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Positive definite Toeplitz matrices, the Arnoldi process for isometric operators, and Gaussian quadrature on the unit circle *

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Abstract

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We show that the well-known Levinson algorithm for computing the inverse Cholesky factorization of positive definite Toeplitz matrices can be viewed as a special case of a more general process. The latter process provides a very efficient implementation of the Arnoldi process when the underlying operator is isometric. This is analogous with the case of Hermitian operators where the Hessenberg matrix becomes tridiagonal and results in the Hermitian Lanczos process. We investigate the structure of the Hessenberg matrices in the isometric case and show that simple modifications of them move all their eigenvalues to the unit circle. These eigenvalues are then interpreted as abscissas for analogs of Gaussian quadrature, now on the unit circle instead of the real line. The trapezoidal rule appears as the analog of the Gauss–Legendre formula.

Keywords: Toeplitz matrices; unitary Hessenberg matrices; Szegő polynomials.

1. Generalities

The linear spaces $\mathbb{P}_{\mathbb{C}}$, of complex polynomials α , and \mathbb{C}_0^{∞} , of simply infinite (column) vectors a with finitely many nonnull elements, are isomorphic under the correspondence

$$\alpha(\zeta) = v(\zeta)^T a, \quad v(\zeta) := (1, \zeta, \zeta^2, \dots)^T.$$

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* This paper was presented during a visit to the Scientific Research Computing Center of Moscow State University on September 6–18, 1981. A Russian translation was published in: E.S. Nikolaev, Ed., *Numerical Methods in Linear Algebra* (Moscow Univ. Press, Moscow, 1982) 16–32. The original English version of the paper, of which only a few copies have been circulating, had great impact on some subsequent work by Greg Ammar, Bill Gragg, Lothar Reichel and others. It therefore seems appropriate to make it here available to a broader audience.

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Let

$$M = (\mu_{i,j})_{i,j=0}^{\infty} = M^H$$

be positive definite in the sense that its n th sections

$$M_n := (\mu_{i,j})_{i,j=0}^{n-1}, \quad n = 1, 2, 3, \dots,$$

are all positive definite. Then M determines inner products $(\cdot, \cdot)_{\mu}$ and $(\cdot, \cdot)_M$ for $\mathbb{R}_{\mathbb{C}}$ and \mathbb{C}_0^{∞} , respectively, by

$$(\alpha, \beta)_{\mu} := (a, b)_M := a^H M b.$$

The superscripts T and H denote transposition and conjugate transposition, respectively. We have

$$\mu_{i,j} = (\zeta^i, \zeta^j)_{\mu} = (e_{i+1}, e_{j+1})_M,$$

where

$$e_j := (\delta_{i,j})_{i=1}^{\infty}, \quad j = 1, 2, 3, \dots,$$

is the j th axis vector in \mathbb{C}_0^{∞} . Hence, M is the *moment matrix* of $(\cdot, \cdot)_{\mu}$ with respect to the standard basis $\{\zeta^k\}_0^{\infty}$ for $\mathbb{P}_{\mathbb{C}}$. When the context dictates, e_j will also denote the j th column of the $n \times n$ identity matrix

$$I_n = (e_1, e_2, \dots, e_n).$$

The *inverse Cholesky decomposition*

$$R^H M R = D = \text{diag}(\delta_0, \delta_1, \delta_2, \dots),$$

with R an upper right triangular unit matrix, can be computed recursively. Equivalently,

$$R_n^H M_n R_n = D_n, \quad n = 1, 2, 3, \dots$$

Setting

$$M_{n+1} := \begin{pmatrix} M_n & m_n \\ m_n^H & \mu_{n,n} \end{pmatrix}, \quad R_{n+1} := \begin{pmatrix} R_n & r_n \\ 0^T & 1 \end{pmatrix},$$

we require

$$\begin{pmatrix} M_n & m_n \\ m_n^H & \mu_{n,n} \end{pmatrix} \begin{pmatrix} R_n & r_n \\ 0^T & 1 \end{pmatrix} = \begin{pmatrix} * & 0 \\ * & 1 \end{pmatrix} \begin{pmatrix} D_n & 0 \\ 0^T & \delta_n \end{pmatrix},$$

or equivalently

$$M_n r_n + m_n = 0, \quad \delta_n = \mu_{n,n} + m_n^H r_n.$$

Since

$$M_n^{-1} = R_n D_n^{-1} R_n^H,$$

we see that r_n and then δ_n are easily computed. This uses $O(n^3)$ arithmetic operations to decompose M_n and is (presumably) a numerically stable process. We also have

$$\delta_n = \frac{\det M_{n+1}}{\det M_n} = \mu_{n,n} - m_n^H M_n^{-1} m_n > 0.$$

The columns of R are orthogonal vectors in \mathbb{C}_0^∞ ; the columns of $RD^{-1/2}$ are orthonormal. The *monic* polynomials $\{\psi_n(\zeta)\}_0^\infty$ defined by

$$(\psi_0(\zeta), \psi_1(\zeta), \psi_2(\zeta), \dots) := v(\zeta)^T R,$$

or equivalently by

$$\psi_n(\zeta) := v_n(\zeta)^T r_n + \zeta^n, \quad v_n(\zeta) := (1, \zeta, \dots, \zeta^{n-1})^T,$$

satisfy

$$(\psi_m, \psi_n)_\mu = \begin{cases} 0 & m \neq n, \\ \delta_n & m = n. \end{cases}$$

The scaled polynomials $\psi_n(\zeta)/\delta_n^{1/2}$ are orthonormal with respect to $(\cdot, \cdot)_\mu$. Thus, each positive definite M determines an inner product for $\mathbb{P}_\mathbb{C}$ and a set of monic orthogonal polynomials for which $\|\psi_n\|_\mu^2 = \delta_n > 0$. Conversely, any sequence $\{\psi_n(\zeta)\}_0^\infty$ with $\psi_n(\zeta) = \zeta^n + \dots$ is orthogonal with respect to such an inner product $(\cdot, \cdot)_\mu$, where the norms $\|\psi_n\|_\mu = \sqrt{\delta_n}$ can be arbitrary positive numbers.

