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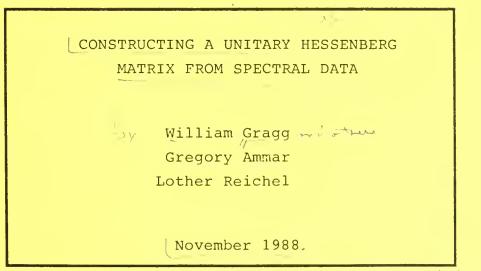
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Constructing a Unitary Hessenberg Matrix from Spectral Data

Gregory Ammar¹, William Gragg², Lothar Reichel³

In memory of Peter Henrici

Abstract

We consider the numerical construction of a unitary Hessenberg matrix from spectral data using an inverse QR algorithm. Any unitary upper Hessenberg matrix H with nonnegative subdiagonal elements can be represented by 2n - 1 real parameters. This representation, which we refer to as the *Schur parameterization* of H, facilitates the development of efficient algorithms for this class of matrices. We show that a unitary upper Hessenberg matrix H with positive subdiagonal elements is determined by its eigenvalues and the eigenvalues of a rank-one unitary perturbation of H. The eigenvalues of the perturbation strictly interlace the eigenvalues of H on the unit circle.

AMS(MOS) Subject Classification: 15A18, 65F15.

Keywords: inverse eigenvalue problem, unitary matrix, orthogonal polynomial.

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1. Introduction

In this paper we focus on an inverse eigenvalue problem for unitary Hessenberg matrices with positive subdiagonal elements. Throughout this paper all Hessenberg matrices are upper Hessenberg matrices. This class of matrices bears many similarities with the class of Jacobi matrices, i.e. real symmetric tridiagonal matrices with positive subdiagonal elements. Any matrix in either class is normal and has distinct eigenvalues. Both $n \times n$ Jacobi matrices and $n \times n$ unitary Hessenberg matrices with positive subdiagonal elements can be parameterized by 2n - 1 real parameters. This is obvious for Jacobi matrices; for unitary Hessenberg matrices this parameterization is described below. Since unitary Hessenberg matrices with positive subdiagonal elements are determined by O(n) parameters, one can develop efficient algorithms for this class of matrices. These algorithms are analogous with algorithms for Jacobi matrices. For example, the unitary QR algorithm, described in [Gr2], has many similarities with the QR algorithm for Jacobi matrices. Another example is provided by the divide-and-conquer methods that have been developed for both the tridiagonal and unitary eigenproblems [Cu], [DS], [GR1], [GR2].

In this paper we show another analogy of unitary Hessenberg matrices with Jacobi matrices, namely, that a unitary Hessenberg matrix H with positive subdiagonal elements is uniquely determined by its eigenvalues and the eigenvalues of a unitary rank-one perturbation of H. The matrix H can be constructed using $O(n^2)$ arithmetic operations using an inverse unitary QR algorithm. Similar results for Jacobi matrices are well-established [BG1], [BG2], [GH]. The inverse unitary QR algorithm is analogous with the algorithm described in [GH] for Jacobi matrices.

2. Unitary Hessenberg Matrices and Szegö Polynomials

We refer to a finite Schur parameter sequence of length n as a sequence of complex numbers $\{\gamma_j\}_{j=1}^n$ with $|\gamma_j| < 1$ for $1 \le j < n$ and $|\gamma_n| = 1$. Also define the complementary Schur parameters $\{\sigma_j\}_{j=1}^{n-1}$ by $\sigma_j := \sqrt{1 - |\gamma_j|^2}$. Associated with the finite Schur parameter sequence $\{\lambda_j\}_{j=1}^n$ is a unitary Hessenberg matrix H with positive subdiagonal elements

$$H = H(\gamma_1, \dots, \gamma_{n-1}, \gamma_n) := G_1(\gamma_1) G_2(\gamma_2) \dots G_{n-1}(\gamma_{n-1}) \tilde{G}_n(\gamma_n),$$
(2.1)

where the Givens reflector $G_j(\gamma_j)$ is the identity matrix of appropriate size except for the 2 × 2 principal submatrix

$$G_{j}\begin{bmatrix} j & j+1\\ j & j+1 \end{bmatrix} = \begin{bmatrix} -\gamma_{j} & \sigma_{j}\\ \sigma_{j} & \bar{\gamma}_{j} \end{bmatrix},$$

with the bar denoting complex conjugation. The matrix on the right in the product (2.1) is defined by $\tilde{G}_n(\gamma_n) := \text{diag}[1, 1, \dots, 1, -\gamma_n]$. The nonzero entries of $H = [\eta_{j,k}]_{j,k=1}^n$ are then given by $\eta_{j+1,j} := \sigma_j$ and $\eta_{j,k} := -\bar{\gamma}_{j-1}\sigma_j\sigma_{j+1}\dots\sigma_{k-1}\gamma_k$ for $1 \le j \le k$, where $\gamma_0 := 1$.

