds a compact set in $\mathbb{R}^d$. Hence, every convergence result that holds in $\mathbb{R}^d$ must also hold in the abstract setting, in view of the homeomorphism between one space and the other. ■

Chapter 5

An application to spectrum estimation

5.1 A spectral estimation procedure

Following the purposes of the THREE method presented in [7], now we describe an application of the above approximation algorithm to the estimation of spectral densities. Consider first the scalar case, and suppose that the finite sequence $y_1, ..., y_N$ is extracted from a realization of a zero-mean, weakly stationary discrete-time process $\{y_t\}_{t=-\infty}^{+\infty}$. We want to estimate the spectral density $\Phi_y(e^{j\vartheta})$ of y. The idea is the following:

- Fix a transfer function $G(z) = (zI - A)^{-1}B$, feed the data $\{y_i\}$ to it, and collect the output data $\{x_i\}$.
- Compute a consistent, and possibly unbiased, estimate $\hat{\Sigma}$ of the covariance matrix of the outputs $\{x_i\}$. Note that some output samples $x_1, ..., x_M$ should be discarded so that the filter can be considered to operate in steady state.
- Choose as "prior" spectrum $\hat{\Phi}_y$ a coarse, low-order, estimate of the true spectrum of y obtained by means of another (simple) identification method.
- "Refine" the estimate $\hat{\Phi}_y$ by solving the approximation problem (3.5.1) with respect to $G(z)$, $\Sigma = \hat{\Sigma}$, and $\Psi = \hat{\Phi}_y$ ("rescaling" $G(z)$ in order to obtain $\Sigma \to I$, as in Remark 1.2.1).

To be clear, the result of the above procedure is *the only spectrum, compatible with the output variance $\hat{\Sigma}$, which is closest to the rough estimate $\hat{\Phi}_y$ in the d_H distance.* Note that we are left with significant degrees of freedom in applying the above procedure: The method for estimating $\hat{\Phi}_y$, in particular its degree, and the whole structure of $G(z) = (zI - A)^{-1}B$, which has no contraints other than A being a stability matrix and (A, B) being reachable.

The coarsest possible estimate of Φ_y is the constant spectrum equal to the sample variance of the $\{y_i\}$, i.e. $\hat{\Phi}_y(\mathrm{e}^{\mathrm{j}\vartheta}) \equiv \hat{\sigma}_y^2$, where $\hat{\sigma}_y^2 = \frac{1}{N-1}\sum_{i=1}^{N}|y_i|^2$. The resulting spectrum has the form $\hat{\sigma}_y^2(1+G^*\hat{\Lambda}G)^{-2}$. Another simple choice is $\hat{\Phi}_y = W(z)W^*(z)$, where $W(z) = \hat{\sigma}_e\frac{c(z)}{a(z)}$ is a low-order AR, MA or ARMA model estimated from $y_1, ..., y_N$ by means of predictive error minimization methods or the like.

The flexibility in the choice of $G(z)$ is more essential, and has more profound implications. As described in [7], [34], [22] and [21], Moreover, the following choice:

$$A = \begin{bmatrix} 0 & 1 & 0 & \dots & 0 \\ 0 & 0 & 1 & \dots & 0 \\ \vdots & \vdots & & \ddots & \vdots \\ 0 & 0 & 0 & \dots & 1 \\ 0 & 0 & 0 & \dots & 0 \end{bmatrix}, \quad B = \begin{bmatrix} 0 \\ 0 \\ \vdots \\ 0 \\ 1 \end{bmatrix} \tag{5.1}$$

implies that the steady-state variance Σ is a Toeplitz matrix whose diagonals contain the lags $c_0, c_1, ..., c_{n-1}$ of the covariance signal of the input, and the corresponding problem of finding *any* spectrum that satisfies (3.52) is a covariance extension problem.

