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Inner–outer factorization and the inversion of locally finite systems of equations

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Abstract

We consider the problem of computing the inverse of a large class of infinite systems of linear equations, which are described by a finite set of data. The class consists of equations in which the linear operator is represented by a discrete time-varying dynamical system whose local state space is of finite dimension at each time point k, and which reduces to time invariant systems for time points $k \to \pm\infty$. In this generalization of classical matrix inversion theory, inner–outer factorizations of operators play the role that QR-factorization plays in classical linear algebra. Numerically, they lead to so-called 'square root' implementations, for which attractive algorithms can be derived, which do not require the determination of spurious multiple eigenvalues, as would be the case if the problem was converted to a discrete time Riccati equation by squaring. We give an overview of the theory and the derivation of the main algorithms. The theory contains both the standard LTI case and the case of a finite set of linear equations as special instances, a particularly instance of which is called 'matrices of low Hankel rank', recently sometimes called 'quasi-separable matrices'. However, in the general case considered here, new phenomena occur which are not observed in these classical cases, namely the occurrence of 'defect spaces'. We describe these and give an algorithm to compute them as well. In all cases, the algorithms given are linear in the amount of data.

Keywords: Inner–outer factorization; URV decomposition; QR factorization; Square-root algorithm; Riccati equation; Lyapunov–Stein equation; System inversion; Time-varying systems; Quasi-separable matrices; Doubling algorithm

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1. Introduction

The problem of computing the inverse of an infinite system of linear equations can be tackled attractively with (low complexity) numerical methods if the parameters that describe the system satisfy certain broad finiteness constrains. A particularly interesting case is when the finite set of data consists of a 'state realization' of the system of equations akin to a state-space representation of a time-varying linear dynamical system.

Let the operator T represent a linear map mapping a (possibly infinite) sequence of vectors $u = [u_i]_{i=-\infty}^{\infty}$ to a (possibly infinite) sequence of vectors $y = [y_k]_{k=-\infty}^{\infty}$

$$y = uT.$$

Each u_i (y_k) is a vector belonging to a finite dimensional vector space of dimension m_i (respectively n_k). These dimensions may vary and even vanish, in which case the entry simply disappears, it is replaced by a 'placeholder' ('$\cdot$' – with the convention that the product of a matrix of dimensions $m \times 0$ with one of dimensions $0 \times n$ is a matrix of dimensions $m \times n$ consisting of zeros). This formalism has the advantage that it includes finite systems of linear equations, but also regular linear time invariant systems as special cases. T has a matrix representation $T = [T_{i,k}]$ with $T_{i,k}$ a matrix of dimension $m_i \times n_k$. If all input entries $u_\ell = 0$ except u_i, then the output y is such that $y_k = u_i T_{i,k}$. In the sequel we shall assume that T is bounded as an operator on ℓ_2 sequences, i.e. that

$$\|T\| = \sup_{\|u\|_2=1} \|uT\|_2 < \infty$$

for $\|u\|_2 = \sqrt{\sum_{i=-\infty}^{\infty} \|u_i\|_2^2}$ with $\|u_i\|_2$ the standard Euclidean norm (and for y likewise). We assume furthermore that T is locally finite, that is, it possesses a time-varying state-space representation. If T is block-upper triangular (i.e. if $T_{i,k} = 0$ for $i > k$), then that means that there exist matrices $\{A_k, B_k, C_k, D_k\}$ for each k, such that

$$\begin{aligned} T_{k,k} &= D_k, \\ T_{i,k} &= B_i A_{i+1} \cdots A_{k-1} C_k \quad (\text{for } i < k). \end{aligned}$$

Underlying this representation, there is a time-varying 'system realization' that produces the operator T via the 'local' state equations:

$$\begin{aligned} x_{k+1} &= x_k A_k + u_k B_k, \\ y_k &= x_k C_k + u_k D_k. \end{aligned}$$

The dimensions of all the matrices in the realization must of course be compatible. If $[b_k]$ is the sequence of dimensions of the x_k's (the state), then the dimensions of A_k, B_k, C_k, and D_k are respectively $b_k \times b_{k+1}$, $m_k \times b_{k+1}$, $b_k \times n_k$ and $m_k \times n_k$. We shall also assume that the realization for T is uniformly exponentially stable (ues) in the classical sense for linear time varying systems, i.e. that there are uniform bounds

on the norms of the matrices A_k, B_k, C_k and D_k, and that there exists a real number ρ with $0 \leqslant \rho < 1$ such that, also uniformly over k,

$$\limsup_{\ell\to\infty} \|A_{k+1}\cdots A_\ell\| \leqslant \rho^{\ell-k}.$$

These conditions make T automatically a bounded operator on ℓ_2 sequences.

In the case that T has both upper and lower parts, we shall assume that also its lower part has a ues realization, i.e. there exist matrices $\{A'_k, B'_k, C'_k\}$ such that for $i > k$,

$$T_{i,k} = B'_i A'_{i-1}\cdots A'_{k+1}C'_k,$$

corresponding to a (backward) realization

$$\begin{aligned} x'_{k-1} &= x'_k A'_k + u'_k B'_k, \\ y'_k &= x'_k C'_k \end{aligned}$$

and satisfying the boundedness requirements for ues.

It is notationally convenient to collect the local realization operators in global 'diagonal' operators. Connected to the series $[A_k]$ we define the operator A as

$$A = \begin{bmatrix} \ddots & & & & \\ & A_{-1} & & & \\ & & \boxed{A_0} & & \\ & & & A_1 & \\ & & & & \ddots \end{bmatrix},$$

in which we distinguish the $(0,0)$th element by boxing it. Likewise for B, C and D. If, moreover, we introduce the 'causal shift' Z by the rule $[\cdots, u_{-1}, \boxed{u_0}, u_1, \cdots]Z = [\cdots, \boxed{u_{-1}}, u_0, u_1, \cdots]$ and by Z^* the inverse, backward shift, then T will have the representation

$$T = B'Z^*(I - A'Z^*)^{-1}C' + D + BZ(I - AZ)^{-1}C \tag{1}$$

in terms of its realization. The property of uniform exponential stability assures the existence of the inverse of $I - AZ$ as an upper operator and $I - A'Z^*$ as a lower operator.

In this paper, we assume that a system representation is given. The algorithms will also lead to system representations. It is rather easy to find a realization for T, either from the structure of the problem that leads to T itself, from standard realization theory or from approximating the operator with a low complexity realization, minimizing a Hankel norm doing so. We refer to the recently published book [12] for extensive information and examples. Very attractive cases are structured matrices, e.g. banded matrices, their inverses, Toeplitz matrices, matrices that are 'close to Toeplitz', products and sums of those. In this paper, we shall especially be interested in the inversion of systems for which the representation for T becomes LTI for $k \to \pm\infty$. In that case,

T is represented by a finite amount of data, although it is an operator on spaces with infinite dimensions. There are other cases, e.g. when the variation for $k \to \pm\infty$ is of the 'low-displacement type', but those are beyond the present paper. Although we shall not make specific provisions for the case where the system is periodic at its extremities, that case is covered in principle by the theory presented, since a periodic system can be converted to an LTI-system, by concatenating a complete period, or, if possible, by applying a Fréchet transformation (practically speaking, however, a lot of additional mileage can be obtained from the periodicity [6,20]).

The method that we present has some kinship with the classical '*QR*-factorization' method for matrices, in which Q is an orthogonal or unitary matrix, and R is an upper matrix with some special invertibility properties. The (non-finite) substitute of a unitary matrix in our theory is called an *inner* operator. Isometric and co-isometric operators will play an important role as well. If T is an operator, then its adjoint T^* is defined e.g. via the property $[T^*]_{i,k} = T^*_{k,i}$, in which the latter is the usual hermitian conjugate of a matrix. The operator U is isometric if $UU^* = I$ and co-isometric if $U^*U = I$ (that is for application to operands at the left side of the operator indicated by '$\cdot U$'). It is *inner* if it is upper, isometric *and* co-isometric. An inner operator which is ues and locally finite has a unitary state realization, i.e. a state realization for which the transition matrices

$$\begin{bmatrix} A_k & C_k \\ B_k & D_k \end{bmatrix}$$

are themselves unitary. The converse is also true, namely that a ues unitary realization represents an inner matrix. The qualification 'ues' in the statement is important: a realization which is unitary but not ues does *not necessarily* lead to an inner operator due to the probable existence of a defect space, see the discussion and the computation of the defect space in Section 5.

Equivalence. Two upper realizations $\{A_k, B_k, C_k, D_k\}$ and $\{\hat{A}_k, \hat{B}_k, \hat{C}_k, \hat{D}_k\}$ are *strictly or Lyapunov equivalent* if there exists a uniformly bounded sequence of invertible square matrices $\{R_k\}$ such that the $\{R_k^{-1}\}$ are uniformly bounded as well, and such that $\hat{A}_k = R_k^{-1} A_k R_{k+1}$, $\hat{B}_k = B_k R_{k+1}$, $\hat{C}_k = R_k^{-1} C_k$ and $\hat{D}_k = D_k$ (the collection of $\{R_k\}$'s is called a Lyapunov state transformation). In other words, an equivalent realization is given by the quadruple

$$\begin{bmatrix} R_k^{-1} A_k R_{k+1} & R_k^{-1} C_k \\ B_k R_{k+1} & D_k \end{bmatrix}.$$

A realization is minimal if the dimension of all A_k's is as small as possible. Minimal realizations can always be found through either a minimal realization procedure, or a reduction of an existing one [12]. A realization is in *input normal form* if all the pairs $\left[\begin{smallmatrix} A_k \\ B_k \end{smallmatrix}\right]$ are co-isometric. It is in *output normal form* if all the pairs $[A_k \; C_k]$ are isometric. It is an interesting question, in general, whether a given realization can be brought to input, respectively, output normal form through a strict equivalency. If

one starts out from a ues realization $\{A, B, C, D\}$, then the answer is as follows. Let $\{M_k\}$ be the bounded solution of the collection of Lyapunov–Stein equations

$$M_{k+1} = A_k^* M_k A_k + B_k^* B_k.$$

The classical Lyapunov–Stein theorem states that these equations will indeed have a unique bounded solution given by the (fixed point) series expansion

$$M_k = \sum_{i=1}^{\infty} \left(A_{k-1}^* \cdots A_{k-i+1}^* B_{k-i}^* B_{k-i} A_{k-i+1} \cdots A_{k-1} \right),$$

when the collection $\{A_k\}$ is ues (there may be many unbounded solutions but those are not interesting in the present context). The bounded solution will of course be positive semidefinite as can be seen from the series expansion. If the solution is actually uniformly positive definite, i.e. if there exists a positive ϵ so that for all k, $M_k > \epsilon I$, then we call the system *strictly reachable* and an adequate set of state transformation matrices $\{R_k\}$ can be derived from $M_k = R_k^{-*} R_k^{-1}$. The corresponding strictly equivalent realization $\{\hat{A}_k, \hat{B}_k, \hat{C}_k, \hat{D}_k\}$ will be both ues and in input normal form. The M_k obtained in the procedure have an important physical interpretation, they form the Gramians of the reachability operators at each time point, of the system under consideration. The case for the output normal form is dual: the observability Gramians are given by the backward equations:

$$N_{k-1} = A_k N_k A_k^* + C_k C_k^*.$$

If the $\{N_k\}$ form a strict transformation, then the system is *strictly observable* and the resulting state transformation to bring the system in output normal form is defined by $N_k = R_{k+1} R_{k+1}^*$.

The case for the lower part is similar, the state transformation then is given by

$$\begin{bmatrix} \hat{A}_k' & \hat{C}_k' \\ \hat{B}_k' & 0 \end{bmatrix} = \begin{bmatrix} R_k^{-1} A' R_{k+1} & R_k^{-1} C' \\ B_k' R_{k+1} & 0 \end{bmatrix}$$

and the transformation to input and output normal form are similar as before, mutatis mutandis.

The solution method. Starting out from an operator given in the form of (1), we wish to compute the inverse T^{-1} of T, or, if T is not invertible, its Moore–Penrose pseudoinverse, $T^\dagger$, which gives the minimal norm solution for $\inf_{u \in \ell_2} \|y - uT\|_2$ as $u = yT^\dagger$. Our method consists in the following steps:

1. First we convert the general (upper–lower) operator to the upper form, using a minimal inner operator U chosen such that UT is upper. This will convert (1) to the form

$$T = D + BZ(I - AZ)^{-1}C, \tag{2}$$

in which the realization is minimal, and T is bounded. This step is equivalent to the classical QR-factorization step.

2. T in the form (2) is not necessarily upper invertible or does not necessarily have an upper Moore–Penrose pseudoinverse—this provides for the added interest of the

inversion problem considered here. The next, and central part of the strategy then consists in a system theoretical equivalent of the *URV*-factorization of numerical linear algebra. We shall show how T can be factored as $T = V_\ell T_o V_r$, in which V_ℓ is co-isometric ($V_\ell^* V_\ell = I$), V_r is isometric ($V_r V_r^* = I$) and T_o is 'outer', i.e. it is causally invertible in a sense to be made precise (although T_o will be well defined, it will not necessarily be boundedly invertible, but it will be invertible in a weaker sense—see Section 7 on the relation between 'outerness' and 'invertibility'). The Moore–Penrose pseudo-inverse for T then follows as

$$T^\dagger = V_r^* T_o^{-1} V_\ell^*$$

and it will satisfy the minimality requirement for the same reason as in the algebraic case (we have: $\|y - uT\|_2^2 = \|y - uV_\ell T_o V_r\|_2^2 = \|y(I - V_r^* V_r) + (yV_r^* - uV_\ell T_o)V_r\|_2^2 = \|y(I - V_r^* V_r)\|_2^2 + \|(yV_r^* - uV_\ell T_o)V_r\|_2^2$. The first term cannot be influenced by u, while the second will be zero if $u = yV_r^* T_o^{-1} V_\ell^*$ whenever defined, i.e. on a dense subset. Minimality of this u is easily established). The procedure goes in two sub-steps. First we compute a so-called left outer–inner factorization of T: $T = T_{o\ell} V_r$, in which V_r is causal isometric (hence not necessarily inner), and $T_{o\ell}$ is left invertible, there is an acceptable causal operator T'_ℓ such that $T'_\ell T_{o\ell} = I$ (as already mentioned before, it may occur that $T_{o\ell}$ does not have a bounded causal left inverse, but only one that can be approximated with a sequence of bounded operators, but that is inherent to the situation). It turns out that $T_{o\ell}$ is IVI when T is—this follows immediately from its state-space realization which we derive further on. Next, we factor, in a dual way: $T_{o\ell} = V_\ell T_o$ to yield the desired overall factorization. We shall derive state-space realizations for the factors. The state-space realizations for the inverses then follow immediately. V_r^* and V_ℓ^* are anticausal and have realizations which are the Hermitian conjugates of those for V_r and V_ℓ, respectively, while for T_o^{-1} it is given in terms of the realization $\{A_{ok}, B_{ok}, C_{ok}, D_{ok}\}$ of T_o as $\{A_{ok} - C_{ok} D_{ok}^{-1} B_{ok}, -D_{ok}^{-1} B_{ok}, C_{ok} D_{ok}^{-1}, D_{ok}^{-1}\}$, in which D_{ok} is invertible because of the outerness assumption. In other words, the state complexity of the inverse is of the same order as the state complexity of the original.

3. However, there is more. As in the classical case, we may want to extend the operators V_ℓ and V_r so that they become unitary, and (try to) construct the 'row-nullspace' and the 'column-nullspace' for T. In doing so, we shall encounter new phenomena. In contrast to the classical algebraic case, the operators V_ℓ and V_r may be such that they cannot be extended to causal unitary operators, although their realizations can indeed be extended to unitary. When that happens, there is an additional nullspace which we call a 'defect space'. We shall show how a basis for it can be computed, yielding a complete solution to the inversion problem.

Minimal state-space realizations for the operators encountered are advantageous, not only because they allow us to find inverses of systems with an infinite number of equations using a finite number of computations, but also because they are economical, even for finite systems of equations, when the dimension of the state-space is small. Calculations on finite matrices form a special simplified case of the theory

presented here. When such matrices have scalar entries (which is not necessary for the theory to go through) and can be represented by a low order model, say maximized by b, then matrix–vector multiplication becomes of $O(nb)$ (if n is the dimension of the matrix), while inversion goes with a complexity of at most $O(nb^2)$, although this figure can be reduced if a proper representation of the original system is choosen. The idea of using time varying system theory for the purpose of manipulating matrices is probably due to the work of the authors in the late 1980s, in conjunction with Alpay and Dym, as exemplified in the papers [1,2,11,13,14,31–34]. A comprehensive treatment is the subject of the thesis [29]. Of course, there were forerunners. We mention the extension theory for general positive definite band matrices based on a generalization of the Levinson and Schur algorithms to the time-varying case [7,8,15] and the treatment of a (restricted) class of matrices that decompose in a sum of a diagonal matrix, an upper and a lower matrix whose rows are partial multiples of each other called 'semiseparable matrices' by the authors [17]. However, these publications do not use the general time-varying state-space model for matrices. The first publication to do so seems to be [14], which solves the minimal Hankel norm approximation problem for general matrices. The first comprehensive publication settling the inversion problem for time-varying systems and matrices described by a time-varying state-space formalism seems to be [30], whose method we adopt and extend here. Recently, in [16] a new term 'quasiseparable matrices' was introduced to indicate matrices whose lower and upper parts admit representations as time-varying systems. This class of matrices is of course identical to the class of 'matrices with low Hankel rank' considered in [12,34], and the references given earlier. The authors of [16] give some invertibility theorems for a sub-class of such matrices based on determinantal theory. They follow another approach than the URV approach we follow here, and which has an interest in its own right, but whose scope is more restricted.

