

Chapter 6

The Generalized **Eigenvalue Problem**

Many eigenvalue problems that arise in applications are most naturally formulated as *generalized* eigenvalue problems

$$Av = \lambda Bv$$

where A and B are $n \times n$ matrices. In this chapter we will discuss how the standard and generalized eigenvalue problems are similar and how they are different. We will introduce GZ algorithms, generalizations of GR algorithms, for solving the generalized eigenvalue problem, and we will show how GZ algorithms can be implemented by bulge-chasing.

6.1 Introduction

Consider an ordered pair (A, B) of matrices in $\mathbb{C}^{n \times n}$. A nonzero vector $v \in \mathbb{C}^n$ is called an *eigenvector* of the pair (A, B) if there exist $\mu, \nu \in \mathbb{C}$, not both zero, such that

$$\mu A v = \nu B v. \tag{6.1.1}$$

The scalars μ and ν are not uniquely determined by ν , but their ratio is (except in the *singular* case $A\nu = B\nu = 0$, which we will mention again below). If $\mu \neq 0$, (6.1.1) is equivalent to

$$Av = \lambda Bv, \tag{6.1.2}$$

where $\lambda = v/\mu$. The scalar λ is then called an *eigenvalue* of the pair (A, B) associated with the eigenvector v. If (6.1.1) holds with $\mu = 0$ and $v \neq 0$, then (A, B) is said to have an *infinite eigenvalue*; the eigenvalue of (A, B) associated with v is ∞ .

This is the generalized eigenvalue problem. In the case B = I it reduces to the standard eigenvalue problem. The following proposition records some fairly obvious facts.

Proposition 6.1.1. Let $A, B \in \mathbb{C}^{n \times n}$, and let $\lambda \in \mathbb{C}$ be nonzero.

- (a) λ is an eigenvalue of (A, B) if and only if $1/\lambda$ is an eigenvalue of (B, A).
- (b) ∞ is an eigenvalue of (A, B) if and only if 0 is an eigenvalue of (B, A).
- (c) ∞ is an eigenvalue of (A, B) if and only if B is a singular matrix.

(d) If B is nonsingular, the eigenvalues of (A, B) are exactly the eigenvalues of AB^{-1} and $B^{-1}A$. If v is an eigenvector of (A, B) with associated eigenvalue λ , then v is an eigenvector of $B^{-1}A$ with eigenvalue λ , and Bv is an eigenvector of AB^{-1} with eigenvalue λ .

The expression $A - \lambda B$ with indeterminate λ is commonly called a *matrix pencil*. The terms "matrix pair" and "matrix pencil" are used more or less interchangeably. For example, if v is an eigenvector of the pair (A, B), we also say that v is an eigenvector of the matrix pencil $A - \lambda B$.

Clearly $\lambda \in \mathbb{C}$ is an eigenvalue of (A, B) if and only if the matrix $A - \lambda B$ is singular, and this is in turn true if and only if

$$\det(\lambda B - A) = 0. \tag{6.1.3}$$

This is the *characteristic equation* of the pair (A, B). From the definition of the determinant it follows easily that the function $\det(\lambda B - A)$ is a polynomial in λ of degree n or less. We call it the *characteristic polynomial* of the pair (A, B).

It can happen that the characteristic polynomial is identically zero. For example, if there is a $v \neq 0$ such that Av = Bv = 0, then $(\lambda B - A)v = 0$ for all λ , and $\det(\lambda B - A)$ is identically zero. Every λ is an eigenvalue. The pair (A, B) is called a *singular pair* if its characteristic polynomial is identically zero. Otherwise it is called a *regular pair*. We will focus mainly on regular pairs. An example of a singular pair that does not have a common null vector is given in Exercise 6.1.2. For more on singular pairs see [92, 73, 206, 231].

If B is nonsingular, then the pair (A, B) is certainly regular. $\det(\lambda B - A) = \det(B) \det(\lambda I - B^{-1}A)$, so the characteristic polynomial is the same as that of the matrix $B^{-1}A$, except for a constant factor. The pair (A, B) has n finite eigenvalues, and they are the same as the eigenvalues of $B^{-1}A$. The pair (A, B) is also guaranteed regular if A is nonsingular. An example of a regular pencil for which neither A nor B is nonsingular is given in Exercise 6.1.4.

Two pairs (A, B) and (\tilde{A}, \tilde{B}) are *strictly equivalent* if there exist nonsingular matrices U and V such that $A = U\tilde{A}V$ and $B = U\tilde{B}V$. This is the same as to say that $A - \lambda B = U(\tilde{A} - \lambda \tilde{B})V$ for all $\lambda \in \mathbb{C}$. Two pairs that are strictly equivalent have the same eigenvalues, and their eigenvectors satisfy simple relationships (Exercise 6.1.5).

Two pairs are strictly equivalent if and only if they have the same *Kronecker canonical form*. You can read about this generalization of the Jordan canonical form in [92, Ch. XII]. For stable computational techniques, see [206] and [73].

Two pairs (A, B) and (\tilde{A}, \tilde{B}) are strictly unitarily equivalent if there exist unitary matrices U and V such that $A = U\tilde{A}V$ and $B = U\tilde{B}V$.

Theorem 6.1.2 (generalized Schur theorem). Let $A, B \in \mathbb{C}^{n \times n}$. Then there exist unitary $Q, Z \in \mathbb{C}^{n \times n}$ and upper triangular $T, S \in \mathbb{C}^{n \times n}$ such that $A = QTZ^*$ and $B = QSZ^*$. In other words,

$$A - \lambda B = Q(T - \lambda S)Z^*.$$

Thus every pair is strictly unitarily equivalent to an upper triangular pair. A proof is worked out in Exercise 6.1.6.

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The eigenvalues of an upper triangular pair (S, T) are evident. The characteristic equation is clearly

$$\det(\lambda T - S) = \prod_{j=1}^{n} (\lambda t_{jj} - s_{jj}) = 0.$$

If $t_{jj} = 0$ and $s_{jj} = 0$ for some j, the pair (S,T) is singular; otherwise it is regular (Exercise 6.1.7). In the regular case, each factor for which $t_{jj} \neq 0$ yields a finite eigenvalue $\lambda_j = s_{jj}/t_{jj}$. If there is a factor with $t_{jj} = 0$ (and hence $s_{jj} \neq 0$), then ∞ is an eigenvalue. We define the algebraic multiplicity of the infinite eigenvalue to be the number of factors $\lambda t_{jj} - s_{jj}$ for which $t_{jj} = 0$. With this convention, each regular pair has exactly n eigenvalues, some of which may be infinite.