These facts justify the theoretical interest in algorithms for constrained spectrum approximation, if for no other reason, as tools to compute at least *one* solution to a Nevanlinna-Pick interpolation or to a covariance extension problem, respectively. But the freedom in choosing $G(z)$ has implications also in the above practical application to spectral estimation, where the key properties, not surprisingly, depend on the poles of $G(z)$, i.e., the eigenvalues of A. In general, as described in [7], the *magnitude* of the latter has implications on the variance of the sample covariance $\hat{\Sigma}$: The closer the eigenvalues to the origin, the smaller that variance (see [7, Section II.D]). Moreover, at least as far as THREE [7] is concerned, the *phase* of the eigenvalues influences resolution capability: More precisely, *the spectrum estimation procedure has higher resolution in those sectors of the unit circle where more eigenvalues are located.* According to simulations, the latter statement appears to be true also in our setting (the fundamental difference being that the metric which is minimized is the Hellinger distance instead of the Kullback-Leibler one).

Remark 5.1.1 *In the above setting $\hat{\Sigma}$ is a consistent estimate of the true steady-state variance. Although $\hat{\Sigma}$ must belong to* Range Γ *as $N \to +\infty$ (this being the case even if y is the sum of a purely nondeterministic process and some sinusoids, as in the simulations that follow), it is almost certainly not the case that $\hat{\Sigma} \in$ Range Γ when we have available only the finitely many data $x_{M+1}, ..., x_N$. Strictly speaking, this implies that the contraint (3.52) with $\Sigma = \hat{\Sigma}$ is almost always not feasible. It turns out that, increasing the tolerance threshold in its step 5, the Newton algorithm exhibits some kind of robustness in this respect. That is, it leads to a Λ whose corresponding spectrum $\hat{\Phi}$ is* close *to satisfying the constraint.*

Nevertheless, we prefer a clear understanding of what the resulting spectrum really is. Thus, we choose to enforce feasibility of the approximation problem, at least as permitted by machine number representation, before starting the optimization procedure.

To this end, following the same approach employed in [7], we pose the approximation problem not in terms of the estimated $\hat{\Sigma}$*, but in terms of its* orthogonal projection $\hat{\Sigma}_\Gamma$ *onto* $\operatorname{Range}\Gamma$*, which can be easily computed by means of algebraic methods. That is to say: We cannot approximate in the preimage* $\Gamma^{-1}(\hat{\Sigma})$*, because that set is empty, thus we choose to approximate in* $\Gamma^{-1}(\hat{\Sigma}_\Gamma)$*, where* $\hat{\Sigma}_\Gamma$ *is the matrix closest to* $\hat{\Sigma}$ *such that its preimage is not empty. This seems a reasonable choice and by the way it is,* mutatis mutandis*, what the Moore-Penrose pseudoinverse does for the "solution"* $\hat{x} = A^\dagger b$*, when the linear system* $Ax = b$ *is not solvable.*

Note that it is not guaranteed at all that the projection of a positive definite matrix onto a subspace of the Hermitian matrices is itself positive definite. In practice, this is not really a problem, inasmuch $\hat{\Sigma}$ *is "sufficiently positive" and close to* $\operatorname{Range}\Gamma$*. The positivity of* $\hat{\Sigma}_\Gamma$ *must anyway be checked before proceeding. This approach and the considerations on the positivity issue should be compared to [7, Section II.D], which deals with the particular case when* $\operatorname{Range}\Gamma$ *is the space of Toeplitz matrices, and to [31, Section 4], where, to find a matrix a* $\hat{\Sigma}_\Gamma$ *close to* $\hat{\Sigma}$*, a Kullback-Leibler criterion is adopted instead of least squares.*