As announced, we concentrate our efforts on the inversion of systems which become LTI for $k \to \pm\infty$, a case which we shall call 'the IVI case' (a special instant of which are just finite matrices). If there is indeed a non-trivial LTI part at $\pm\infty$, then it will turn out that we must find the inner–outer factorization of an LTI-system in state-space form. During the redaction of this paper it was brought to our attention that the inner–outer factorization of rational LTI systems was recently considered by Oară and Varga [26]. These authors use a method based on the determination of eigenvalues of a related pencil characteristic for the zeros of the system, followed by a regular spectral factorization of a reduced system via the solution of a regular Riccati equation. They face the problem of the removal of boundary zeros which they address by what they call 'a recently developed technique of pole dislocation'. The procedure presented by these authors parallels to a certain extent the presentation in this paper, although it does not make use of the square root form. Although their approach seems to yield good results, it strikes us as unnecessarily complex (we believe that too many dislocations are performed, which must have a negative effect on the overall performance).

In the present paper, we endeavour to present direct inner–outer factorization algorithms based on the square-root equation which results directly from the translation of the inner–outer factorization to state-space terms. As in the pencil approach, we are forced to consider a number of cases. There is a dichotomy between cases which lead to a restricted eigenvalue problem (Cases I and II), and cases which lead to a completion problem (Cases III and IV). It turns out that in the first two cases only a simple direct eigenvalue problem needs to be solved, no conversion to a spectral factorization is needed at all. In Cases III and IV we are also forced to consider possible zeros on the boundary separately, but we believe that we can do that in an elementary, classical way (pole and zero dislocation techniques were developed in the 1960s and must by now be considered as standard system theoretical techniques—we give the basic algorithm in appendix). Once the dislocation of zeros on the boundary is done, a regular reduced spectral factorization problem remains, which can be solved in a classical way. But here also, the square root equation yields an attractive alternative and just as classical route. It results in a doubling algorithm which is capable of quick convergence. This method is well known from Kalman filtering theory and has been pioneered by Kailath and his students, we reproduce it here for the sake of completeness (see the references further on in the text).

All in all, it turns out that inner–outer factorization can indeed be solved generally, for LTI and IVI cases, using attractive, stable and elementary algorithms, which need no recourse to potentially ill-conditioned eigenvalue determination on the Hamiltonian matrix.

2. From general to upper operator

The first step in the algorithmic treatment of the general operator T is the conversion of its lower part to upper. The goal is to compute an inner operator U so that UT is upper. We summarize the basic result from [12].

Theorem 1. *Suppose that T has the realization* (1) *and that the pair $\{A', B'\}$ is strictly reachable, then there exist inner operators U such that UT is upper. A U with minimal state dimension has a realization given by*

$$\begin{bmatrix} [R_k^{-1} A'_k R_{k+1}]^* & [B'_k R_{k+1}]^* \\ C'^*_{uk} & D'^*_{uk} \end{bmatrix},$$

in which $M_k = R_k^{-*} R_k^{-1}$, $\{M_k\}$ is the solution of the collection of Lyapunov–Stein equations

$$M_{k-1} = A'^*_k M_k A'_k + B'^*_k B'_k$$

and C'_{uk} and D'_{uk} are matrices derived from the isometries $[[R_k^{-1} A'_k R_{k+1}]^* \ [B'_k R_{k+1}]^*]$ by an orthogonal completion procedure which makes the completed matrix at stage k unitary.

The derivation of the upper form is easy and goes as follows. An equivalent, non-unitary realization for U is

$$\begin{bmatrix} A'^*_k & B'^*_k \\ C'^*_{uk} R^*_k & D'^*_{uk} \end{bmatrix}.$$

If we compute UT by brute force (dropping the indices k for ease of computation), and utilize the identity

$$\begin{aligned}(I - ZA'^*)^{-1} ZB'^* B' Z^* (I - A'Z^*)^{-1} C' \\ = (I - ZA'^*)^{-1} M + M(I - A'Z^*)^{-1} A'Z^*\end{aligned}$$

with M defined above, we obtain

$$\begin{aligned}UT &= [D'^*_u + C'^*_u R^* Z(I - A'^* Z)^{-1} B'^*] \cdot [B'(I - Z^* A')^{-1} Z^* C' \\ &\quad + D + BZ(I - AZ)^{-1} C] \\ &= C'^*_u R^{-1} C' + D'^*_u D + C'^*_u R^* Z(I - A'^* Z)^{-1} [A'^* M C' + B'^* D] \\ &\quad + D'^*_u BZ(I - AZ)^{-1} C + C'^*_u R^* Z(I - A'^* Z)^{-1} B'^* BZ(I - AZ)^{-1} C.\end{aligned}$$

This transfer operator expression corresponds to the realization:

$$\begin{bmatrix} \hat{A} & \hat{C} \\ \hat{B} & \hat{D} \end{bmatrix} \triangleq \left[\begin{array}{cc|c} A'^* & B'^* B & A'^* M C' + B'^* D \\ 0 & A & C \\ \hline C'_u R^* & D'^*_u B & C'^*_u R^{-1} C' + D'^*_u R \end{array}\right].$$

The Lyapunov–Stein equation has the appearance of a recursive equation. However, if the system is locally LTI (e.g. for $k \to \pm\infty$), then the equation can be made non-recursive, and the time invariant or 'algebraic' solution, in which $M_{k-1} = M_k$ should be used. It is worth observing that the property 'the system is LTI for $k \to \pm\infty$' is preserved under the transformation $T \mapsto UT$. This case we shall call 'the IVI case' henceforth. We see also that all the calculations are purely local, in the case of finite matrices with scalar entries, the upper form can be computed in at most $O(nb^2)$ calculations, where n is the dimension of the matrix and b an upper bound on the size of the state space. If care is exercised to make the realizations algebraically minimal (see [12, Chapter 14]), then the complexity can be reduced to $O(nb)$.

The strict reachability assumption can always be satisfied in the IVI case. To see that, it suffices to choose a minimal realization at each time point. The reachability operator will then automatically be strictly positive definite, because $\lim_{k\to\infty} M_k$ becomes a square non-singular matrix and likewise for (the different) $\lim_{k\to-\infty} M_k$. As a global operator, M will then be boundedly invertible, since the inverse is given by a diagonal matrix consisting of the local inverses $\{M_k^{-1}\}$ and hence will be bounded.

3. Outer–inner factorization

The computation of the left-inner–outer factorization. We are now given T upper in minimal state-space form (2). We wish to find $T_{o\ell}$ and V such that $T = T_{o\ell}V$, V is upper isometric and $T_{o\ell}$ is left outer. The basis for the algorithm is given by the following theorem.

Theorem 2. *Let, for each k, W_k be a unitary matrix, and Y_k a uniformly bounded sequence of matrices which satisfy the following equalities* (*for all k*):

$$\begin{bmatrix} A_k Y_{k+1} & C_k \\ B_k Y_{k+1} & D_k \end{bmatrix} = \begin{bmatrix} 0 & Y_k & C_{ok} \\ 0 & 0 & D_{ok} \end{bmatrix} W_k, \tag{3}$$

and which are such that
(1) *Y_k is such that* $\ker(Y_k \cdot) = 0$ *and has maximal dimension, and*
(2) $\ker(D_{ok}\cdot) = 0$.
Let

$$W_k = \begin{bmatrix} B_{Uk} & D_{Uk} \\ A_{Vk} & C_{Vk} \\ B_{Vk} & D_{Vk} \end{bmatrix}$$

be a conformal decomposition of W_k. Then $\{A_{Vk}, B_{Vk}, C_{Vk}, D_{Vk}\}$ is an isometric realization for V, $\{A_k, B_k, C_{ok}, D_{ok}\}$ is a realization for $T_{o\ell}$ and $\{A_{Vk}, B_{Vk}, C_{Uk}, D_{Uk}\}$ is a realization for a (*maximal*) *causal isometric operator for which $TU^* = 0$.*

Proof (*Sketch*). The proof of the theorem is given in [12]. It is based on the Beurling–Lax theorem (first proven in this context in [29]) and a system theoretical interpretation of the operator $Y = \mathrm{diag}[Y_k]$ in terms of bases for the observability spaces of T and V. If $(I - A_V Z)$is invertible, then Eq. (3) can easily be obtained from a state-space expansion of $T_o = TV^*$:

$$\begin{aligned} &D_o + BZ(I - AZ)^{-1}C_o \\ &\quad = [D + BZ(I - AZ)^{-1}C][D_V^* + C_V^*(I - Z^*A_V^*)^{-1}Z^*B_V^*] \end{aligned} \tag{4}$$

and the application of the following basic mixed partial factorization lemma.

Lemma 1. *Suppose that U is a unitary operator, and A_1 and A_2 are contractive operators such that the spectral radius of either A_1U or A_2U (or both) is less than* 1, *$(I - A_1U)$ and $(I - A_2U)$ are boundedly invertible. Let Γ be an otherwise arbitrary operator of appropriate dimensions. Then*

$$\begin{aligned} &(I - A_1U)^{-1}\Gamma(I - U^*A_2^*)^{-1} \\ &\quad = (I - A_1U)^{-1}M - M + M(I - U^*A_2^*)^{-1} \\ &\quad = (I - A_1U)^{-1}A_1UM + M + MU^*A_2^*(I - U^*A_2^*)^{-1}, \end{aligned} \tag{5}$$

in which M is the unique bounded solution of the (*generalized*) *Lyapunov–Stein equation*

$$M - A_1 U M U^* A_2^* = \Gamma. \tag{6}$$

The proof of the lemma is immediate, by pre- and post-multiplication with the invertible operators $(I - A_1 U)$ and $(I - U^* A_2^*)$. A closed form expression for M is given by the converging summation

$$M = \sum_{k=0}^{\infty} (A_1 U)^k \Gamma (U^* A_2^*)^k.$$

Expansion of the quadratic term in (4) and equating members leads to

$$\begin{bmatrix} A_k Y_{k+1} & C_k \\ B_k Y_{k+1} & D_k \end{bmatrix} \begin{bmatrix} A_{V_k}^* & B_{V_k}^* \\ C_{V_k}^* & D_{V_k}^* \end{bmatrix} = \begin{bmatrix} 0 & Y_k & C_{ok} \\ 0 & 0 & D_{ok} \end{bmatrix}.$$

Completion of the second factor to unitary and inversion produces (3). The diagonal matrix Y satisfies the Lyapunov–Stein equation

$$Y_k = C_k C_{V_k}^* + A_k Y_{k+1} A_{V_k}^*.$$

The proof of the theorem proceeds by showing that (3) is indeed solvable and produces a bounded $Y = \mathrm{diag} Y_k$, and that the kernel and maximality requirements on Y and D_o indeed produce an outer factor T_o. □

Eq. (3) indeed gives an algorithm which is capable to compute W_k, Y_k, C_{ok} and D_{ok} from the knowledge of Y_{k+1} and the original system matrices $\{A_k, B_k, C_k, D_k\}$. In fact, W_k is a generalized (unitary) Jacobi transformation which brings

$$\begin{bmatrix} A_k Y_{k+1} & C_k \\ B_k Y_{k+1} & D_k \end{bmatrix}$$

to block upper echelon form, taking care of trivial zero columns in the process. For self-containment of this paper the elementary algorithm is given in Appendix B. It assumes that for some large, positive value of k, Y_{k+1} is known. This will be the case if the system is LTI for large k, but other instances are conceivable, e.g. the system is of finite displacement rank, or it is almost periodic for large k. These instances are quite interesting but beyond the scope of this paper.

Eq. (3) can be squared to eliminate W_k by right multiplication with its complex conjugate, and this leads to a recursive Riccati equation in $M_k \triangleq Y_k Y_k^*$ (the connection of inner–outer factorization and Riccati equations is classical, see e.g. [3], for treatments of the time-varying case, see [18,29]),

$$\begin{aligned} M_k = {} & A_k M_{k+1} A_k^* + C_k C_k^* \\ & - [A_k M_{k+1} B_k^* + C_k D_k^*](D_k D_k^* + B_k M_{k+1} B_k^*)^\dagger \\ & \times [D_k C_k^* + B_k M_{k+1} A_k^*]. \end{aligned} \tag{7}$$

One may be tempted to solve the Riccati equation to solve the outer–inner factorization problem, but that leads to great difficulties as is amply documented in the literature [22]. It is already not advisable numerically to square an equation to solve it, and the discrete time Riccati equation has some nasty properties in addition. We shall thus endeavour to solve what we shall henceforth call the 'square root equations' (following the terminology of [24]). We do it for the time invariant case in the next section, and then generalize to the case where the system is only LTI for $k \to \pm\infty$. In the latter case, the LTI theory form the essential starting point.

The kernel conditions mentioned in the theorem are necessary for the following reasons:

(1) The maximality condition on Y_k only makes sense if at the same time one requires that $\ker(Y_k \cdot) = 0$. In that case the column dimension of Y_k corresponds to the dimension of a minimal realization for V. In fact, Y so defined has a nice interpretation as the 'angle operator' between the observability spaces of V and T, see [12] for further details. Interestingly enough, this dimension can have a value ranging from zero to the dimension of the state space of T. When it is zero, Y_k just disappears.

(2) The kernel condition on D_{ok} is certainly necessary, $T_{o\ell}$ could not possibly be left-outer if any D_{ok} would not have a left inverse. That the condition is also sufficient is the subject matter of the theorem.

4. Outer–inner factorization in the LTI-case

Now we turn to the algebraic, i.e. non-recursive or fixed point version of the square root equation (3), to be used for the LTI left-outer–inner factorization $T(z) = T_{o\ell}(z)v(z)$, in which $T_{o\ell}(z)$is left-outer and $v(z)$ causal isometric. Let $\{A, B, C, D\}$ be a minimal realization for $T(z)$. Then one has to solve the algebraic (i.e. non-recursive or fixed point) version of (3), i.e. the set of equations

$$\begin{bmatrix} A & C \\ B & D \end{bmatrix} \begin{bmatrix} Y & \\ & I \end{bmatrix} = \begin{bmatrix} 0 & Y & C_o \\ 0 & 0 & D_o \end{bmatrix} W \tag{8}$$

for a Y of maximal dimension such that $\ker(Y \cdot) = 0$, a D_o such that $\ker(D_0 \cdot) = 0$ and a W that is unitary, in fact

$$W = \begin{bmatrix} B_u & D_u \\ A_v & C_v \\ B_v & D_v \end{bmatrix}$$

is such that $\{A_v, B_v, C_v, D_v\}$ defines an isometric realization of $v(z)$, while $\{A_v, B_u, C_v, D_u\}$ defines an isometric realization for $u(z)$, which is such that

$$\begin{bmatrix} v(z) \\ u(z) \end{bmatrix}$$

is inner, and $T(z)u^*(z) \equiv 0$. $u(z)$ defines the orthogonal complementary range space of $v(z)$, which in this case turns out to have a basis which is analytic in the unit disc. Finally, a minimal realization for $T_{o\ell}$ is given by $\{A, B, C_o, D_o\}$. The existence of all these matrices has been shown a long time ago in complex function theory, for a very attractive treatment see [19], our purpose here is to derive an economical solution to the 'LTI square root equations' (8). The zeros of $T(z)$ play an essential role at least in part of the treatment (Cases I and II). They can be studied via the Smith–McMillan form, or directly via appropriate Hankel matrices connected to Laurent series expansions in the relevant point of the complex plane, see [35] where also the ensuing factorization theory is developed. We recall some facts. Let $\sup_z(\text{rank}(T(z))$ be called the 'normal rank of T', it is the normal rank of the Smith–McMillan form. $T(z)$ will have that rank almost everywhere. Points of exceptions are points where one or more of the minimal factors of T have a zero. Such points are called 'zeros' of $T(z)$ (they may be poles as well, when some other minimal factor has a pole at that point). The Smith–McMillan theory defines poles and zeros properly, except in the point $z = \infty$, which plays a special role in the theory because of its utilization of unimodular matrices—if it is of interest, it can be displaced to some other point in the complex plane through a bilinear transformation, but we shall avoid having to work 'at infinity' in this paper, we shall solely be concerned with zeros in the open unit disc of the complex plane, where $T(z)$ does not have any poles by definition. In the theory to follow, an anomaly can occur if T does not have normal rank at the point $z = 0$, for which we have to make the provision explained in the following paragraph.

