

(HESSENBERG) EIGENVALUE-EIGENMATRIX RELATIONS*

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Abstract. Explicit relations between eigenvalues, eigenmatrix entries and matrix elements are derived. First, a general, theoretical result based on the TAYLOR expansion of the adjugate of $zI - A$ on the one hand and explicit knowledge of the JORDAN decomposition on the other hand is proven. This result forms the basis for several, more practical and enlightening results tailored to non-derogatory, diagonalizable and normal matrices, respectively. Finally, inherent properties of (upper) HESSENBERG, resp. tridiagonal matrix structure are utilized to construct computable relations between eigenvalues, eigenvector components, eigenvalues of principal submatrices and products of lower diagonal elements.

Key words. Algebraic eigenvalue problem, eigenvalue-eigenmatrix relations, JORDAN normal form, adjugate, principal submatrices, HESSENBERG matrices, eigenvector components

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1. Introduction. Eigenvalues and eigenvectors are defined using the relations

$$Av = v\lambda \quad \text{and} \quad V^{-1}AV = J. \quad (1.1)$$

We speak of a *partial* eigenvalue problem, when for a given matrix $A \in \mathbb{C}^{n \times n}$ we seek scalar $\lambda \in \mathbb{C}$ and a corresponding nonzero vector $v \in \mathbb{C}^n$. The scalar λ is called the *eigenvalue* and the corresponding vector v is called the *eigenvector*. We speak of the *full* or *algebraic* eigenvalue problem, when for a given matrix $A \in \mathbb{C}^{n \times n}$ we seek its JORDAN normal form $J \in \mathbb{C}^{n \times n}$ and a corresponding (not necessarily unique) eigenmatrix $V \in \mathbb{C}^{n \times n}$.

Apart from these constitutional relations, for some classes of structured matrices several more intriguing relations between components of eigenvectors, matrix entries and eigenvalues are known. For example, consider the so-called JACOBI matrices. A JACOBI matrix is a symmetric tridiagonal matrix $T \in \mathbb{R}^{n \times n}$ with positive off-diagonal entries. For these matrices it is well known [23, (Theorem 7.9.2, Corollary 7.9.1)] that the squares of the last eigenvector components v_{ni} to an eigenvalue λ_i ,

$$Tv_i = v_i\lambda_i \quad (1.2)$$

are given by the algebraic expression

$$v_{ni}^2 = \frac{\det(\lambda_i I - \tilde{T})}{\det'(\lambda_i I - T)}, \quad (1.3)$$

where \tilde{T} denotes the leading principal submatrix of T of dimension $n - 1$ times $n - 1$.

A few comments are in order. Given an eigenvalue, we obtain a simple rational expression for a product of two eigenmatrix entries, in this case, the square of the last eigenvector component. The numerator is the characteristic polynomial of a submatrix of T and the denominator is a polynomial made of components of T , to be precise, the derivative of the characteristic polynomial of T . Both these polynomial terms are evaluated at the corresponding eigenvalue.

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This case is conceptually simple, since JACOBI matrices are normal, thus have orthogonal eigenvectors, and moreover have no multiple eigenvalues. Nevertheless, it already suggests that given information on *eigenvalues* we might be able to predict something about *eigenmatrix* entries. It is for this reason that we have chosen to use the term *eigenvalue-eigenmatrix* relation, despite some authors refer to simpler relations as eigenvector-eigenvalue relations.

In this note we intend to broaden and deepen results of aforementioned type to apply to more general matrices and to hold for more general cases, like multiple eigenvalues and principal vector components. All the relations we have in mind typically utilize knowledge on (principal) submatrices of A . This typical occurrence of submatrices follows upon the basic, broad, yet simple derivation of generalized eigenvalue-eigenmatrix relations we present in this note. This derivation is heavily based on the TAYLOR expansion of the adjugate of $zI - A$.

We remark that known relations between different submatrices of a specially structured matrix A often give (possibly not yet known) information on the eigenvector structure. One of the interesting cases is when structural constraints on A , for instance the sparsity of A , allow to obtain an *explicit* expression for the adjugate of $zI - A$ other than the rather technical definition as transposed matrix of cofactors. This explicit expression can be obtained for the class of unreduced HESSENBERG matrices, JACOBI matrices being merely a special subclass of this class.

1.1. Overview. This note is organized as follows. In the first section we briefly touch some historical landmarks in the field of eigenvalue-eigenmatrix relations and its close relative, the field of inverse eigenvalue problems. Due to the enormous amount of references, we refuse to be exhaustive and just give some first, subjective impression. Afterwards, we motivate why we need a rather technical and self-contained note that gathers and extends the relations. We conclude the first section by introducing the main portion of notations.

The second section covers the general case of $A \in \mathbb{C}^{n \times n}$ being a general square matrix with arbitrary, but known JORDAN structure. In this section the (analytic) TAYLOR expansion of the adjugate of $zI - A$ is linked to (algebraic) eigeninformation.

The third section specializes the general result to the case of non-derogatory eigenvalues. Major achievement is the introduction of shortened notation that allows to simplify the statement of the general result to be stated in more intuitive, straightforward and conceivable manner.

The fourth section is included for the sake of completeness and contains some rather well known results for diagonalizable matrices. The already thoroughly investigated subclasses of normal and HERMITEAN matrices are similarly just briefly touched.

Sections two, three and four are based on simplifications of the information related to the algebraic eigeninformation. The fifth section raises the level for the special class of HESSENBERG matrices from a purely theoretical investigation to an applicable one. This is achieved by rewriting the adjugate, and thus the TAYLOR expansion of the adjugate, of $zI - A$. Section five includes the main results of this note, even though the results of previous sections may serve as a platform for other important generalizations.

Some other paths of generalizations as well as some implications and applications of the HESSENBERG eigenvalue-eigenmatrix relations are briefly outlined in the concluding section six.

1.2. Historical Remarks. From the variety of references we mention as classical reference the treatise on determinants by MUIR [21] dating back to 1928. Even though at that time the use of HESSENBERG matrices was of no importance due to the lack of computers and thus of numerical algorithms, part of this famous treatise is closely related to the field of eigenvalue-eigenmatrix relations. We mention explicitly Section 13 on continuants. Continuants are determinants of tridiagonal matrices. The section contains plenty of results on eigenvalue-eigenvector relations in hidden form, relying on the intimate connection between determinantal recursions and eigenvalue relations to become obvious in this note.

Another inspiring source is the book by GANTMACHER and KREIN [14]. Despite the fact that the main focus is on knot-lines in eigenvectors and eigenfunctions for so-called oscillation matrices, respectively oscillation kernels, they focus partly on the already mentioned JACOBI matrices and corresponding relations for eigenvectors. Such knowledge on JACOBI matrices finds its counterpart in linear functional analysis in STURM-LIOUVILLE eigenvalue problems. This topic is also covered in their book.

Knowing the intimate relations in more detail enables analysis of what is known as inverse eigenvalue problems; concerning JACOBI matrices this is part of the work of HOCHSTADT [17, 18], HALD [16] and GRAGG [15]. For more details on inverse eigenvalue problems we refer the reader to the extensive list of references compiled in 1998 by MOODY T. CHU [11]. An early collection of results for the field of inverse STURM-LIOUVILLE problems has been compiled in 1946 by BORG [5].

Newer references include a summarizing paper by ELHAY, GLADWELL, GOLUB and RAM [13], where the authors gathered relations for tridiagonal matrices (JACOBI matrices) and STURM-LIOUVILLE problems. A large portion of the material on JACOBI matrices is collected in the book by PARLETT on the symmetric eigenvalue problem [23]. The book covers the same results that are dealt with in PAIGE's thesis [22], where these results find their natural application in the error analysis of the (symmetric) LANCZOS method.

It is interesting that both PAIGE and PARLETT cite a paper by THOMPSON and MCENTEGGERT as being the origin of the relations refined by them to the tridiagonal case. To be more precise, the origin of the relations is a *sequel* of altogether nine papers by R. C. THOMPSON [24, 32, 25, 28, 26, 29, 27, 31, 30]. The second paper in that row, the only one published with co-author MCENTEGGERT [32], is cited in the aforementioned book by PARLETT and the thesis by PAIGE. Yet, the results of interest to us are already contained in the first paper [24].

The THOMPSON sequel is an inspirational source for results concerning Hermitian and symmetric matrices, clarifying the relations between eigenvalues and eigenvalues of principal submatrices. This includes a proof for the well known result that the eigenvalues of a principal submatrix of a normal matrix are contained in the convex hull of the eigenvalues. More fascinating, the results are even sharpened to theorems about the position of the other eigenvalues, when additional knowledge on some eigenvalues is given.

Results have mostly been obtained for JACOBI matrices and STURM-LIOUVILLE problems. This, of course, can be explained on the one hand by the historical development, on the other hand by the importance of these two closely linked areas in several applications.