It is easy to see that every $n \times n$ unitary Hessenberg matrix $H = [\eta_{j,k}]_{j,k=1}^n$ with $\eta_{j+1,j} > 0$ is uniquely determined by a finite Schur parameter sequence of length n. In fact, the Schur parameters $\{\gamma_j\}_{j=1}^n$ and the complementary Schur parameters $\{\sigma_j\}_{j=1}^{n-1}$ can be determined from H by

$$\sigma_j = \eta_{j+1,j}, \qquad 1 \le j < n; \qquad \gamma_j = -\eta_{1,j}/\sigma_1\sigma_2\cdots\sigma_{j-1}, \qquad 1 \le j \le n.$$

Hence, we have a one-to-one correspondence between Schur parameter sequences of length n and $n \times n$ unitary Hessenberg matrices with positive subdiagonal elements. This Schur parameterization of unitary Hessenberg matrices with positive subdiagonal elements shows that these matrices are determined by 2n - 1 real parameters: the real and imaginary parts of γ_j for $1 \le j < n$, and the

argument of γ_n . To avoid numerical instability, however, we also retain the complementary Schur parameters.

Let $H = H_n := H(\gamma_1, \ldots, \gamma_{n-1}, \gamma_n)$, and let $H_k := G_1(\gamma_1)G_2(\gamma_2)\ldots G_{k-1}(\gamma_{k-1})\tilde{G}_k(\gamma_k)$ be the leading principal submatrix of $H = H_n$ of order k. Introduce the functions

$$\phi_k(\lambda) := e_1^T (\lambda I - H_k)^{-1} e_1,$$

$$\psi_k(\lambda) := \det(\lambda I - H_k),$$

$$\pi_k(\lambda) := \det(\lambda I - H_{k-1}'').$$

where $e_1 := [1, 0, ..., 0]^T$, and H_{k-1}'' denotes the trailing principal submatrix of H_k of order k-1. Thus, $\phi_k(\lambda) = \pi_k(\lambda)/\psi_k(\lambda)$. The following proposition can be verified by induction.

Proposition 2.1. The polynomials $\psi_k(\lambda)$ and $\pi_k(\lambda)$, k > 0, satisfy

$$\begin{bmatrix} \psi_k(\lambda) & \pi_k(\lambda) \\ \tilde{\psi}_k(\lambda) & \tilde{\pi}_k(\lambda) \end{bmatrix} = \begin{bmatrix} \lambda & \gamma_k \\ \bar{\gamma}_k \lambda & 1 \end{bmatrix} \begin{bmatrix} \psi_{k-1}(\lambda) & \pi_{k-1}(\lambda) \\ \tilde{\psi}_{k-1}(\lambda) & \tilde{\pi}_{k-1}(\lambda) \end{bmatrix}; \begin{bmatrix} \psi_0(\lambda) & \pi_0(\lambda) \\ \tilde{\psi}_0(\lambda) & \tilde{\pi}_0(\lambda) \end{bmatrix} = \begin{bmatrix} 1 & 1/\lambda \\ 1 & 0 \end{bmatrix}.$$

It follows that for each k, the polynomials $\tilde{\psi}_k(\lambda) := \lambda^k \bar{\psi}_k(1/\lambda)$ are obtained by reversing and conjugating the coefficients of $\psi_k(\lambda)$. From the initial conditions we recognize $\psi_k(\lambda)$ to be the kth *Szegö polynomial* determined by the Schur parameter sequence $\{\gamma_j\}_{j=1}^n$. \Box

The Szegö polynomials $\{\psi_k\}_{k=0}^n$ are orthogonal with respect to a discrete measure on the unit circle. This measure assigns a positive weight ω_k to each zero λ_k of $\psi_n(\lambda)$. These weights are the numerators in the partial fraction decomposition

$$\phi_n(\lambda) =: \sum_{k=1}^n \frac{\omega_k}{\lambda - \lambda_k},$$

see [Gr1] for details.