If $T(0)$ does not have normal rank, then it can be brought to the generic case where it does, through a simple bilinear transformation on the variable z. Let a be a point in the complex plane $\mathbf{C}$ such that $|a| < 1$, and let

$$T_1(z) \triangleq T\left(\frac{a - z}{1 - \bar{a}z}\right).$$

Then T_1 has the new realization:

$$\begin{aligned}
A_1 &= (\bar{a}I - A)(I - aA)^{-1},\\
B_1 &= -\sqrt{1 - |a|^2}B(I - aA)^{-1},\\
C_1 &= \sqrt{1 - |a|^2}(I - aA)^{-1}C,\\
D_1 &= D + Ba(I - aA)^{-1}C \ (= T(a)).
\end{aligned}$$

If a is chosen as a point in the open unit disc where $T(a)$ has normal rank, then $T_1(z)$ will have normal rank at $z = 0$. Properties like outerness and innerness are preserved under this bilinear transformation—a well-known fact from Hardy space theory. Alternatively, and preferably, the zero at $z = 0$ can be factored out as an inner factor using the technique described in Appendix C. For brevity, we skip this technical point.

Generic case: $T(0) = D$ *has normal rank*. Let $\{A, B, C, D\}$ be a minimal realization for T, and let

$$D = [u_1\ u_2]\begin{bmatrix} d & 0 \\ 0 & 0 \end{bmatrix}\begin{bmatrix} v_1^* \\ v_2^* \end{bmatrix} \tag{9}$$

with d square invertible, $u = [u_1\ u_2]$ and $v = [v_1\ v_2]$ unitary (an SVD would do but is not really needed, just orthonormal bases for kernels and ranges of D and D^*). Let $T'(z) \triangleq u^* T(z) v$. Let $\beta = u^* B$ and $\gamma = Cv$. Then a minimal realization for T' is given by

$$\left\{A,\ \begin{bmatrix} \beta_1 \\ \beta_2 \end{bmatrix},\ [\gamma_1\ \gamma_2],\ \begin{bmatrix} d & 0 \\ 0 & 0 \end{bmatrix}\right\}, \tag{10}$$

in which β and γ have been partitioned according to the sub-division of u and v. Let $\Delta \triangleq A - \gamma_1 d^{-1}\beta_1$.

Lemma 2. $T'(0)$ *will have normal rank iff* $\beta_2(I - \Delta z)^{-1}\gamma_2 \equiv 0$.

A proof of the lemma is given below under 'Case IV'. The condition given in the lemma may serve as a test to determine whether $T(z)$ satisfies the condition itself, else one can apply the bilinear transformation of the previous paragraph. It should be clear that an outer–inner factorization for T' will produce one for T and vice versa (see further for the precise formulas). We assume from now on that T is in the normalized form of (10) and that it has normal rank at $z = 0$.

The treatment of the inner–outer factorization will differ greatly according to whether β_2 disappears, or γ_2, or both. The last case corresponds to D being square, non-singular and can be solved in a particularly simple way, involving only a partial eigenvalue decomposition of the matrix $\Delta = A - CD^{-1}B$ and the solution of a Lyapunov–Stein equation. No recursion is needed nor is it necessary to convert to a Riccati equation. The procedure can be extended in a rather straightforward way to the case where γ_2 is empty, but not β_2.

The next case, γ_2 not empty, β_2 not present, is fundamentally different. It corresponds to the determination of a 'range function'—a well-known problematic question in classical Hardy space theory. The standard way to tackle it is to construct a corresponding Riccati equation and then to solve the latter using an eigenvalue decomposition of a pencil constructed on an Hamiltonian matrix derived from the data [22]. The problem with that approach is that the method requires the numerically unstable determination of intrinsically multiple eigenvalues on the unit circle. Different approaches are possible. One consists in first reducing the problem to a regular Riccati equation, which then can be solved in a classical, stable way. The reduction consists in the determination of the eigenstructure of the zeros of $T(z)$ on the unit circle followed by a polynomial extraction. This step can be done in an as stable way as possible, the multiplicity of the eigenvalues is not doubled as would be the case if one would work on the original data. An alternative approach was proposed by Kailath e.a. as a square root algorithm to solve the Kalman filtering problem

[21]. This recursive solution has an interesting connection with the Szegö theory of orthonormal polynomials on the unit circle. Although the theory is classical, we give the recursive solution and its doubling version as the preferred method both from a numerical point of view and because it solves the square root equations in a reasonably direct way.

Finally, Case IV is the general case, which combines the previous cases in a reasonably direct way. It may seem a little convoluted to distinguish all these different cases, but there are very good numerical and mathematical reasons to do so. We shall go into these in the discussion at the end of the paper.

4.1. Case I: The square non-singular case

We assume that $T(z) = D + Bz(I - Az)^{-1}C$ is minimal with D square and non-singular. Since the Y sought is such that $\ker(Y\cdot) = 0$, we can always express it as

$$Y = V\begin{bmatrix}\sigma\\0\end{bmatrix},$$

in which σ is square non-singular and V unitary, e.g. by an RQ-factorization or an SVD.

Proposition 1. *Let $\Delta = A - CD^{-1}B$ and let Y be expressed as*

$$Y = V\begin{bmatrix}\sigma\\0\end{bmatrix}$$

with σ square and non-singular and V unitary. Let moreover

$$V^*\Delta V \triangleq \begin{bmatrix}\delta_{11} & \delta_{12}\\ \delta_{21} & \delta_{22}\end{bmatrix}.$$

Then Y will be a solution of (8) *with* $\ker(Y\cdot) = 0$ *iff*

(a) $\delta_{21} = 0$;

(b) δ_{11} *is invertible and has its eigenvalues strictly outside the unit disc of the complex plane*;

(c) $M \triangleq \sigma^{-*}\sigma^{-1}$ *is the unique non-singular solution of the Lyapunov–Stein equation*

$$M = \beta^*\beta + \delta_{11}^{-*}M\delta_{11}^{-1}$$

in which $\beta = D^{-1}BV\left[\begin{smallmatrix}\delta_{11}^{-1}\\0\end{smallmatrix}\right]$.

The solution will be maximal if δ_{11} contains all the eigenvalues of Δ which are located outside the open unit disc (*multiplicities counted*).

Proof. We first establish *necessity* (i.e. we assume the solution Y given).

Since D is assumed square invertible, we can write down a block upper–lower factorization

$$\begin{bmatrix} A & C \\ B & D \end{bmatrix} = \begin{bmatrix} I & CD^{-1} \\ & I \end{bmatrix} \begin{bmatrix} \Delta & \\ & D \end{bmatrix} \begin{bmatrix} I & \\ D^{-1}B & I \end{bmatrix},$$

in which $\Delta \triangleq A - CD^{-1}B$ is the celebrated Schur complement of D in the realization matrix. Hence (8) can be rewritten as

$$\begin{bmatrix} \Delta & \\ B & D \end{bmatrix} \begin{bmatrix} Y & \\ & I \end{bmatrix} W^* = \begin{bmatrix} I & -CD^{-1} \\ & I \end{bmatrix} \begin{bmatrix} 0 & Y & C_o \\ 0 & 0 & D_o \end{bmatrix}. \tag{11}$$

Looking at the second block column of this equation, we find

$$\begin{bmatrix} \Delta & 0 \\ B & D \end{bmatrix} \begin{bmatrix} Y & \\ & I \end{bmatrix} \begin{bmatrix} W_{21}^* \\ W_{22}^* \end{bmatrix} = \begin{bmatrix} Y \\ 0 \end{bmatrix} \tag{12}$$

and hence

$$\Delta Y W_{21}^* = Y.$$

It follows that W_{21} must be invertible, since it is square by definition ($W_{21} = A_v$) and $W_{21}^* x = 0 \Rightarrow Yx = 0 \Rightarrow x = 0$ by the kernel hypothesis on Y. Hence

$$\Delta Y = Y W_{21}^{-*}$$

and since Y has the left (Moore–Penrose) inverse $Y^\dagger = [\sigma^{-1} \;\; 0]V^*$,

$$\begin{aligned} W_{21}^{-*} &= Y^\dagger \Delta Y, \\ &= [\sigma^{-1} \;\; 0] V^* \Delta V \begin{bmatrix} \sigma \\ 0 \end{bmatrix}, \\ &= \sigma^{-1} \delta_{11} \sigma, \end{aligned}$$

and we have that δ_{11} is invertible with W_{21}. Hence $W_{21} = \sigma^* \delta_{11}^{-*} \sigma^{-*}$ and since $W_{21} = A_v$, the state transition matrix of an inner operator, δ_{11}^{-*}, must have its eigenvalues strictly inside the unit disc. From (12) and after multiplication with $Y^\dagger$ we find

$$\begin{bmatrix} \sigma^{-1}\delta_{11}\sigma & 0 \\ BY & D \end{bmatrix} \begin{bmatrix} W_{21}^* \\ W_{22}^* \end{bmatrix} = \begin{bmatrix} I \\ 0 \end{bmatrix}.$$

Introducing $\beta = D^{-1}BV \begin{bmatrix} \delta_{11}^{-1} \\ 0 \end{bmatrix}$ and inverting the leftmost matrix, we find finally

$$\begin{bmatrix} W_{21}^* \\ W_{22}^* \end{bmatrix} = \begin{bmatrix} \sigma^{-1}\delta_{11}^{-1}\sigma & 0 \\ -\beta\sigma & D^{-1} \end{bmatrix} \begin{bmatrix} I \\ 0 \end{bmatrix}.$$

Expressing the isometry of $[W_{21} \;\; W_{22}]$ and puting $M \triangleq \sigma^{-*}\sigma^{-1}$, we obtain the Lyapunov–Stein equation

$$M = \beta^* \beta + \delta_{11}^{-*} M \delta_{11}^{-1}. \tag{13}$$

Since δ_{11}^{-1} has its eigenvalues strictly inside the unit disc of the complex plane, this equation has a unique solution given by

$$M = \sum_{k=0}^{\infty} [\delta_{11}^{-*}]^k \beta^* \beta [\delta_{11}^{-1}]^k. \tag{14}$$

M is strictly positive definite since σ is assumed non-singular. Hence we find

$$[W_{21} \quad W_{22}] = [\sigma^* \delta_{11}^{-*} \sigma^{-*} \quad -\sigma^* \beta^*].$$

If we plow this result back into the original equation, we obtain

$$\begin{bmatrix} AY & C \\ BY & D \end{bmatrix} \begin{bmatrix} W_{21}^* \\ W_{22}^* \end{bmatrix} = \begin{bmatrix} V \begin{bmatrix} \sigma \\ \delta_{21}\delta_{11}^{-1}\sigma \end{bmatrix} \\ 0 \end{bmatrix},$$

which will be equal to $\left[\begin{smallmatrix} Y \\ 0 \end{smallmatrix}\right]$ only if $\delta_{21} = 0$. This proves necessity.

Sufficiency will follow if we show that the algorithm derived from the conditions of the theorem produce a Y which solves (3), and which is left invertible ($\ker(Y\cdot) = 0$). Let

$$\Delta^* = V \begin{bmatrix} \delta_{11}^* & 0 \\ \delta_{12}^* & \delta_{22}^* \end{bmatrix} V^* \tag{15}$$

be a block Schur eigenspace decomposition for Δ, in which δ_{11} collects (the) eigenvalues of Δ which are strictly outside the unit disc. Let now β be defined as given in the statement of the theorem, and let next M be the solution of the Lyapunov–Stein equation (13). We claim that M is strictly positive definite as a consequence of the minimality of the original system T. This can be seen as follows. Since the eigenvalues of δ_{11}^{-1} are strictly inside the unit disc of the complex plane, the solution of the Lyapunov–Stein equation given by (14) is unique. It will be non-singular, iff the reachability pair $[\delta_{11}^{-1} \quad \beta]$ is minimal, which means that there does not exist a vector $x \neq 0$ such that $\forall k \geqslant 0 : \beta \delta_{11}^{-k} x = 0$. Let $\delta_{11}^{-1} x \triangleq y$. Then $x = 0 \Leftrightarrow y = 0$, and we find that the condition is equivalent to

$$D^{-1} B V \begin{bmatrix} y \\ 0 \end{bmatrix} = 0,$$
$$D^{-1} B V \begin{bmatrix} \delta_{11} & \delta_{12} \\ 0 & \delta_{22} \end{bmatrix}^k \begin{bmatrix} y \\ 0 \end{bmatrix} = 0 \quad \text{for } k \geqslant 1.$$

Let $V\left[\begin{smallmatrix} y \\ 0 \end{smallmatrix}\right] = y_1$. Then $y_1 = 0 \Leftrightarrow x = 0$, and the condition becomes $\forall k \geqslant 0 : \ B\Delta^k y_1 = 0$ for $\Delta = A - C D^{-1} B$. It is now not hard to see (recursively) that this condition is equivalent to $\forall k \geqslant 0 : \ B A^k y_1 = 0$. Since the realization was assumed strictly reachable, we find $y_1 = 0$ and subsequently $y = 0$ and $x = 0$. (The proof boils down to the fact that if the realization for a system is minimal, then the derived realization for the inverse system is minimal as well, but in the present case the inverse system is partially unstable so that the corresponding Lyapunov–Stein equation for the reachability Gramian cannot simply be summed.) Factor now $M = \sigma^{-*}\sigma^{-1}$ and put

$$Y = V \begin{bmatrix} \sigma \\ 0 \end{bmatrix}.$$

Y satisfies all the necessary conditions by construction and is hence the solution sought. □

4.2. Case II: $T(0)$ has full column rank—γ_2 is empty

Let

$$D = u \begin{bmatrix} d \\ 0 \end{bmatrix} v^*$$

be a decomposition of D with u and v unitary matrices and d square non-singular. We find

$$\begin{bmatrix} A & C \\ B & D \end{bmatrix} = \begin{bmatrix} I & 0 & 0 \\ 0 & u_1 & u_2 \end{bmatrix} \begin{bmatrix} A & \gamma \\ \beta_1 & d \\ \beta_2 & 0 \end{bmatrix} \begin{bmatrix} I & 0 \\ 0 & v^* \end{bmatrix},$$

where $u = [u_1\ u_2]$ is a decomposition of u conformal to the partitioning of D. Let $T'(z) \triangleq u^* T(z)$ and let $T'(z) = T'_o(z)V'(z)$ be a left-outer–inner decomposition of $T'(z)$. Then $T_o(z) = uT'(z)$ and $V(z) = V'v^*$ will produce the left-outer–inner decomposition of $T(z)$. We may just as well take $T(z)$ in the $T'(z)$ form to start with, for simplicity of notation. $T(z)$ then has the form

$$T(z) = \begin{bmatrix} T_1(z) \\ T_2(z) \end{bmatrix}$$

with $T_1(z)$ a 'Case I' matrix, and $T_2(0) = 0$. A left-outer–inner factorization of $T_1(z) = T_{1o}V_1(z)$ produces, via the techniques of Case I, an inner factor $V_1(z)$ which, however, may be 'too large' for $T_2(z)$ in the sense that $T_2(z)V_1^*(z)$ may not be analytic in the open unit disc. The true right inner factor $V(z)$ will be the largest inner factor such that both $T_1(z)V^*(z)$ and $T_2(z)V^*(z)$ are analytic in the open unit disc at the same time. To establish the relation between V_1 and V, let now n temporarily be the dimension of the output space and H_2^n the Hardy space of dimension n [27]. We must have $H_2^n V_1(z) \subset H_2^n V$ and hence $V_1(z) = V_r(z)V(z)$, $V(z)$ is a right-inner factor of $V_1(z)$ with remainder $V_r(z)$. We determine $V_1(z)$ first using the method of case I, then compute the part of $V_1(z)$ that makes $T_2(z)V_1^*(z)$ non-analytic, and finally compute a minimal V_r so that $T_2(z)V_1^*(z)V_r(z)$ is analytic. The square root equation now has the form

$$\left[\begin{array}{cc} A & \gamma \\ \hline \beta_1 & d \\ \beta_2 & 0 \end{array}\right] \begin{bmatrix} Y & \\ & I \end{bmatrix} = \begin{bmatrix} 0 & Y & C_o \\ 0 & 0 & D_o \end{bmatrix} W. \tag{16}$$

We apply the Case I procedure on

$$\begin{bmatrix} A & \gamma \\ \beta_1 & d \end{bmatrix} \begin{bmatrix} Y_1 & \\ & I \end{bmatrix} = \begin{bmatrix} 0 & Y_1 & C_{o1} \\ 0 & 0 & D_d \end{bmatrix} W_1. \tag{17}$$