Denote by $\mathbb{P}_\mathbb{C}^n$ the subspace of $\mathbb{P}_\mathbb{C}$ of polynomials of degree $\leq n$. The Fourier expansion of $\alpha \in \mathbb{P}_\mathbb{C}$ is

$$\alpha(\zeta) = \sum_{k=0}^n \alpha_k \psi_k(\zeta), \quad \alpha_k = \frac{(\psi_k, \alpha)_\mu}{\delta_k}.$$

Moreover, we have

$$(\alpha, \alpha) = \sum_{k=0}^n |\alpha_k|^2 \delta_k = \sum_{k=0}^n \frac{|(\psi_k, \alpha)_\mu|^2}{\delta_k}.$$

It follows that

$$\min\{(\alpha, \alpha)_\mu : \alpha(\zeta) = \zeta^n + \dots\} = (\psi_n, \psi_n)_\mu = \delta_n,$$

and that this *extremal property* uniquely determines the monic polynomial ψ_n .

The *kernel polynomial* $\kappa_n(\zeta, \omega)$, of degree $\leq n$ in ζ and ω^H , may be defined as the generating function of M_{n+1}^{-1} :

$$\begin{aligned} \kappa_n(\zeta, \omega) &:= v_{n+1}(\zeta)^T M_{n+1}^{-1} v_{n+1}(\omega^H) = \frac{-1}{\det M_{n+1}} \det \begin{pmatrix} M_{n+1} & v_{n+1}(\omega^H) \\ v_{n+1}(\zeta)^T & 0 \end{pmatrix} \\ &= \sum_{k=0}^n \frac{\psi_k(\zeta) \psi_k(\omega)^H}{\delta_k}, \end{aligned}$$

the determinant representation following from Sylvester's determinant identity

$$\det \begin{pmatrix} A_{1,1} & A_{1,2} \\ A_{2,1} & A_{2,2} \end{pmatrix} = \det A_{1,1} \det(A_{2,2} - A_{2,1} A_{1,1}^{-1} A_{1,2}),$$

and the third from $M_{n+1}^{-1} = R_{n+1} D_{n+1}^{-1} R_{n+1}^H$. By means of elementary operations we also have

$$\kappa_n(\sigma, \tau) = \frac{\det M_n(\sigma, \tau)}{\det M_{n+1}}, \quad \text{with } M_n(\sigma, \tau) := ((\zeta^i(\zeta - \tau), \zeta^j(\zeta - \sigma))_\mu)_{i,j=0}^{n-1}.$$

For $\alpha \in \mathbb{P}_{\mathbb{C}}^n$ we have

$$(\kappa_n(\cdot, \omega), \alpha)_{\mu} = \alpha(\omega),$$

the *reproducing property* of $\kappa_n(\zeta, \omega)$, and it is not difficult to show, by Cauchy's inequality, that

$$\max\{|\alpha(\omega)|^2 : \alpha \in \mathbb{P}_{\mathbb{C}}^n, (\alpha, \alpha)_{\mu} = 1\} = \kappa_n(\omega, \omega),$$

with the extremal polynomials the unimodular multiples of

$$\alpha(\zeta) = \frac{\kappa_n(\zeta, \omega)}{\kappa_n(\omega, \omega)^{1/2}}.$$

Let $E : \mathbb{C}_0^{\infty} \rightarrow \mathbb{C}_0^{\infty}$ be the *downshift operator*; specifically,

$$E := (e_2, e_3, e_4, \dots) = (\delta_{i,j+1})_{i,j=0}^{\infty}.$$

The corresponding operator on $\mathbb{P}_{\mathbb{C}}$ is multiplication by ζ :

$$\zeta\alpha(\zeta) = v(\zeta)^T E a.$$

We have

$$M' := (\mu_{i,j+1})_{i,j=0}^{\infty} = ME.$$

The finite analog of this is

$$M'_n = N_n F_n, \quad F_n := E_n - r_n e_n^T.$$

F_n is the Frobenius matrix, or companion matrix, associated with $\psi_n(\zeta)$. Now, as is easily verified using the above results,

$$e_n \psi_n(\zeta) + F_n^T v_n(\zeta) = v_n(\zeta) \zeta \quad \text{and} \quad e_1 \psi_n(\zeta) + F_n y_n(\zeta) = y_n(\zeta) \zeta,$$

where

$$y_n(\zeta) := U_n v_n(\zeta), \quad U_n := (E_n^T r_n, E_n^{2T} r_n, \dots, E_n^{nT} r_n) + J_n$$

and

$$J_n := (e_n, e_{n-1}, \dots, e_1) = J_n^T = J_n^{-1}$$

is the $n \times n$ *reversal matrix*. It follows that

$$\psi_n(\zeta) = \det(\zeta I_n - F_n) = \frac{\det(\zeta M_n - M'_n)}{\det M_n} = \frac{1}{\det M_n} \det \begin{pmatrix} M_n & m_n \\ v_n(\zeta)^T & \zeta^n \end{pmatrix}$$

is the characteristic polynomial of F_n , and that if

$$\lambda \in \lambda(F_n) := \{\lambda_{n,1}, \lambda_{n,2}, \dots, \lambda_{n,n}\},$$

the *spectrum* of F_n , then $y_n(\lambda)$ and $v_n(\lambda)$ are associated eigenvectors of F_n and F_n^T , respectively. Moreover, we have

$$F_n^T V_n = V_n \Lambda_n, \quad F_n \cdot U_n V_n = U_n V_n \cdot \Lambda_n,$$