One nice exception is the investigation of unitary HESSENBERG matrices by AMMAR et al. ([1, 2]). In this case the relations can not be simply based on principal submatrices, since a principal submatrix of a unitary HESSENBERG matrix in most

cases is no longer unitary, even if obviously HESSENBERG structure is inherited.

The author knows of no result for non-diagonalizable matrices, with the remarkable exception of knowledge on the JORDAN structure of FROBENIUS companion matrices and so-called double companion matrices.

The full treatment of the former class can be found in WILKINSON's Algebraic Eigenvalue Problem, [33], sections 11 and 12 entitled "Non-derogatory matrices", pages 13–15, equations (11.6) and (12.6). Parts of it are contained in most textbooks on ordinary differential equations, see for instance the book by CODDINGTON and CARLSON [12].

The latter class is considered in the construction process of stable general linear methods for ordinary differential equations, see [8, 34, 9]. It is remarkable that apart from purely theoretical investigations both non-diagonalizable cases stem from applications in the context of ordinary differential equations.

1.3. Motivation. The focus of this note lies on a topic in the field of matrix analysis that appears to be a well researched and quite old one. This suggests that most things are surely known and raises the question if we really need yet another paper addressing this topic. There are at least three reasons for this note:

1) Certain instances of eigenvalue-eigenmatrix relations are frequently re-derived and re-proven. The goal of this note is to gather, unify and generalize the derivation of the relations in the finite dimensional setting in such a way that a toolkit is at hand to construct precisely the relation needed without digging through a vast amount of papers on the subject.

2) When eigenvalue-eigenmatrix relations were first derived, HESSENBERG matrices have not been of interest to the matrix analysis community. Nowadays, HESSENBERG matrices occupy a position at the center of numerical analysis, but the focus of most matrix analysts has shifted significantly from eigenvalue-eigenmatrix relations to other topics. Yet, the relations for the HESSENBERG case enable better understanding and error analysis of KRYLOV subspace methods [35] and might be fruitful in understanding properties of modern QR algorithms like multi-shift QR with aggressive early deflation [6, 7].

3) With the generalizations to multiple eigenvalues and principal vector components achieved in the present note, eigenvalue-eigenmatrix relations have entered a new stage of completeness and can be presented using only simple mathematics in self-contained form.

For simplicity of presentation two of the possible generalizations, namely, the generalization to the general eigenvalue problem, i.e., to relations involving matrix pencils, and to the infinite dimensional setting, i.e., to STURM-LIOUVILLE eigenvalue problems, have been neglected.

1.4. Notation. We derive and present the results in the field of complex numbers denoted by \mathbb{C} . Let a matrix $A \in \mathbb{C}^{n \times n}$ be given. In the following, we are interested in inherited characteristics and cross-relations of solutions to the algebraic eigenvalue problem

$$Av = v\lambda, \quad 0 \neq v \in \mathbb{C}^n, \lambda \in \mathbb{C}. \quad (1.4)$$

The spectrum of A is denoted by Λ . Let the JORDAN decomposition of A be given by $V^{-1}AV = J$. The JORDAN matrix J is the direct sum of JORDAN boxes J_λ , which in turn are direct sums of JORDAN blocks $J_{\lambda\iota}$:

$$J = \bigoplus_{\lambda \in \Lambda} J_\lambda, \quad J_\lambda = \bigoplus_{\iota=1}^{\gamma} J_{\lambda\iota}. \quad (1.5)$$

Here, $\gamma = \gamma(\lambda)$ denotes the *geometric* multiplicity of λ and $\iota \in \{1, \dots, \gamma\}$ is the *index* of the JORDAN block to eigenvalue λ . The *algebraic* multiplicity of λ is denoted by $\alpha = \alpha(\lambda)$. The *size* of the ι th JORDAN block to eigenvalue λ is denoted by $\sigma = \sigma(\lambda, \iota)$. With these definitions the matrices defined in (1.5) have dimensions

$$J_\lambda \in \mathbb{C}^{\alpha \times \alpha}, \quad J_{\lambda_\iota} \in \mathbb{C}^{\sigma \times \sigma}. \quad (1.6)$$

Moreover, α , γ and σ satisfy the relations

$$\sum_{\iota=1}^{\gamma(\lambda)} \sigma(\lambda, \iota) = \alpha(\lambda) \quad \forall \lambda \in \Lambda, \quad \sum_{\lambda \in \Lambda} \alpha(\lambda) = n. \quad (1.7)$$

We need special matrices associated with the JORDAN matrices and boxes, respectively. First, nilpotent matrices N_{λ_ι} are defined by splitting single JORDAN blocks J_{λ_ι} into diagonal and nilpotent part,

$$J_{\lambda_\iota} = \lambda I + N_{\lambda_\iota}, \quad N_{\lambda_\iota} \in \mathbb{C}^{\sigma \times \sigma} \quad (1.8)$$

Here and in what follows, I denotes the identity matrix of appropriate dimension. When necessary, a subscript is used to denote dimension. The letter O denotes a zero matrix, while O with double subscript O_{mn} denotes a rectangular $m \times n$ zero matrix. The nilpotent matrix N_{λ_ι} has elements

$$[N_{\lambda_\iota}]_{ij} = \delta_{i,j-1}, \quad (1.9)$$

where δ_{ij} denotes KRONECKER delta, i.e., δ_{ij} denotes the elements of the identity matrix. Nilpotent matrices N_λ are defined by an analog splitting of JORDAN boxes J_λ into diagonal and nilpotent part,

$$J_\lambda = \lambda I + N_\lambda, \quad N_\lambda \in \mathbb{C}^{\alpha \times \alpha}. \quad (1.10)$$

Obviously, N_λ is the direct sum of all N_{λ_ι} to the eigenvalue λ ,

$$N_\lambda = \bigoplus_{\iota=1}^{\gamma} N_{\lambda_\iota}. \quad (1.11)$$

For later purposes, we stress the fact that in any case $N_\lambda^\alpha = 0$, and that $N_\lambda^{\alpha-1} \neq 0$ precisely when λ is non-derogatory, in which case $N_\lambda^{\alpha-1} = e_1 e_\alpha^T$. As usual, e_j , $j \in \mathbb{N}$ denotes the j th column of the identity matrix of appropriate dimension.

The columns of V are right eigenvectors or right principal vectors (if any). In order to have access to *left* eigenvectors and *left* principal vectors, we define a special *left* eigenmatrix \hat{V} by $\hat{V} \equiv V^{-H}$. These matrices satisfy the three relations

$$AV = VJ, \quad \hat{V}^H A = J\hat{V}^H \quad \text{and} \quad \hat{V}^H V = I. \quad (1.12)$$

Later on, we depict the relations for one specific eigenvalue λ . To ease understanding we define additional notation with respect to the chosen eigenvalue λ .

We gather the columns of V and \hat{V} that span the α -dimensional invariant subspace corresponding to the eigenvalue λ in the biorthogonal rectangular matrices $V_\lambda \in \mathbb{C}^{n \times \alpha}$ and $\hat{V}_\lambda \in \mathbb{C}^{n \times \alpha}$. These matrices satisfy the three relations

$$AV_\lambda = V_\lambda J_\lambda, \quad \hat{V}_\lambda^H A = J_\lambda \hat{V}_\lambda^H \quad \text{and} \quad \hat{V}_\lambda^H V_\lambda = I. \quad (1.13)$$

Additionally, we define analog biorthogonal rectangular matrices V_{λ_ℓ} and \hat{V}_{λ_ℓ} , consisting only of the columns corresponding to the (not necessarily unique) invariant subspace to JORDAN block J_{λ_ℓ} .

We refer to the rectangular submatrices $V_\lambda, V_{\lambda_\ell}$ of V (respectively to the rectangular submatrices $\hat{V}_\lambda, \hat{V}_{\lambda_\ell}$ of \hat{V}) as right (respectively as left) *partial* eigenmatrices.

The natural enumeration of *left* eigenvectors and *left* principal vectors given by the column index as columns of \hat{V} is counter-intuitive to common usage. In order to stick close to common use, we define the flip matrix $F_n \in \mathbb{C}^{n \times n}$ by

$$F_n \equiv \begin{pmatrix} & & & 1 \\ & & \cdot & \\ & \cdot & & \\ 1 & & & \end{pmatrix}, \quad f_{ij} = \delta_{i, n-j+1}. \quad (1.14)$$

When the dimension of $F \equiv F_n$ is obvious from the context we leave out the subscript n . We now use F to define the *reordered* left eigenvector matrix $W_{\lambda_\ell} \equiv \hat{V}_{\lambda_\ell} F$. This ensures that when $W \equiv W_{\lambda_\ell}$, the first column of W is the left eigenvector, the second column of W is the first left principal vector, and so forth. For this reason we term W left eigenmatrix with natural ordering.