Let $H = U\Lambda U^*$, with $\Lambda = \text{diag}[\lambda_1, \lambda_2, \dots, \lambda_n]$ and U unitary, be the spectral resolution of $H = H(\gamma_1, \dots, \gamma_{n-1}, \gamma_n)$, where * denotes transposition and complex conjugation. Let $u := U^T \epsilon_1$ be the vector containing the first components of the eigenvectors of H. Since H has nonzero subdiagonal elements, every entry of $u = [v_1, v_2, \dots, v_n]^T$ is nonzero, and we normalize U so that each $v_k > 0$. Then

$$\phi_n(\lambda) = u^* (\lambda I - \Lambda)^{-1} u = \sum_{k=1}^n \frac{v_k^2}{\lambda - \lambda_k}$$

Hence, the weights $\omega_k = v_k^2$ are guaranteed to be positive, and $\sum_{k=1}^n \omega_k = 1$.

3. The Inverse Unitary QR Algorithm

Given *n* distinct unimodular complex numbers $\{\lambda_k\}_{k=1}^n$ and associated positive weights $\{v_k^2\}_{k=1}^n$, we can construct a unitary Hessenberg matrix *H* with the λ_k and v_k equal to the eigenvalues and first components of the corresponding eigenvectors of *H*, respectively. This construction is achieved using an inverse QR algorithm, which is analogous with the procedure of [GH] for real symmetric tridiagonal matrices.

The required Hessenberg matrix is obtained by performing a sequence of elementary unitary similarity transformations to transform the matrix $\begin{bmatrix} \delta & u^* \\ u & \Lambda \end{bmatrix}$ to a Hessenberg matrix $\begin{bmatrix} \delta & \epsilon_1^* \\ \epsilon_1 & H \end{bmatrix}$ without

using or changing the arbitrary entry δ . Then $H = H(\gamma_1, \ldots, \gamma_{n-1}, \gamma_n)$ has the desired eigenvalues and associated eigenvectors.

The idea is to build the Hessenberg matrix by adding weight-abscissa pairs one at a time. Suppose that we have constructed the unitary Hessenberg matrix $H_m := H(\gamma_1, \ldots, \gamma_{m-1}, \gamma_m)$, for some m < n, corresponding with the weight-abscissa pairs $\{(\omega_k, \lambda_k)\}_{k=1}^m$. Let $\sigma_0 := (\sum_{k=1}^m \omega_k)^{1/2}$ and assume that the first components of the eigenvectors of H_m are $\{(v_k/\sigma_0)\}_{k=1}^m$. In order to add the weight-abscissa pair (v^2, λ) and construct the corresponding $(m+1) \times (m+1)$ unitary Hessenberg matrix $H'_{m+1} := H(\lambda'_1, \lambda'_2, \ldots, \lambda'_{m+1})$, we perform a sequence of unitary similarity transformations to put the $(m+2) \times (m+2)$ matrix

into Hessenberg form without changing δ . Let $\sigma'_0 := \sqrt{\sigma_0^2 + v^2}$ and $\alpha_0 := -v/\sigma'_0$. Then

is a Hessenberg matrix with a trailing principal $(m+1) \times (m+1)$ submatrix, which is both unitary and of Hessenberg form. On the completion of the similarity transformation of $\tilde{H}^{(1)}$, we obtain

The circled element in (3.1) forms a "bulge", which is to be chased down along the subdiagonal in order to obtain a matrix of Hessenberg form. Define $G_3(\alpha_1)$ so that $G_3(\alpha_1)\tilde{H}^{(2)}G_2^*(\alpha_0) =: \tilde{H}^{(3)}$ is a Hessenberg matrix. Then $\tilde{H}^{(3)}G_3^*(\alpha_1)$ has a bulge, which we annihilate by multiplying from the left with $G_4(\alpha_2)$. Proceeding in this manner, we ultimately chase the bulge off the bottom of the matrix, and obtain the Hessenberg matrix $\tilde{H}^{(m-1)}G_{m-1}^*(\gamma_{m-3})$, which is unitarily similar to $\tilde{H}^{(1)}$. The trailing principal $(m+1) \times (m+1)$ submatrix of $\tilde{H}^{(m-1)}G_{m-1}^*(\gamma_{m-3})$ is unitarily similar to a unitary Hessenberg matrix with positive subdiagonal elements. The latter matrix is the desired Hessenberg matrix $H'_{m+1} = H(\gamma'_1, \gamma'_2, \dots, \gamma'_{m+1})$.