The proof of Theorem 6.1.2 outlined in Exercise 6.1.6 is nonconstructive; it gives no clue how to compute the triangular pair (S, T) without knowing some eigenvectors in advance. Practical computational procedures will be developed in Sections 6.2 and 6.3.

We have tipped our hand about how we intend to attack the generalized eigenvalue problem. Another method that suggests itself when B is nonsingular is to form either AB^{-1} or $B^{-1}A$ and solve the standard eigenvalue problem for that matrix. As it turns out, this approach is usually inadvisable, as accuracy can be lost through the inversion of B and through formation of the product.

Example 6.1.3. Here is a small MATLAB example in which a superior outcome is obtained by keeping A and B separate.

```
format long e
randn('state',123);
[M,R] = qr(randn(2));
[N,R] = qr(randn(2));
A = [ 2 1; 0 1e-8]; B = [ 1 1; 0 1e-8];
A = M*A*N; B = M*B*N;
Smart_Result = eig(A,B)
Other_Result = eig(A*inv(B))
```

This code produces a 2×2 matrix pair (A, B) for which the eigenvalues are $\lambda_1 = 2$ and $\lambda_2 = 1$. B is ill conditioned, as is A. The eigenvalues are computed two different ways. The command eig(A,B) uses the QZ algorithm (Section 6.3), which works with A and B separately to compute the eigenvalues. The command eig(A*inv(B)) obviously computes AB^{-1} and then finds the eigenvalues. Here are the results:

```
Smart_Result =
    1.999999999475219e+00
    1.000000000557143e+00

Other_Result =
    1.997208963148296e+00
    1.002791036386043e+00
```

We see that the QZ computation got the eigenvalues correct to about ten decimal places. The fact that it did not do better can be attributed to the ill conditioning of the eigenvalues. As we see, the computation that formed AB^{-1} explicitly did much worse.

Exercises

6.1.1. Prove Proposition 6.1.1.

6.1.2. Let

$$A = \left[\begin{array}{rrr} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 1 \end{array} \right]$$

and

$$B = \left[\begin{array}{rrr} 0 & 1 & 0 \\ 0 & 0 & 1 \\ 0 & 0 & 0 \end{array} \right].$$

- (a) Show that $det(\lambda B A)$ is identically zero. Thus (A, B) is a singular pair.
- (b) Show that there is no nonzero v such that Av = Bv = 0.
- (c) For each $\lambda \in \mathbb{C}$, find a nonzero v (depending on λ) such that $(\lambda B A)v = 0$.
- **6.1.3.** Show that if A is nonsingular, then the pair (A, B) is regular.
- **6.1.4.** Let $A = \begin{bmatrix} 1 & 0 \\ 0 & 0 \end{bmatrix}$ and $B = \begin{bmatrix} 0 & 0 \\ 0 & 1 \end{bmatrix}$. Compute the characteristic polynomial of (A, B). Show that (A, B) is a regular pair with eigenvalues 0 and ∞ .
- **6.1.5.** Let (A, B) and (\tilde{A}, \tilde{B}) be equivalent pairs. Let U and V be nonsingular matrices such that $A \lambda B = U(\tilde{A} \lambda \tilde{B})V$.
 - (a) Show that (A, B) and (\tilde{A}, \tilde{B}) have the same characteristic polynomial to within a constant. Thus they have the same eigenvalues.
 - (b) Show that x is an eigenvector of (A, B) associated with eigenvalue λ if and only if Vx is an eigenvector of (\tilde{A}, \tilde{B}) associated with λ .
 - (c) A nonzero vector y^T is called a *left eigenvector* of (A, B) associated with the eigenvalue λ if $y^T A = \lambda y^T B$. Show that y^T is a left eigenvector of (A, B) if and only if $y^T U$ is a left eigenvector of (\tilde{A}, \tilde{B}) .
- **6.1.6.** This exercise proves the generalized Schur theorem (Theorem 6.1.2) by induction on n. Clearly the result holds when n = 1. Now we prove that it holds for matrices of size $n \times n$, assuming that it holds for $(n 1) \times (n 1)$ matrices.
 - (a) The fundamental task is to produce two vectors $x, y \in \mathbb{C}^n$ such that ||x|| = 1, ||y|| = 1, $Ax = \mu y$, $Bx = \nu y$, for some μ , $\nu \in \mathbb{C}$. First assume that B is nonsingular, and let x be an eigenvector of $B^{-1}A$: $B^{-1}Ax = \lambda x$, with ||x|| = 1. Now take y to be an appropriate multiple of Bx, and show that this x and y do the job for some μ and ν satisfying $\lambda = \nu/\mu$.

- (b) Now suppose that B is singular. Then there is a vector x with ||x|| = 1 and Bx = 0. Consider two cases: $Ax \neq 0$ (infinite eigenvalue) and Ax = 0 (singular pencil). Show that in each case there is a vector y satisfying ||y|| = 1 and scalars μ and ν such that $Ax = \mu y$ and $Bx = \nu y$.
- (c) Let $Z_1 \in \mathbb{C}^{n \times n}$ and $Q_1 \in \mathbb{C}^{n \times n}$ be unitary matrices with x and y as first column, respectively. Show that $Q_1^*AZ_1$ and $Q_1^*BZ_1$ are both block triangular:

$$Q_1^*(A-\lambda B)Z_1 = \begin{bmatrix} \begin{array}{c|ccc} \mu & * & \cdots & * \\ \hline 0 & & & \\ \vdots & & \hat{A} & \\ \hline 0 & & & \\ \end{bmatrix} - \lambda \begin{bmatrix} \begin{array}{c|ccc} \nu & * & \cdots & * \\ \hline 0 & & & \\ \vdots & & \hat{B} & \\ \hline 0 & & & \\ \end{bmatrix}.$$

Here you make essential use of the fact that Q_1 is unitary.