We define a *family* of matrices depending on the parameter z by ${}^z A \equiv zI - A$. Then by the previous definitions, the family ${}^z A$ has JORDAN decomposition $V^{-1}({}^z A)V = {}^z J$, where ${}^z J \equiv zI - J$. We define the characteristic polynomial such that the leading coefficient is one, $\chi(z) \equiv \det({}^z A) = \det(zI - A)$. The resolvent is defined accordingly, $R(z) \equiv ({}^z A)^{-1} = (zI - A)^{-1}$. The set of $z \in \mathbb{C}$ where the resolvent is defined is known as the *resolvent set* and is given explicitly by $\mathbb{C} \setminus \Lambda$. For ease of understanding we split the characteristic polynomial into $\chi(z) \equiv \omega(z)(z - \lambda)^\alpha$. Obviously, the polynomial $\omega(z)$ defined this way has degree $n - \alpha$ and $\omega(\lambda) \neq 0$. Multiplication of the TAYLOR expansion

$$\omega(z) = \sum_{k=0}^{n-\alpha} \frac{\omega^{(k)}(\lambda)}{k!} (z - \lambda)^k. \quad (1.15)$$

of $\omega(z)$ at λ with $(z - \lambda)^\alpha$ results in the TAYLOR expansion of $\chi(z)$ at λ . Thus, we can easily switch between TAYLOR coefficients in terms of χ and in terms of ω ,

$$\begin{aligned} \frac{\chi^{(i)}(\lambda)}{i!} &= 0, & \forall i \in \{0, \dots, \alpha - 1\}, \\ \frac{\chi^{(\alpha+i)}(\lambda)}{(\alpha+i)!} &= \frac{\omega^{(i)}(\lambda)}{i!}, & \forall i \in \{0, \dots, n - \alpha\}. \end{aligned} \quad (1.16)$$

The *adjugate* (sometimes named *classical adjoint*) $P(z) \equiv \text{adj}({}^z A)$ of ${}^z A$ is defined as the matrix of cofactors, $p_{ij}(z) \equiv (-1)^{i+j} \det({}^z A_{ji})$, where the submatrix ${}^z A_{ji}$ is defined to be ${}^z A$ without the j th row and the i th column. The matrix $P(z)$ is, by definition, polynomial in z . All subsequent analysis and results rely on expansions of the polynomial matrix $P(z)$ in terms of information stemming from the eigendecomposition of A .

2. The General Case. We first derive our main result for the case of A being a general square matrix. We need the *explicit* knowledge of the JORDAN decomposition of A . The result is of theoretical interest and serves as basis for several improvements.

THEOREM 2.1 (eigenexpansion of $P(z)$). *Let $P(z)$, V and \hat{V} be defined as above. Pick an eigenvalue λ of A . Let α , $\omega(z)$, V_λ , \hat{V}_λ and N_λ be defined with respect to chosen λ .*

Then

$$\frac{P^{(\ell)}(\lambda)}{\ell!} = V_\lambda \left(\sum_{k=0}^{\ell} \frac{\omega^{(k)}(\lambda)}{k!} N_\lambda^{(\alpha-1)-(\ell-k)} \right) \hat{V}_\lambda^H \quad \forall 0 \leq \ell < \alpha \quad (2.1)$$

and

$$\frac{P^{(\alpha)}(\lambda)}{\alpha!} = V_\lambda \left(\sum_{k=1}^{\alpha} \frac{\omega^{(k)}(\lambda)}{k!} N_\lambda^{k-1} \right) \hat{V}_\lambda^H + V S(\lambda) \hat{V}^H, \quad (2.2)$$

where $S(\lambda)$ is defined by

$$S(\lambda) \equiv \omega(\lambda) \left(\bigoplus_{\mu \neq \lambda} ({}^{\lambda}J_\mu)^{-1} \oplus O \right). \quad (2.3)$$

REMARK 2.1. *The proof follows upon multiplication of the well known representation of the resolvent as sum of LAURENT expansions at the eigenvalues, see [10, Corollary 2.2.12]. This representation of the adjugate of zA can be viewed as a special case of utilizing SCHWERDTFEGER's formula, see [19, (6.1.39)].*

Since the proof based on the representation of the resolvent or on SCHWERDTFEGER's formula is for notational reasons almost as long as a direct proof, we decided to give a direct proof.

Proof. Applying the CAUCHY-BINET formula to zA for all z in the resolvent set,

$$P(z) = \text{adj}({}^zA) = \det({}^zA)({}^zA)^{-1} = \chi(z)R(z). \quad (2.4)$$

Since we are interested in eigenvalues and eigenmatrices, we express the resolvent using the JORDAN decomposition,

$$R(z) = V ({}^zJ)^{-1} \hat{V}^H = V \left(\bigoplus_{\mu \in \Lambda} ({}^zJ_\mu)^{-1} \right) \hat{V}^H. \quad (2.5)$$

The inverse of a single block ${}^zJ_\mu$ with block size σ is easily computed as

$$({}^zJ_\mu)^{-1} = \begin{pmatrix} (z - \mu)^{-1} & \cdots & (z - \mu)^{-\sigma} \\ & \ddots & \vdots \\ & & (z - \mu)^{-1} \end{pmatrix} = \sum_{\ell=1}^{\sigma} (z - \mu)^{-\ell} N_\mu^{\ell-1}. \quad (2.6)$$

Thus, by adding for the sake of simplicity some zero terms in the sum, the inverse of a single box can be written as

$$({}^zJ_\mu)^{-1} = \gamma_\mu \bigoplus_{\iota=1}^{\sigma(\mu, \iota)} ({}^zJ_{\mu\iota})^{-1} = \gamma_\mu \bigoplus_{\iota=1}^{\sigma(\mu, \iota)} \left(\sum_{\ell=1}^{\sigma(\mu, \iota)} (z - \mu)^{-\ell} N_\mu^{\ell-1} \right) = \sum_{\ell=1}^{\alpha(\mu)} (z - \mu)^{-\ell} N_\mu^{\ell-1}. \quad (2.7)$$

We define the matrix $Q(z)$ by

$$Q(z) \equiv \chi(z) \left(\bigoplus_{\mu \in \Lambda} ({}^zJ_\mu)^{-1} \right). \quad (2.8)$$

By preceding considerations, $Q(z)$ is *polynomial* in z , since the rational factors in the inverted blocks cancel with the appropriate factors in the characteristic polynomial. After canceling terms $Q(z)$ can be expressed as follows:

$$Q(z) = \left(\sum_{\ell=1}^{\alpha} \omega(z)(z-\lambda)^{\alpha-\ell} (N_{\lambda}^{\ell-1} \oplus O) \right) + S(z)(z-\lambda)^{\alpha}. \quad (2.9)$$

Here we have defined the polynomial matrix $S(z)$ by

$$S(z) \equiv \omega(z) \left(\bigoplus_{\mu \neq \lambda} (zJ_{\mu})^{-1} \oplus O \right), \quad (2.10)$$

compare with equation (2.3).

We insert the TAYLOR expansion (1.15) of $\omega(z)$ at λ . This results in

$$Q(z) = \left(\sum_{\ell=1}^{\alpha} \sum_{k=0}^{n-\alpha} \frac{\omega^{(k)}(\lambda)}{k!} (z-\lambda)^{\alpha+k-\ell} (N_{\lambda}^{\ell-1} \oplus O) \right) + S(z)(z-\lambda)^{\alpha}. \quad (2.11)$$

Changing the order of summation by introducing variable $j = \alpha + k - \ell$, i.e., $\ell = \alpha + k - j$, we arrive at

$$Q(z) = \left[\sum_{j=0}^{n-1} \left(\sum_k \frac{\omega^{(k)}(\lambda)}{k!} (N_{\lambda}^{\alpha+k-j-1} \oplus O) \right) (z-\lambda)^j \right] + S(z)(z-\lambda)^{\alpha}, \quad (2.12)$$

where k in the second sum runs from $\max\{0, j - (\alpha - 1)\}$ to $\min\{j, n - \alpha\}$. We can safely replace the upper bound by j , since ω has degree $n - \alpha$ and all additional terms are zero. The first α terms in the TAYLOR expansion

$$Q(z) = \sum_{\ell=0}^n \frac{Q^{(\ell)}(\lambda)}{\ell!} (z-\lambda)^{\ell} \quad (2.13)$$

of $Q(z)$ at λ are given as corresponding terms in the inner brackets of (2.12), the $(\alpha + 1)$ th term has an additional summand $S(\lambda)$,

$$\frac{Q^{(\ell)}(\lambda)}{\ell!} = \sum_{k=0}^{\ell} \frac{\omega^{(k)}(\lambda)}{k!} (N_{\lambda}^{\alpha+k-\ell-1} \oplus O), \quad \forall \ell \in \{0, \dots, \alpha - 1\} \quad (2.14)$$

$$\frac{Q^{(\alpha)}(\lambda)}{\alpha!} = \sum_{k=1}^{\alpha} \frac{\omega^{(k)}(\lambda)}{k!} (N_{\lambda}^{k-1} \oplus O) + S(\lambda). \quad (2.15)$$

We compare the TAYLOR coefficients on both sides of $P(z) = VQ(z)\hat{V}^H$,

$$P^{(\ell)}(\lambda) = VQ^{(\ell)}(\lambda)\hat{V}^H \quad \forall \ell \geq 0. \quad (2.16)$$

Inserting the explicit expressions (2.14) and (2.15) and restricting attention to the invariant subspace of interest where possible,

$$V(N_{\lambda}^j \oplus O)\hat{V}^H = V_{\lambda} N_{\lambda}^j \hat{V}_{\lambda}^H, \quad (2.17)$$

finishes the proof. \square

The proof reveals that proceeding in this manner, relations may also be derived for the higher derivatives. Focusing on the leading α coefficients in the TAYLOR expansion gives rise to very simple and intuitive relations.