This procedure for adding a weight-abscissa pair to H_m , if implemented by directly manipulating the elements of the matrices $\tilde{H}^{(k)}$, for $1 \leq k < m$, would require $O(m^2)$ arithmetic operations. However,

we note that for each k the trailing $(m+1)\times(m+1)$ principal submatrix of $\tilde{H}^{(k)}$ is unitary and of Hessenberg form, and, therefore, is unitarily similar to a unitary Hessenberg matrix. denoted by $\hat{H}_{m+1}^{(k)}$, with positive subdiagonal elements. Hence, we can carry out the similarity transformations by manipulating the Schur parameters of the matrices $\hat{H}_{m+1}^{(k+2)} = H(\gamma'_1, \gamma'_2, \ldots, \gamma'_k, \bar{\lambda}^k \alpha_k, \gamma_{k+1}, \ldots, \gamma_m)$. This gives rise to a method that requires only O(m) arithmetic operations in order to add a weightabscissa pair to H_m . We refer to this method as the *inverse unitary QR algorithm* because of its relationship with the unitary QR algorithm presented in [Gr2].

Inverse Unitary QR Algorithm: adding a weight-abscissa pair (v^2, λ) , where $|\lambda| = 1$. v > 0.

$$\sigma'_{0} := \sqrt{\sigma_{0}^{2} + v^{2}};$$

$$\alpha_{0} := -v/\sigma'_{0}; \ \beta_{0} := \sigma_{0}/\sigma'_{0};$$
for $k := 1, 2, ..., m$

$$\begin{bmatrix} \sigma'_{k} := \beta_{k-1}\sqrt{\sigma_{k}^{2} + |\alpha_{k-1} + \gamma_{k}\lambda^{k-2}\bar{\alpha}_{k-1}|^{2}}; \\ \alpha_{k} := \beta_{k-1}\lambda(\alpha_{k-1} + \gamma_{k}\lambda^{k-2}\bar{\alpha}_{k-1})/\sigma'_{k}; \\ \beta_{k} := \beta_{k-1}\sigma_{k}/\sigma'_{k}; \\ \gamma'_{k} := \beta_{k-1}^{2}\gamma_{k} - \bar{\lambda}^{k-2}\alpha_{k-1}^{2}; \\ \gamma'_{m+1} := \lambda\gamma_{m}; \end{bmatrix}$$

Thus, the inverse unitary QR algorithm can be used to construct the unitary $n \times n$ Hessenberg matrix $H = H(\gamma_1, \ldots, \gamma_{n-1}, \gamma_n)$ from its eigenvalues and the first components of its normalized eigenvectors in $O(n^2)$ arithmetic operations.

4. An Inverse Spectral Problem

Let $H = H(\gamma_1, \dots, \gamma_{n-1}, \gamma_n)$ and $\phi_n(\lambda) = \frac{\pi_n(\lambda)}{\psi_n(\lambda)} = \sum_{k=1}^n \frac{\omega_k}{\lambda - \lambda_k}$. Let $\alpha := e^{i\tau}$ for some $0 < \tau < 2\pi$.

and consider the polynomials

$$\chi_k(\lambda) := (1 - \alpha)\lambda\pi_k(\lambda) + \alpha\psi_k(\lambda), \quad 0 \le k \le n.$$
(4.1)

Proposition 4.1. The polynomials $\{\chi_k(\lambda)\}_{k=0}^n$ are the monic Szegö polynomials corresponding with the Schur sequence $\{\alpha\gamma_k\}_{k=1}^n$.