where

$$\Lambda_n := \text{diag}(\lambda_{n,1}, \lambda_{n,2}, \dots, \lambda_{n,n})$$

and

$$V_n := V_n(\lambda_{n,1}, \lambda_{n,2}, \dots, \lambda_{n,n}) := (v_n(\lambda_{n,1}), v_n(\lambda_{n,2}), \dots, v_n(\lambda_{n,n}))$$

is the *Vandermonde matrix*. If the eigenvalues are all distinct, then V_n and $U_n V_n$ are nonsingular and Λ_n is the Jordan canonical form of F_n . If some of the eigenvalues are repeated, then V_n must be replaced by the corresponding *confluent Vandermonde matrix*, in which the corresponding columns are replaced by successive (Taylor) derivatives. In such cases F_n is not diagonalizable and has only one normalized eigenvector associated with each distinct eigenvalue.

We have

$$U_n =: (v_{i,j})_{i,j=1}^n,$$

with

$$v_{i,j} = e_i^T U_n e_j = \begin{cases} e_{i+j}^T r_n, & i+j \leq n, \\ 1, & i+j = n+1, \\ 0, & i+j > n+1. \end{cases}$$

That is, U_n is a *unit upper triangular Hankel matrix*. It follows that

$$F_n U_n = U_n F_n^T,$$

that is, F_n is *symmetrically similar* with F_n^T . This can be used to show that any matrix $A \in \mathbb{C}^{n \times n}$ is symmetrically similar with A^T , and equivalently, that every $A \in \mathbb{C}^{n \times n}$ is the product of two symmetric matrices, either one of which can be taken nonsingular. The elements of

$$y_n(\zeta) =: (\eta_{1,n}(\zeta), \eta_{2,n}(\zeta), \dots, \eta_{n,n}(\zeta))^T$$

are *Horner polynomials*. They satisfy the recursion

$$\begin{aligned} \eta_{n,n}(\zeta) &= 1, \\ \text{for } k &\leftarrow n-1, n-2, \dots, 0, 1 \\ \eta_{k,n}(\zeta) &= \zeta \eta_{k+1,n}(\zeta) + \rho_{k,n}, \\ \psi_n(\zeta) &= \eta_{0,n}(\zeta), \end{aligned}$$

where

$$r_n =: (\rho_{0,n}, \rho_{1,n}, \dots, \rho_{n-1,n})^T.$$

Define the matrices H_n by

$$R_n H_n := F_n R_n.$$

Then F_n and H_n are similar matrices and

$$D_n H_n = R_n^H M_n' R_n.$$

Moreover

$$H_{n+1} =: \begin{pmatrix} H_n & h_n \\ e_n^T & \eta_n \end{pmatrix}$$

is unit right Hessenberg (nearly triangular) and

$$r_{n+1} = \begin{pmatrix} 0 \\ r_n \end{pmatrix} - \begin{pmatrix} R_n & r_n \\ 0^T & 1 \end{pmatrix} \begin{pmatrix} h_n \\ \eta_n \end{pmatrix}.$$

Equivalently,

$$\psi_{n+1}(\zeta) = (\zeta - \eta_n)\psi_n(\zeta) - (\psi_0(\zeta), \psi_1(\zeta), \dots, \psi_{n-1}(\zeta))h_n.$$

If we put

$$h_n =: (\eta_{0,n}, \eta_{1,n}, \dots, \eta_{n-1,n})^T, \quad \eta_{n,n} =: \eta_n,$$

then by the orthogonality,

$$\eta_{i,n} = \frac{(\psi_i, \zeta \psi_n)_\mu}{\delta_i}.$$

This is the (generalized) Arnoldi reduction of the operator $\zeta: \mathbb{P}_\mathbb{C} \rightarrow \mathbb{P}_\mathbb{C}$ to Hessenberg form, with respect to the inner product $(\cdot, \cdot)_\mu$. If we define

$$Q_n := R_n^T V_n = (\psi_{i-1}(\lambda_{n,j}))_{i,j=1}^n,$$

then we have

$$H_n^T Q_n = Q_n \Lambda_n, \quad H_n \cdot S_n Q_n = S_n Q_n \cdot \Lambda_n,$$

with

$$S_n := R_n^{-1} U_n R_n^{-T} = S_n^T$$

(R_n^{-1} is upper right triangular, U_n is upper left triangular, R_n^{-T} is lower left triangular).

The rational matrix function

$$\mathcal{R}_n(\zeta) := (\zeta I_n - H_n)^{-1}$$

will be called the *n*th resolvent. The sequence $\{\phi_n(\zeta)\}_1^\infty$ of scaled (1, 1)-elements

$$\phi_n(\zeta) := \mu_{0,0} e_1^T \mathcal{R}_n(\zeta) e_1$$

is a *generalized continued fraction* associated with the moment matrix M . We have

$$\phi_n(\zeta) = \frac{\pi_n(\zeta)}{\psi_n(\zeta)}, \quad \text{with } \pi_n(\zeta) = \mu_{0,0} \det(\zeta I_{n-1} - H'_{n-1}), \quad H_n =: \begin{pmatrix} \eta_0 & * \\ * & H'_{n-1} \end{pmatrix}.$$