3. The Non-derogatory Case. In what follows, we assume without loss of generality that the eigenvalue of interest corresponds to the first JORDAN box. Explicit knowledge of the JORDAN decomposition is usually not at hand. So, we may ask for improvements for the most prominent classes of matrices. First, we still allow eigenvalues to be multiple. These matrices are non-derogatory with probability one [3]. To proceed, we need additional notations and a few definitions.

For the sake of simplicity, we introduce the notion of *natural restrictions* of the JORDAN block J_λ and the corresponding right and left eigenmatrices $V_\lambda, \hat{V}_\lambda$. These natural restrictions are identified by a superscript $[\ell]$, where ℓ is the number of *principal* vectors involved. We define the natural restrictions of the JORDAN block to be a JORDAN block to the same eigenvalue λ that has only ℓ principal vectors, i.e.,

$$J_\lambda^{[\ell]} \equiv (I_{\ell+1} \quad O_{\ell+1, \alpha - (\ell+1)}) J_\lambda \begin{pmatrix} I_{\ell+1} \\ O_{\alpha - (\ell+1), \ell+1} \end{pmatrix} \in \mathbb{C}^{(\ell+1) \times (\ell+1)} \quad (3.1)$$

is a JORDAN block of dimension $\ell + 1$. The natural restrictions of the partial eigenmatrices V_λ and \hat{V}_λ are defined to be the matrices

$$\begin{aligned} V_\lambda^{[\ell]} &\equiv V_\lambda \begin{pmatrix} I_{\ell+1} \\ O_{\alpha - (\ell+1), \ell+1} \end{pmatrix} \in \mathbb{C}^{n \times (\ell+1)}, \\ \hat{V}_\lambda^{[\ell]H} &\equiv (O_{\ell+1, \alpha - (\ell+1)} \quad I_{\ell+1}) \hat{V}_\lambda^H \in \mathbb{C}^{(\ell+1) \times n}. \end{aligned} \quad (3.2)$$

We stress the fact that the ordering of the principal vectors as columns of the restrictions is the converse of each other.

COROLLARY 3.1 (non-derogatory eigenexpansion of $P(z)$). *Let $A \in \mathbb{C}^{n \times n}$. Let λ be non-derogatory, i.e., geometrically simple. Let α denote the algebraic multiplicity of λ . Let J_λ denote the unique JORDAN block, V_λ the corresponding right eigenbasis and \hat{V}_λ^H the corresponding biorthogonal left eigenbasis. Let natural restrictions of JORDAN block, right, and left eigenbasis be defined as above for all $\ell < \alpha$.*

Then, for all $\ell < \alpha$

$$\frac{P^{(\ell)}(\lambda)}{\ell!} = V_\lambda^{[\ell]} \omega \left(J_\lambda^{[\ell]} \right) \hat{V}_\lambda^{[\ell]H}. \quad (3.3)$$

We denote the columns of the right eigenbasis and the columns of the flipped left eigenbasis by

$$V_\lambda \equiv (v_1, \dots, v_\alpha) \quad \text{and} \quad \hat{V}_\lambda^H \equiv W_\lambda \equiv (w_1, \dots, w_\alpha). \quad (3.4)$$

Then, for all $\ell < \alpha$

$$\begin{aligned} \frac{P^{(\ell)}(\lambda)}{\ell!} &= \frac{\omega^{(\ell)}(\lambda)}{\ell!} v_1 w_1^H + \frac{\omega^{(\ell-1)}(\lambda)}{(\ell-1)!} (v_1 w_2^H + v_2 w_1^H) + \dots \\ &\quad + \omega(\lambda) \left(\sum_{k=1}^{\ell+1} v_k w_{(\ell+1)-k+1}^H \right). \end{aligned} \quad (3.5)$$

Proof. Theorem 2.1, equation (2.1) shows that

$$\frac{P^{(\ell)}(\lambda)}{\ell!} = V_\lambda \left(\sum_{k=0}^{\ell} \frac{\omega^{(k)}(\lambda)}{k!} N_\lambda^{(\alpha-1)-(\ell-k)} \right) \hat{V}_\lambda^H \quad \forall 0 \leq \ell < \alpha.$$

Since λ is non-derogatory, N_λ is given by one single nilpotent matrix $N_{\lambda 1}$. The powers of N_λ are given by shifted unit diagonal matrices,

$$N^{(k)} \equiv N_\lambda^k, \quad n_{ij}^{(k)} = \delta_{i,j-k}. \quad (3.6)$$

Carefully looking at the term in brackets reveals that

$$\sum_{k=0}^{\ell} \frac{\omega^{(k)}(\lambda)}{k!} N_\lambda^{(\alpha-1)-(\ell-k)} = \begin{pmatrix} 0 & \cdots & 0 & & & & \\ \vdots & \ddots & \vdots & \omega(J_\lambda^{[\ell]}) & & & \\ 0 & \cdots & 0 & & & & \\ 0 & \cdots & 0 & 0 & \cdots & 0 & \\ \vdots & \ddots & \vdots & \vdots & \ddots & \vdots & \\ 0 & \cdots & 0 & 0 & \cdots & 0 & \end{pmatrix}, \quad (3.7)$$

where

$$\omega(J_\lambda^{[\ell]}) \equiv \begin{pmatrix} \omega(\lambda) & \cdots & \omega^{(\ell)}(\lambda)/\ell! \\ & \ddots & \vdots \\ & & \omega(\lambda) \end{pmatrix} \in \mathbb{C}^{(\ell+1) \times (\ell+1)} \quad (3.8)$$

is the polynomial ω evaluated at the *natural restriction* of the JORDAN block J_λ of dimension $\ell + 1$. The zero blocks ensure that only the $\ell + 1$ *leading* columns of V_λ and the $\ell + 1$ *trailing* columns of \hat{V}_λ play a rôle. This is where the natural restrictions of the left and right partial eigenmatrices emerge. Stripping off zero blocks proves the first claim of equation (3.3). The second claim, equation (3.5), follows upon splitting the polynomial matrix in the middle into rank-one matrices and sorting terms by the degree of the derivative of ω . \square

REMARK 3.1. *The relation for $\ell = 0$, namely,*

$$\text{adj}(\lambda I - A) = P(\lambda) = \omega(\lambda) \cdot vw^H = \left(\prod_{\mu \neq \lambda} (\lambda - \mu) \right) vw^H, \quad (3.9)$$

is well known and states that the adjugate of $\lambda I - A$ in case of a non-derogatory eigenvalue λ is a rank-one matrix whose columns and rows are multiples of the right eigenvector and left eigenvector, respectively.

To the authors knowledge, the similarly simple relations for $\ell \neq 0$ did not appear in the open literature.

4. Diagonalizable Matrices. Matrices with principal vectors form a zero-set. Thus, it is natural to restrict the investigations to the diagonalizable case. This implies that $N_\lambda = 0$, and only terms with $N_\lambda^0 = I$ are of interest.