Proof. The definition (4.1) and Proposition 2.1 yield

$$\begin{bmatrix} \chi_k(\lambda) \\ \xi_k(\lambda) \end{bmatrix} = \begin{bmatrix} \lambda & \gamma_k \\ \bar{\gamma}_k \lambda & 1 \end{bmatrix} \begin{bmatrix} \chi_{k-1}(\lambda) \\ \xi_{k-1}(\lambda) \end{bmatrix}, \begin{bmatrix} \chi_0(\lambda) \\ \xi_0(\lambda) \end{bmatrix} = \begin{bmatrix} 1 \\ \alpha \end{bmatrix},$$

where $\xi_k(\lambda) := (1 - \alpha)\lambda \tilde{\pi}_k(\lambda) + \alpha \tilde{\psi}_k(\lambda)$. On setting $\tilde{\chi}_k(\lambda) = \bar{\alpha}\xi_k(\lambda)$, we obtain

$$\begin{bmatrix} \chi_k(\lambda) \\ \tilde{\chi}_k(\lambda) \end{bmatrix} = \begin{bmatrix} \lambda & \alpha \gamma_k \\ \bar{\alpha} \bar{\gamma}_k \lambda & 1 \end{bmatrix} \begin{bmatrix} \chi_{k-1}(\lambda) \\ \tilde{\chi}_{k-1}(\lambda) \end{bmatrix}, \begin{bmatrix} \chi_0(\lambda) \\ \tilde{\chi}_0(\lambda) \end{bmatrix} = \begin{bmatrix} 1 \\ 1 \end{bmatrix}.$$

An immediate consequence of Proposition 4.1 is that each zero of $\chi_n(\lambda)$ has unit modulus. When $\alpha = -1$ the polynomials $\{\chi_k(\lambda)\}_{k=0}^n$ are known as the Szegö polynomials of the second kind corresponding with $\{\gamma_k\}_{k=1}^n$.

Proposition 4.2. The zeros $\{\mu_k\}_{k=0}^n$ of $\chi_n(\lambda)$ strictly interlace the zeros $\{\lambda_k\}_{k=0}^n$ of $\psi_n(\lambda)$ on the unit circle. Moreover, $\prod_{k=1}^n (\mu_k/\lambda_k) = \alpha$.

Proof. Let $\lambda := e^{i\theta}$ for some $0 \le \theta < 2\pi$, and let $\alpha =: e^{i\tau}$ for some $0 < \tau < 2\pi$. Then

$$\Phi_n(\lambda) := \frac{\chi_n(\lambda)}{\psi_n(\lambda)} = \sum_{k=1}^n \omega_k \frac{\lambda - \alpha \lambda_k}{\lambda - \lambda_k}$$
$$= \sum_{k=1}^n \omega_k \frac{1 - \lambda \bar{\lambda}_k + \alpha (1 - \bar{\lambda} \lambda_k)}{|\lambda - \lambda_k|^2}$$
$$= \sum_{k=1}^n 2 e^{i\tau/2} \omega_k \frac{\operatorname{Re}(e^{i\tau/2}(1 - \bar{\lambda} \lambda_k))}{|\lambda - \lambda_k|^2}$$

Thus, $\operatorname{Im}(e^{-i\tau/2}\Phi_n(e^{i\theta})) \equiv 0$ for $0 \leq \theta < 2\pi$. Let $\lambda_k =: e^{i\theta_k}$. We may assume that $0 \leq \theta_1 < \theta_2 < \cdots < \theta_n < 2\pi$. Then

$$e^{-i\tau/2}\Phi_n(\epsilon^{i\theta}) = \sum_{k=1}^n 2\omega_k \frac{\cos(\tau/2) - \cos(\tau/2 + \theta_k - \theta)}{(1 - \cos(\theta_k - \theta))^2 + \sin^2(\theta_k - \theta)}$$
$$= \sum_{k=1}^n \omega_k \frac{\cos(\tau/2) - \cos(\tau/2)\cos(\theta_k - \theta) + \sin(\tau/2)\sin(\theta_k - \theta)}{1 - \cos(\theta_k - \theta)}$$
$$= \sum_{k=1}^n \omega_k \left(\cos(\tau/2) + \sin(\tau/2)\cot((\theta_k - \theta)/2)\right).$$

From $0 < \tau < 2\pi$ and $\omega_k > 0$ for all k, it follows that

$$e^{-i\tau/2}\frac{d}{d\theta}\Phi_n(e^{i\theta}) = \frac{1}{2}\sin(\tau/2)\sum_{k=1}^n \omega_k / \sin^2((\theta_k - \theta)/2) > 0 \quad \text{for} \quad \theta \neq \theta_k, \ 1 \le k \le n.$$