- (d) Finish the proof of the theorem by induction on n.
- **6.1.7.** Let (S, T) be a pair in which both S and T are upper triangular.
 - (a) Show that $\det(\lambda T S) = \prod_{j=1}^{n} (\lambda t_{jj} s_{jj})$.
 - (b) Show that the pair is regular if and only if there is no j for which $s_{ij} = t_{ij} = 0$.
 - (c) Suppose that the pair (S, T) is regular and has ∞ as an eigenvalue. Show that the algebraic multiplicity of the eigenvalue ∞ (the number of j for which $t_{jj} = 0$) is equal to the algebraic multiplicity of 0 as an eigenvalue of (T, S).
 - (d) Give an example of a pair (S, T) that is regular but has no finite eigenvalues.

6.2 Reduction to Hessenberg-Triangular Form

According to Theorem 6.1.2, every pair (A, B) is strictly unitarily equivalent to an upper triangular pair (S, T). If we know (S, T), then we know the eigenvalues of (A, B). We now begin to tackle the question of how to compute (S, T). The solution of the standard eigenvalue problem usually begins by reducing the matrix to a condensed form, usually upper Hessenberg form. An analogous procedure works for the generalized eigenvalue problem: We can transform (A, B) to (H, T), where H is upper Hessenberg and T is upper triangular. We call this *Hessenberg-triangular* form.

Theorem 6.2.1. Let $A, B \in \mathbb{C}^{n \times n}$. Then the pair (A, B) is strictly equivalent to a pair (H, T) that can be computed by a direct algorithm in $O(n^3)$ flops, where H is upper Hessenberg and T is upper triangular. That is, A = UHV and B = UTV, where U and V are nonsingular, and U, V, H, and T can be computed in $O(n^3)$ flops. U and V can be taken to be unitary.

Proof: We will outline a class of algorithms that transform (A, B) to the Hessenberg-triangular form. Each of the matrices U and V will be constructed as a product of elimination

matrices. If unitary transformations are desired, each elimination matrix should be taken to be unitary.

The first step is to transform B immediately to triangular form. Let B = GR be any decomposition of B for which G is nonsingular and R is upper triangular. (If you insist on a unitary transformation, do a QR decomposition.) As we know, this can be done in $O(n^3)$ flops. Then the pair $(G^{-1}A, R)$ is strictly equivalent to (A, B). The computation of $G^{-1}A$ also costs $O(n^3)$ flops. G will become a factor in the transforming matrix U.

In light of the previous paragraph, let us now consider a pair (A, B) in which B is already upper triangular. The following algorithm transforms A to upper Hessenberg form while defending the upper triangular form of B. In what follows, the symbols A and B will refer to the transformed matrices that are on their way to becoming B and B which an elimination matrix (e.g., a rotator) that acts on rows B and B which transforms B and B which transforms and to B and when it is, the upper triangular form is disturbed: B and when it is, the upper triangular form is disturbed: B and B when it is a right transformation; it will become a part of B and B and B and B are a part of B. This is a right transformation; it will become a part of B. This transformation must also be applied to B and B and B and does not disturb the zero that was introduced at position B and B and B and does not disturb the zero that was introduced at position B and B and B and B and B and does not disturb the zero that was introduced at position B and B and B and B and B and B and does not disturb the zero that was introduced at position B and B are a part of B.

The next step is to apply an elimination matrix acting on rows n-2 and n-1 to transform $a_{n-1,1}$ to zero. When this transformation is applied to B, it disturbs the triangular form, creating a nonzero in position $b_{n-1,n-2}$. This can be eliminated by a transformation on the right that acts on columns n-2 and n-1. When this transformation is applied to A, it does not disturb the zeros that were introduced previously.

Continuing in this manner, we transform the entries $a_{n-2,1}, \ldots, a_{31}$ to 0 one by one. This is as far as we can go in column one. If we try to transform a_{21} to 0, we will end up destroying all the zeros that we previously created. (We cannot violate Galois theory.) We move on to the second column and transform $a_{n,2}, a_{n-1,2}, \ldots, a_{42}$ to 0. Then we move on to the third column, the fourth column, and so on. In the end, A will have been transformed to upper Hessenberg form, and B will still be upper triangular. It is easy to check that the total computational effort is $O(n^3)$ (Exercise 6.2.1).

Second Reduction Algorithm

The proof of Theorem 6.2.1 outlines a direct method for transforming a matrix pair to Hessenberg-triangular form. We now develop a second procedure that is less efficient in general but is useful in special cases. We will use it for bulge-chasing in Section 6.3.

Unlike the first method, the second method does not begin by transforming B to upper triangular form. Instead it transforms A and B to Hessenberg and triangular form together. Transformations on the right (resp., left) are used to create zeros in B (resp., A). The first step creates the desired zeros in the first columns of A and B, beginning with B. Needed is a transformation $BH^* = \tilde{B}$ such that $\tilde{b}_{21} = \cdots = \tilde{b}_{n1} = 0$. This is a different sort of elimination than those we studied in Section 3.1, but fortunately it is not hard to accomplish, at least in theory. In fact, it can be seen as an elimination on the first column of B^{-1} in the sense of Section 3.1 (Exercise 6.2.2). Fortunately the elimination can be done even if

 B^{-1} does not exist. The conditions $\tilde{b}_{21} = \cdots = \tilde{b}_{n1} = 0$ just mean that the first row of H must be orthogonal to the second through nth rows of B, so we need to build an H with this property. A stable way to do this is to compute a decomposition B = RQ, where R is upper triangular and Q is unitary. This can be done by a process analogous to that of computing a QR decomposition (Exercise 6.2.3). Then the equation $BQ^* = R$ (first column) shows that the first row of Q is orthogonal to rows 2 through n of B. Now we just need to take H to be a matrix whose first row is proportional to the first row of Q. We could take H to be Q itself, but in general Q is quite an expensive transformation. We prefer to build a cheap transformation to do the same task. This is just a matter of building an H^* with a specified first column. We have seen in Section 3.1 how to do this economically. Once we have H, we can make the updates $B \leftarrow BH^*$, $A \leftarrow AH^*$, creating the desired zeros in B.