COROLLARY 4.1. *Let $A \in \mathbb{C}^{n \times n}$ be diagonalizable. Let λ be an eigenvalue of A with multiplicity α . Let $P(z)$, $\chi(z)$, V_λ and \hat{V}_λ be defined as above.*

Then, the first $\alpha - 1$ derivatives of $P(z)$ at λ are all zero,

$$P^{(\ell)}(\lambda) = 0 \quad \forall \ell \leq \alpha - 2, \quad (4.1)$$

and the derivative $\alpha - 1$ of P at λ is a scalar multiple of the spectral projector,

$$\frac{P^{(\alpha-1)}(\lambda)}{\chi^{(\alpha)}(\lambda)} = \frac{1}{\alpha} V_\lambda \hat{V}_\lambda^H = \frac{1}{\alpha} \sum_i v_i \hat{v}_i^H. \quad (4.2)$$

Proof. This is an immediate consequence of Theorem 2.1, equation (2.1). Due to $N_\lambda = 0$, the only terms that are non-zero in the sum in equation (2.1) are the terms such that $(\alpha - 1) - (\ell - k) = 0$. This can only be solved for nonnegative k when $\ell \geq \alpha - 1$, which proves equation (4.1). The only solution for $\ell = \alpha - 1$ is given for $k = 0$:

$$\frac{P^{(\alpha-1)}(\lambda)}{(\alpha-1)!} = V_\lambda \left(\omega(\lambda) I \right) \hat{V}_\lambda^H.$$

Rewritten in terms of χ instead of ω and sorted according to polynomials in λ and constant matrices this is equation (4.2). \square

4.1. Normal Matrices. Now we restrict our attention to the case that A is a normal matrix. This implies that we can choose the eigenmatrix such that $\hat{V} = V$ is unitary and that $N_\lambda = 0$. Normal matrices are members of the best investigated class of matrices concerning behavior of eigenvalues and eigenvectors. In order not to double any work, we just briefly touch this large and interesting area. Since we have no need for an artificial left eigenmatrix with natural ordering, we use the letter W in this subsection to denote a nonnegative doubly stochastic matrix.

An immediate consequence of Corollary 4.1 is the following remark:

REMARK 4.1. *Let $A \in \mathbb{C}^{n \times n}$ be normal. Then the diagonal elements of equation (4.2) give information where the eigenspace is “thin” or “thick”, i.e., where the eigenvalue “lives” in the following strict mathematical sense:*

$$\left(\frac{\sum_{i=1}^{\alpha} |v_{i1}|^2}{\alpha}, \dots, \frac{\sum_{i=1}^{\alpha} |v_{in}|^2}{\alpha} \right)^T = \text{diag} \left(\frac{P^{(\alpha-1)}(\lambda)}{\chi^{(\alpha)}(\lambda)} \right). \quad (4.3)$$

This gives information, since the columns of V_λ are all scaled to unit length, because we assume $V_\lambda^H V_\lambda = I_\alpha$.

Another, more useful consequence was used by Thompson in his sequel of nine principal submatrices papers.

COROLLARY 4.2 (THOMPSON, [24], equations (7) and (8)). *Let $A \in \mathbb{C}^{n \times n}$ be normal. Denote the characteristic polynomial by $\chi(z) = \det(zA) = \det(zI - A)$ and define characteristic polynomials $\chi_i(z) \equiv \det(zA_{ii}) = \det(zI - A_{ii})$ for the principal submatrices A_{ii} , $i = 1, \dots, n$ of A . Define the nonnegative and doubly stochastic matrix W by $w_{ij} \equiv |v_{ij}|^2$.*

Then

$$\begin{pmatrix} \chi_1(z) \\ \vdots \\ \chi_n(z) \end{pmatrix} = W \begin{pmatrix} \frac{\chi(z)}{z - \lambda_1} \\ \vdots \\ \frac{\chi(z)}{z - \lambda_n} \end{pmatrix} \quad (4.4)$$

Proof. Row i of equation (4.4) is given by

$$\chi_i(z) = \sum_{j=1}^n |v_{ij}|^2 \frac{\chi(z)}{z - \lambda_j}. \quad (4.5)$$

But this is just the element in position i in the diagonal of the equation $P(z) = VQ(z)V^H$ for the special case of A being diagonalizable, where $Q(z)$ defined in equation (2.8) takes the simple form

$$Q(z) = \chi(z) \left(\bigoplus_{\lambda \in \Lambda} (zI_\alpha - \lambda I_\alpha)^{-1} \right). \quad (4.6)$$

□

THOMPSON used this result and more general results for smaller principal submatrices to derive several statements on the positions of eigenvalues of normal, HERMITEAN and symmetric matrices. This includes among various other results an alternative simple proof of CAUCHY's interlacing inequalities, see [32], page 213. Since most results obtained by THOMPSON are based on the fact that W is *nonnegative* and doubly stochastic, they can not be easily adopted to a more general case.

5. Hessenberg Matrices. In this section we denote the matrix of interest by H instead of A to emphasize that we restrict attention to *unreduced upper* HESSENBERG matrices. Before we proceed, we briefly remind of the structure of inverses of HESSENBERG matrices. This knowledge in mind we might suspect similar knowledge on the structure of the resolvent and thus of the adjugate of zH .

Beginning with the pioneering work by ASPLUND [4] in 1959 on matrices that satisfy $a_{ij} = 0$ for $j > i + p$, much knowledge has been gained for inverses of HESSENBERG matrices. The main branch of research soon specialized to tridiagonal matrices, see the 1992 review [20] by MEURANT.

Summarizing their results in a simplified manner, we may state that the lower triangular part of the inverse is the lower triangular part of a certain rank-one matrix. Similarly, the HESSENBERG eigenvalue-eigenmatrix relations turn out to be conceptually simple for the lower triangular part of the adjugate of zH .

Instead of merely doubling the work for inverses to fit for the adjugate, we give a full expression for the adjugate in terms of principal submatrices and products of lower diagonal elements. To be more precise, we intend to show that $P(z) \equiv \text{adj}({}^zH)$ is expressible in terms of what we refer to as *leading*, *trailing* and *middle* characteristic polynomials of the underlying HESSENBERG matrix.

To state the result in full generality, we first prove two lemmata and introduce additional notations. We define polynomial vectors $\nu(z)$ and $\check{\nu}(z)$ by

$$\nu(z) \equiv \left(\frac{\chi_{i+1:n}(z)}{\prod_{l=i+1}^n h_{l,l-1}} \right)_{i=1}^n \quad \text{and} \quad \check{\nu}(z) \equiv \left(\frac{\chi_{1:j-1}(z)}{\prod_{l=1}^{j-1} h_{l+1,l}} \right)_{j=1}^n, \quad (5.1)$$

with the usual convention that the empty product is one and where $\chi_{i:j}(z)$ is defined by

$$\chi_{i:j}(z) \equiv \begin{cases} \det({}^zH_{i:j}), & 1 \leq i \leq j \leq n, \\ 1, & i - 1 = j. \end{cases} \quad (5.2)$$

Here, ${}^zH_{i:j}$ is the principal submatrix of zH consisting of the elements indexed by rows and columns i to j . Thus,

$$\det({}^zH_{i:j}) \equiv \det(zI - H_{i:j})$$

is a characteristic polynomial which we term *leading*, when $i = 1$ and $j < n$, *trailing*, when $i > 1$ and $j = n$, and *middle*, when $i > 1$ and $j < n$. Hence, $\nu(z)$ consists of all (scaled) trailing and $\check{\nu}(z)$ of all (scaled) leading characteristic polynomials. Let constant h_{Π} be given by

$$h_{\Pi} \equiv \prod_{l=1}^{n-1} h_{l+1,l}. \quad (5.3)$$

Now we are able to state and prove the first lemma.

LEMMA 5.1 (row index less than column index). *Let $H \in \mathbb{C}^{n \times n}$ be unreduced upper HESSENBERG. Let $P(z)$ denote the adjugate of ${}^zH \equiv zI - H$. Let $\nu(z)$, $\check{\nu}(z)$ and h_Π be defined as denoted above. Furthermore, let $\text{tril}(A)$ denote the restriction of A to its triangular lower part.*

Then

$$\text{tril}(P(z)) = \text{tril}(h_\Pi \nu(z) \check{\nu}(z)^T). \quad (5.4)$$

Especially, we have validity of the relations

$$({}^zH)\nu(z) = \frac{\chi(z)}{h_\Pi} e_1, \quad \check{\nu}(z)^T ({}^zH) = \frac{\chi(z)}{h_\Pi} e_n^T. \quad (5.5)$$