It follows that if we put $\phi_0(\zeta) := 0$, then also

$$\pi_{n+1}(\zeta) = (\zeta - \eta_n)\pi_n(\zeta) - (\pi_0(\zeta), \pi_1(\zeta), \dots, \pi_{n-1}(\zeta))h_n,$$

with initial conditions

$$\pi_0(\zeta) := 0, \quad \pi_1(\zeta) = \mu_{0,0}.$$

We can give an explicit formula for $\phi_n(\zeta)$, solely in terms of the moments $\mu_{i,j}$. This is analogous with what is known as *Nuttall's compact formula* in the theory of the Padé table. First of all, it is easy to get

$$\mathcal{R}_n(\zeta) = R_n^{-1} (\zeta M_n - M'_n)^{-1} R_n^{-H} D_n.$$

Then from

$$R_n^{-H}e_1 = M_n R_n D_n^{-1}e_1 = \frac{M_n e_1}{\mu_{0,0}},$$

we conclude that

$$\phi_n(\zeta) = e_1^T M_n (\zeta M_n - M_n')^{-1} M_n e_1.$$

From this we find, by means of Sylvester's identity, elementary operations and the determinant formula for $\psi_n(\zeta)$, that

$$\pi_n(\zeta) = \frac{1}{\det M_n} \det \begin{pmatrix} M_n e_1 & M_n' - \zeta M_n \\ 0 & e_1^T M_n \end{pmatrix}.$$

Further elementary operations now reduce this to

$$\pi_n(\zeta) = \frac{1}{\det M_n} \det \begin{pmatrix} M_n e_1 & M_n' \\ 0 & u_n(\zeta)^T \end{pmatrix}, \quad \text{with } u_n(\zeta)^T e_j = \sum_{k=0}^{j-1} \mu_{0,j-k-1} \zeta^k.$$

Letting

$$\phi(\zeta) := \sum_{k=0}^{\infty} \frac{\mu_{0,k}}{k+1}$$

be the formal Laurent series determined by the first row of M , we now arrive at

$$\begin{aligned} \det M_n [\phi(\zeta)\psi_n(\zeta) - \pi_n(\zeta)] &= \sum_{k=1}^{\infty} \det \begin{pmatrix} \mu_{0,0} & \mu_{0,1} & \cdots & \mu_{0,n} \\ \mu_{1,0} & \mu_{1,1} & \cdots & \mu_{1,n} \\ \vdots & \vdots & & \vdots \\ \mu_{n-1,0} & \mu_{n-1,1} & \cdots & \mu_{n-1,n} \\ \mu_{0,k} & \mu_{0,k+1} & \cdots & \mu_{0,k+n} \end{pmatrix} \frac{1}{\zeta^{k+1}} \\ &= \det \begin{pmatrix} M_n & m_n \\ e_1^T M_n' & \mu_{0,n+1} \end{pmatrix} \frac{1}{\zeta^2} + O\left(\frac{1}{\zeta^3}\right), \quad \zeta \rightarrow \infty. \end{aligned}$$

Since

$$\begin{aligned} \mu_{0,0} \eta_{0,n} = (\psi_0, \zeta \psi_n)_\mu &= e_1^T M_n' r_n + \mu_{0,n+1} = \mu_{0,n+1} - e_1^T M_n' M_n^{-1} m_n \\ &= \frac{1}{\det M_n} \det \begin{pmatrix} M_n & m_n \\ e_1^T M_n' & \mu_{0,n+1} \end{pmatrix}, \end{aligned}$$

we conclude that, in general,

$$\phi(\zeta) - \phi_n(\zeta) = \mu_{0,0} \frac{\eta_{0,n}}{\zeta^{n+2}} + O\left(\frac{1}{\zeta^{n+3}}\right), \quad \zeta \rightarrow \infty.$$

Let A be a linear transformation on the inner product space \mathcal{X} , with inner product (\cdot, \cdot) . If $0 \neq k_0 \in \mathcal{X}$, we could, in theory, form the Krylov sequence $k_n = A k_{n-1} = A^n k_0$, the moments

$$\mu_{i,j} = (k_i, k_j) = (A^i k_0, A^j k_0)$$

and, as long as M_n remains positive definite, we could form the polynomial ψ_{n+1} . *Transplantation of the Arnoldi process from $\mathbb{P}_{\mathbb{C}}$ to \mathcal{H} allows us to avoid construction of all these entities, and this is very important for numerical stability.* We put

$$x_n := \psi_n(A)k_0 \quad \text{and} \quad X_n := (x_0, x_1, \dots, x_{n-1}),$$

an n -tuple of vectors in \mathcal{H} . Then

$$AX_n = X_n H_n + x_n e_n^T \quad \text{and} \quad ((x_i, x_j))_{i,j=0}^{n-1} = D_n.$$

Moreover, setting

$$\chi_n := X_n D_n^{-1/2}, \quad \mathcal{H}_n := D_n^{1/2} H_n D_n^{-1/2},$$

we see that

$$A\chi_n = \chi_n \mathcal{H}_n + \frac{x_n e_n^T}{\delta_{n-1}^{1/2}}$$

and that the vectors of χ_n are orthonormal. If $\delta_n = \|x_n\|^2 = 0$, that is, if M_{n+1} is singular, then these vectors form an orthonormal basis for an invariant subspace of A . However, this event is more unlikely in practice than it is in theory, and the study of how the spectra of \mathcal{H}_n and A are related is of great interest. We have

$$K_n R_n = X_n, \quad K_n := (k_0, k_1, \dots, k_{n-1}),$$

and this represents an (inverse) Gram–Schmidt orthogonalization of the Krylov vectors $\{k_j\}_0^{n-1}$. The Arnoldi process for A , in the *modified* Gram–Schmidt formulation, is as follows:

$$\begin{aligned} x_0 &= k_0, \quad \delta_0 = (x_0, x_0), \\ \text{for } n &\leftarrow 1, 2, \dots \text{ until } \delta_n = 0 \\ x_n &\leftarrow Ax_{n-1}, \\ \text{for } k &\leftarrow 0, 1, \dots, n-1 \\ \eta_{k,n-1} &= (x_k, x_n) / \delta_k, \\ x_n &\leftarrow x_n - x_k \eta_{k,n-1}, \\ \delta_n &= (x_n, x_n). \end{aligned}$$

In practice, the use of *reorthogonalization* may be required. If $\mathcal{H} = \mathbb{C}^N$, $A \in \mathbb{C}^{N \times N}$, $(y, x) = y^H x$, and the process goes to stage n , the cost is n applications of A and about $n^2 N$ arithmetic operations when no reorthogonalizations are used.