This produces a realization $V_1(z) = D_{v1} + zB_{v1}(I - zA_{v1})^{-1}C_{v1}$. Applying $V_1^*(z)$ to the right of $T_2(z)$ gives

$$T_2(z)V_1^*(z) = \beta_2 z(I - Az)^{-1}\gamma[D_{v1}^* + C_{v1}^*(I - z^*A_{v1}^*)^{-1}z^*B_{v1}^*]. \tag{18}$$

Reduction of this equation necessitates a 'partial fraction decomposition' of a matrix quadratic term. Lemma 1 applies. Let M be the unique solution of the Lyapunov–Stein equation

$$M - AMA_{v_1}^* = \gamma C_{v_1}^*,$$

which is well defined since A and A_{v_1} both have spectral radius less than one (and hence also zA and zA_{v_1}). Then we find in sequence:

$$(I - Az)^{-1})\gamma C_{v_1}^*(I - z^*A_{v_1}^*)^{-1} = (I - Az)^{-1}M - M + M(I - z^*A_{v_1}^*)^{-1},$$

$$\begin{aligned} T_2(z)V_1^*(z) = {} & z^*\beta_2 M(I - z^*A_{v_1}^*)^{-1}B_{v_1}^* - \beta_2 MB_{v_1}^* \\ & + \beta_2(I - Az)^{-1}[MB_{v_1}^* + \gamma D_{v_1}^*]. \end{aligned}$$

We see that $T_2(z)V_1^*(z)$ may have an anticausal part

$$z^*\beta_2 M(I - z^*A_{v_1}^*)^{-1}B_{v_1}^*.$$

The computation of V_r and V is now a straightforward application of factorization theory for unitary realizations, intended to remove this anticausal part. We give the essential steps. Let $C_\ell^* \triangleq \beta_2 M$, and let us find a unitary matrix u which reduces the possibly non-minimal observability pair $[A_{v_1}\ C_\ell]$, thereby defining the A_{v_r} and A_v sought:

$$[u^*A_{v_1}u \mid u^*C_\ell] = \left[\begin{array}{cc|c} A_{v_r} & A' & C'_\ell \\ 0 & A_v & 0 \end{array}\right].$$

If we now apply the state transformation $u^* \cdots u$ on the realization $\{A_{v_1}, B_{v_1}, C_{v_1}, D_{v_1}\}$, then unitarity is preserved, and an equivalent realization is obtained, which will factor in the desired way. Let us denote this new realization as follows:

$$\left[\begin{array}{c|c} u^*A_{v_1}u & u^*C_{v_1} \\ \hline B_{v_1}u & D_{v_1} \end{array}\right] = \left[\begin{array}{cc|c} A_{v_r} & A' & C'_{v_r} \\ 0 & A_v & C_v \\ \hline B_{v_r} & B'_v & D'_{v_1} \end{array}\right],$$

in which we have anticipated notationwise on the destination of the sub-matrices. Because of the reduction of the strictly non-causal part of $T_2(z)V_1^*(z)$ to minimality, we have

$$z^*C_\ell^*(I - A_{v_1}^*z^*)^{-1}B_{v_1}^* = z^*C_\ell'^*(I - A_{v_r}^*z^*)^{-1}B_{v_r}^*.$$

The equivalent unitary realization of $V_1(z)$ factors now

$$\left[\begin{array}{cc|c} A_{v_r} & A' & C'_{v_r} \\ 0 & A_v & C_v \\ \hline B_{v_r} & B'_v & D'_{v_1} \end{array}\right] = \left[\begin{array}{cc|c} A_{v_r} & & C_{v_r} \\ & I & \\ \hline B_{v_r} & & D_{v_r} \end{array}\right] \left[\begin{array}{cc|c} I & & \\ & A_v & C_v \\ \hline & B_v & D_v \end{array}\right],$$

in which the quantities to the left of the equal sign are known, and the quantities to the right must be such that two unitary factors are obtained, this being always possible due to the unitarity of the original matrix and its partial block triangularization. $V(z)$ and $V_r(z)$ are now fully determined (up to equivalence), and it is readily verified that

$$z^* C_\ell'^* (I - A_{v_r}^* z^*)^{-1} B_{v_r}^* V_r(z)$$

has become causal (analytic in the unit disc), so that $T_2 V^*$ is analytic as well. In addition, minimality of V is also readily established, thanks to standard inner–outer factorization theory. The procedure shown is a handy technique to compute common factors in inner functions. This completely solves Case II in the square root form. However, criticism on the method is still possible, since in many instances it may lead to too many computations: first the determination of a realization for $V_1(z)$ via the determination of a Schur eigenvalue form, followed by a further reduction.

4.3. *Case III: T(0) has full row rank – β_2 is empty*

This case is fundamentally different from the previous cases — it corresponds to the determination of the orthogonal basis of a range function and its completion to a unitary matrix. We shall see that a special case of this instance is found in the classical square root algorithm for the Kalman filter. If m is the input dimension of $T(z)$ (dimensions $m \times \underline{(n_1 + n_2)}$, with $n_1 = m$), then the range function for T is defined as the space $\mathscr{R} \triangleq \overline{H_m^2[T_1(z)\ T_2(z)]}$, in which H_m^2 is the m-dimentional Hardy space of the unit disc. The subject of range functions is both a very essential part of classical Hardy space theory [19], and one in which major problems occur in general, because an analytic range function (that is a range function with a basis that is analytic in the unit disc) need not have an analytic orthogonal complement. However, for the rational case such an anomality cannot occur and complete results are available, a rational range function that has an orthonormal basis consisting of elements analytic in the unit disc has an analytic orthogonal complement. Our goal will be to give numerically stable algorithms that compute both the orthogonal basis and its complement. It turns out that the most attractive algorithm is based on the square root equation, this time in the recursive form of the Kalman filter. It will have exactly the same appearance as the time-varying equation (3), executed as a 'doubling procedure'. A traditional alternative is the solution of the related Riccati equation. No numerically stable solution for the discrete time Riccati equation is possible if the zeros on the unit circle of $T(z)$ are not removed first. It may seem that the recursive square root solution does not suffer from the presence of these zeros, but that is not true, as we shall see later in this section. Therefore, it is necessary to perform a 'reduction of zeros on the boundary' first. This can be done in a rather elementary way, using the characterization of zeros of general transfer function as originally done in [35].

As in the previous section we may assume $T(z) = [T_1(z)\ T_2(z)]$ with the realization

$$\left[\begin{array}{c|cc} A & \gamma_1 & \gamma_2 \\ \hline \beta & d_1 & 0 \end{array}\right] \triangleq \left[\begin{array}{c|c} A & \gamma \\ \hline \beta & d \end{array}\right] \tag{19}$$

in which d_1 is square invertible and $\gamma_2 \neq 0$. Let

$$T_o(z)T_o^*(z) = T_1(z)T_1^*(z) + T_2(z)T_2^*(z) \triangleq R(z) \tag{20}$$

be a (left) spectral factorization of $T(z)T^*(z)$ with $T_o(z)$ the (left-)outer factor. Then $T(z) = T_o(z)[V_1(z)\ V_2(z)]$ in which, of course, $V(z) = [V_1(z)\ V_2(z)] = T_o^{-1}(z)$ $[T_1(z)\ T_2(z)]$ defines a causal isometric matrix function whose rows actually form an analytic basis for the range space $\mathscr{R}$. V can then further be embedded in an inner factor

$$W(z) = \begin{bmatrix} V(z) \\ U(z) \end{bmatrix}, \tag{21}$$

in which it forms the first block row. As before, we wish to have T_o, V and W in state-space form, the realization for the latter can be chosen isometric, augmentable to a unitary matrix.

Two observations are in order at this point. First, the zeros in the unit disc of $V(z)$ (i.e. points where its rank drops) often have no relation with the zeros in the unit disc of $T(z)$, in contrast to case I. They will appear in the right inner factor, but in a trivial way. Even if T has no zeros in the unit disc, the embedding will have such zeros as is exemplified by

$$T(z) = \begin{bmatrix} \frac{1}{1+\frac{1}{2}z} & \frac{z}{1+\frac{1}{2}z} \end{bmatrix} \tag{22}$$

for which

$$W(z) = \begin{bmatrix} \frac{1}{\sqrt{2}} & \frac{z}{\sqrt{2}} \\ \frac{-1}{\sqrt{2}} & \frac{z}{\sqrt{2}} \end{bmatrix}. \tag{23}$$

The zero of W is at $z = 0$, a point at which $T(z)$ has no zero. Second, the execution of the spectral factorization shown in (20) appears to be essential in as much as T_o is normalizing the rows of T to produce V. The classical way of doing this in state-space terms is to convert the problem to the solution of a Riccati equation, in this case a discrete time (algebraic) Riccati equation. It is well known (see e.g. [22] for a comprehensive exposition) that this Riccati equation can only be solved in a numerical stable way when T has no zeros on the unit circle, because zeros on the unit circle will appear double in the subsequent Hamiltonian eigenvalue problem, making it unnecessarily ill-conditioned. In case there are no zeros (and of course no poles) on the unit circle, one speaks of a regular problem. Although we shall not solve the Riccati equation directly—we shall work on the square root form—the same problem with boundary zeros appears. Moreover, it appears advantageous to work on a modified system representation in which an obvious factor of the inner

part has been taken out first. Therefore, a couple of preliminary steps have to be executed first.

4.3.1. Preliminary inner reduction of $T_1(z)$

We start out by using the simple procedure of Case I to reduce $T_1(z)$ to an outer matrix

$$T_1(z) = T_{1o}(z)V_1(z)$$

in which T_{1o} is outer and $V_1(z)$ inner. Then

$$T(z) = [T_{1o}(z)\ T_2(z)]\begin{bmatrix} V_1(z) & \\ & I \end{bmatrix}$$

and a realization for $[T_{1o}(z)\ T_2(z)]$, given by

$$\begin{bmatrix} A & \gamma_{1o} & \gamma_2 \\ \beta & d_{1o} & 0 \end{bmatrix}$$

is such that $A - \gamma_{1o}d_{1o}^{-1}\beta$ has no eigenvalues larger than 1. Once an outer–inner factorization

$$[T_{1o}(z)\ T_2(z)] = [T_o(z)\ 0]W(z)$$

has been found, then

$$T(z) = [T_o(z)\ 0]\left(W(z)\begin{bmatrix} V_1(z) & \\ & I \end{bmatrix}\right)$$

will be an outer–inner factorization of the original matrix, and

$$\deg\left(W(z)\begin{bmatrix} V_1(z) & \\ & I \end{bmatrix}\right) = \deg W(z) + \deg V_1(z)$$

(a well-known property of inner matrices). Hence, this part of the procedure is minimal. We may and shall now assume that the original matrix for Case III is such that $T_1(z)$ is outer, and hence has a realization with d non-singular and $A - \gamma d^{-1}\beta$ such that it has no eigenvalues of modulus larger than 1.

4.3.2. Removal of zeros on the boundary

We shall now reduce the spectral factorization problem to a regular problem. This is done in an as stable as possible way, by computing a square non-singular polynomial matrix $P(z)$ of dimensions $m \times m$ which is such that

$$T(z) = P(z)T'(z) = P(z)[T_1'(z)\ T_2'(z)] \tag{24}$$

for $T'(z)$ stable with no zeros (and of course no poles) on the unit circle. The procedure requires first the determination of candidate zeros on the unit circle. Since a zero of $T(z)$ must a fortiori be a zero of $T_1(z)$, we find a complete collection of candidates by computing the eigenvalues on the unit circle of $A - \gamma_1 d_1^{-1}\beta$. If $\{a_i : i = 1 \cdots\}$ is the set so obtained, then we must find $P(z)$ so that it incorporates

all these zeros, multiplicities and directional data included. This can be done in a recursive fashion on the candidates $\{a_i\}$—one extracts first the complete zero at a_1 as a polynomial matrix $P_1(z)$, and then proceeds on the remainder $P_1^{-1}T(z)$ for which the set of zeros is now $\{a_2 \cdots\}$, because the extraction will not affect the location nor the multiplicity structure of the zeros at the other points. The extraction of a polynomial with a single zero at a point a is an 'elementary' procedure, which can be based on an invariant sub-space structure of T characteristic for that zero. An efficient computation is based e.g. on the theory of surplus spaces as originally proposed in [35]. We give the algorithm in Appendix C.

4.3.3. The recursive solution

The attractive way of solving the regular problem is provided by setting up a recursive solution as has been proposed for the computation of the classical Kalman filter in the square root form [25]. The method can be approached via a continuous Cholesky factorization as explained in [12, pp. 65–71].

Let a minimal realization for $T(z)$ (with $T_1(z)$ outer) be as before, and let us denote a realization for an outer T_o such that $T(z)T^*(z) = T_o(z)T_o^*(z)$ by

$$T_o = \left[\begin{array}{c|c} A & \gamma_o \\ \hline \beta & d_o \end{array}\right].$$

We assume that a realization for $T_o(z)$ exists with $\{A, \beta\}$ as reachability pair—a well-known fact, which is constructively proven by the procedure to be derived now.

Applying Lemma 1 on the product $T(z)T^*(z)$ with $A_1 = A_2 \triangleq A$, $U \triangleq z$ and $\mu = \gamma\gamma^* + A\mu A^*$ we obtain a mixed realization

$$\begin{aligned} R(z) \triangleq T(z)T^*(z) = {} & dd^* + \beta\mu\beta^* + \beta z(I - Az)^{-1}[\gamma d^* + A\mu\beta^*] \\ & + [d\gamma^* + \beta\mu A^*](I - z^*A^*)^{-1}z^*\beta^*. \end{aligned}$$

Let $\gamma_r \triangleq \gamma d^* + A\mu\beta^*$, $R(z)$ is the transfer function corresponding to the doubly infinite Toeplitz operator

$$\begin{bmatrix} \ddots & \ddots & \ddots & \ddots & \ddots \\ \ddots & dd^* + \beta\mu\beta^* & \beta\gamma_r & \beta A\gamma_r & \ddots \\ \ddots & \gamma_r^*\beta^* & \boxed{dd^* + \beta\mu\beta^*} & \beta\gamma_r & \ddots \\ \ddots & \gamma_r^*A^*\beta^* & \gamma_r^*\beta^* & dd^* + \beta\mu\beta^* & \ddots \\ \ddots & \ddots & \ddots & \ddots & \ddots \end{bmatrix},$$

in which the (0, 0)th entry has been boxed for orientation purposes. The simplest trick to find a realization for $T_o(z)$ recursively is to consider a Cholesky factorization of a strategically choosen sub-operator of $R(z)$, namely of the operator

$$\mathbf{R}_- = \begin{bmatrix} \ddots & \ddots & \ddots & \ddots \\ \ddots & dd^* + \beta\mu\beta^* & \beta\gamma_r & \beta A\gamma_r \\ \ddots & \gamma_r^*\beta^* & dd^* + \beta\mu\beta^* & \beta\gamma_r \\ \ddots & \gamma_r^* A^*\beta^* & \gamma_r^*\beta^* & \boxed{dd^* + \beta\mu\beta^*} \end{bmatrix}$$

A motivation for this choice can be found in [12, pp. 65–71, 369 and 370], where use is made of the partial factorization lemma in the time-varying setting. We attempt to find a Cholesky factorization for $\mathbf{R}_-$, as follows:

$$\mathbf{R}_- = \begin{bmatrix} \ddots & \ddots & \ddots & \vdots \\ \ddots & d_{-2} & \beta c_{-1} & \beta A c_0 \\ \ddots & 0 & d_{-1} & \beta c_0 \\ \cdots & 0 & 0 & \boxed{d_0} \end{bmatrix} \begin{bmatrix} \ddots & \ddots & \ddots & \vdots \\ \ddots & d_{-2}^* & 0 & 0 \\ \ddots & c_o^*\beta^* & d_{-1}^* & 0 \\ \cdots & c_o^* A^*\beta^* & c_{-1}^*\beta^* & d_0^* \end{bmatrix}. \quad (25)$$

In other words, we look for a collection of $\{d_{-k} : k = 0, \cdots, \infty\}$ and $\{c_{-k} : k = 0, \cdots, \infty\}$ so that $\{A, \beta, c_{-k}, d_{-k}\}$ form a partially time-varying realization for the Cholesky factor sought. All products in the factorization (25) are finite—for any finite sub-block of $\mathbf{R}_-$ in its bottom right corner, there is a finite upper–lower traditional Cholesky factorization. Each such factorization exists and is unique, since $\mathbf{R}_-$ is strictly positive definite, and so is each finite main square sub-block. Starting with the right bottom (0,0)th element, we find d_0 such that $d_0 d_0^* = dd^* + \beta M\beta^*$. Next, an adequate c_0 follows: $c_0 = \gamma_r d_0^{-*}$. This initializes the recursion. Let us now define an intermediate quantity for $k = 1, \ldots, \infty$,

$$M_{-k} = \sum_{i=0}^{k} A^i c_{k-i} c_{k-i}^* A^{*i} (= c_{-k} c_{-k}^* + A M_{-k+1} A^*),$$

with $M_0 = c_0 c_0^*$. Then it is easy to check directly that the upper–lower Cholesky factorization of the block $(-k \cdots 0) \times (-k \cdots 0)$ leads to the following recursion on the state-space data:

$$\begin{aligned} &(1)\ d_{-k} d_{-k}^* = d_0 d_0^* - \beta M_{-k+1}\beta^*, \\ &(2)\ c_{-k} = [\gamma_r - A M_{-k+1}\beta^*] d_{-k}^{-*}, \\ &(3)\ M_{-k} = c_{-k} c_{-k}^* + A M_{-k+1} A^*, \end{aligned} \quad (26)$$

in which Eq. (1) gives a strictly positive definite value for $d_{-k} d_{-k}^*$ simply because of the existence of the Cholesky factorization, Eq. (2) provides an adequate value for c_{-k}, and Eq. (3) updates M. We show that the recursion converges for $k \to \infty$. An attractive proof is derived from the Szegö theory of orthormal polynomials (although other proofs based on the Wiener–Masani theory for spectral factorization are equally

well possible, we give the basic proof in Appendix D because it may not be too well known).