The second part of the first step creates zeros in the first column of A in positions $(3, 1), \ldots, (n, 1)$. This is a routine elimination that can be done as described in Section 3.1. The elimination matrix has the form $G^{-1} = \text{diag}\{1, \tilde{G}^{-1}\}$. The transformation $A \leftarrow G^{-1}A$, $B \leftarrow G^{-1}B$ creates the desired zeros in the first column of A without disturbing the zeros that were previously created in B. This completes the first step, which can be summarized as follows.

Second reduction to Hessenberg-triangular form (first step)

Compute decomposition
$$B = RQ$$
.
Compute elimination matrix H with $H^*e_1 = \alpha Q^*e_1$.
 $A \leftarrow AH^*$
 $B \leftarrow BH^*$ (creating zeros in B)
Let $x = [a_{21} \ a_{31} \ \cdots \ a_{n1}]^T$
Compute \tilde{G} such that $\tilde{G}e_1 = x$
let $G = \text{diag}\{1, \tilde{G}\}$
 $A \leftarrow G^{-1}A$ (creating zeros in A)
 $B \leftarrow G^{-1}B$

The second step introduces zeros in the second columns of A and B. It is identical to the first step, except that its action is restricted to the submatrix obtained by ignoring the first row and column of each matrix. One easily checks that the operations of the second step do not disturb the zeros that were created in the first step. The third step operates on even smaller submatrices, and so on. After n-1 steps, the pair has been transformed to Hessenberg-triangular form. The final step creates a single zero in B and no zeros in A.

This algorithm is uneconomical in general. If it is implemented in the obvious way, there is an RQ decomposition costing $O(n^3)$ work at each step. Thus the total work will be $O(n^4)$.²

¹The first reduction process that we described began with a QR decomposition of B, but it could just as well have begun with an RQ decomposition. Now, in our second reduction process, we are proposing to start with an RQ decomposition of B. Since we are going to all that expense, why don't we just use the RQ decomposition to triangularize B and then proceed as in the first reduction? Good question! The answer is that we are just developing an approach here that is not economical in general but will be useful later when we talk about bulge-chasing.

²There is a way to bring the flop count down to $O(n^3)$. A new RQ decomposition does not need to be computed from scratch at each step. Instead it can be obtained by an $O(n^2)$ updating procedure from the RQ decomposition from the previous step [134]. The resulting algorithm seems still to be somewhat more expensive than the first reduction algorithm that we described.

Exercises

- **6.2.1.** This exercise checks out some of the details of the reduction to Hessenberg-triangular form (Theorem 6.2.1).
 - (a) Check that the algorithm sketched in the proof of Theorem 6.2.1 succeeds in transforming *A* to upper Hessenberg form. In particular, none of the right transformations, which are required to preserve the triangular form of *B*, destroys any of the zeros that have been previously introduced into *A*.
 - (b) Show that the total number of elimination matrices that are used (not counting the preliminary reduction of B to triangular form) is approximately n^2 .
 - (c) Show that each of the transformations requires O(n) (or less) computational effort. Thus the total computational effort to produce H and T is $O(n^3)$.
 - (d) Describe how the transforming matrices U and V can be accumulated. Show that the total work to construct U and V is $O(n^3)$.

6.2.2.

(a) Suppose that $T \in \mathbb{C}^{n \times n}$ is nonsingular and block upper triangular:

$$T = \left[\begin{array}{cc} T_{11} & T_{12} \\ 0 & T_{22} \end{array} \right],$$

where T_{11} is square. Show that T^{-1} has the same block triangular structure as T. You will probably find it useful to apply this fact to the matrix \tilde{B} in part (c) of this exercise.

- (b) Give formulas for the blocks of T^{-1} .
- (c) Suppose that $B \in \mathbb{C}^{n \times n}$ is nonsingular, let Z be a nonsingular matrix, and let $\tilde{B} = BZ$. Show that $\tilde{b}_{21} = \cdots = \tilde{b}_{n1} = 0$ if and only if Z^{-1} is an elimination matrix for the first column of B^{-1} .
- **6.2.3.** Outline an algorithm that computes a decomposition B = RQ, where R is upper triangular and Q is unitary. Use unitary elimination matrices to transform B to upper triangular form. Start with one that produces the desired zeros in the bottom row of R. Show that this decomposition takes the same amount of work as a QR decomposition.
- **6.2.4.** Let $B, H \in \mathbb{C}^{n \times n}$, and suppose $BH^* = \tilde{B}$. Let b_1, \ldots, b_n and h_1, \ldots, h_n denote the *rows* of B and G, respectively.
 - (a) Show that the conditions $\tilde{b}_{21} = \cdots = \tilde{b}_{n1} = 0$ just mean that h_1 is orthogonal to b_2, \ldots, b_n .
 - (b) Suppose B = RQ, where R is upper triangular and Q is unitary with rows q_1, \ldots, q_n . Show that q_1 is orthogonal to b_2, \ldots, b_n .
- **6.2.5.** Check that the second and subsequent steps of the algorithm outlined in (6.2.1) do not disturb the zeros that were created in the earlier steps.

6.3 GZ Algorithms

Consider a pair (A, B) for which B is nonsingular. In this section we describe a family of iterative methods called GZ algorithms that transform A and B to triangular form. For our initial description it is crucial that B be nonsingular, but later on we will see that nothing bad happens if B is singular. We draw substantially from [228].

Before we begin our iterations of the GZ algorithm, we transform the pair to some initial form

$$A_0 = G_0^{-1} A Z_0, \qquad B_0 = G_0^{-1} B Z_0.$$

For example, (A_0, B_0) could be in Hessenberg-triangular form. Later on we will assume that (A_0, B_0) does have this form, but for now we allow them to have any form. For example, we could take $G_0 = Z_0 = I$.

The explicit form of the generic GZ algorithm can be described as follows. The ith iteration transforms (A_{i-1}, B_{i-1}) to (A_i, B_i) by a strict equivalence transformation determined by A_{i-1} , B_{i-1} , a shift polynomial p_i , and two GR decompositions. Specifically, let G_i and Z_i be nonsingular matrices, and let R_i and S_i be upper triangular matrices such that

$$p_i(A_{i-1}B_{i-1}^{-1}) = G_iR_i$$
 and $p_i(B_{i-1}^{-1}A_{i-1}) = Z_iS_i$. (6.3.1)

Then let

$$A_i = G_i^{-1} A_{i-1} Z_i$$
 and $B_i = G_i^{-1} B_{i-1} Z_i$. (6.3.2)

In the special case $B_{i-1} = I$, $Z_i = G_i$, $S_i = R_i$, this algorithm reduces to the GR algorithm (4.3.1).