2. Toeplitz matrices M

Suppose now that $A: \mathcal{H} \rightarrow \mathcal{H}$ is *isometric* with respect to (\cdot, \cdot) , that is, $(Ay, Ax) \equiv (y, x)$ for $x, y \in \mathcal{H}$. Then

$$\mu_{i,j} = (A^i x_0, A^j x_0) = \begin{cases} (x_0, A^{j-i} x_0) =: \mu_{j-i}, & i \leq j, \\ (A^{i-j} x_0, x_0) = (x_0, A^{i-j} x_0)^H = \mu_{i-j}^H =: \mu_{j-i}, & i \geq j, \end{cases}$$

so $M = (\mu_{j-i})$ is a positive definite Toeplitz matrix. We also have $(\zeta\alpha, \zeta\beta)_\mu = (\alpha, \beta)_\mu$ and $(Ea, Eb)_M = (a, b)_M$, that is, $E^TME = M$. M is *persymmetric* in the sense that

$$J_n M_n^T J_n = M_n,$$

or equivalently, since $M_n = M_n^H$,

$$J_n M_n J_n = \overline{M}_n.$$

This means that if we define

$$\alpha^*(\zeta) := \zeta^n \overline{\alpha}(\zeta^{-1}), \quad \text{for } \alpha \in \mathbb{P}_\mathbb{C}^n,$$

then we have

$$(\alpha, \beta)_\mu = (\beta^*, \alpha^*)_\mu, \quad \alpha, \beta \in \mathbb{P}_\mathbb{C}^n.$$

In particular, we put

$$\psi_n^*(\zeta) := \zeta^n \overline{\psi}_n(\zeta^{-1})$$

and have

$$(\psi_n^*, \psi_n^*)_\mu = (\psi_n, \psi_n)_\mu = \delta_n.$$

Let us put

$$\gamma_n := \psi_n(0).$$

Since $\psi_n^*(0) = 1$, we can write

$$\frac{1 - \psi_n^*(\zeta)}{\zeta} := \sum_{k=0}^{n-1} \overline{\alpha}_k \psi_k(\zeta), \quad \alpha_k := \alpha_{n,k},$$

that is,

$$\psi_n^*(\zeta) = 1 - \sum_{k=0}^{n-1} \overline{\alpha}_k \zeta \psi_k(\zeta).$$

Now the polynomials $\{\zeta \psi_k(\zeta)\}_0^\infty$ are also orthogonal, so

$$(\zeta \psi_k, \psi_n^*)_\mu (\zeta \psi_k, 1)_\mu - \overline{\alpha}_k \delta_k = (\psi_n, (\zeta \psi_k)^*)_\mu = (\psi_n, \zeta^{n-k-1} \psi_k^*)_\mu = 0, \quad \text{for } k < n.$$

Hence the numbers

$$\alpha_k = \frac{(1, \zeta \psi_k)_\mu}{\delta_k}$$

are indeed independent of n . One sees also that $\gamma_n = -\alpha_{n-1}$. Hence,

$$\psi_{n+1}^*(\zeta) = \psi_n^*(\zeta) + \overline{\gamma}_{n+1} \zeta \psi_n(\zeta),$$

and equivalently

$$\psi_{n+1}(\zeta) = \zeta \psi_n(\zeta) + \gamma_{n+1} \psi_n^*(\zeta).$$

Finally, from

$$(\psi_n^*, \zeta \psi_n)_\mu = (\psi_n^*, \psi_{n+1} - \gamma_{n+1} \psi_n^*)_\mu = -\gamma_{n+1} \delta_n,$$

we see that

$$\delta_{n+1} = \|\psi_n^* + \bar{\gamma}_{n+1}\zeta\psi_n\|_\mu^2 = \delta_n(1 - |\gamma_{n+1}|^2).$$

Hence we have the *Levinson algorithm*:

$$\begin{aligned} \psi_0(\zeta) &= 1, \delta_0 = \mu_0, \\ \text{for } n &= 0, 1, 2, \dots \\ \gamma_{n+1} &= -(1, \zeta\psi_n)_\mu / \delta_n, \\ \psi_{n+1}(\zeta) &= \zeta\psi_n(\zeta) + \gamma_{n+1}\psi_n^*(\zeta), \\ \delta_{n+1} &= \delta_n(1 - |\gamma_{n+1}|^2). \end{aligned}$$

This computes the inverse Cholesky factorization of M_n in $O(n^2)$ operations. It follows that

$$\delta_n = \mu_0 \prod_{k=1}^n (1 - |\gamma_k|^2), \quad \mu_0 = \delta_0 > \delta_1 > \delta_2 > \dots > \delta_n \rightarrow \delta^* \geq 0, \quad |\gamma_n| < 1, \text{ for } n \geq 1.$$

If $\mu_n = \theta^{n^2}$, $-1 < \theta < 1$, then we have $\gamma_n = \theta^n$,

$$\delta_n = \prod_{k=1}^n (1 - \theta^{2k}) \rightarrow \prod_{k=1}^{\infty} (1 - \theta^{2k}) = \delta^* > 0 \quad \text{and} \quad \psi_n^*(\zeta) = \sum_{k=0}^n \begin{bmatrix} n \\ k \end{bmatrix}_{\theta^2} (-\theta\zeta)^k,$$

where

$$\begin{bmatrix} n \\ k \end{bmatrix}_{\theta} := \frac{(1 - \theta^n)(1 - \theta^{n-1}) \dots (1 - \theta^{n-k+1})}{(1 - \theta)(1 - \theta^2) \dots (1 - \theta^k)}$$

are the Gauss binomial coefficients. This can be shown by noting that $M = \text{diag}(\theta^{k^2})(\theta^{-2ij})\text{diag}(\theta^{k^2})$ is diagonally equivalent with a symmetric Vandermonde matrix whose Cholesky and inverse Cholesky factors are known from polynomial interpolation theory. Of course the simplest example is $\mu_n = \delta_{n,0}$, for which $\psi_n(\zeta) = \zeta^n$, $\psi_n^*(\zeta) \equiv 1$.