Proposition 2. *The Cholesky recursions* (26) *converge for* $k \to \infty$ *and produce a realization* $\{A, \beta, c_o, d_o\}$ *of the outer factor* $T_o(z)$ *as*

$$c_o = \lim_{k\to\infty} c_{-k},$$
$$d_o = \lim_{k\to\infty} d_{-k}.$$

The rate of convergence can also be deduced from the Szegö theory, see in this connection [10].

It is now straightforward to turn this recursion into a recursive square root algorithm. We reintroduce the original data ($\mu = \gamma\gamma^* + A\mu A^*$ and $\gamma_r = \gamma d^* + A\mu\beta^*$) to find:

$$\begin{aligned} &dd^* + \beta(\mu - M_{-k+1})\beta^* = d_{-k}d_{-k}^*, \\ &\gamma d^* + A(\mu - M_{-k+1})\beta^* = c_{-k}d_{-k}^*, \\ &\gamma\gamma^* + A(\mu - M_{-k+1})A^* = c_{-k}c_{-k}^* + (\mu - M_{-k}). \end{aligned} \tag{27}$$

It is not hard to show that $m_k \triangleq \mu - M_{-k}$ is (not necessarily strictly) positive define for all k, inductively. With $m_k = r_k r_k^*$ a minimal factorization of m_k, we can write (27) in factored form

$$\begin{bmatrix} Ar_{k-1} & \gamma \\ Br_{k-1} & d \end{bmatrix} \begin{bmatrix} r_{k-1}^* A^* & r_{k-1}^*\beta^* \\ \gamma^* & d^* \end{bmatrix} = \begin{bmatrix} r_k & c_{-k} \\ 0 & d_{-k} \end{bmatrix} \begin{bmatrix} r_k^* & 0 \\ c_{-k}^* & d_{-k}^* \end{bmatrix}. \tag{28}$$

Eq. (28) will be solved if we find unitary matrices Q_k for $k = 1, 2, \ldots$ such that, starting with $M_0 = c_0 c_0^*$,

$$\begin{bmatrix} Ar_{k-1} & \gamma \\ \beta r_{k-1} & d \end{bmatrix} = \begin{bmatrix} 0 & r_k & c_{-k} \\ 0 & 0 & d_{-k} \end{bmatrix} Q_k \tag{29}$$

i.e. an *RQ* procedure computing the upper echelon form and producing the desired quantities c_{-k}, d_{-k} and r_k and of course also M_{-k} recursively. In (29) we recognize the square root algorithm for the Kalman filter as proposed by Kailath and Morf, adapted to our circumstances (in the Kalman filter, d and γ have a special form). For an account with references, see [21]. Since we are only interested in the end result $T_o(z)$, the doubling procedure, also proposed by Morf and Kailath together with Dobbins and Friedlander [23], yields a particularly fast and attractive method—we give the doubling procedure in Appendix E. Further refinements of these procedures have been derived by Kailath and Morf, and are known as Chandrasekhar equations. Instead of inductively computing the M_{-k}'s, they actually compute the increments $M_{-k} - M_{-k+1}$. In our case, these are all positive definite. The complexity of the

incremental matrix is usually (much) smaller than that of the matrix itself. Both inductive and square root versions are possible here, and lead to a further improvement in complexity, at the cost of numerical stability. We refer to the literature for further information [21].

With $T_o(z)$ determined, the result for Case III is now written down easily. The outer factor is already known, and we have for the inner factor

$$V(z) = T_o^{-1}(z)T(z).$$

Since $T_o(z)$ is outer (with no zeros on the unit circle if the zero extraction has been done first, an advisable procedure), it has a straight inverse, and a simple, direct calculation gives, with $\Delta = A - c_o d_o^{-1}\gamma$

$$\begin{aligned} V(z) &= [d_o^{-1} - d_o^{-1}\beta z(I - \Delta z)^{-1}c_o d_o^{-1}][d + \beta z(I - Az)^{-1}\gamma] \\ &= d_o^{-1}d + d_o^{-1}\beta z(I - \Delta z)^{-1}(c_o d_o^{-1}d - \gamma). \end{aligned}$$

Hence,

$$\begin{bmatrix} \Delta & c_o d_o^{-1}d - \gamma \\ \beta & d_o d^{-1} \end{bmatrix}$$

is a realization of the isometric system $V(z)$. It is not necessarily minimal, e.g. if the zeros on the boundary have not been taken out, then it is certainly non-minimal, because the zeros on the boundary will appear as eigenvalues of Δ, and these zeros have to cancel out in $V(z)$. Hence, if the reduction procedure of boundary zeros of the beginning of this section would not have been carried out, numerical instability would result even in case the recursive square root algorithm (in its doubling version) is used. There may be cancellations in the realization of $T_o(z)$, but these should not give rise to additional difficulties.

4.4. Case IV: the general LTI case

The general case is now a reasonably straightforward generalization of the preceeding cases. We assume normal rank at zero, and the transition matrix for T given by

$$\begin{bmatrix} A & \gamma_1 & \gamma_2 \\ \beta_1 & d & 0 \\ \beta_2 & 0 & 0 \end{bmatrix},$$

in which d is square, non-singular. Corresponding to this realization is the decompostion of $T(z)$ in four blocks:

$$\begin{aligned} T(z) &= \begin{bmatrix} T_{11}(z) & T_{12}(z) \\ T_{21}(z) & T_{22}(z) \end{bmatrix} \\ &= \begin{bmatrix} d + \beta_1 z(I - Az)^{-1}\gamma_1 & \beta_1 z(I - Az)^{-1}\gamma_2 \\ \beta_2 z(I - Az)^{-1}\gamma_1 & \beta_2 z(I - Az)^{-1}\gamma_2 \end{bmatrix}. \end{aligned}$$

The normal rank conditions makes the bottom rows in this representation linearly dependent on the top rows. This can be seen as follows. Since d is square non-singular, T_{11} is invertible (in fact, with $\Delta = A - \gamma_1 d^{-1}\beta_1$,

$$T_{11}^{-1}(z) = d^{-1} - d^{-1}\beta_1 z(I - \Delta z)^{-1}\gamma_1 d^{-1})$$

and hence:

$$T(z) = \begin{bmatrix} I & \\ T_{21}T_{11}^{-1} & I \end{bmatrix} \begin{bmatrix} T_{11} & \\ & T_{22} - T_{21}T_{11}^{-1}T_{12} \end{bmatrix} \begin{bmatrix} I & T_{11}^{-1}T_{12} \\ & T_{22} \end{bmatrix}.$$

Since $T(z)$ has normal rank at $z = 0$ and $T_{11}(z)$ is guaranteed non-singular in a neighborhood of $z = 0$, we must have that

$$T_{22}(z) - T_{21}(z)T_{11}^{-1}(z)T_{12}(z) \equiv 0.$$

It follows that

$$[T_{21}\ T_{22}] = T_{21}T_{11}^{-1}[T_{11}\ T_{12}].$$

Suppose that the outer factor T_o' and the isometric range function $[V_{11}\ V_{12}]$ for $[T_{11}\ T_{12}]$ have been found by the method of Case III above, then we find

$$T = \begin{bmatrix} T_o' \\ T_{21}V_{11}^{-1} \end{bmatrix} [V_{11}\ V_{12}].$$

It turns out that the left factor may have poles in the open unit disc. If it is brought back to analyticity in a minimal way, then the desired left-inner–outer factorization will follow. The procedure is simple and similar to what is done in Case II above. Let $s(z)$ be a minimal inner factor which pushes $T_{21}V_{11}^{-1}$ to analyticity, i.e. the $s(z)$ with lowest possible degree such that

$$T_{12}(z)V_{11}^{-1}(z)s(z) \in H_\infty^{m_1 \times m_1}.$$

Then

(1) $[s_*(z)V_{11}(z)\ s_*(z)V_{12}(z)]$ is analytic in the open unit disc and isometric;

(2) $\begin{bmatrix} T_o(z)s(z) \\ T_{21}V_{11}^{-1}(z)s(z) \end{bmatrix}$ is outer;

(3) the left inner–outer factorization for $T(z)$ is given by

$$T(z) = \begin{bmatrix} T_o'(z)s(z) \\ T_{21}(z)V_{11}^{-1}(z)s(z) \end{bmatrix} [s^*(z)V_{11}(z)\ s^*(z)V_{12}(z)].$$

As before, the proof is based on standard Hardy space theory. Numerically the procedure boils down to cancelling the anticausal part of $T_{21}(z)V_{11}^{-1}$, which is done exactly in the same way as in Case II above.

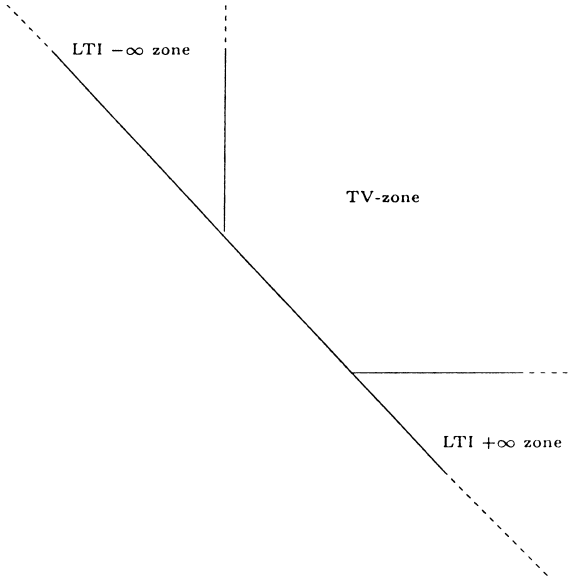

Fig. 1. The general structure of an IVI-system: it is a time-varying system which is essentially LTI for very small and very large index points.

5. The LTI/LTV/LTI or IVI case

We now turn to the case where the system is time-varying, but has a form which is described by a finite number of parameters, i.e. the system begins as LTI for very small time points, then starts varying, and ends up again as LTI for very large times. The dimension of the state space need not stay constant, and the degree of the limiting systems, which also have an LTI representations $T_{\pm\infty}(z)$ may be different. The simplest example is a system which switches from one type to the other at some time t_s. The general appearance of such a system is given in Fig. 1. It should be remarked that such a system is truly LTI only in the top-left and bottom-right triangular block. We keep assuming that the overall system is ues, so that the norm of the $T_{i,j}$ drops uniformly and exponentially to zero when $\inf(i, j) \to \infty$. Again, we shall be interested in the computation of the left-outer–inner factorization $T = T_o V$ in which V is causal isometric ($V V^* = I$), since the other cases can be brought to it via the procedures of Section 2. The recursive equation (3) specialized to this case shows that for $k \approx +\infty$, the solution Y_∞ is time-invariant and to be obtained by the techniques of the previous section. We assume now that we know Y_∞, and hence we can start up the recursion given by (3), going back in time, and computing Y_k from Y_{k+1}, which is done by a simple QR-factorization. Interesting things start to happen when we reach the LTI part for $k \to -\infty$. The present case is substantially different from the LTI-case in that the isometric factor V does not necessarily become LTI again, but will have a special structure closely related to the invertibility properties of T. Our goal in this section is to determine that structure.

Two simple examples, taken from [12], should illustrate the point.

Example 1. Let

$$T = \left[\begin{array}{ccc|ccccc} \ddots & \ddots & & & & & & \\ & 1 & -\frac{1}{2} & & & & & \\ & & 1 & -\frac{1}{2} & & & & \\ \hline & & & \boxed{1} & -2 & & & \\ & & & & 1 & -2 & & \\ & & & & & 1 & -2 & \\ & & & & & & \ddots & \ddots \end{array}\right].$$

Then it is easy to see that $Ty = 0$ for $y^* = [\cdots, \frac{1}{4}, \frac{1}{2}, \boxed{1}, \frac{1}{2}, \frac{1}{4}, \cdots]$, hence T is not invertible, $\cdot T^*$ has a non-trivial kernel. T does have a right inverse, namely

$$T_r' = \left[\begin{array}{cccc|ccccc} \ddots & \ddots & \ddots & \vdots & & & & & \\ & 1 & \frac{1}{2} & \frac{1}{4} & & & & & \\ & & 1 & \frac{1}{2} & & & & & \\ & & & 1 & & & & & \\ \hline & & & & \boxed{0} & & & & \\ & & & & -\frac{1}{2} & 0 & & & \\ & & & & -\frac{1}{4} & -\frac{1}{2} & 0 & & \\ & & & & \vdots & \ddots & \ddots & \ddots & \end{array}\right].$$

However, this is not the Moore–Penrose pseudo-inverse. To obtain the latter we should compute $T = T_o V$ to find $T^\dagger = V^* T_o^{-1}$, since in this case T_o will already be outer. The computation of V starts out LTI for $k > 0$ (Case I). If we choose for T the realization:

$$\begin{aligned} A_k &= 0 \quad \forall k, \\ B_k &= 1 \quad \forall k, \\ C_k &= \begin{cases} -\frac{1}{2} & \text{for } k \leqslant 0, \\ -2 & \text{for } k > 0, \end{cases} \\ D_k &= 1 \quad \forall k, \end{aligned}$$

then $Y_\infty = \sqrt{3}$. We find $\lim_{k\to-\infty} Y_k = 0$, from which follows that for $k \to -\infty$,

$$\lim_{k\to-\infty} \begin{bmatrix} A_{Vk} & B_{Vk} \\ C_{Vk} & D_{Vk} \end{bmatrix} = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}.$$

In other words, the state of the isometric system 'disappears', it becomes (almost) uncontrollable and unobservable, although the transition matrix stays unitary. Although V has at all times a unitary realization, it is not an inner system because it shares the right kernel with T and hence has no inverse.

Example 2. The second example is much like the first except that the numerical values are now reversed:

$$T = \left[\begin{array}{ccc|ccccc} \ddots & \ddots & & & & & & \\ & 1 & -2 & & & & & \\ & & 1 & -2 & & & & \\ \hline & & & \boxed{1} & -\frac{1}{2} & & & \\ & & & & 1 & -\frac{1}{2} & & \\ & & & & & 1 & -\frac{1}{2} & \\ & & & & & & \ddots & \ddots \end{array}\right].$$

The $+\infty$ LTI system is now outer. Hence $Y_\infty = [\cdot]$ is empty, and it will stay that way all through the recursion $k \to -\infty$. Hence, this T is already left-outer—a fact that we could have guessed from the existence of the right-inverse in the preceeding example, adapted to the present case.