5.2 Simulation results

5.2.1 Simulation results: Scalar case

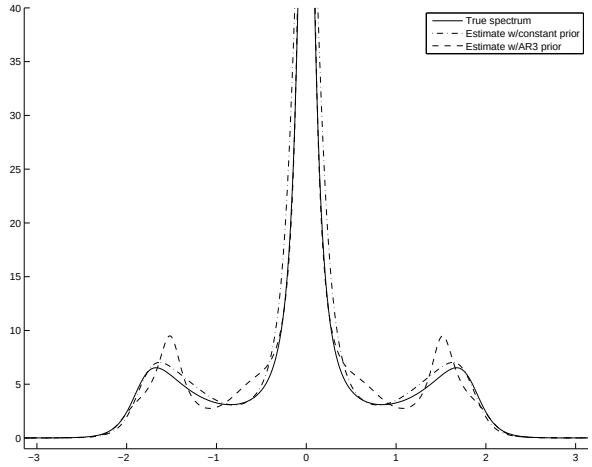

Figure 5.1: Estimation of an ARMA(6,4) spectrum by means of Hellinger-distance spectrum approximation, constant prior and AR(3) prior.

Figure 5.1 shows the results of the above estimation procedure with $G(z)$ structured according to the covariance extension setting (5.1) with 6 covariance lags (i.e.

$n = 6$, A is 6×6), run over 500 samples of the following ARMA process:

$$\begin{aligned} y(t) &= 0.5y(t-1) - 0.42y(t-2) + 0.602y(t-3) \\ &\quad - 0.0425y(t-4) + 0.1192y(t-5) \\ &\quad + e(t) + 1.1e(t-1) + 0.08e(t-2) - 0.15e(t-3) \end{aligned}$$

(poles in $0.9, -0.2 \pm 0.7\mathrm{j}, \pm 0.5\mathrm{j}$) where $e(t)$ is a zero-mean Gaussian white noise with unit variance. Two priors, both estimated from data, have been considered: the constant spectrum $\hat{\Phi}_y(\mathrm{e}^{\mathrm{j}\vartheta}) \equiv \hat{\sigma}_y^2$ and the spectrum $\hat{\Phi}_y = W_{AR}(z)W_{AR}^*(z)$, where $W_{AR}(z) = \frac{\hat{\sigma}_e}{a(z)}$ is an AR model of order 3 obtained from the data by means of the Predictive Error Method procedure in Matlab's System Identification toolbox.

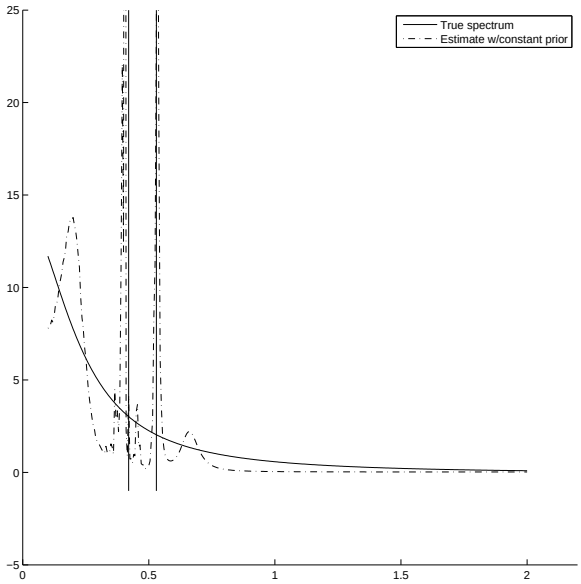

Figure 5.2: Spectral estimates of two sinusoids with superimposed noise by means of Hellinger-distance spectrum approximation, constant prior. Compare with [7, Section IV.B, Example 1].

Figure 5.2 shows the performance of the above procedure in a setting that resembles that of [7, Section IV.B, Example 1]. The estimation procedure was run on 300 samples of a superposition of two sinusoids in colored noise:

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

with ϕ_1, ϕ_2 and $\nu(t)$ independent normal random variables with zero mean and unit variance, $\omega_1 = 0.42$ and $\omega_2 = 0.53$. The prior here considered is the constant spectrum equal to the sample variance of the $\{y_i\}$ data. Following [7], A was chosen real block-diagonal with the following poles (equispaced in a narrow range where the frequencies

of the two sinusoids lie, to increase resolution in that region):

$$0, 0.85, -0.85,$$
$$0.9\mathrm{e}^{\pm \mathrm{j}0.42}, 0.9\mathrm{e}^{\pm \mathrm{j}0.44}, 0.9\mathrm{e}^{\pm \mathrm{j}0.46}, 0.9\mathrm{e}^{\pm \mathrm{j}0.48}, 0.9\mathrm{e}^{\pm \mathrm{j}0.50}$$