Proof. By definition of $P(z)$, the matrix elements $p_{ij}(z)$ can be expressed for the lower triangular part ($i \geq j$) in terms of cofactors as follows:

$$p_{ij}(z) = (-1)^{i+j} \begin{vmatrix} zI - H_{1:j-1} & & \star \\ & R_{j:i-1} & \\ 0 & & zI - H_{i+1:n} \end{vmatrix} \quad (5.6)$$

$$= \chi_{1:j-1}(z) \left(\prod_{l=j}^{i-1} h_{l+1,l} \right) \chi_{i+1:n}(z) \quad (5.7)$$

$$= \underbrace{\left(\frac{\chi_{i+1:n}(z)}{\prod_{l=i}^{n-1} h_{l+1,l}} \right)}_{\equiv \nu_i(z)} \underbrace{\left(\prod_{l=1}^{n-1} h_{l+1,l} \right)}_{\equiv h_\Pi} \underbrace{\left(\frac{\chi_{1:j-1}(z)}{\prod_{l=1}^{j-1} h_{l+1,l}} \right)}_{\equiv \check{\nu}_j(z)} \quad (5.8)$$

$$= h_\Pi e_i^T (\nu(z) \check{\nu}(z)^T) e_j, \quad (5.9)$$

This establishes equality between triangular lower parts of $P(z)$ and the outer product representation (5.9). We know (by definition) that the adjugate satisfies the relations

$${}^zHP(z) = P(z){}^zH = \chi(z)I. \quad (5.10)$$

Since the first column and last row are included in the triangular lower part and $\check{\nu}_1 \equiv \nu_n \equiv 1$,

$$\begin{aligned} P(z)e_1 &= h_\Pi \nu(z) \check{\nu}(z)^T e_1 = h_\Pi \nu(z), \\ e_n^T P(z) &= e_n^T \nu(z) \check{\nu}(z)^T h_\Pi = h_\Pi \check{\nu}(z)^T. \end{aligned}$$

Now, (5.5) follows upon multiplication of (5.10) with e_1 and e_n^T . \square

COROLLARY 5.2. *Let H , $\nu(z)$ and $\check{\nu}(z)$ be defined as before. Let λ denote an eigenvalue of H with (algebraic) multiplicity α .*

Then, complete chains of (unscaled) right and left principal vectors of H to the eigenvalue λ are given by

$$\left\{ \frac{\nu^{(\ell)}(\lambda)}{\ell!} \right\}_{\ell=0}^{\alpha-1} \quad \text{and} \quad \left\{ \frac{\check{\nu}^{(\ell)}(\lambda)^T}{\ell!} \right\}_{\ell=0}^{\alpha-1}. \quad (5.11)$$

The last (first) ℓ entries in the right (left) unscaled principal vector of step ℓ are zero. The entry $n-\ell$ of the unscaled right principal vector and the entry $\ell+1$ of the unscaled left principal vector are nonzero and these are given explicitly by

$$\frac{\nu_{n-\ell}^{(\ell)}(\lambda)}{\ell!} \equiv \frac{1}{\ell! \cdot \prod_{n-\ell+1}^n h_{\ell, \ell-1}} \quad \text{and} \quad \frac{\check{\nu}_{\ell+1}^{(\ell)}(\lambda)}{\ell!} \equiv \frac{1}{\ell! \cdot \prod_1^\ell h_{\ell+1, \ell}}. \quad (5.12)$$

Proof. The result stated in equation (5.5) already proves that the vectors $\nu(\lambda)$ and $\check{\nu}(\lambda)^T$ are left and right eigenvectors, respectively, since $z = \lambda$ is a zero of $\chi(z)$. We have to show that the consecutive terms in the TAYLOR expansion of $\nu(z)$ and $\check{\nu}(z)$ at λ provide specially scaled chains of principal vectors. With ${}^zH' = I$ and ${}^zH'' = 0$ and LEIBNIZ identity we conclude that

$$\begin{aligned} ({}^zH) \frac{\nu^{(\ell)}(z)}{\ell!} + \frac{\nu^{(\ell-1)}(z)}{(\ell-1)!} &= \frac{\chi^{(\ell)}(z)}{\ell! \cdot h_{\Pi}} e_1 \quad \text{and} \\ \frac{\check{\nu}^{(\ell)}(z)^T}{\ell!} ({}^zH) + \frac{\check{\nu}^{(\ell-1)}(z)^T}{(\ell-1)!} &= \frac{\chi^{(\ell)}(z)}{\ell! \cdot h_{\Pi}} e_n^T \quad \forall \ell > 1. \end{aligned}$$

Thus, for every $1 < \ell < \alpha$ we have at $z = \lambda$ that $\chi^{(\ell)}(\lambda) = 0$, and thus

$$\begin{aligned} (\lambda I - H) \frac{\nu^{(\ell)}(\lambda)}{\ell!} + \frac{\nu^{(\ell-1)}(\lambda)}{(\ell-1)!} &= 0 \quad \text{and} \\ \frac{\check{\nu}^{(\ell)}(\lambda)^T}{\ell!} (\lambda I - H) + \frac{\check{\nu}^{(\ell-1)}(\lambda)^T}{(\ell-1)!} &= 0. \end{aligned}$$

Reordering terms finishes the proof of claim (5.11). Inserting the explicit representation (5.1) of the polynomial vectors ν and $\check{\nu}$, and using the fact that the characteristic polynomials involved have leading term one, proves equations (5.12). \square

We have found complete chains of right and left principal vectors. We have not clarified yet the relation of the chains to the biorthogonal matrices V_λ and \hat{V}_λ , even if they might be constructed from explicit knowledge of the chains. This fault is removed by constructing an explicit formula for the adjugate $P(z)$ of zH . First, we take a closer look at the elements of $P(z)$ to grasp some intuitive understanding why we only could determine the entries in the lower triangular part.

COROLLARY 5.3. *The polynomials $p_{ij}(z)$ have (maximal) degree*

$$\begin{aligned} \deg(p_{ij}(z)) &= n - 1 + j - i, & i \geq j, \\ \deg(p_{ij}(z)) &\leq n - 2, & i < j. \end{aligned} \quad (5.13)$$

The latter inequality is an equality precisely when h_{ij} is nonzero.

Proof. Equality (5.13) follows from (5.7) since the elements are products of characteristic polynomials of degrees $n-i$ and $j-1$ (with leading coefficient one) and a nonzero constant (due to the unreduced HESSENBERG structure). Inequality (5.13) follows since when $i \neq j$ in the expansion of the determinant of ${}^zH_{ji}$ the maximal number of occurrences of the variable z is given by $n-2$. When $i < j$, the only element in the submatrix ${}^zH_{ji}$ where no variable z occurs in the corresponding row and column is given by $-h_{ij}$ in the shifted position $(i, j-1)$. Thus, for $i < j$, $p_{ij}(z)$ has an expansion

$$p_{ij}(z) = (-1)^{i+j} \cdot (-1)^{i+(j-1)} \cdot (-h_{ij}) z^{n-2} \pm \dots = h_{ij} z^{n-2} \pm \dots$$

□

The elements in the strictly upper part of $P(z)$ have a lower degree than the corresponding elements in the outer product of ν and $\check{\nu}^T$. Still, it turns out that we can relate $P(z)$ to the outer product in such a way that they are equal *precisely* at the eigenvalues (counting algebraic multiplicity). To proceed, we need the following auxiliary lemma, in which the middle characteristic polynomials first enter the scene.

LEMMA 5.4. *The elements of the inverse $M^\Delta(z)$ of the regular upper triangular matrix $H^\Delta(z) \in \mathbb{C}^{(n-1) \times (n-1)}$ obtained from zH upon deletion of the first row and the last column are given by*

$$m_{ij}^\Delta(z) = \begin{cases} -\frac{\chi_{i+1;j}(z)}{\prod_{l=i}^j h_{l+1,l}}, & i \leq j, \\ 0, & i > j. \end{cases} \quad (5.14)$$

Proof. We express the inverse of $H^\Delta(z)$ using the adjugate and the determinant:

$$m_{ij}^\Delta(z) = (-1)^{i+j} \begin{vmatrix} R_{1:i-1} & & \star \\ & zI - H_{i+1;j} & \\ 0 & & R_{j+1:n-1} \end{vmatrix} / \left(\prod_{l=1}^{n-1} -h_{l+1,l} \right) \quad (5.15)$$

$$= (-1)^{i+j} \frac{\left(\prod_{l=1}^{i-1} -h_{l+1,l} \right) \chi_{i+1;j}(z) \left(\prod_{l=j+1}^{n-1} -h_{l+1,l} \right)}{\prod_{l=1}^{n-1} -h_{l+1,l}} \quad (5.16)$$

$$= (-1)^{i+j} \frac{\chi_{i+1;j}(z)}{\prod_{l=i}^j -h_{l+1,l}} = -\frac{\chi_{i+1;j}(z)}{\prod_{l=i}^j h_{l+1,l}}. \quad (5.17)$$

□

Now we are able to give an explicit simple expression for the adjugate $P(z)$ of zH in terms of characteristic submatrices and products of sub-diagonal elements. This is one of our main results, since it allows us to switch from purely *analytic* properties of (characteristic) polynomials to purely *algebraic* properties of eigen- and principal vectors, once an eigenvalue λ is known.