The left outer–inner factorization for T produces $T = T_{o\ell}V$ in which V has an isometric realization $A_{Vk}, B_{Vk}, C_{Vk}, D_{Vk}$. The square root algorithm given in Theorem 2 produces a unitary right factor

$$\mathbf{W}_k = \begin{bmatrix} A_{Wk} & C_{Wk} \\ B_{Wk} & D_{Wk} \end{bmatrix} = \begin{bmatrix} A_{Vk} & C_{Vk} \\ B_{Vk} & D_{Vk} \\ B_{Uk} & D_{Uk} \end{bmatrix}$$

and contains a causal isometric sub-operator U with realization $\{A_{Vk}, B_{Uk}, C_{Vk}, D_{Uk}\}$. This operator satisfies $UT^* = 0$—outputs of the type yU belong to the kernel of $\cdot T^*$ (the 'column-nullspace'). But, as we saw in the examples, the kernel of $\cdot T^*$ can be larger. We shall say that signals in $\ell_2(-\infty, \infty)$, which are in the kernel of $\cdot T^*$ and are not contained in any $\ell_2(k, \infty)$ for any k belong to the 'right defect space of T', an orthonormal basis for which we shall denote with $\mathbf{q}_o(T)$. The following properties hold and are proven in [12]:

(1) $\mathbf{q}_o(T) = \mathbf{q}_o(W)$;
(2) W will be inner iff $\mathbf{q}_o(T)(= \mathbf{q}_o(W))$ vanishes;
(3) In the recursion (3) for $k \to -\infty$, Y_k can be chosen in such a way that

$$\lim_{k\to-\infty} Y_k = \begin{bmatrix} Y_{-\infty} \\ 0 \end{bmatrix},$$

and the realization $\{A_{Wk}, B_{Wk}, C_{Wk}, D_{Wk}\}$ for $\mathbf{W}_k$ converges for $k \to -\infty$ to the form

$$\begin{aligned} A_{Wk} &= \begin{bmatrix} A_{W,-\infty} & 0 \\ 0 & I \end{bmatrix}, \qquad B_{Wk} = \begin{bmatrix} B_{W,-\infty} & 0 \end{bmatrix}, \\ C_{Wk} &= \begin{bmatrix} C_{W,-\infty} \\ 0 \end{bmatrix}, \qquad D_{Wk} = D_{W,-\infty}, \end{aligned} \tag{30}$$

in which $\{A_{W,-\infty}, B_{W,-\infty}, C_{W,-\infty}, D_{W,-\infty}\}$ defines an LTI inner function $V_{-\infty}(z)$, which is such that $T_{-\infty}(z)V^*_{-\infty}(z)$ is analytic in the open unit disc (i.e. $V_{-\infty}(z)$ is a right factor of the full right inner factor $v_{-\infty}$ of $T_{-\infty}(z) = T_{o,-\infty}(z)v_{-\infty}(z)$—Example 2 shows readily that the two inner functions do not necessarily coincide).

To complete the characterization of the inverse, we must give an explicit computation of the defect space. We propose an algorithm based on a characterization of the observability space of W due to [12].

Proposition 3. *Let P_k be the orthogonal projection of $\ell_2(-\infty, +\infty)$ onto $\ell_2[k, \infty)$ (i.e. $(yP_k)_\ell = y_\ell$ for $\ell \geqslant k$ and otherwise zero). Then $\mathbf{q}_o(T)P_k$ spans a sub-space of the k*th *observability space of W, which is given by*

$$\text{span}[C_{Wk}, A_{Wk}C_{W,k+1}, A_{Wk}A_{W,k+1}C_{W,k+2}, \ldots).$$

The backward recursive computation starts with an orthonormal basis for $\mathbf{q}'_\infty$ of the LTI system at $+\infty$ given by (we use the notation $(\cdot)'$ for vectors whose right-hand zeros have been chopped off):

$$\mathbf{q}'_\infty = [C_V,\ A_V C_V,\ A_V^2 C_V,\ \cdots),$$

and proceeds recursively as follows:

Assume that at point $k+1$ an orthonormal basis of the observability space is

$$\mathbf{q}'_{k+1} \triangleq [C_{W,k+1}, A_{W,k+1}C_{W,k+2}, \ldots),$$

then after the recursive step of the square root algorithm, the kth basis is given by:

$$\mathbf{q}'_k = [C_{Wk}, A_{Wk}\mathbf{q}'_{k+1}),$$

until it reaches a time point k in the $-\infty$-LTI zone, where Y_k has converged to a stable value (see the properties detailed in the previous paragraph). This is evaluated numerically as follows. When k progresses towards $-\infty$, we find as SVD for Y_k determined by (3):

$$Y_k = U_k \begin{bmatrix} \Sigma_k & \\ & E_k \end{bmatrix} V_k,$$

in which the singular values captured by the diagonal matrix E_k are negligible and can be put to zero for practical purposes (in principle, Y_k should be right invertible, but that does not preclude near-zero singular values, corresponding to a part of it that goes to zero). From the limiting theory we know that $\text{span}(V_{k+1}) \approx \text{span}(V_k)$ when k has become small enough, this property can be tested, e.g. by checking whether $V_{k+1}V_k^*$ is nearly unitary. When that is the case, convergence has been established, and Y_k can be chosen equal to Y_{k+1}. In fact, U_k can then be absorbed in A_{Vk} and the value of

$$Y_{-\infty} = \begin{bmatrix} \Sigma_{k+1} & \\ & 0 \end{bmatrix} W_{k+1} \triangleq \begin{bmatrix} \Sigma_{-\infty} & \\ & 0 \end{bmatrix} W_{-\infty}$$

has been reached,

$$A_{W,-\infty} = \begin{bmatrix} A'_{W,-\infty} & \\ & I \end{bmatrix},$$

as well as limiting values for the other realization matrices, yielding the values for the matrices in (30). With k in the convergence zone, we find for the defect space

$$\mathbf{q}_o P_k = [0\ I]\mathbf{q}'_k,$$

in which $[0\ I]$ is conformal the decomposition for $Y_{-\infty}$. The actual $\mathbf{q}_o$ is then found simply by extending $\mathbf{q}_o P_k$ to the left with zeros (the 'tail' goes to zero geometrically, see the formula in Proposition 3). The examples in Section 6 should clarify the procedure.

6. Example

Let T be given by the realization

$$\mathbf{T}_k = \left[\begin{array}{cc|c} 0.5 & 1 & 1 \\ 0 & 0.5 & 1 \\ \hline 2.5 & 1 & 1 \end{array}\right] (k \leqslant 0), \qquad \mathbf{T}_k = \left[\begin{array}{cc|c} 0.5 & 2.333 & 1 \\ 0 & 0.333 & 1 \\ \hline 2.5 & 2.333 & 1 \end{array}\right] (k \geqslant 1).$$

For $k > 0$, the LTI realization has a double zero at $-\frac{1}{2}$, for $k \leq 0$, the LTI part has a zero at $-\frac{1}{2}$ and one at -2. The inner factor will keep only the zero at $-\frac{1}{2}$ as a pole, whereas the squelching of the second zero will generate a defect space of dimension 1.

An initial point Y_∞ for the backward recursion (3) is given by the procedure in Section 4, Case I. This gives

$$Y_k = \begin{bmatrix} 0.891 & 0.530 \\ 0 & 0.742 \end{bmatrix}, \quad k = +\infty, \ldots, 1.$$

Continuing now the recursion, we find successively

$$Y_0 = \begin{bmatrix} 0.733 & 0.824 \\ 0 & 0.298 \end{bmatrix}, \quad Y_{-1} = \begin{bmatrix} 0.536 & 0.781 \\ 0 & 0.143 \end{bmatrix}, \quad Y_{-2} = \begin{bmatrix} 0.461 & 0.735 \\ 0 & 0.071 \end{bmatrix},$$

$$Y_{-3} = \begin{bmatrix} 0.432 & 0.711 \\ 0 & 0.035 \end{bmatrix}, \quad Y_{-4} = \begin{bmatrix} 0.422 & 0.700 \\ 0 & 0.018 \end{bmatrix}, \quad Y_{-5} = \begin{bmatrix} 0.418 & 0.695 \\ 0 & 0.009 \end{bmatrix},$$

$$Y_{-6} = \begin{bmatrix} 0.416 & 0.694 \\ 0 & 0.004 \end{bmatrix}, \quad Y_{-7} = \begin{bmatrix} 0.416 & 0.693 \\ 0 & 0.002 \end{bmatrix}, \quad Y_{-8} = \begin{bmatrix} 0.416 & 0.693 \\ 0 & 0.001 \end{bmatrix},$$

$$Y_{-9} = \begin{bmatrix} 0.416 & 0.693 \\ 0 & 0.001 \end{bmatrix}, \quad Y_{-10} = \begin{bmatrix} 0.416 & 0.693 \\ 0 & 0.000 \end{bmatrix}.$$

At this point, we decide that the second row of Y is too small to keep. It is dropped: we continue with

$$Y_{-11} = \begin{bmatrix} 0.416 & 0.693 \end{bmatrix}$$

and we have reached a stationary value for Y_k, $k \to -\infty$.

The corresponding outer factor has a realization given by

$$\mathbf{T}_{ok} = \left[\begin{array}{cc|c} 0.5 & 1 & 1.280 \\ 0 & 0.5 & 0.800 \\ \hline 2.5 & 1 & 2 \end{array}\right] \quad (k \leqslant -12), \quad \mathbf{T}_{o-11} = \left[\begin{array}{cc|c} 0.5 & 1 & 1.280 \\ 0 & 0.5 & 0.800 \\ \hline 2.5 & 1 & 2 \end{array}\right],$$

$$\mathbf{T}_{o-10} = \left[\begin{array}{cc|c} 0.5 & 1 & 1.280 \\ 0 & 0.5 & 0.800 \\ \hline 2.5 & 1 & 2 \end{array}\right], \quad \mathbf{T}_{o-9} = \left[\begin{array}{cc|c} 0.5 & 1 & 1.280 \\ 0 & 0.5 & 0.800 \\ \hline 2.5 & 1 & 2 \end{array}\right],$$

$$\mathbf{T}_{o-8} = \left[\begin{array}{cc|c} 0.5 & 1 & 1.280 \\ 0 & 0.5 & 0.800 \\ \hline 2.5 & 1 & 2.001 \end{array}\right], \quad \mathbf{T}_{o-7} = \left[\begin{array}{cc|c} 0.5 & 1 & 1.281 \\ 0 & 0.5 & 0.800 \\ \hline 2.5 & 1 & 2.002 \end{array}\right],$$

$$\mathbf{T}_{o-6} = \left[\begin{array}{cc|c} 0.5 & 1 & 1.282 \\ 0 & 0.5 & 0.800 \\ \hline 2.5 & 1 & 2.007 \end{array}\right], \quad \mathbf{T}_{o-5} = \left[\begin{array}{cc|c} 0.5 & 1 & 1.287 \\ 0 & 0.5 & 0.799 \\ \hline 2.5 & 1 & 2.019 \end{array}\right],$$

$$\mathbf{T}_{o-4} = \left[\begin{array}{cc|c} 0.5 & 1 & 1.297 \\ 0 & 0.5 & 0.798 \\ \hline 2.5 & 1 & 2.052 \end{array}\right], \quad \mathbf{T}_{o-3} = \left[\begin{array}{cc|c} 0.5 & 1 & 1.323 \\ 0 & 0.5 & 0.794 \\ \hline 2.5 & 1 & 2.137 \end{array}\right],$$

$$\mathbf{T}_{o-2} = \left[\begin{array}{cc|c} 0.5 & 1 & 1.381 \\ 0 & 0.5 & 0.783 \\ \hline 2.5 & 1 & 2.349 \end{array}\right], \quad \mathbf{T}_{o-1} = \left[\begin{array}{cc|c} 0.5 & 1 & 1.490 \\ 0 & 0.5 & 0.749 \\ \hline 2.5 & 1 & 2.855 \end{array}\right],$$

$$\mathbf{T}_{o0} = \left[\begin{array}{cc|c} 0.5 & 1 & 1.402 \\ 0 & 0.5 & 0.663 \\ \hline 2.5 & 1 & 3.025 \end{array}\right], \quad \mathbf{T}_{ok} = \left[\begin{array}{cc|c} 0.5 & 2.333 & 2.457 \\ 0 & 0.333 & 0.510 \\ \hline 2.5 & 2.333 & 4 \end{array}\right] \quad (k \geqslant 1).$$

The inner factor has realization (note the change of state dimension induced by the dimension change of Y_k)

$$\mathbf{V}_k = \left[\begin{array}{cc|c} -0.500 & 0.866 \\ \hline 0.866 & 0.500 \end{array}\right] \quad (k \leqslant -12), \quad \mathbf{V}_{-11} = \left[\begin{array}{cc|c} -0.500 & 0 & 0.866 \\ \hline 0.866 & 0 & 0.500 \end{array}\right],$$

$$\mathbf{V}_{-10} = \left[\begin{array}{cc|c} -0.500 & 0 & 0.866 \\ 0 & -1 & 0.001 \\ \hline 0.866 & 0 & 0.500 \end{array}\right], \quad \mathbf{V}_{-9} = \left[\begin{array}{cc|c} -0.500 & 0.001 & 0.866 \\ 0 & -1 & 0.001 \\ \hline 0.866 & 0.001 & 0.500 \end{array}\right],$$

$$\mathbf{V}_{-8} = \left[\begin{array}{cc|c} -0.500 & 0.002 & 0.866 \\ 0 & -1 & 0.002 \\ \hline 0.866 & 0.001 & 0.500 \end{array}\right], \quad \mathbf{V}_{-7} = \left[\begin{array}{cc|c} -0.499 & 0.004 & 0.866 \\ 0 & -1 & 0.004 \\ \hline 0.866 & 0.002 & 0.499 \end{array}\right],$$

$$\mathbf{V}_{-6} = \left[\begin{array}{cc|c} -0.498 & 0.008 & 0.867 \\ 0 & -1 & 0.009 \\ \hline 0.867 & 0.004 & 0.498 \end{array}\right], \quad \mathbf{V}_{-5} = \left[\begin{array}{cc|c} -0.495 & 0.015 & 0.869 \\ 0 & -1 & 0.018 \\ \hline 0.869 & 0.009 & 0.495 \end{array}\right],$$

$$\mathbf{V}_{-4} = \left[\begin{array}{cc|c} -0.488 & 0.031 & 0.873 \\ 0 & -0.999 & 0.035 \\ \hline 0.873 & 0.017 & 0.487 \end{array}\right], \quad \mathbf{V}_{-3} = \left[\begin{array}{cc|c} -0.469 & 0.062 & 0.881 \\ 0 & -0.998 & 0.071 \\ \hline 0.883 & 0.033 & 0.468 \end{array}\right],$$

$$\mathbf{V}_{-2} = \left[\begin{array}{ccc} -0.430 & 0.128 & 0.894 \\ 0 & -0.990 & 0.141 \\ \hline 0.903 & 0.061 & 0.426 \end{array}\right], \quad \mathbf{V}_{-1} = \left[\begin{array}{ccc} -0.365 & 0.266 & 0.892 \\ 0 & -0.958 & 0.286 \\ \hline 0.931 & 0.104 & 0.350 \end{array}\right],$$

$$\mathbf{V}_0 = \left[\begin{array}{ccc} -0.412 & 0.543 & 0.732 \\ 0 & -0.803 & 0.596 \\ \hline 0.911 & 0.245 & 0.331 \end{array}\right],$$

$$\mathbf{V}_k = \left[\begin{array}{ccc} -0.500 & 0.750 & 0.433 \\ 0 & -0.500 & 0.866 \\ \hline 0.866 & 0.433 & 0.250 \end{array}\right] \quad (k \geqslant 1).$$

Note that $\mathbf{V}_{-\infty}$ is equal to the LTI solution, but only after we drop the state corresponding to the defect space. From the observability space of V, we deduce that a basis for this space is

$$\mathbf{q}_o = \begin{bmatrix} \cdots & 0.001 & -0.001 & 0.002 & -0.004 & 0.009 & -0.018 & 0.035 & -0.070 \\ & 0.141 & -0.282 & \boxed{0.564} & -0.658 & 0.329 & -0.164 & 0.082 & -0.041 \\ & 0.021 & -0.010 & 0.005 & -0.003 & 0.001 & \cdots & & \end{bmatrix}$$

7. Discussion

The representation of systems of equations by state-space models opens up new perspectives for system inversion. The classical *QR* or *LQ* algorithm gets replaced by upper–lower transformations, inner–outer factorizations and combinations of these. The inner–outer factorization determines in all cases how the inverse or pseudo-inverse is divided between the upper and lower part, and necessitates an eigenvalue decomposition, or, in the worst case, either the solution of a regular, discrete-time Riccati equation or a doubling procedure. At no point in the procedure eigenvalues on the boundary of a Hamiltonian matrix have to be determined. In the IVI-case—the main point of interest in the present paper—the LTI theory plays an important role as starting point for the recursions. However, as the recursion proceeds, a new phenomenon starts to appear, called the defect space. Its incidence has been neglected in the literature, sometimes leading to incorrect statements.