(and B a column of ones). It can be seen that Hellinger-distance based approximation does a good job, as does the THREE algorithm, at detecting the spectral lines at frequencies ω_1 and ω_2.

5.2.2 Simulation results: Multivariate case

We now consider spectral estimation for a multivariate process. Here, 100 samples of a bivariate process with a high order spectrum were generated by feeding a bivariate Gaussian white noise with mean 0 and variance I to a square (stable) shaping filter of order 40. The latter was constructed with random coefficients, except for one fixed conjugate pair of poles with radius 0.9 and argument 0.52, and one fixed conjugate pair of zeros with radius $1-10^{-5}$ and argument 0.2. The transfer function $G(z)$ was chosen with one pole in the origin and 4 complex pole pairs with radius 0.9 and frequencies equispaced in the range $[0, \pi]$. Then the above estimating procedure was applied, with prior spectrum chosen as the constant density equal to the sample covariance of the bivariate process y. Figure 5.3 shows a plot of $\Phi_{11}(\mathrm{e}^{\mathrm{j}\vartheta})$, $\mathrm{Re}\,\Phi_{12}(\mathrm{e}^{\mathrm{j}\vartheta})$, $\mathrm{Im}\,\Phi_{12}(\mathrm{e}^{\mathrm{j}\vartheta})$ and $\Phi_{22}(\mathrm{e}^{\mathrm{j}\vartheta})$, respectively for the true spectrum and for the estimation of the latter based on one run of 100 samples. In Figure 5.4 we compare the performances of various spectral estimation methods in the following way. We consider four estimates $\hat{\Phi}_{\mathrm{H}}$, $\hat{\Phi}_{\mathrm{ME}}$, $\hat{\Phi}_{\mathrm{PEM}}$, and $\hat{\Phi}_{\mathrm{N4SID}}$ of Φ. The spectral density $\hat{\Phi}_{\mathrm{H}}$ is the estimate obtained by the procedure described above in Subsection 5.1. The spectral density $\hat{\Phi}_{\mathrm{ME}}$ is the maximum entropy estimate [27] obtained using the same $G(z)$ employed to obtain our estimate. The spectral densities $\hat{\Phi}_{\mathrm{PEM}}$ and $\hat{\Phi}_{\mathrm{N4SID}}$ are the estimates of Φ obtained by using "off-the-shelf" Matlab procedures for the Prediction Error Method (see i.e. [55] or [43]) and for the N4SID method (see [58] or [43]): The former is a multivariable extension of the classical approach to ARMAX identification, while the latter is a standard algorithm in the modern field of subspace identification. In order to obtain a comparison reasonably independent of the specific data set, we have performed 50 independent runs each with 100 samples of y. In such a way we have obtained 50 different estimates $\hat{\Phi}_{\mathrm{M},i}$, $\mathrm{M} = \mathrm{H}, \mathrm{ME}, \mathrm{PEM}, \mathrm{N4SID}$, $i = 1, 2, \ldots, 50$, for each method.