The analogs of the *Cristoffel–Darboux formula* (which occurs in the case of Hermitian A and Hankel M) are

$$\begin{aligned} \kappa_n(\zeta, \omega) &= v_{n+1}(\zeta)^T M_{n+1}^{-1} v_{n+1}(\bar{\omega}) = \sum_{k=0}^n \frac{\psi_k(\zeta)\overline{\psi_k(\omega)}}{\delta_k} \\ &= \frac{\psi_{n+1}^*(\zeta)\overline{\psi_{n+1}^*(\omega)} - \psi_{n+1}(\zeta)\overline{\psi_{n+1}(\omega)}}{\delta_{n+1}(1 - \zeta\bar{\omega})} = \frac{\psi_n^*(\zeta)\overline{\psi_n^*(\omega)} - \zeta\bar{\omega}\psi_n(\zeta)\overline{\psi_n(\omega)}}{\delta_n(1 - \zeta\bar{\omega})}. \end{aligned}$$

These follow from the recursion formulas for the polynomials ψ_n and ψ_n^* . The matrix interpretation is that M_n^{-1} can be expressed in two ways as the difference of products of left and right triangular Toeplitz factors (so-called Gohberg–Semenecul formulas). These formulas form the basis of recent work on superfast, $O(n \log_2^2 n)$, methods for solving (Hankel and) Toeplitz systems $M_n x = b$. The numerical stability of such methods seems not to have been determined. Examples like the one above may aid in assessing the effect of numerical cancellation when forming $x = M_n^{-1} b$ using such formulas.

The transliteration of the Levinson algorithm from $\mathbb{P}_{\mathbb{C}}$ to \mathcal{H} gives an *isometric analog of the Hermitian Lanczos process*. The latter is the specialization of the Arnoldi process to Hermitian

A ; in that case the matrix H is tridiagonal, making the simplification apparent. Setting

$$x_n := \psi_n(A)k_0, \quad x_n^* := \psi_n^*(A)k_0$$

and noting that

$$(\psi_n^*, \zeta \psi_n)_\mu = (x_n^*, Ax_n),$$

we get the algorithm

$$\begin{aligned} x_0 &= x_0^* = k_0, \quad \delta_0 = (x_0, x_0), \\ \text{for } n &= 0, 1, 2, \dots \text{ until } \delta_{n+1} = 0 \\ \gamma_{n+1} &= -(x_n^*, Ax_n)/\delta_n, \\ x_{n+1} &= Ax_n + \gamma_{n+1}x_n^*, \\ x_{n+1}^* &= x_n^* + \bar{\gamma}_{n+1}Ax_n, \\ \delta_{n+1} &= \delta_n(1 - |\gamma_{n+1}|^2). \end{aligned}$$

If $\mathcal{H} = \mathbb{C}^N$, $A \in \mathbb{C}^{N \times N}$ and $(y, x) = y^H x$, then A is unitary. If the process goes to stage n , the cost is n applications of A and about $2nN$ arithmetic operations.

Let us look at the structure of the Hessenberg matrices H_n and \mathcal{H}_n . First of all we note that the finite analogs of $E^T M E = M$ are

$$M_n - F_n^H M_n F_n = \delta_n e_n e_n^T, \quad D_n - H_n^H D_n H_n = \delta_n e_n e_n^T, \quad \text{and} \quad I_n - \mathcal{H}_n^H \mathcal{H}_n = \frac{\delta_n}{\delta_{n-1}} e_n e_n^T,$$

that is,

$$\mathcal{H}_n^H \mathcal{H}_n = \text{diag}(1, 1, \dots, 1, |\gamma_n|^2).$$

Hence, \mathcal{H}_n has orthogonal columns and *singular values*

$$\sigma(\mathcal{H}_n) = \{1, 1, \dots, 1, |\gamma_n|\}.$$

Putting $\omega = 0$ in the Christoffel–Darboux formula, we get

$$\kappa_n(\zeta, 0) = \sum_{k=0}^n \frac{\bar{\gamma}_k \psi_k(\zeta)}{\delta_k} = \frac{1}{\delta_n} \psi_n^*(\zeta).$$

Hence,

$$\begin{aligned} \gamma_{n+1} \delta_n \kappa_n(\zeta, 0) &= \sum_{k=0}^n \frac{\bar{\gamma}_k \gamma_{n+1} \delta_n}{\delta_k} \psi_k(\zeta) \\ &= \gamma_{n+1} \psi_n^*(\zeta) = -(\psi_0(\zeta), \psi_1(\zeta), \dots, \psi_n(\zeta)) \begin{pmatrix} h_n \\ \eta_n \end{pmatrix}. \end{aligned}$$

It follows that

$$D_{n+1} \begin{pmatrix} h_n \\ \eta_n \end{pmatrix} = -\bar{g}_n \gamma_{n+1} \delta_n,$$

where

$$g_n^T := (\gamma_0, \gamma_1, \dots, \gamma_{n-1}) := e_1^T R_n, \quad \gamma_0 := 1.$$

We conclude that the unit right Hessenberg matrix

$$H_n := (\eta_{i,j})_{i,j}^{n-1} = 0$$

has its nontrivial elements

$$\eta_{i,j} = \frac{-\bar{\gamma}_i \gamma_{j+1} \delta_j}{\delta_i}, \quad i \leq j.$$