An easy computation shows that

$$A_i B_i^{-1} = G_i^{-1} (A_{i-1} B_{i-1}^{-1}) G_i.$$

Since G_i was obtained from the decomposition $p_i(A_{i-1}B_{i-1}^{-1}) = G_iR_i$, we see that the transformation $A_{i-1}B_{i-1}^{-1} \to A_iB_i^{-1}$ is an iteration of the GR algorithm (4.3.1). At the same time we have

$$B_i^{-1}A_i = Z_i^{-1}(B_{i-1}^{-1}A_{i-1})Z_i,$$

where $p_i(B_{i-1}^{-1}A_{i-1}) = Z_iS_i$, so the transformation $B_{i-1}^{-1}A_{i-1} \to B_i^{-1}A_i$ is also a GR iteration.

Since the GZ algorithm automatically effects GR iterations on AB^{-1} and $B^{-1}A$, we expect the sequences $(A_iB_i^{-1})$ and $(B_i^{-1}A_i)$ to converge to (block) triangular form. If the shifts are chosen well, we expect quadratic convergence. In [228] it is shown that under suitable conditions the sequences (A_i) and (B_i) separately converge to (block) triangular form, exposing the eigenvalues. With a suitable choice of shifts, quadratic convergence can be obtained. The developments of Chapter 8 show that, at least in the Hessenberg-triangular case, convergence of the GZ algorithm follows immediately from the convergence of the GR algorithm.

The generic GZ algorithm is actually a large class of algorithms. Specific instances are obtained by specifying the exact form of the GR decompositions and how the p_i are to be chosen. The choice of p_i is generally the same as it is for GR iterations: The zeros of p_i , which are called the *shifts* for the *i*th iteration, should be estimates of eigenvalues. The

degree of p_i is called the *degree* of the *i*th GZ iteration. If the G_i and Z_i are always taken to be unitary, implying that the decompositions in (6.3.1) are (more or less unique) QR decompositions, the algorithm is called the QZ algorithm [156]. If the G_i and Z_i are lower triangular, it is an LZ algorithm. If they are products of lower triangular and permutation matrices, it is an LZ algorithm with pivoting [129].

The Generic Bulge-Chasing Algorithm

If we execute the generic GZ algorithm as shown in (6.3.1) and (6.3.2), each step will be very expensive. We have to invert B_{i-1} , multiply it by A_{i-1} in both orders, and compute $p_i(A_{i-1}B_{i-1}^{-1})$ and $p_i(B_{i-1}^{-1}A_{i-1})$. These are all expensive operations, as are the two GR decompositions that follow. It is imperative that we find a more efficient way to do these iterations. We do not want to do any of the operations explicitly; in particular, we want to avoid inverting B_{i-1} . In the end we hope to have an algorithm that works well even if B_{i-1} does not have an inverse. To this end we introduce the generic bulge-chasing algorithm.

Since we are now going to consider just a single iteration, we drop the subscripts (so that we can reintroduce subscripts for a different purpose) and consider a single iteration that starts with a pair (A, B) and ends with a strictly equivalent pair (\hat{A}, \hat{B}) via

$$p(AB^{-1}) = GR, p(B^{-1}A) = ZS$$
 (6.3.3)

and

$$\hat{A} = G^{-1}AZ, \qquad \hat{B} = G^{-1}BZ.$$
 (6.3.4)

At this point we will assume that *A* is upper Hessenberg and *B* is upper triangular. The iteration will preserve the Hessenberg-triangular form. We may assume further that *A* is a proper upper Hessenberg matrix, since otherwise the eigenvalue problem can be decoupled to produce two or more smaller eigenvalue problems.

We will begin by describing the generic bulge-chasing algorithm. Then we will show that it effects an iteration of the generic GZ algorithm. (Thus the generic bulge-chasing algorithm is also known as an *implicit* GZ algorithm.) To get the algorithm started, we just need a vector proportional to the first column of $p(AB^{-1})$. This can be computed inexpensively if, as we shall assume, the degree of p (call it m) satisfies $m \ll n$. Since A is upper Hessenberg, so is AB^{-1} . Thus $p(AB^{-1})$ is m-Hessenberg, which implies that only the first m+1 entries of the first column of $p(AB^{-1})$ can be nonzero. Let ρ_1, \ldots, ρ_m denote the zeros of p (the *shifts*). Then the first column of $p(AB^{-1})$ is

$$p(AB^{-1})e_1 = (AB^{-1} - \rho_m I)(AB^{-1} - \rho_{m-1} I) \cdots (AB^{-1} - \rho_1 I)e_1,$$

so a vector x proportional to the first column of $p(AB^{-1})$ can be computed by the following algorithm:

$$x \leftarrow e_1$$
for $k = 1, ..., m$

$$\begin{bmatrix} y \leftarrow B^{-1}x \\ x \leftarrow \alpha_k (Ay - \rho_k x) \end{bmatrix}$$
(6.3.5)

Here α_k can be any convenient scaling factor. The step $y \leftarrow B^{-1}x$ looks like it might be expensive, but fortunately it is not. For example, consider what happens on the first

time through the loop. Initially we have $x = e_1$, so $B^{-1}x = b_{11}^{-1}e_1$, because B is upper triangular. The operation $x \leftarrow \alpha_1(Ay - \rho_1x)$ results in a new x whose first two components are (potentially) nonzero, all other components being zero. On the second time through the loop, the operation $y \leftarrow B^{-1}x$ results in a y whose first two components are the only ones that can be nonzero because B^{-1} is upper triangular. The operation $x \leftarrow \alpha_2(Ay - \rho_2x)$ then results in an x that can be nonzero only in the first three components. Each time through the loop adds one more nonzero to x. On the kth time through the loop, the current x has zeros everywhere except in the first k positions. The operation $y \leftarrow B^{-1}x$ results in a y that is also zero everywhere except in the first k positions. y can be computed in $O(k^2)$ flops by back substitution (Exercise 6.3.1). The operation $x \leftarrow \alpha_k(Ay - \rho_kx)$ also costs $O(k^2)$ flops and results in an x that is zero except in the first k + 1 components. After m steps, the final x is nonzero only in the first m + 1 components. The total cost of producing x is $O(m^3)$, which is small if $m \ll n$.