We have then defined

$$E_{\mathrm{H}}(\vartheta) := \frac{1}{50} \sum_{i=1}^{50} \|\hat{\Phi}_{\mathrm{H},i}(\mathrm{e}^{j\vartheta}) - \Phi(\mathrm{e}^{j\vartheta})\|, \tag{5.2}$$

where $\|\cdot\|$ denotes the spectral norm. This is understood as the average estimation error of our method at each frequency. Similarly, we have defined the average errors $E_{\mathrm{ME}}(\vartheta)$, $E_{\mathrm{PEM}}(\vartheta)$, and $E_{\mathrm{N4SID}}(\vartheta)$ of the other methods. In the each of the plots

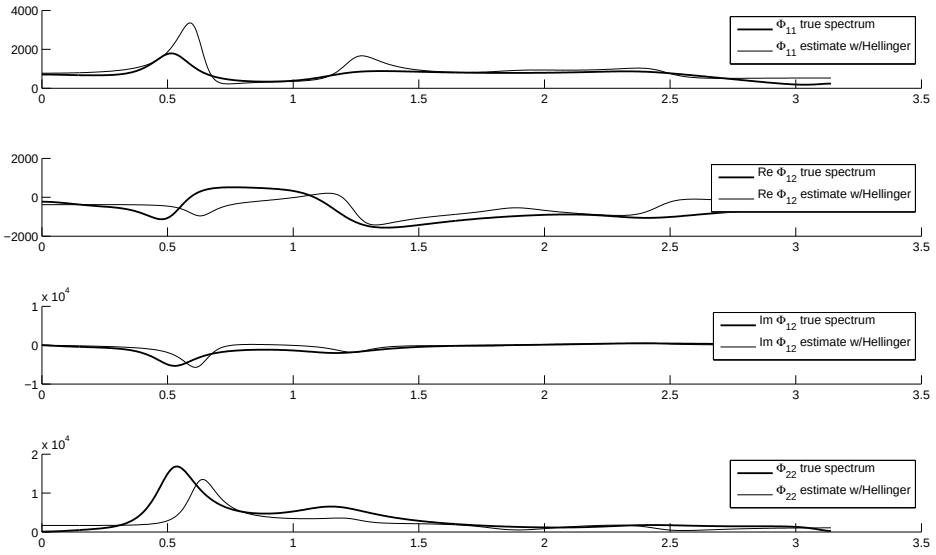

Figure 5.3: Estimation of the spectrum of a bivariate process with rich dynamics by means of Hellinger-distance spectrum approximation, constant prior.

of Figure 5.4, we depict the average error of our method $E_{\mathrm{H}}(\vartheta)$ together with the average error of one of the other methods. More explicitly, the first diagram shows the error for the Hellinger approximation method and for the maximum entropy spectrum described in [27]. The second diagram shows the error for the Hellinger approximation and for the spectrum obtained via MATLAB's PEM identification method. The third diagram shows the same for Hellinger approximation and MATLAB's N4SID method. The Hellinger approximation based approach appears to perform better or much better than the other methods. The simulation yields similar results with $N = 200$ data points. With $N = 300$ data samples, PEM and N4SID perform as well as our method.

Of course, one should always take into account the complexity of the resulting spectrum. In this example, $G(z)$ being of order 9, the resulting spectral factor (or "model") produced by the Hellinger approximation has order 18, whereas the corresponding maximum entropy model has order 9 and both N4SID and PEM usually choose order 10.

In our simulation, the norm of the difference of two estimates produced by PEM or by N4SID is sometimes very large when compared to the norm of the difference between any two of the estimates produced by our method. That is, although PEM and N4SID are provably consistent as $N \to \infty$, when few data are available both of them may introduce occasional artifacts, which are well visible as "peaks" in figure