From the recurrence relations,

$$\frac{\psi_n(\zeta)}{\psi_n^*(\zeta)} = t_n \left(\zeta \frac{\psi_{n-1}(\zeta)}{\psi_{n-1}^*(\zeta)} \right), \quad t_n(\omega) := \frac{\psi_n + \omega}{1 + \bar{\gamma}_n \omega}.$$

Since $|\gamma_n| < 1$, the well-known mapping properties of $t_n(\omega)$ give

$$|\zeta| < 1 \Rightarrow \left| \frac{\psi_n(\zeta)}{\psi_n^*(\zeta)} \right| < 1, \quad \psi_n(\zeta) = 0 \Rightarrow |\zeta| < 1.$$

Moreover, clearly,

$$\left| \frac{\psi_n(\zeta)}{\psi_n^*(\zeta)} \right| = 1, \quad \text{for } |\zeta| = 1.$$

Hence

$$\frac{\psi_n(\zeta)}{\psi_n^*(\zeta)} = \prod_{k=1}^n \frac{\zeta - \lambda_{n,k}}{1 - \bar{\lambda}_{n,k} \zeta}$$

is a *Blaschke product* and $\lambda(\mathcal{H}_n)$ lies in the open unit disk. Now, for fixed n , replace γ_n by a general parameter τ , call the resulting matrix $\tilde{\mathcal{H}}_n(\tau)$, and replace $t_n(\omega)$ by

$$t(\tau; \omega) := \frac{\tau + \omega}{1 + \bar{\tau} \omega}.$$

Then also $|\lambda(\tilde{\mathcal{H}}_n(\tau))| < 1$ for $|\tau| < 1$. Now, the eigenvalues of $\tilde{\mathcal{H}}_n(\tau)$ are the zeros of

$$t \left(\tau; \zeta \frac{\psi_{n-1}(\zeta)}{\psi_{n-1}^*(\zeta)} \right) = t \left(\tau; t_n^{-1} \left(\frac{\psi_n(\zeta)}{\psi_n^*(\zeta)} \right) \right),$$

that is, they are the zeros of

$$\psi_n(\zeta) - t_n(-\tau) \psi_n^*(\zeta).$$

Now we have

$$t_n^{-1}(\omega) = -t_n(-\omega).$$

Hence, on replacing τ by $t_n(\tau)$ we see that *the eigenvalues of*

$$\mathcal{H}_n(\tau) := D_n^{1/2} H_n(\tau) D_n^{-1/2},$$

with

$$H_n(\tau) := D_n^{-1} \begin{pmatrix} -\bar{\gamma}_0\gamma_1 & -\bar{\gamma}_0\gamma_2 & -\bar{\gamma}_0\gamma_3 & \cdots & -\bar{\gamma}_0\gamma_{n-1} & -\bar{\gamma}_0t_n(\tau) \\ 1 - |\gamma_1|^2 & -\bar{\gamma}_1\gamma_2 & -\bar{\gamma}_1\gamma_3 & \cdots & -\bar{\gamma}_1\gamma_{n-1} & -\bar{\gamma}_1t_n(\tau) \\ & 1 - |\gamma_2|^2 & -\bar{\gamma}_2\gamma_3 & \cdots & -\bar{\gamma}_2\gamma_{n-1} & -\bar{\gamma}_2t_n(\tau) \\ & & \ddots & \ddots & \vdots & \vdots \\ & & & & -\bar{\gamma}_{n-2}\gamma_{n-1} & -\bar{\gamma}_{n-2}t_n(\tau) \\ & & & & 1 - |\gamma_{n-1}|^2 & -\bar{\gamma}_{n-1}t_n(\tau) \end{pmatrix} D_n,$$

are the zeros of

$$\psi_n(\tau, \zeta) := \psi_n(\tau) + \tau\psi_n^*(\zeta) = (1 + \tau\bar{\gamma}_n)\zeta^n + \cdots,$$

a polynomial of degree $\leq n$ in ζ . But $\mathcal{H}_n(\tau)$ is unitary for $|\tau| = 1$, so has its eigenvalues on $|\lambda| = 1$. Since $\psi_n(\zeta)/\psi_n^*(\zeta)$ has all its zeros in $|\zeta| < 1$, and poles in $|\zeta| > 1$, it has winding number n with respect to $|\zeta| = 1$. Hence, for $|\tau| = 1$, the eigenvalues $\{\lambda_{n,k}(\tau)\}_{k=1}^n$ of $\mathcal{H}_n(\tau)$ are all distinct and lie on $|\lambda| = 1$.

The eigenvalues of $\mathcal{H}_n := \mathcal{H}_n(0)$ can be of the highest possible multiplicity. For example, with $\mu_n = \delta_{n,0}$, we have $\psi_n(\zeta) = \zeta^n$, $\psi_n^*(\zeta) \equiv 1$, and the $\{\lambda_{n,k}(\tau)\}_{k=1}^n$ are the n th roots of $-\tau$. The motivation behind the Arnoldi process is that the spectrum of the matrices $\mathcal{H}_n(0)$ should, in some sense, approximate that of A as n becomes (hopefully only moderately) large. For $A: \mathbb{C}^N \rightarrow \mathbb{C}^N$ unitary, with respect to y^Hx , we have $|\lambda(A)| = 1$. At least in this simplest case it seems natural to force the approximating spectrum to also lie on $|\lambda| = 1$. This can be done by working with $\mathcal{H}_n(\tau): |\tau| = 1$, which can be viewed as a rank-one modification of $\mathcal{H}_n(0)$. In fact, $\mathcal{H}_n(\tau)$ is not even normal, with respect to y^Hx , for $|\tau| < 1$ and $|\gamma_k| < 1, 1 \leq k \leq n$.