Once x has been produced, we build an elimination matrix G_1 such that $G_1e_1 = \beta_1x$. Because of the form of x, G_1 can take the form

$$G_1 = \left[\begin{array}{cc} \tilde{G}_1 \\ & I_{n-m-1} \end{array} \right].$$

Let

$$A_{1/2} = G_1^{-1}A$$
 and $B_{1/2} = G_1^{-1}B$.

The action of G_1^{-1} affects the first m+1 rows of A and B, disturbing the Hessenberg-triangular form. For example, in the case m=2, $A_{1/2}$ and $B_{1/2}$ have the forms

$$\begin{bmatrix} a & a & a & a & a \\ a & a & a & a & a \\ + & a & a & a & a \\ & & & a & a \end{bmatrix} \text{ and } \begin{bmatrix} b & b & b & b & b \\ + & b & b & b & b \\ + & + & b & b & b \\ + & + & b & b & b \\ & & & & b \end{bmatrix},$$

respectively. The plus symbols indicate bulges that have crept into the matrices.

The rest of the iteration consists of returning the pair to Hessenberg-triangular form using the second algorithm discussed in Section 6.2, whose first step is sketched in (6.2.1). As we shall see, this amounts to a bulge-chase. The first task is to return the first column of $B_{1/2}$ to upper triangular form. From (6.2.1) we recall that this requires an RQ decomposition of $B_{1/2}$, which is normally an expensive process. In this case it is not, because $B_{1/2}$ is nearly triangular to begin with. We can write $B_{1/2}$ in the partitioned form

$$B_{1/2} = \left[\begin{array}{cc} B_{11} & B_{12} \\ & B_{22} \end{array} \right],$$

where B_{11} is $(m + 1) \times (m + 1)$ and B_{22} is upper triangular. If $B_{11} = R_{11}Q_{11}$ is an RQ decomposition of B_{11} , then an RQ decomposition of $B_{1/2}$ is given by

$$B_{1/2} = \begin{bmatrix} B_{11} & B_{12} \\ & B_{22} \end{bmatrix} = \begin{bmatrix} R_{11} & B_{12} \\ & B_{22} \end{bmatrix} \begin{bmatrix} Q_{11} & \\ & I \end{bmatrix}.$$

Thus the decomposition costs only $O(m^3)$ flops, which is negligible if m is small. Let $\tilde{Z}_1 \in \mathbb{C}^{(m+1)\times (m+1)}$ be an elimination matrix such that the first row of \tilde{Z}_1^* is proportional to the first row of Q_{11} , let $Z_1 = \operatorname{diag}\{\tilde{Z}_1, I_{n-m-1}\}$, and let

$$A_1 = A_{1/2}Z_1, \qquad B_1 = B_{1/2}Z_1.$$

This completes the first part of (6.2.1). The first column of B_1 has zeros below the main diagonal. The transforming matrix Z_1 acts on the first m+1 columns of $A_{1/2}$, with the result that one row is added to the bottom of the bulge. In the case m=2, A_1 and B_1 have the forms

$$\begin{bmatrix} a & a & a & a & a \\ a & a & a & a & a \\ + & a & a & a & a \\ + & + & a & a & a \\ & & & a & a \end{bmatrix} \text{ and } \begin{bmatrix} b & b & b & b & b \\ b & b & b & b & b \\ + & b & b & b & b \\ & & & b & b \end{bmatrix},$$

respectively. The bulge in B has been shrunk at the expense of expanding the bulge in A. The second half of (6.2.1) transforms the first column of A_1 to Hessenberg form. This is done by a transformation

$$A_{3/2} = G_2^{-1} A_1, \qquad B_{3/2} = G_2^{-1} B_1,$$

where $G_2 = \text{diag}\{1, \tilde{G}_2, I_{n-m-2}\}$. The transformation $B_{3/2} = G_2^{-1}B_1$ acts on rows 2 through m+2 of B, adding a row to the bulge. In the case m=2, $A_{3/2}$ and $B_{3/2}$ have the forms

respectively. The bulge in A has been shrunk and the bulge in B expanded. Both bulges have now been moved down one row and over one column. The pattern should now be clear. The next transformation, Z_2 , clears out the second column of $B_{3/2}$. This requires another RQ decomposition, but this is again inexpensive, because the part of $B_{3/2}$ that is not already upper triangular is only $(m+1) \times (m+1)$. This acts on columns 2 through m+2 of $A_{3/2}$, adding a row to the bottom of the bulge. Next, a transformation G_3^{-1} clears out the second column of A_2 , adding a row to the bottom of the bulge in B_2 . Continuing in this manner, we chase the bulges downward and eventually off of the bottom of the matrices, returning the pair to Hessenberg-triangular form, at which point we have completed an iteration of the generic bulge-chasing algorithm. This takes a total of n-1 transformations on left and right. The result is

$$\hat{A} = A_{n-1} = G_{n-1}^{-1} \cdots G_1^{-1} A Z_1 \cdots Z_{n-1},$$

$$\hat{B} = B_{n-1} = G_{n-1}^{-1} \cdots G_1^{-1} B Z_1 \cdots Z_{n-1}.$$

In the case B = I and $Z_i = G_i$ for all i, this algorithm reduces to the generic bulge-chasing algorithm for the standard eigenvalue problem described in Section 4.5.