THEOREM 5.5. *Let $H \in \mathbb{C}^{n \times n}$ be unreduced upper HESSENBERG. Let polynomial vectors $\nu(z)$, $\check{\nu}(z)$ and constant h_Π be defined as above. Let the strictly upper triangular polynomial matrix $M(z)$ be defined by*

$$M(z) \equiv \begin{pmatrix} 0 & & \\ \vdots & M^\Delta(z) & \\ 0 & \dots & 0 \end{pmatrix}. \quad (5.18)$$

Then

$$P(z) = h_\Pi \nu(z) \check{\nu}(z)^T + \chi(z) M(z), \quad i.e., \quad (5.19)$$

$$p_{ij}(z) = \begin{cases} \chi_{1;j-1}(z) \left(\prod_{l=j}^{i-1} h_{l+1,l} \right) \chi_{i+1;n}(z) & j \leq i, \\ \frac{\chi_{1;j-1}(z) \chi_{i+1;n}(z) - \chi_{i+1;j-1}(z) \chi_{1;n}(z)}{\prod_{l=i}^{j-1} h_{l+1,l}} & i < j. \end{cases} \quad (5.20)$$

REMARK 5.1. *The theorem implies the slightly weaker, but easier to remember and thus remarkable result*

$$P(z) = h_{\Pi}\nu(z)\check{\nu}(z)^T \pmod{\chi(z)}. \quad (5.21)$$

Proof. The adjugate of zH is uniquely defined by property (5.10), i.e., it suffices to prove that

$$\begin{aligned} & [h_{\Pi}\nu(z)\check{\nu}(z)^T + \chi(z)M(z)] {}^zH = \chi(z)I \\ \text{and } & {}^zH [h_{\Pi}\nu(z)\check{\nu}(z)^T + \chi(z)M(z)] = \chi(z)I. \end{aligned}$$

We use equation (5.5) to simplify:

$$\begin{aligned} \chi(z) [\nu(z)e_n^T + M(z)({}^zH)] &= \chi(z)I, \\ \chi(z) [e_1\check{\nu}(z)^T + ({}^zH)M(z)] &= \chi(z)I. \end{aligned}$$

Thus, we have to show that $M(z)$ satisfies the following singular systems of equations:

$$M(z)({}^zH) = \nu(z)e_n^T - I, \quad ({}^zH)M(z) = e_1\check{\nu}(z)^T - I \quad (5.22)$$

These singular systems have a very special structure. For convenience, we give a pictorial impression of the first system of equations (5.22):

$$\begin{aligned} \left(\begin{array}{c|ccc} 0 & & & \\ \vdots & M^{\Delta}(z) & & \\ 0 & & & \\ \hline 0 & 0 & \dots & 0 \end{array} \right) & \left(\begin{array}{ccc|c} z-h_{11} & -h_{12} & \dots & -h_{1n} \\ & & & \vdots \\ & H^{\Delta}(z) & & -h_{n-1,n} \\ & & & z-h_{nn} \end{array} \right) \\ &= \left(\begin{array}{c|ccc} & & & -\nu_1(z) \\ & I & & \vdots \\ & & & -\nu_{n-1}(z) \\ \hline 0 & \dots & 0 & 0 \end{array} \right) \quad (5.23) \end{aligned}$$

We can now safely remove the last rows of the first and the last matrix in this equation, since they correspond to blocks that are trivially satisfied due to the zero elements. We can also remove the first column of the first matrix and the first row of the second matrix, since multiplication in these positions only introduces zero elements. We end up with the following simpler system of equations:

$$M^{\Delta}(z) \left(\begin{array}{c|ccc} & & -h_{2n} & \\ & H^{\Delta}(z) & \vdots & \\ & & -h_{n-1,n} & \\ & & z-h_{nn} & \end{array} \right) = \left(\begin{array}{c|ccc} & & & -\nu_1(z) \\ & I & & \vdots \\ & & & -\nu_{n-1}(z) \end{array} \right) \quad (5.24)$$

The first block collapses to the definition of $M^{\Delta}(z)$, i.e., to $M^{\Delta}(z)H^{\Delta}(z) = I$. We

only have to prove consistency by proving that also the second block equation

$$M^\Delta(z) \begin{pmatrix} -h_{2n} \\ \vdots \\ -h_{n-1,n} \\ z - h_{nn} \end{pmatrix} = \begin{pmatrix} -\nu_1(z) \\ \vdots \\ -\nu_{n-1}(z) \end{pmatrix} \quad (5.25)$$

$$\Leftrightarrow \begin{pmatrix} -h_{2n} \\ \vdots \\ -h_{n-1,n} \\ z - h_{nn} \end{pmatrix} = H^\Delta(z) \begin{pmatrix} -\nu_1(z) \\ \vdots \\ -\nu_{n-1}(z) \end{pmatrix} \quad (5.26)$$

holds true. This follows trivially by reordering, since $\nu_n(z) \equiv 1$ and thus we only have to prove that

$$\left(H^\Delta(z) \left| \begin{array}{c} -h_{2n} \\ \vdots \\ -h_{n-1,n} \\ z - h_{nn} \end{array} \right. \right) \begin{pmatrix} \nu_1(z) \\ \vdots \\ \nu_{n-1}(z) \\ \nu_n(z) \end{pmatrix} = 0 \quad (5.27)$$

But these equations correspond to the second to last row of the first equation of (5.5), which finishes the proof for the first singular system of equations in (5.22). The proof for the second singular system of equations in (5.22) is analogous. \square

To express the final relations in matrix form we gather the derivatives of the vectors ν and $\check{\nu}$ into matrices. We define rectangular matrices $\mathcal{V}_\ell(z)$ and $\check{\mathcal{V}}_\ell(z)$ by

$$\mathcal{V}_\ell(z) \equiv \left[\nu(z), \nu'(z), \dots, \frac{\nu^{(\ell)}(z)}{\ell!} \right], \quad \check{\mathcal{V}}_\ell(z) \equiv \left[\check{\nu}^{(\ell)}(z), \dots, \check{\nu}'(z), \check{\nu}(z) \right]. \quad (5.28)$$

Now we can prove the main theorem stating the explicit relation between the (analytic) polynomial and the (algebraic) subspace point of view for unreduced HESSENBERG matrices.

THEOREM 5.6 (HESSENBERG eigenvalue-eigenmatrix relations). *Let $H \in \mathbb{C}^{n \times n}$ be an unreduced HESSENBERG matrix. Let λ be an arbitrary eigenvalue of H . Let α be the multiplicity of λ . Let ω be the corresponding reduced characteristic polynomial. Let natural restrictions of the JORDAN block and the partial eigenmatrices corresponding to the chosen λ be defined by (3.1) and (3.2). Let the constant h_Π be defined by (5.3) and let \mathcal{V}_ℓ and $\check{\mathcal{V}}_\ell$ be defined by (5.28).*

Then

$$V_\lambda^{[\ell]} \omega \left(J_\lambda^{[\ell]} \right) \hat{V}_\lambda^{[\ell]H} = h_\Pi \cdot \mathcal{V}_\ell(\lambda) \check{\mathcal{V}}_\ell(\lambda)^T. \quad (5.29)$$

Proof. Theorem 2.1 is already tailored to the non-derogatory case, see Corollary 3.1. This is the left hand side of equation (5.29). It only remains to prove that the terms in the TAYLOR expansion of $P(z)$ around λ are indeed given by the outer product of the matrices gathering the derivatives. But this is again LEIBNIZ identity,

this time applied to the consecutive derivatives of $\nu(z)\check{\nu}(z)$:

$$\frac{(\nu(z)\check{\nu}(z)^T)^{(\ell)}}{\ell!} = \frac{1}{\ell!} \sum_{k=0}^{\ell} \binom{\ell}{k} \nu(z)^{(k)} (\check{\nu}(z)^T)^{(\ell-k)} \quad (5.30a)$$

$$= \sum_{k=0}^{\ell} \frac{\nu(z)^{(k)}}{k!} \cdot \frac{(\check{\nu}(z)^T)^{(\ell-k)}}{(\ell-k)!} = \mathcal{V}_{\ell} \check{\mathcal{V}}_{\ell}^T \quad (5.30b)$$

□

To proceed, we need two additional simple lemmata. The first clarifies uniqueness issues of partial eigenmatrices to non-derogatory eigenvalues, the second investigates square roots of upper triangular (regular) TOEPLITZ matrices.