We henceforth assume that $|\tau| = 1$. Let

$$V_n(\tau) := (v_n(\lambda_{n,1}(\tau)), v_n(\lambda_{n,2}(\tau)), \dots, v_n(\lambda_{n,n}(\tau))).$$

The Christoffel–Darboux formula shows that

$$V_n(\tau)^T M_n^{-1} \overline{V_n(\tau)} = W_n(\tau)^{-1},$$

with

$$W_n(\tau) := \text{diag}(\omega_{n,1}(\tau), \omega_{n,2}(\tau), \dots, \omega_{n,n}(\tau)) \quad \text{and}$$

$$\omega_{n,k}(\tau)^{-1} := \sum_{j=0}^{n-1} \frac{|\psi_j(\lambda_{n,k}(\tau))|^2}{\delta_j} > 0.$$

Hence

$$M_n = \overline{V_n(\tau)} W_n V_n(\tau)^T.$$

For $|\tau| = 1$ this is equivalent with

$$\mu_k = \sum_{j=1}^n \omega_{n,j}(\tau) \lambda_{n,j}(\tau)^k, \quad |k| < n,$$

since then $\lambda_{n,j}(\tau)^H = \lambda_{n,j}(\tau)^{-1}$. For $|\tau| = 1$ we put

$$2\pi\nu_n(\tau; \theta) = \sum_j \{\omega_{n,j}(\tau): 0 \leq \arg \lambda_{n,j}(\tau) < \theta\},$$

to get

$$\mu_k = \frac{1}{2\pi} \int_0^{2\pi} e^{ik\theta} d\nu_n(\tau; \theta), \quad |k| < n.$$

Since

$$\int_0^{2\pi} d\nu_n(\tau; \theta) \equiv 2\pi\mu_0, \quad n = 0, 1, 2, \dots,$$

we may apply the Helly theorems to conclude the existence of a bounded nondecreasing function $\nu(\theta)$, with infinitely many points of increase, for which

$$\mu_k = \frac{1}{2\pi} \int_0^{2\pi} e^{ik\theta} d\nu(\theta), \quad -\infty < k < +\infty.$$

Then the “Gauss–Szegő” quadrature formula

$$\sum_{k=1}^n \omega_{n,k}(\tau) f(\lambda_{n,k}(\tau)) = \frac{1}{2\pi} \int_0^{2\pi} f(\theta) d\nu(\theta)$$

is exact for trigonometric polynomials of $f(e^{i\theta})$ of degree $< n$. Conversely, every such $\nu(\theta)$ determines, in this manner, a positive definite Toeplitz matrix M . If $\nu(\theta) = \theta$, then $\mu_n = \delta_{n,0}$, $\psi_n(\zeta) = 1$, and $\omega_{n,k}(\tau) \equiv 1/n$, $1 \leq k \leq n$. Hence, the Gauss–Szegő quadrature formulas for $\nu(\theta) = \theta$, which are analogs of the classical Gauss–Legendre quadrature formulas for the interval $(-1, 1)$, are the trapezoidal rule and its rotations.

Let us now put

$$Q_n(\tau) := R_n^T V_n(\tau) = \left(\psi_{i-1}(\lambda_{n,j}(\tau)) \right)_{i,j=1}^n$$

and

$$\Lambda_n(\tau) := \text{diag}(\lambda_{n,1}(\tau), \lambda_{n,2}(\tau), \dots, \lambda_{n,n}(\tau)).$$

Then,

$$Q_n(\tau) W_n(\tau) Q_n(\tau)^H = D_n$$

and, because $H_n(\tau)$ is obtained from $H_n(0)$ by replacing γ_n by $t_n(\tau)$, we have already shown that

$$H_n(\tau)^T Q_n(\tau) = Q_n(\tau) \Lambda_n(\tau).$$

It follows that the matrix

$$\mathcal{Q}_n(\tau) := D_n^{-1/2} Q_n(\tau) W_n(\tau)^{1/2}$$

is unitary, and that

$$\mathcal{H}_n(\tau)^T \mathcal{Q}_n(\tau) = \mathcal{Q}_n(\tau) \Lambda_n(\tau).$$

We now wish to show that

$$\rho_n := \mu_n - \sum_{k=1}^n \omega_{n,k}(\tau) \lambda_{n,k}(\tau)^n \neq 0.$$

We have

$$\begin{aligned}\rho_n &= e_1^T M_n' e_n - e_1^T \overline{V_n(\tau)} W_n(\tau) \Lambda_n(\tau) V_n(\tau)^T e_n \\ &= e_1^T [M_n F_n(0) - \overline{V_n(\tau)} W_n(\tau) V_n(\tau) F_n(\tau)] e_n \\ &= e_1^T M_n [F_n(0) - F_n(\tau)] e_n,\end{aligned}$$

where $F_n(\tau)$ is the companion matrix of $\psi_n(\tau, \zeta)$. If we put

$$\begin{pmatrix} r_n \\ 1 \end{pmatrix} := \begin{pmatrix} \gamma_n \\ s_n \end{pmatrix},$$

then we have

$$F_n(\tau) = E_n - \frac{1}{1 + \overline{\gamma}_n \tau} (r_n + \tau J_n \bar{s}_n) e_n^T.$$

The use of $M_n r_n + m_n = 0$ now gives

$$\begin{aligned}\rho_n &= \frac{\tau}{1 + \overline{\gamma}_n \tau} e_1^T (\overline{\gamma}_n m_n + M_n J_n \bar{s}_n) = \frac{\tau}{1 + \overline{\gamma}_n \tau} e_1^T M_{n+1} J_{n+1} \begin{pmatrix} \bar{r}_n \\ 1 \end{pmatrix} \\ &= \frac{\tau}{1 + \overline{\gamma}_n \tau} (m_m^T \bar{r}_n + \mu_0) = \frac{\tau \delta_n}{1 + \overline{\gamma}_n \tau} \neq 0,\end{aligned}$$

as required.

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