Letting

$$G = G_1 G_2 \cdots G_{n-1}$$
 and $Z = Z_1 Z_2 \cdots Z_{n-1}$, (6.3.6)

we have

$$\hat{A} = G^{-1}AZ$$
 and $\hat{B} = G^{-1}BZ$,

as in (6.3.4). To show that the generic bulge-chasing algorithm effects a GZ iteration, we must show that the matrices G and Z of (6.3.6) satisfy equations of the form (6.3.3). To this end we begin by noting that the form of the matrices G_2, \ldots, G_{n-1} implies that the first column of G is the same as the first column of G [Exercise 6.3.2). Thus the first column of G is proportional to the first column of $P(AB^{-1})$; that is, $P(AB^{-1}) = P(AB^{-1}) = P(AB^{-1})$

Proposition 6.3.1. Suppose the matrix pair (A, B) is properly Hessenberg-triangular; that is, A is properly upper Hessenberg and B is upper triangular and nonsingular. Suppose further that

$$\hat{A} = G^{-1}AZ$$
 and $\hat{B} = G^{-1}BZ$,

where G and Z are nonsingular, and that the pair (\hat{A}, \hat{B}) is also Hessenberg-triangular. Finally, suppose $Ge_1 = \alpha p(AB^{-1})e_1$ for some $\alpha \neq 0$. Then there exist upper triangular matrices R and S such that

$$p(AB^{-1}) = GR$$
 and $p(B^{-1}A) = ZS$.

Proof: Applying Lemmas 4.5.3 and 4.5.2 with A replaced by AB^{-1} , and recalling that $G(\hat{A}\hat{B}^{-1}) = (AB^{-1})G$, we find that

$$p(AB^{-1})\kappa(AB^{-1}, e_1) = \kappa(AB^{-1}, p(AB^{-1})e_1)$$

$$= \alpha^{-1}\kappa(AB^{-1}, Ge_1) = \alpha^{-1}G\kappa(\hat{A}\hat{B}^{-1}, e_1).$$
(6.3.7)

By Lemma 4.5.4, $\kappa(AB^{-1}, e_1)$ and $\kappa(\hat{A}\hat{B}^{-1}, e_1)$ are both upper triangular, and the former is nonsingular. Letting $R = \alpha^{-1}\kappa(\hat{A}\hat{B}^{-1}, e_1)\kappa(AB^{-1}, e_1)^{-1}$, we see that R is upper triangular and, by (6.3.8),

$$p(AB^{-1}) = GR.$$

To get the equation $p(B^{-1}A) = ZS$, we start by figuring out what the first column of Z is. Noting that $Z = B^{-1}G\hat{B}$, we have

$$Ze_1 = B^{-1}G\hat{B}e_1 = \hat{b}_{11}B^{-1}Ge_1 = \hat{b}_{11}\alpha B^{-1}p(AB^{-1})e_1$$
$$= \hat{b}_{11}\alpha p(B^{-1}A)B^{-1}e_1 = \hat{b}_{11}\alpha b_{11}^{-1}p(B^{-1}A)e_1.$$

Thus $Ze_1 = \beta p(B^{-1}A)e_1$, where $\beta = \hat{b}_{11}\alpha b_{11}^{-1}$: The first column of Z is proportional to the first column of $p(B^{-1}A)$. Now we can use Lemmas 4.5.3, 4.5.2, and 4.5.4, just as in the previous paragraph, to show that $p(B^{-1}A) = ZS$, where $Z = \beta^{-1}\kappa(\hat{B}^{-1}\hat{A}, e_1)\kappa(B^{-1}A, e_1)^{-1}$ is upper triangular. \square

We have shown that the generic bulge-chasing algorithm satisfies (6.3.4), where G and Z are from GR decompositions (6.3.3). Therefore an iteration of the generic bulge-chasing algorithm effects an iteration of the generic GZ algorithm. It is not hard to show (Exercise 6.3.3) that the cost of a generic bulge-chasing iteration is $O(n^2m)$ if m is small, so this is much less expensive than if we did the generic GZ step explicitly.

A more thorough exposition of the connection between explicit and implicit GZ algorithms is given in [228]. There it is shown, by arguments like those in Section 4.7, that the transformations used in explicit and implicit (bulge-chasing) GZ iterations on a Hessenberg-triangular pair are essentially identical.

Repeatedly applying the generic bulge-chasing algorithm with appropriate shifts, we normally get rapid convergence, which is reflected in convergence of the subdiagonal entries $a_{j+1,j}$ to zero. Monitoring these entries and setting each one to zero once it has become sufficiently small, we repeatedly deflate and decouple the problem until all of the eigenvalues have been found.

If the generic bulge-chasing algorithm is effected using only unitary elimination matrices, it becomes an implicit QZ algorithm, as exemplified by Moler and Stewart's original QZ algorithm [156]. If only Gaussian elimination transformations with permutations are used, it becomes the LZ algorithm with partial pivoting, as exemplified by Kaufman [129]. There is nothing to rule out hybrids that mix unitary and Gauss transforms. For example, in [130], Kaufman proposed an algorithm that uses unitary elimination matrices for the "G" transformations and Gaussian elimination matrices with pivoting for the "Z" transformations.

In Section 4.9, we discussed a number of practical details for the implementation of GR algorithms for the standard eigenvalue problem. Most of these apply to GZ algorithms for the generalized eigenvalue problem as well. Ward [212] showed how to balance the generalized eigenvalue problem. Once balancing has been done, the standard software for general regular pairs uses only unitary transformations in the interest of numerical stability. Shift blurring is a problem if m is made too large. However, large numbers of small bulges can be chased in pipeline fashion to achieve improved performance due to better cache use, resulting in significant performance improvements on large matrices. Performance can also be improved by aggressive early deflation [123]. These innovations will be incorporated in the large-matrix QZ code in a future release of LAPACK.

Exercises

- **6.3.1.** The operation $y \leftarrow B^{-1}x$ in (6.3.5) is effected by solving the system By = x. Show that if all but the first k entries of x are zero, then the same will be true of y, y can be computed in $O(k^2)$ flops by back substitution, and only the upper left-hand $k \times k$ submatrix of B participates in the computation. An easy way to work this problem is to partition the equation By = x appropriately.
- **6.3.2.** This exercise addresses some of the details of the generic bulge-chasing algorithm.
 - (a) Describe the kth step of the generic bulge-chasing algorithm, transforming A_k and B_k to $A_{k+1} = G_k^{-1} A_k Z_k$ and $B_{k+1} = G_k^{-1} B_k Z_k$. What can you say about the form of each of A_k , B_k , G_k , Z_k , A_{k+1} , and B_{k+1} ?
 - (b) Show that the first column of $G = G_1 \cdots G_{n-1}$ is the same as the first column of G_1 .
 - (c) Check the details in the argument that shows that $p(AB^{-1}) = GR$, where R is upper triangular.
 - (d) Show that $B^{-1}p(AB^{-1}) = p(B^{-1}A)B^{-1}$ for any polynomial p. Using the upper triangularity of B and \hat{B} , show that $p(B^{-1}A)e_1 = \delta Ze_1$, where $\delta = \gamma b_{11}\hat{b}_{11}^{-1}$.