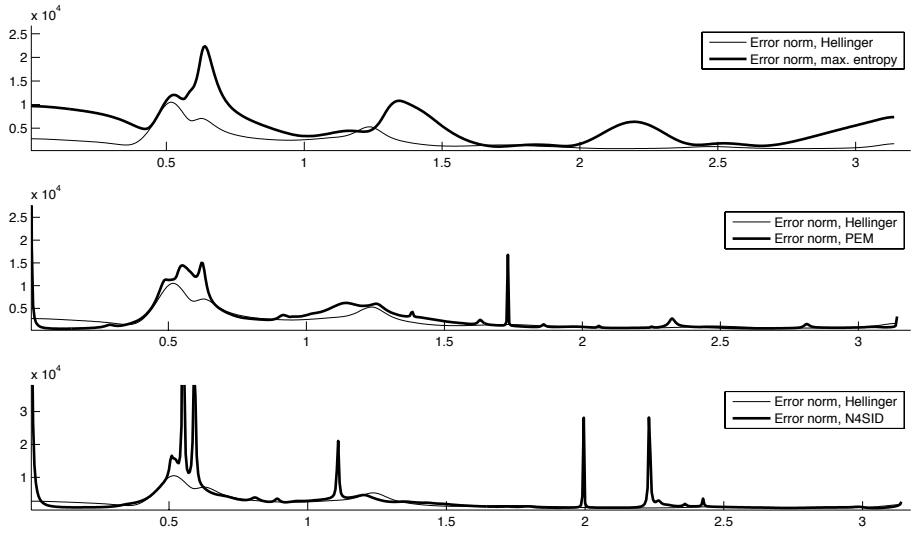

Figure 5.4: Estimation of the spectrum of a bivariate process with rich dynamics by means of various methods. Comparison between the spectral norm of the differences $\hat{\Phi}_{\mathrm{H}} - \Phi$, $\hat{\Phi}_{\mathrm{ME}} - \Phi$, $\hat{\Phi}_{\mathrm{PEM}} - \Phi$, and $\hat{\Phi}_{\mathrm{N4SID}} - \Phi$ (average over 50 simulations).

5.4 (a "peak" in the 50-run average is due to a very high error in one of the runs, not to a systematic error). Our method appears to be more robust in this respect.

Appendix A

Proofs of some technical lemmas

Lemma A.0.1 *Let $H \in \mathcal{H}(n)$ and m be its minimum eigenvalue. The map $H \mapsto m$ is continuous.*

Proof. The map from a matrix H to the vector of coefficients of its characteristic polynomial $a(s) = \det(sI - H) = a_0 + ... + a_{n-1}s^{n-1} + s^n$ is continuous. Indeed, each of the coefficients of $a(s)$ is obtained by means of sums and products of elements of H. Moreover, it is a well-known fact (see for example [45]) that the mapping from the coefficients of a monic polynomial to its roots is continuous, in the following sense: Given $a(s) = s^n + \sum_{i=0}^{n-1} a_i s^i$, let λ_i be the zeros of $a(s)$ and ν_i the respective multiplicities. For all $\varepsilon > 0$, there exists $\delta > 0$ such that if $b(s) = s^n + \sum_{i=0}^{n-1} b_i s^i$ and $|b_i - a_i| < \delta$ for all $i = 0, 1, \ldots, n-1$, then $b(s)$ has ν_i zeros in the ball centered in λ_i with radius ε. In conclusion, if H is Hermitian, the mapping from H to its minimum (real) eigenvalue is continuous. ∎

Lemma A.0.2 *Let A be a stability matrix and $H(z) = C(zI - A)^{-1}B + D$ be a minimal realization. Let P be the solution of the Lyapunov equation*

$$P - A^*PA = C^*C. \tag{A.1}$$

Let $\begin{bmatrix} K \\ J \end{bmatrix}$ *be an ortho-normal basis of* $\ker \begin{bmatrix} A^*P^{1/2} & C^* \end{bmatrix}$ *i.e.*

$$\begin{bmatrix} A^*P^{1/2} & C^* \end{bmatrix} \begin{bmatrix} K \\ J \end{bmatrix} = 0, \qquad \begin{bmatrix} K^* & J^* \end{bmatrix} i \begin{bmatrix} K \\ J \end{bmatrix} = I. \tag{A.2}$$

Let $G := P^{-1/2}K$ and

$$H_1(z) := (D^*C + B^*PA)(zI - A)^{-1}G + B^*PG + D^*J. \tag{A.3}$$

Then, $H^*H = H_1H_1^*$.