LEMMA 5.7. *Let λ be a non-derogatory eigenvalue of algebraic multiplicity α of $A \in \mathbb{C}^{n \times n}$. As before, let $J_{\lambda} \in \mathbb{C}^{\alpha \times \alpha}$ denote the unique JORDAN block and let V_{λ} denote a fixed partial eigenmatrix.*

Then the set of all partial eigenmatrices is given by the α -dimensional set

$$\{V_{\lambda}T : T \in \mathbb{C}^{\alpha \times \alpha} \text{ is upper triangular regular TOEPLITZ}\}. \quad (5.31)$$

Proof. Let $\tilde{V}_{\lambda} \in \mathbb{C}^{n \times \alpha}$ denote an arbitrary partial eigenmatrix. This together with the assumption that λ is non-derogatory implies that \tilde{V}_{λ} has full rank and spans the same space as V_{λ} , i.e., $\tilde{V}_{\lambda} = V_{\lambda}T$, where $T \in \mathbb{C}^{\alpha \times \alpha}$ is regular. Additionally, the relation

$$A\tilde{V}_{\lambda} = \tilde{V}_{\lambda}J_{\lambda}. \quad (5.32)$$

holds true, since \tilde{V}_{λ} by definition is a partial eigenmatrix. This implies that

$$A\tilde{V}_{\lambda} = AV_{\lambda}T = V_{\lambda}J_{\lambda}T = V_{\lambda}TJ_{\lambda} = \tilde{V}_{\lambda}J_{\lambda}, \quad (5.33)$$

i.e., the set of all T is the subset of regular matrices described by the additional constraint $J_{\lambda}T = TJ_{\lambda}$. In other words, we are looking for the regular matrices T in the *centralizer* of the JORDAN block J_{λ} . The centralizer of a JORDAN block is easily computed regardless of the value of λ , since

$$0 = J_{\lambda}T - TJ_{\lambda} = (\lambda I + N)T - T(\lambda I + N) = NT - TN. \quad (5.34)$$

When we interpret the nilpotent matrix N as a shift matrix, we observe that T has to be upper triangular TOEPLITZ. Thus, the set of matrices T we are looking for consists of the upper triangular regular TOEPLITZ matrices. The dimension of the set follows upon the parameterization of the TOEPLITZ matrices by their first row. □

Now, having parameterized the set of all partial eigenmatrices to a non-derogatory eigenvalue, we can choose in light of Theorem 5.6 left and right partial eigenmatrices such that they are *biorthogonal*. This could be achieved by setting

$$V_{\lambda} = \mathcal{V}_{\alpha-1}(\lambda) \quad \text{and} \quad \check{V}_{\lambda} = h_{\Pi} \check{\mathcal{V}}_{\alpha-1}(\lambda) (\omega(J_{\lambda}))^{-T}, \quad (5.35)$$

or

$$V_{\lambda} = h_{\Pi} \mathcal{V}_{\alpha-1}(\lambda) (\omega(J_{\lambda}))^{-1} \quad \text{and} \quad \check{V}_{\lambda} = \check{\mathcal{V}}_{\alpha-1}(\lambda). \quad (5.36)$$

Here, we have used for purely esthetic reasons the notation

$$\check{V}_\lambda \equiv \overline{\check{V}_\lambda}. \quad (5.37)$$

To obtain a more symmetric and more appropriate choice, we need the following lemma on square roots of regular upper triangular TOEPLITZ matrices. It is easy to see that a regular upper triangular TOEPLITZ matrix has exactly two upper triangular TOEPLITZ square roots. The square roots can be distinguished by the usual scalar square root of the diagonal element.

We remark that in the proof of the following lemma, σ is used to denote the first row of a upper triangular TOEPLITZ matrix, instead the size of a JORDAN block.

LEMMA 5.8 (TOEPLITZ square roots). *Let $T \in \mathbb{C}^{n \times n}$ be an upper triangular TOEPLITZ matrix. Let T be parameterized by the first row denoted by τ , such that $t_{ij} = \tau_{j-i+1}$ for all $i \leq j$.*

Then, when T is regular, which is precisely when $\tau_1 \neq 0$, exactly two upper triangular TOEPLITZ square roots $S_1, S_2 \in \mathbb{C}^{n \times n}$ exist. These square roots are both regular and are related by $S_1 = -S_2$.

When T is singular, i.e., when τ_1 is equal zero, no upper triangular TOEPLITZ square root exists.

Proof. We give a constructive proof. Let S be upper triangular TOEPLITZ. Let S be parameterized by first row, denoted by σ , $s_{ij} = \sigma_{j-i+1}$. For S being a square root of T , i.e., a matrix such that $SS = T$, necessarily

$$\tau_i = (T)_{1i} = (SS)_{1i} = \sum_{j=1}^n s_{1j}s_{ji} = \sum_{j=1}^i \sigma_j\sigma_{i-j+1}. \quad (5.38)$$

Thus, for $i = 1$, $\sigma_1\sigma_1 = \tau_1$. Here, we can choose one of the two branches of the square root, denoted by $\sigma_1 = \pm\sqrt{\tau_1}$. Then we can successively compute uniquely all other σ_i , $i = 2, \dots, n$ using the triangular structure, precisely when $\sigma_1 \neq 0$:

$$\sigma_i = \frac{\tau_i - \sum_{j=2}^{i-1} \sigma_j\sigma_{i-j+1}}{2\sigma_1} \quad (5.39)$$

It is easy to verify that both computed S indeed satisfy $SS = T$. Since the branch ± 1 of the square root enters only linearly, $S_1 = -S_2$. Since $\sigma_1 \neq 0$ precisely when $\tau_1 \neq 0$, we have proven all assertions of the lemma. \square

In the following, we will denote the square roots S_1 and S_2 of Lemma 5.8 simply by $\pm\sqrt{T}$.

Since $\omega(\lambda)$ is non-zero, $\omega(J_\lambda)$ is regular. $\omega(J_\lambda)$ is upper triangular TOEPLITZ. Thus, we can utilize the last two lemmata to define unique biorthogonal matrices V_λ and \check{V}_λ . This is achieved by the following definition:

DEFINITION 5.9 (HESSENBERG natural eigenbasis). *We define the natural eigenbasis of an unreduced HESSENBERG matrix $H \in \mathbb{C}^{n \times n}$ by defining the special partial left and right eigenmatrices*

$$V_\lambda = \sqrt{h_\Pi} \mathcal{V}_{\alpha-1}(\lambda) \left(\sqrt{\omega(J_\lambda)} \right)^{-1} \quad (5.40)$$

$$\check{V}_\lambda = \sqrt{h_\Pi} \check{\mathcal{V}}_{\alpha-1}(\lambda) \left(\sqrt{\omega(J_\lambda)} \right)^{-T} \quad (5.41)$$

for all eigenvalues λ of H .

We note the interesting fact that the conditioning of the eigenspaces concerning the angles between the subspaces depends only on the leading and trailing characteristic polynomials and the eigenvalue λ , i.e., the point of evaluation. The distance to the other eigenvalues enters the scene afterwards in some sort of normalization of the eigen- and principal vectors by the inverse of the square roots of $\omega(J_\lambda)$.

5.1. Particular Cases. We briefly collect implications on some particular cases of HESSENBERG matrices. When the HESSENBERG matrix H is diagonalizable all eigenvalues are simple and the results collapse to a very simple special case. When H is furthermore normal, $\hat{V} = V$ and we can utilize all results on normal matrices, e.g., the results of THOMPSON, and insert the explicit representation of P .

At first glance, it seems difficult to find unreduced normal HESSENBERG matrices. Two known remarkable exceptions are unitary (or real orthogonal) HESSENBERG matrices and HERMITEAN (or real symmetric) tridiagonal matrices.

The former naturally arise as the Q factor from the QR decomposition of a HESSENBERG matrix and when we use the ARNOLDI method to compute a HESSENBERG normal form of an arbitrary unitary matrix. Unitary HESSENBERG matrices are treated in more detail in several articles by AMMAR et al., [1, 2]. In this context, what we named *leading characteristic polynomials* are known as *Szegő polynomials*.

The latter are not only *upper* HESSENBERG matrices, but at the same time also *lower* HESSENBERG matrices. Thus, we obtain forward and backward expressions for the eigenvectors. This symmetric case (up to scaling) corresponds to the aforementioned JACOBI matrices.

Two conceptual simple cases of special HESSENBERG matrices deserve some attention. These are the FROBENIUS companion and doubly companion matrices. The first case has already been mentioned in the historical remarks and is exemplified in great detail in the classical work of WILKINSON [33] and in less detail applied in the context of ordinary differential equations in several textbooks, see for instance [12]. The latter case arises in the construction of stable general linear methods for ordinary differential equations, see [8, 34, 9].

6. Conclusion and Outlook. We have shown how to construct eigenvalue-eigenmatrix relations. The main new contribution is the construction of explicit relations in case of HESSENBERG matrices. These relations may be generalized to the case when we have a matrix pencil that still has HESSENBERG form.

It remains an open and challenging question how to generalize the results, especially those involving principal vectors to the infinite dimensional setting.

To develop eigenvalue-eigenmatrix relations for other matrix structures, we *only* need an explicit representation of the adjugate $P(z) = \text{adj}(zA) = \text{adj}(zI - A)$ for the matrix structure of interest, of course in terms of quantities that might be of interest in applications. This is the area of future research.

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