Thus, $\Phi_n(e^{i\theta}) \to -\infty$ as $\theta \searrow \theta_k$, and $\Phi_n(e^{i\theta}) \to \infty$ as $\theta \nearrow \theta_{k+1}$. This shows that $\theta \to \Phi_n(e^{i\theta})$ has precisely one zero in $]\theta_k, \theta_{k+1}[$. Consequently, the zeros μ_j of $\Phi_n(\lambda)$ strictly interlace the λ_j on the unit circle. The second statement of the Proposition follows from the fact that $\chi_n(0)/\psi_n(0) = \alpha$.

Let $\lambda_k =: e^{i\theta_k}$ and $\mu_k =: e^{i\nu_k}$ for $0 \le \theta_k, \nu_k < 2\pi$. Then we have $\sum_{k=1}^n (\nu_k - \theta_k) = \tau$. We may assume that the arguments have been ordered so that

$$0 \le \theta_1 < \nu_1 < \theta_2 < \dots < \nu_{n-1} < \theta_n < \nu_n < \theta_1 + 2\pi.$$
(4.2)

Proposition 4.3. With the above notation, and the ordering (4.2), the weights ω_k are given by

$$\omega_k = \frac{1}{\sin(\tau/2)} \frac{\prod_{\substack{j=1\\j\neq k}}^n \sin((\nu_j - \theta_k)/2)}{\prod_{\substack{j=1\\j\neq k}}^n \sin((\theta_j - \theta_k)/2)}$$

Proof. We have

$$(1-\alpha)\lambda_k\omega_k = \lim_{\lambda \to \lambda_k} (\lambda - \lambda_k) \frac{\chi_n(\lambda)}{\psi_n(\lambda)} = \frac{\chi_n(\lambda_k)}{\psi'_n(\lambda_k)} = \frac{\prod_{j=1}^n (\lambda_k - \mu_j)}{\prod_{\substack{j=1\\j \neq k}}^n (\lambda_k - \lambda_j)}$$

since $\chi_n(\lambda)$ and $\psi_n(\lambda)$ are monic. Thus,

$$(1-\alpha)\omega_{k} = e^{-i\theta_{k}} \frac{\prod\limits_{j=1}^{n} (e^{i\theta_{k}} - e^{i\nu_{j}})}{\prod\limits_{\substack{j=1\\j\neq k}}^{n} (e^{i\theta_{k}} - e^{i\theta_{j}})} = \frac{\prod\limits_{j=1}^{n} (1 - e^{i(\nu_{j} - \theta_{k})})}{\prod\limits_{\substack{j=1\\j\neq k}}^{n} (1 - e^{i(\theta_{j} - \theta_{k})})} = -2i\epsilon^{i\tau/2} \frac{\prod\limits_{j=1}^{n} \sin((\nu_{j} - \theta_{k})/2)}{\prod\limits_{\substack{j=1\\j\neq k}}^{n} \sin((\theta_{j} - \theta_{k})/2)}, \quad (4.3)$$

because

$$1 - \epsilon^{i\beta} = -2i\sin(\beta/2), \tag{4.4}$$

and $\sum_{j=1}^{n} (\nu_j - \theta_j) = \tau$. The formula for the weights now follows by substituting (4.4) with $\beta := \tau$ into (4.3).

We can now state the inverse spectral problem and its solution.

Problem: Given two sets of *n* mutually interlacing points on the unit circle $\{\lambda_k\}_{k=1}^n$ and $\{\mu_k\}_{k=1}^n$. determine the unique unitary Hessenberg matrix $H = H(\gamma_1, \ldots, \gamma_{n-1}, \gamma_n)$ and $|\alpha| = 1$ such that the spectrum of *H* is $\{\lambda_k\}_{k=1}^n$ and the spectrum of $H(\alpha\gamma_1, \ldots, \alpha\gamma_{n-1}, \alpha\gamma_n)$ is $\{\mu_k\}_{k=1}^n$.

Solution: Let $\alpha := \prod_{k=1}^{n} (\mu_k / \lambda_k)$, calculate the weights by Proposition 4.3, and use the inverse unitary QR algorithm to construct $H = H(\gamma_1, \ldots, \gamma_{n-1}, \gamma_n)$.

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