Proof. Let $Q := C(zI - A)^{-1}G + J$. We first show that $QQ^* = I$, so that Q is inner. We then prove that $Q^*H = H_1^*$, concluding the proof. We have

$$\begin{aligned} Q^*Q = {} & G^*(z^{-1}I - A^*)^{-1}C^*C(zI - A)^{-1}G + \\ & + G^*(z^{-1}I - A^*)^{-1}C^*J + J^*C(zI - A)^{-1}G + J^*J \end{aligned} \tag{A.4}$$

Now let $P > 0$ be the solution of the Lyapunov equation (A.1). Then,

$$\begin{aligned} C^*C = {} & -(z^{-1}I - A^*)P(zI - A) + \\ & + (z^{-1}I - A^*)Pz + z^{-1}P(zI - A) \end{aligned} \tag{A.5}$$

Substituting (A.5) into (A.4) we obtain

$$\begin{aligned} Q^*Q = {} & -G^*PG + G^*Pz(zI - A)^{-1}G + \\ & + G^*(z^{-1}I - A^*)^{-1}z^{-1}PG + \\ & + G^*(z^{-1}I - A^*)^{-1}C^*J + J^*C(zI - A)^{-1}G + J^*J \end{aligned} \tag{A.6}$$

Moreover,

$$\begin{aligned} & z(zI - A)^{-1} = I + A(zI - A)^{-1} \quad \text{and} \\ & (z^{-1}I - A^*)^{-1}z^{-1} = I + (z^{-1}I - A^*)^{-1}A^* \end{aligned} \tag{A.7}$$

so that

$$\begin{aligned} Q^*Q = {} & (J^*C + G^*PA)(zI - A)^{-1}G + \\ & + \big((J^*C + G^*PA)(zI - A)^{-1}G\big)^* + G^*PG + J^*J \end{aligned} \tag{A.8}$$

Taking (A.2) into account, it is easy to see that $Q^*Q = I$. Therefore, $H^*H =$

H^*QQ^*H. Recalling (A.5) and (A.7), we eventually get

$$
\begin{aligned}
& Q^*H = \\
= \; & (G^*(z^{-1}I - A^*)^{-1}C^* + J^*)(C(zI - A)^{-1}B + D) \\
= \; & -G^*(z^{-1}I - A^*)^{-1}(z^{-1}I - A^*)P(zI - A)(zI - A)^{-1}B \\
& +G^*(z^{-1}I - A^*)^{-1}(z^{-1}I - A^*)Pz(zI - A)^{-1}B \\
& +G^*(z^{-1}I - A^*)^{-1}z^{-1}P(zI - A)(zI - A)^{-1}B \\
& +G^*(z^{-1}I - A^*)^{-1}C^*D + J^*C(zI - A)^{-1}B + J^*D \\
= \; & -G^*PB + G^*Pz(zI - A)^{-1}B \\
& +G^*(z^{-1}I - A^*)^{-1}z^{-1}PB \\
& +G^*(z^{-1}I - A^*)^{-1}C^*D + J^*C(zI - A)^{-1}B + J^*D \\
= \; & -G^*PB + G^*P\left(I + A(zI - A)^{-1}\right)B \\
& +G^*\left(I + (z^{-1}I - A^*)^{-1}A^*\right)PB \\
& +G^*(z^{-1}I - A^*)^{-1}C^*D + J^*C(zI - A)^{-1}B + J^*D \\
= \; & G^*PB + G^*PA(zI - A)^{-1}B \\
& +G^*(z^{-1}I - A^*)^{-1}A^*PB \\
& +G^*(z^{-1}I - A^*)^{-1}C^*D + J^*C(zI - A)^{-1}B + J^*D \\
= \; & G^*(z^{-1}I - A^*)^{-1}(C^*D + A^*PB) \\
& +(G^*PA + J^*C)(zI - A)^{-1}B + G^*PB + J^*D \\
= \; & G^*(z^{-1}I - A^*)^{-1}(C^*D + A^*PB) + G^*PB + J^*D \\
= \; & H_1^* \qquad\qquad (A.9)
\end{aligned}
$$

■

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