An important point deserves attention: the relation between 'outer' and 'invertible'. Throughout the paper, we have assumed the two notions to be equivalent. This statement must be mitigated. If we consider classical Hardy space theory on the unit disc $\mathbf{T}$ of the complex plane, then $f \in H_\infty$ is said to be outer if $\overline{H_2 f} = H_2$. If it is true that also $H_2 f = H_2$, then f has an inverse which is in H_∞, and we can say that f is 'strictly outer'. However, the more general case often occurs. For example, $f = 1 - z$ is outer, but its inverse is not in H_∞ (not even in L_2 of the unit circle). However, it can be approximated by functions in H_2, e.g. by $g_\rho = 1/(z - \rho)$ for $\rho > 1$ in the sense that $g_\rho f$ can be made as close to 1 as desired in the $L_2(\mathbf{T})$ sense. Clearly, f then has a practical inverse, i.e. a function that approximates the inverse as closely as desired, in a strong sense. In such a case f cannot have zeros inside

the unit disc. Surprisingly, this theory generalizes to the matrix case and even to the time-varying case as is amply discussed in the book [12]. Suppose now that we have a (time-varying) realization of an outer operator

$$T_o = D + BZ(I - AZ)^{-1}C,$$

then a bounded, approximate inverse will be given by

$$T'_\rho = D^{-1} - D^{-1}BZ(I - \rho\Delta Z)^{-1}CD^{-1},$$

in which $\Delta = A - CD^{-1}B$, $\rho > 1$ and $\rho \approx 1$. In practice, people will just put $\rho = 1$, of course, the resulting transfer function will not be ues anymore, but will be stable for some weaker criteria.

We terminate with some words on the discrete time Riccati equation. If one attempts to solve the algebraic Riccati equation (7) directly for the LTI case, then the chance that one will hit a singular case, i.e. a case with zeros on the boundary is very high. We have shown in this paper that we can always avoid this, by approaching the problem from the square root viewpoint. We cannot avoid the Riccati equation or spectral factorization altogether, in Case III we have to solve an instance of it, but it is a regular one, without zeros on the boundary. Case III is very interesting because of the connection to Kalman filtering, Darlington synthesis and range function theory.

Although we do present a consistent and complete set of algorithms, a number of points are not well settled yet. We believe that our solution for Case I is the most efficient and stable one can device, although an argument can be made that the doubling procedure of Case III could simply be used for Case I as well. This would not be advisable numerically. The main interest of doing Case I the way we have presented (by solving a restricted eigenvalue problem) is that a reduced degree for the inner factor is guaranteed to come out. If one would use the doubling procedure (or the Riccati method), then the resulting inner function would automatically be of full degree, and a lot of cancellations would occur. This would introduce a very undesirable numerical instability. In Case II, the resulting degree of the inner factor is even lower. Here a procedure which would directly determine the zeros inside the unit disc of the overall system would certainly be an improvement. The most problematic are Cases III and IV. Although the algorithms given are valid and effective, the essential polynomial extraction (zero displacement procedure from the unit circle) could be done in a global way. It is possible to combine the sequence of zero extractions, but the resulting formulas are complex and messy. Furthermore, the doubling algorithm looks nice in first instance, but from a numerical point of view it should be refined. First, the matrix Δ should be put in Schur form, and kept that way in the succeeding steps. Attention to a minimal number of algebraic operations is essential, utilization of Hessenberg forms might be a solution. Still this seems to be much better than the determination of eigenvalues on the Hamiltonian matrix, because the recursive algorithm is inherently stable and therefore can always refine a result that has been obtained by a quick and dirty procedure.

The final word on what are the best numerical methods for inner–outer factorization requires further investigations!

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Appendix A. Solving the LTI Lyapunov–Stein equation

Let us assume that we want to solve the Lyapunov–Stein equation

$$M = AMA^* + CC^*,$$

in which A is strictly stable. There are two classical ways. One solves it in quadratic form by first performing a Schur eigenvalue decomposition on A and then expressing the solution in terms of the eigenvalues and the component vectors of the Schur decomposition [5]. (The Bartels–Stewart method handles the 'continuous time' problem $AX + XB = C$ problem but can easily be adapted to the present case. The method does not require A to be ues, a solution will exist if there are no pairs of eigenvalues λ_j and λ_k such that $1 - \lambda_j \lambda_k^* = 0$. For further evolution of the method, see the papers in the survey book [28].) The other solves the equation iteratively in square root form, and uses a doubling procedure, for efficiency. Since the latter procedure may not be so well known, we give a brief survey. Let $M = RR^*$. Then the square root equivalent of the Lyapunov–Stein equation is

$$[A\,R\;C] = [R\;0]V, \tag{A.1}$$

in which V is unitary. If R were known and lower triangular, then (A.1) would amount to an LQ-factorization, with V for Q. But R is not known except for the general theoretical expression

$$M = RR^* = \sum_{i=0}^{\infty} A^i CC^* A^{*i}.$$

The doubling iteration works as follows:

Step 0. Initialize R_0 square by either extending C, $R_0 = [C\;0]$ if C has more rows than columns, or else by computing $C = LQ$ in which L is lower triangular and Q orthogonal, in which case one puts $R_0 = L$.

Step 1. $[A\,R_0\;R_0] = [R_1\;0]V_1$ by an LQ-factorization which makes R_1 lower; also, compute $A_2 = A^2$,

General step n. $[A_n\,R_{n-1}\;R_{n-1}] = [R_n\;0]V_n$, $A_{n+1} = A_n^2$ to produce a lower R_n, again using an LQ factorization.

It is easy to see, by squaring, that the algorithm computes the square root of the partial sum of M consisting of the first 2^n terms. It converges very quickly, and is very well suited for 'stiff' problems, i.e. problems in which A has eigenvalues of widely different amplitudes. Several variations are possible, depending on the structure of A, and a combination with the algorithm that computes eigenvalues of A is also possible.

Appendix B. Computation of the upper echelon form

A matrix has the *strict upper echelon form* if it looks like

$$\begin{bmatrix} \vdots & \vdots & & \vdots \\ * & \cdot & & \cdot \\ \text{`0'} & \vdots & \ddots & \vdots \\ 0 & * & & \cdot \\ \text{`0'} & \text{`0'} & & \vdots \\ 0 & 0 & & * \\ \text{`0'} & \text{`0'} & & \text{`0'} \end{bmatrix}$$

in which the entries indicated by $*$ must be non-zero (they can be chosen strictly positive), and the entries between '0' indicate a vertical sequence of zeros, which may disappear. Notice that such a matrix has right-kernel zero and hence a left (pseudo-) inverse. A matrix will have upper echelon form if it consists of columns of zeros followed by a strict upper echelon matrix. The defining property for a matrix X to be in upper echelon form is that for each column i there is an index k_i such that k_i is either zero or $k_i > k_{i-1}$, $X_{k_i,i} \neq 0$, and $X_{\ell,i} = 0$ for $\ell > k_i$. An arbitrary matrix can be brought to upper echelon form through a sequence of Jacobi transformations applied to the right to the columns of the matrix. For example, suppose

$$\begin{bmatrix} a_1 & b_1 \\ \vdots & \vdots \\ a_n & b_n \end{bmatrix}$$

are two columns such that $|a_n|^2 + |b_n|^2 > 0$, then

$$\begin{bmatrix} a_1 & b_1 \\ \vdots & \vdots \\ a_n & b_n \end{bmatrix} \frac{1}{\sqrt{|a_n|^2 + |b_n|^2}} \begin{bmatrix} b_n & a_n^* \\ -a_n & b_n^* \end{bmatrix} = \begin{bmatrix} a'_1 & b'_1 \\ \vdots & \vdots \\ a'_{n-1} & b'_{n-1} \\ 0 & \sqrt{|a_n|^2 + |b_n|^2} \end{bmatrix},$$

which is in upper echelon form. It should be clear that recursive applications of such transformations on the rows of a general matrix can bring it to echelon form. One starts the algorithm bottom up from the right and annihilates as many entries as possible while accumulating 'energy' towards the upper-right corner. Notice that the algorithm actually defines the unitary transformations needed and also yields the right-hand side of the equation as a result. In our case, the matrix block decomposition, and some reordering of block rows produces

$$\left[\begin{array}{c|c} A_k Y_{k+1} & C_k \\ \hline B_k Y_{k+1} & D_k \end{array}\right] W_k^* = \left[\begin{array}{c|c|c} 0 & Y_k & C_{ok} \\ \hline 0 & 0 & D_{ok} \end{array}\right],$$

in which the unitary matrix W_k has the conformal block decomposition

$$W_k = \left[\begin{array}{c|c} B_{Uk} & D_{Uk} \\ \hline A_{Vk} & C_{Vk} \\ \hline B_{Vk} & D_{Vk} \end{array}\right]$$

and quite a few entries are possibly empty (even Y_k or Y_{k+1} can be empty, they are rectangular matrices in general), but the algorithm certainly produces Y_k and D_{ok} in strict upper echelon form, hence satisfying the required kernel condition. Q_k^* and the right-hand side are defined by the procedure. They are 'essentially' unique, i.e. unique except for trivial transformations, which we do not wish to make explicit here.

Appendix C. Extraction of a multiple zero on the unit circle

Let a be a (candidate) zero on the unit circle. The procedure to extract a poynomial $P(z)$ from $T(z)$ such that $T(z) = P(z)T'(z)$, $P(z)$ is a minimal polynomial and $T'(z)$ has no zero at a (i.e. has full rank at a) can best be explained if a linear coordinate transformation that puts a at the origin of the complex plane is first executed. It makes the notation easier, and as we shall see, it allows us also to use classical Hardy space results directly. Thus, we first make the transformation $\xi = z - a$. Then, with $A_a = A(I - aA)^{-1}$

$$\begin{aligned} T = {} & [d + \beta a(I - aA)^{-1}\gamma] \\ & + \beta(I - aA)^{-1}\xi(I - \xi A_a)^{-1}(I - aA)^{-1}\gamma \end{aligned} \tag{C.1}$$

or the transition matrix changes to

$$\begin{bmatrix} A(I - aA)^{-1} & (I - aA)^{-1}\gamma \\ \beta(I - aA)^{-1} & d + \beta a(I - aA)^{-1}\gamma \end{bmatrix}.$$

The surplus theory alluded to before produces a characterization of the zero now at $\xi = 0$ from a Maclaurin series expansion at zero. Let

$$T = T_0 + \xi T_1 + \xi^2 T_2 + \cdots \in \mathbb{C}^{m\times n}[\xi].$$

We wish to find $P(\xi)$ polynomial such that $P(\xi)^{-1}T = T'$ has rank m at $\xi = 0$. We look for (and will find) a $P(\xi)$ which has zeros at zero and poles at ∞, i.e. $P^{-1}(\xi)$ is a polynomial in ξ^{-1}. We go a step further and require that $P(\xi)$ be inner (this restriction makes the solution essentially unique). Let $\{A_P, B_P, C_P, D_P\}$ be a realization for $P(\xi)$ ($P(\xi) = D_P + B_P\xi(I - A_P\xi)^{-1}C_P$). Let $\mathbf{D}$ be a small enough disc centered around $\xi = 0$ so that there are no other zeros of T in it, and let us denote by T_ξ the expression of T in terms of ξ. Then $\xi = 0$ is the only zero of T_ξ in $\mathbf{D}$,

we have $T_\xi H_2^n(\mathbf{D}) \subset H_2^m(\mathbf{D})$ and $P(\xi)$ will have to meet the condition $T_\xi H_2^n(\mathbf{D}) = P(\xi)H_2^m(\mathbf{D})$. It turns out that this latter space is actually fully characterized by the reachability parameters of P when P is unitary:

Lemma C.1. *A_P and B_P are a maximal reachable pair such that*

$$\xi^*(I - \xi^* A_P^*)^{-1} B_P^* T_\xi$$

is analytic in a neighborhood of $\xi = 0$.

Working out, we must find a maximal observable pair and order k such that

$$\begin{bmatrix} A_P^{*(k-1)}B_P^* & \cdots & B_P^* \\ & \ddots & \vdots \\ 0 & & A_P^{*(k-1)}B_P^* \end{bmatrix} \begin{bmatrix} T_0 & T_1 & \cdots & T_{k-1} \\ & T_0 & & \vdots \\ & & \ddots & \vdots \\ & & & T_0 \end{bmatrix} = 0. \tag{C.2}$$

To solve this set of structured equations in a non-redundant way, we proceed in two phases. First we construct elements of a basis for the right nullspace of the right Toeplitz matrix recursively. Next, we shall order these components in such a way that they fit the shift invariant structure of the reachability space sought.

C.1. Phase 1: components of the nullspace

Step 0. Find U_{00} whose rows form a basis for the right nullspace $\mathscr{R}_0$ of T_0

$$U_{00}T_0 = 0.$$

Finding a nullspace is a classical procedure in numerical analysis, it is done using either an SVD or a rank-revealing QR-factorization on T_0.

Step 1. Find $[U_{10} \;\; U_{11}]$ whose rows form a basis and which is such that (1) $U_{10}T_0 = 0$ and (2) $U_{10}T_1 + U_{11}T_0 = 0$. Since U_{10} will span a sub-space of the span of the rows of U_{00}, there will be a right invertible matrix X_1 such that $U_{10} = X_1 U_{00}$. The rows of X_1 constitute a basis for the space

$$\mathscr{R}_1 = \mathscr{R}(\cdot U_{00}T_1) \cap \mathscr{R}(\cdot T_0)$$

(where '$\mathscr{R}(\cdot X)$' denotes the range of the rows of the matrix X).

The determination of X_1 is a little more elaborate than the computation of a simple nullspace since the intersect of two spaces is involved, a simple numerically stable algorithm uses an RQ-transformation to determine an adequate basis of one of the row-spaces and to rotate that basis to the span of the first natural base vectors. If the same rotation is applied to the other span, then the intersection can be determined via a simple range-kernel decomposition or an SVD on the remaining entries.

Step ℓ. This step is generic. When it delivers an empty space, then the procedure has terminated (the last non-trivial step gives the order $k = \ell$ of the zero). Find $[U_{\ell 0}\ U_{\ell 1}\ \cdots\ U_{\ell\ell}]$ such that $U_{\ell 0}$ has zero left kernel and is such that it lays in the kernel of the blok Toeplitz operator with $\ell + 1$ blocks

$$\begin{bmatrix} T_0 & \cdots & T_\ell \\ & \ddots & \vdots \\ & & T_0 \end{bmatrix}.$$

Since this condition implies that $[U_{\ell 0}\ \cdots\ U_{\ell\ell-1}]$ lays in the kernel of a similar block Toeplitz operator with one block row and column less, there must exist a right invertible matrix X_ℓ such that

$$[U_{\ell 0}\ \cdots\ U_{\ell,\ell-1}] = X_\ell [U_{\ell-1,0}\ \cdots\ U_{\ell-1,\ell-1}].$$

X_ℓ will be a solution if its rows form a basis for the space

$$\mathscr{R}(\cdot[U_{\ell 0}T_\ell + \cdots + U_{\ell,\ell-1}T_1]) \cap \mathscr{R}(\cdot T_0).$$

This is can again be done by the intersection procedure described above.

C.2. Phase 2: construction of A_P, B_P

Starting from a basis for $U_{\ell 0}$ and the corresponding basis of order ℓ, $[U_{\ell 0}\ U_{\ell 1}\ \cdots\ U_{\ell\ell}]$, we transform the lower order bases so that they incorporate the base vectors of the higher order elements already defined. This leads to the following tableau, in which we denote the elements of B_P so obtained by lower case 'b's:

$$\begin{aligned} \begin{bmatrix} b^*_{\ell 0} & b^*_{\ell 1} & \cdots & b^*_{\ell\ell} \end{bmatrix} &= [U_{\ell 0}\ U_{\ell 1}\ \cdots\ U_{\ell\ell}] \\ \begin{bmatrix} b^*_{\ell-1,0} & \cdots & b^*_{\ell-1,\ell-1} \\ b^*_{\ell 0} & \cdots & b_{\ell,\ell-1} \end{bmatrix} &\approx [U_{\ell-1,0}\ \cdots\ U_{\ell-1,\ell-1}] \\ &\cdots \\ \begin{bmatrix} b^*_{\ell,0} \\ \vdots \\ b^*_{00} \end{bmatrix} &\approx [U_{00}]. \end{aligned} \tag{C.3}$$

The result is:

$$B_P = \left[b^*_{\ell,0}\ \ b^*_{\ell,1}\ \cdots\ b^*_{\ell,\ell} \,\middle|\, b^*_{\ell-1,0}\ \ b^*_{\ell-1,1}\ \cdots\ b^*_{\ell-1,\ell-1} \,\middle|\, \cdots \,\middle|\, b^*_{00} \right]$$

and A_P is a block Jordan matrix of the form:

$$A_P = \left[\begin{array}{cccc|cccc|c|c} 0 & I & \cdots & 0 & & & & & & \\ & 0 & \ddots & \vdots & & & & & & \\ & & \ddots & I & & & & & & \\ & & & 0 & & & & & & \\ \hline & & & & 0 & I & \cdots & 0 & & \\ & & & & & 0 & \ddots & \vdots & & \\ & & & & & & \ddots & I & & \\ & & & & & & & 0 & & \\ \hline & & & & & & & & \ddots & \\ \hline & & & & & & & & & 0 \end{array}\right].$$

(The proof of these results is of course classical and akin to the construction of the Jordan canonical form.)

Appendix D. Proof of convergence

Let $\mathbf{R}_-[n]$ be the lower-right bottom corner sub-matrix of $\mathbf{R}_-$ of dimensions $(n+1)\times(n+1)$, and let the factorization (25) be specialized to that bottom corner as

$$\mathbf{R}_-[n] = \mathbf{F}[n]\mathbf{F}[n]^*$$

with

$$\mathbf{F}[n] = \begin{bmatrix} d_{-n} & \beta c_{-n+1} & \cdots & \beta A^{n-1}c_0 \\ 0 & d_{-n+1} & \cdots & \beta A^{n-2}c_0 \\ & & \ddots & \vdots \\ & & & d_0 \end{bmatrix}$$

Because of the Cholesky property, $\mathbf{F}[n]$ is an invertible finite upper triangular matrix, and we can write

$$\mathbf{F}[n]^{-1}\mathbf{R}_-[n] = \mathbf{F}[n]^*.$$

Specialising this equation further to the first row, we find

$$\begin{bmatrix} d_{-n}^{-1} & f_{n,n-1} & \cdots & f_{n,0} \end{bmatrix}\mathbf{R}_-[n] = \begin{bmatrix} d_{-n}^* & 0 & \cdots & 0 \end{bmatrix}$$

for some (block) coefficients $f_{n,n-1}\cdots f_{n,0}$ which we leave unspecified. This actually identifies

$$F_n(z) \triangleq d_{-n}^{-1} + f_{n,n-1}z + \cdots f_{n,0}z^n$$

as the Szegö orthonormal (block) polynomial of order n belonging to the spectral function $R(z)$. From the Szegö theory (or Wiener–Masani theory, see [19] last chapter for a nice account), we now have the following properties of the Szegö integrals:

(1) $\int_{-\pi}^{\pi} \log|\det F_n(\mathrm{e}^{\mathrm{i}\theta})|^2 \frac{\mathrm{d}\theta}{2\pi} = \log|\det d_{-n}|^{-2}$.

(2) $\lim_{n\to\infty}(\int_{-\pi}^{\pi} \log|\det F_n(\mathrm{e}^{\mathrm{i}\theta})|^2 \frac{\mathrm{d}\theta}{2\pi}) = \int_{-\pi}^{\pi} \log|\det R(\mathrm{e}^{\mathrm{i}\theta})|\frac{\mathrm{d}\theta}{2\pi}$.

From the recursion (26) it is already clear that the limit $d_{-n}d_{-n}^*$ is bounded from below, the question is whether the limit is non-singular. This now follows from point (2) above, and the fact that $R(z)$ originates from a rational system, for which the Szegö integral is necessarily bounded. Hence $\lim_{n\to\infty} d_{-n} = d_o$ is non-singular. From the Szegö theory it also follows that $f_{n,n-k}$ converge for $n \to \infty$, let us say to f_{ok}, for any number of k (for a proof, see [9]). Let us take k equal to the dimension of A, then we find, for n large enough

$$\begin{bmatrix} \beta \\ \beta A \\ \vdots \\ \beta A^k \end{bmatrix} c_{-n+1} \approx \begin{bmatrix} f_{o1} \\ f_{o2} \\ \vdots \\ f_{ok} \end{bmatrix}$$

to any degree of approximation. Since the pair $\{A, \beta\}$ is assumed reachable by minimality of the realization for $T(z)$, c_{-n+1} must converge to

$$\lim_{n\to\infty} c_{-n+1} = \begin{bmatrix} \beta \\ \beta A \\ \vdots \\ \beta A^k \end{bmatrix}^{\dagger} \begin{bmatrix} f_{o1} \\ f_{o2} \\ \vdots \\ f_{ok} \end{bmatrix}.$$

With the c_{-n} converging, the convergence of M_{-k} becomes automatic since the spectral radius of A is assumed strictly within the unit disc.

Appendix E. The doubling procedure

We start out from expression (29) in which $T(z) = [T_1(z)\ T_2(z)]$ and the preliminary reductions have been done: $T_1(z)$ is outer and common zeros on the unit circle have been removed (this later point being essential in getting a numerically stable outer factor). $T(z)$ has a realization given by

$$\begin{bmatrix} A & \gamma_1 & \gamma_2 \\ \beta & d & 0 \end{bmatrix},$$

in which d is square non-singular. Our goal will be to find $M_o = \lim_{k\to\infty} m_k$ in square root form. The other quantities c_o and d_o then follow easily from the single recursion.

Step 1: *reduction to the 'Kalman case'*. Let

$$\begin{bmatrix} A & \gamma_1 & \gamma_2 \\ \beta & d & 0 \end{bmatrix} \begin{bmatrix} Y & & \\ & I & \\ & & I \end{bmatrix} = \begin{bmatrix} 0 & Y & C_o \\ 0 & 0 & D_o \end{bmatrix} W$$

with $\ker(Y\cdot) = 0$ and D_o square non-singular and W unitary. Then also

$$\begin{bmatrix} \Delta & 0 & \gamma_2 \\ d^{-1}\beta & I & 0 \end{bmatrix} \begin{bmatrix} Y & & \\ & I & \\ & & I \end{bmatrix} = \begin{bmatrix} 0 & Y & C_o - \gamma_1 d^{-1} D_o \\ 0 & 0 & d^{-1} D_o \end{bmatrix} W$$

with $\Delta = A - \gamma_1 d^{-1}\beta$. The equivalence is obtained via by premultiplication with the non-singular transformation matrix

$$\begin{bmatrix} I & -\gamma_1 d^{-1} \\ 0 & d^{-1} \end{bmatrix}.$$

Returning to the recursion for the determination of the outer factor (29) and the notation defined there), an application of the previous lemma brings it to the form

$$\begin{bmatrix} \Delta & 0 & \gamma \\ \beta & I & 0 \end{bmatrix} \begin{bmatrix} r_k & & \\ & I & \\ & & I \end{bmatrix} = \begin{bmatrix} 0 & r_{k+1} & c'_{k+1} \\ 0 & 0 & d'_{k+1} \end{bmatrix} Q_{k+1}$$

for some appropriately modified (and otherwise unimportant) c'_{k+1} and d'_{k+1}. In this expression, Δ is the transfer operator of the inverse of an outer function, and hence has spectral radius less or equal to one – by an appropriate state transformation it can be in fact be made contractive, e.g. by using an input or output normal form, we skip this operational detail. Note also the convenient redefinition of β and γ.

Step 2: *the linearization of the Riccati equation.*

Lemma E.1. *The relation*

$$\begin{bmatrix} \Delta & 0 & \gamma \\ \beta & I & 0 \end{bmatrix} \begin{bmatrix} r_k & & \\ & I & \\ & & I \end{bmatrix} = \begin{bmatrix} 0 & r_{k+1} & c'_{k+1} \\ 0 & 0 & d'_{k+1} \end{bmatrix} Q_{k+1},$$

with Q_{k+1} unitary, is equivalent to

$$\begin{bmatrix} m_{k+1} \\ b_k \end{bmatrix} = \Sigma \begin{bmatrix} m_k b_k \\ I \end{bmatrix}, \tag{E.1}$$

in which $m_k = r_k r_k^*$ is a minimal factorization, $b_k = (I + \beta^*\beta m_k)^{-1}\Delta^*$ is a well-defined intermediate quantity and

$$\Sigma = \begin{bmatrix} \Delta & \gamma\gamma^* \\ -\beta^*\beta & \Delta^* \end{bmatrix}.$$

Proof. $\Leftarrow$: The second equation in (E.1) gives

$$(I + \beta^*\beta m_k)b_k = \Delta^*.$$

It is easy to see that $(I + \beta^*\beta m_k)$ is always invertible, being of the form $(I + MN)$ with M and N positive definite, and hence the expression for b_k follows. Filling b_k in the first equation we obtain

$$m_{k+1} = \gamma\gamma^* + \Delta(I + \beta^*\beta m_k)^{-1}\Delta^*,$$

which can easily be transformed to the equivalent

$$m_{k+1} = \gamma\gamma^* + \Delta m_k\Delta^* - \Delta m_k\beta^*(I + \beta m_k\beta^*)^{-1}\beta m_k\Delta^*.$$

Introduce now a minimal factorization

$$I + \beta m_k\beta^* = d'_{k+1}d'^*_{k+1}$$

and define

$$c'_{k+1} = \Delta\beta^* d'^{-*}_{k+1}.$$

Then

$$\begin{aligned} \Delta m_k\Delta^* + \gamma\gamma^* &= m_{k+1} + c'_{k+1}c'^*_{k+1}, \\ \Delta m_k\beta^* &= c'_{k+1}d'^*_{k+1}, \\ \beta m_k\beta^* + I &= d'_{k+1}d'^*_{k+1}. \end{aligned}$$

Introducing minimal factorizations $m_k = r_k r_k^*$ and padding with zeros to equal out dimensions, we find

$$\begin{bmatrix} \Delta r_k & 0 & \gamma \\ \beta r_k & I & 0 \end{bmatrix} \begin{bmatrix} r_k^* & r_k^* \\ 0 & I \\ \gamma^* & 0 \end{bmatrix} = \begin{bmatrix} 0 & r_{k+1} & c'_{k+1} \\ 0 & 0 & d'_{k+1} \end{bmatrix} \begin{bmatrix} 0 & 0 \\ r_k^* & 0 \\ c'^*_{k+1} & d'^*_{k+1} \end{bmatrix}.$$

This is of the form $MM^* = NN^*$ with M and N matrices of equal dimensions. In that case there exists a unitary matrix Q such that $M = NQ$ and the property follows.

$\Rightarrow$: Retraces the steps in the opposite direction. □

Σ is what is known in classical circuit theory a 'hybrid matrix' linking input quantities at both sides of a circuit to output quantities also occurring at both sides. These quantities are of the 'voltage and current' type and not of the scattering type, see the discussion at the end of this section.

Step 3: *The doubling procedure.* The doubling procedure is obtained by chaining representations of the type (E.1) and is due to [23], for a scattering interpretation, see [4]. We state the property as a lemma.

Lemma E.2. *If*

$$\begin{bmatrix} m_2 \\ b_1 \end{bmatrix} = \Sigma \begin{bmatrix} m_1 b_1 \\ I \end{bmatrix} \tag{E.2}$$

with

$$\Sigma = \begin{bmatrix} \Delta & \gamma\gamma^* \\ -\beta^*\beta & \Delta^* \end{bmatrix},$$

then

$$\begin{bmatrix} m_4 \\ b_1 \end{bmatrix} = \Sigma_2 \begin{bmatrix} m_1 b_1 \\ I \end{bmatrix} \tag{E.3}$$

with

$$\Sigma_2 = \begin{bmatrix} \Delta_2 & \gamma_2\gamma_2^* \\ -\beta_2^*\beta_2 & \Delta_2^* \end{bmatrix},$$

in which

$$\Delta_2 = \Delta(I + \gamma\gamma^*\beta^*\beta)^{-1}\Delta$$

γ_2 *has minimal dimensions and is such that*

$$[\Delta\gamma(I + \gamma^*\beta^*\beta\gamma)^{-1/2} \;\; \gamma]q_1 = [\gamma_2 \;\; 0]$$

for some unitary transformation matrix q_1, *and* β_2 *has minimal dimensions and is such that*

$$[\Delta^*\beta^*(I + \beta\gamma\gamma^*\beta^*)^{-1/2} \;\; \beta^*]q_2 = [\beta_2^* \;\; 0]$$

for some unitary transformation q_2.

Proof (*By chaining*). If

$$\Sigma = \begin{bmatrix} r & s \\ t & u \end{bmatrix}$$

and both $(I - st)$ and $(I - ts)$ are invertible, then

$$\Sigma_2 = \begin{bmatrix} r(I - st)^{-1}r & s + r(I - st)^{-1}u \\ t + u(I - ts)^{-1}tr & u(I - ts)^{-1}u \end{bmatrix}. \tag{E.4}$$

The given formulas then follow by simple evaluation. □

Reverting back to Lemma E.1, we obtain the doubling algorithm for the computation of r_o with $M_o = r_o r_o^*$ as follows.

Algorithm E.1 (*Doubling algorithm*). *Startup:* find μ such that $\mu = \gamma\gamma^* + A\mu A^*$, let $r_1 \triangleq A\mu\beta^*(I + \beta\mu\beta^*)^{-1/2}$ (that is: in the original data, and with a slight renumbering, the new r_i equal the old r_{i-1}).

Generic step i: Given r_i compute r_{2i} via the *RQ* factorization:

$$\begin{bmatrix} \Delta_i r_i & 0 & \gamma_i \\ \beta_i r_i & I & 0 \end{bmatrix} = \begin{bmatrix} 0 & r_{2i} & * \\ 0 & 0 & * \end{bmatrix} Q_i$$

and update the parameters:

$$\begin{aligned} &\Delta_{2i} = \Delta_i (I + \gamma_i \gamma_i^* \beta_i^* \beta_i)^{-1} \Delta_i \\ &\left[\Delta_i \gamma_i (I + \gamma_i^* \beta_i^* \beta_i \gamma_i)^{-1/2} \ \gamma_i \right] q_{1,i} = [\gamma_{2i} \ 0] \\ &\left[\Delta_i^* \beta_i^* (I + \beta_i \gamma_i \gamma_i^* \beta_i^*)^{-1/2} \ \beta_i^* \right] q_{2,i} = [\beta_{2i}^* \ 0]. \end{aligned} \tag{E.5}$$

A number of remarks are in order:

1. When Δ is strictly contractive, the algorithm quickly converges to a limiting value in which $\Delta_\infty = 0$ and which is further given by

$$\begin{bmatrix} 0 & 0 & r_o \\ \beta_\infty r_o & I & 0 \end{bmatrix} = \begin{bmatrix} 0 & r_o & 0 \\ 0 & 0 & (I + \beta_\infty r_o^2 \beta_\infty^*)^{1/2} \end{bmatrix} Q$$

with a (simple) unitary Q. Convergence in the general case was shown in the previous appendix, its form can be derived and is beyond the present paper.

2. Once r_o and M_o are found, then the other quantities c_o and d_o quickly follow from the original recursion, which can also be used to check correctness, and improve on the obtained value.
3. Numerically, one would handle the various inverses by an SVD. Let $\kappa \triangleq \beta\gamma$. Then we must compute $\gamma(I + \kappa^*\kappa)^{-1/2}$, $\beta^*(I + \kappa\kappa^*)^{-1/2}$ and $I - \gamma(I - \kappa^*\kappa)^{-1}\kappa^*\beta$. With $\kappa = u\sigma v^*$ an SVD for κ, we find for these quantities, respectively: $\gamma v(I + \sigma^2)^{-1/2}v^*$, $\beta^* u(I + \sigma^2)^{-1/2}u^*$ and $I - \gamma v(\sigma(I + \sigma^2)^{-1})v^*\beta$.
4. Kailath et al. [4] call the matrix Σ a 'scattering matrix' and the composition (E.4) a 'Redheffer product'. We take issue with this viewpoint. Traditionally, Σ would be called a 'hybrid matrix' by circuit theorists, see e.g. [36, p. 17]. The composition in (E.4) is in fact a composition of hybrid matrices, which is not written down in that form in most classical textbooks, but is usually converted to the chain form and then written as a product, see e.g. [36, p. 22] Further argument for the statement that Σ should be regarded a hybrid matrix is provided by its algebraic properties (related to the algebraic properties of a Hamiltonian). We had, for the propagation of m_k

$$\begin{bmatrix} m_{k+1} \\ b_k \end{bmatrix} = \begin{bmatrix} \Delta & \gamma\gamma^* \\ -\beta^*\beta & \Delta^* \end{bmatrix} \begin{bmatrix} m_k b_k \\ I \end{bmatrix}.$$

Introducing a judicious $\mathrm{i} = \sqrt{-1}$ in the propagation chain, we find

$$\begin{bmatrix} \mathrm{i}m_{k+1} \\ b_k \end{bmatrix} = \begin{bmatrix} \Delta & \mathrm{i}\gamma\gamma^* \\ \mathrm{i}\beta^*\beta & \Delta^* \end{bmatrix} \begin{bmatrix} \mathrm{i}m_k b_k \\ I \end{bmatrix}.$$

The matrix

$$H \triangleq \begin{bmatrix} \Delta & \mathrm{i}\gamma\gamma^* \\ \mathrm{i}\beta^*\beta & \Delta^* \end{bmatrix}$$

is skew-Hermitian in the sense that $H^*E = EH$ for

$$E = \begin{bmatrix} 0 & I \\ -I & 0 \end{bmatrix}.$$

This corresponds classically to conservation of energy in the system

$$\begin{bmatrix} v_2 \\ i_1 \end{bmatrix} = H \begin{bmatrix} v_1 \\ i_2 \end{bmatrix},$$

in which v_k is interpreted as a voltage and i_k a current flowing from right to left ($k = 1, 2$). Further interpretations and additional numerical mileage may be obtained by substituting the shift z for i, but this goes beyond the scope of this paper.

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