(e) Use Lemmas 4.5.3 and 4.5.2, with A replaced by $B^{-1}A$, to show that

$$p(B^{-1}A)\kappa(B^{-1}A, e_1) = \delta Z\kappa(\hat{B}^{-1}\hat{A}, e_1).$$

Then use Lemma 4.5.4 to show that the matrix

$$S = \delta \kappa (\hat{B}^{-1} \hat{A}, e_1) \kappa (B^{-1} A, e_1)^{-1}$$

exists and is upper triangular. Then deduce that $p(B^{-1}A) = ZS$.

- **6.3.3.** Show that the cost of an iteration of the generic bulge-chasing algorithm is $O(n^2m)$ if $m \le \sqrt{n}$ by the following steps:
 - (a) Show that the cost of computing the first column of G_1 is $O(m^3) = O(nm)$.
 - (b) Show that the cost of setting up and applying each G_k^{-1} transformation is O(nm).
 - (c) Show that the cost of setting up and applying each Z_k transformation is O(nm). Do not overlook the cost of the RQ decomposition that is used in the setup phase.
 - (d) Show that the entire flop count for an iteration of the generic bulge-chasing algorithm is $O(n^2m)$.
 - (e) At what points did you use the assumption $m \le \sqrt{n}$?
- **6.3.4.** An alternate way of implementing the implicit GZ algorithm can be built on the principle of defending the upper triangular form of B vigorously. In this variant, the "A" matrix carries a bulge of the same size as in the variant described in the text, but a bulge is never allowed to build up in the "B" matrix.
 - (a) Show that each of the transformations G_k (including G_1) can be constructed as a product $G_k = G_{k1}G_{k2}\cdots G_{km}$ of m transformations, each of which operates on two adjacent rows, such that (for k>1) each G_{ki}^{-1} creates one new zero in the "A" bulge. A_{k1}^{-1} zeros the bottom element, A_{k2}^{-1} zeros the next one, and so on upwards.
 - (b) Z_k is created and applied simultaneously with G_k . Supposing that the "B" matrix is upper triangular, show that each G_{ki}^{-1} creates a nonzero in the subdiagonal of B, thus disturbing the upper triangular form. Show that there is a Z_{ki} that acts on two adjacent columns to return B to triangular form. Show that Z_{ki} adds one new entry to the bottom of the bulge in A. Let $Z_k = Z_{k1} \cdots Z_{km}$. This is a bit different from the Z_k of the algorithm described in the text. Let $A_k = G_k^{-1} A_{k-1} Z_k$ and $B_k = G_k^{-1} B_{k-1} Z_k$.

6.4 The *HZ* Algorithm

In Section 4.9 we introduced and briefly discussed the HR algorithm for pseudosymmetric matrices. This can also be formulated as an HZ algorithm for a certain generalized eigenvalue problem. Recall that a matrix $A \in \mathbb{R}^{n \times n}$ that is tridiagonal and pseudosymmetric can be expressed as a product A = TD, where T is tridiagonal and symmetric and D is a signature matrix. That is, D is a diagonal matrix whose main diagonal entries are ± 1 . Since $D = D^{-1}$, we see that the eigenvalue problem for A = TD is the same as the generalized eigenvalue problem for the pair (T, D).

The Explicit HZ Algorithm

Recall that an HR iteration on a pseudosymmetric matrix A = TD is a special kind of GR iteration of the form

$$p(A) = HR, \qquad \hat{A} = H^{-1}AH,$$

where H satisfies $H^TDH = \hat{D}$, with \hat{D} another signature matrix. One easily checks (Exercise 4.9.7) that $\hat{A} = \hat{T}\hat{D}$, where \hat{T} is symmetric and tridiagonal.

Let us now see that we can formulate this as an HZ algorithm, a special structurepreserving GZ algorithm, on the pair (T, D). Referring back to (6.3.1) or (6.3.3), we see that an HZ iteration on (T, D) should begin with a pair of HR decompositions

$$p(TD^{-1}) = HR, \qquad p(D^{-1}T) = \tilde{H}\tilde{R}.$$

These are not independent; each can be derived from the other. Suppose that we have a decomposition $p(TD^{-1}) = HR$, where R is upper triangular and $H^TDH = \hat{D}$ for some signature matrix \hat{D} . Then $p(D^{-1}T) = D^{-1}p(TD^{-1})D = D^{-1}HRD = (DH\hat{D})(\hat{D}RD)$. Let $\tilde{H} = DH\hat{D}$ and $\tilde{R} = \hat{D}RD$. Then clearly \tilde{R} is upper triangular, and \tilde{H} satisfies $\tilde{H}^TD\tilde{H} = \hat{D}$. (See Exercise 6.4.1 for this and other details.) Thus the decomposition $p(D^{-1}T) = \tilde{H}\tilde{R}$ is an HR decomposition. It is easy to check that $\tilde{H} = H^{-T}$, so the decomposition can be written as $p(D^{-1}T) = H^{-T}\tilde{R}$. Thus we can take the HR version of (6.3.3) as

$$p(TD^{-1}) = HR, p(D^{-1}T) = H^{-T}\tilde{R}.$$
 (6.4.1)

Then the HR version of (6.3.4) is

$$\hat{T} = H^{-1}TH^{-T}, \qquad \hat{D} = H^{-1}DH^{-T}.$$
 (6.4.2)

If we invert the second equation here, we recognize it as a variant of the equation $\hat{D} = H^T D H$. Also note that the first equation guarantees that \hat{T} is symmetric. Equations (6.4.1) and (6.4.2) together constitute an iteration of the HZ algorithm. Since $\hat{T} \hat{D}^{-1} = H^{-1}(TD^{-1})H$, the HZ iteration effects an HR iteration on $A = TD^{-1}$.

The Implicit HZ Algorithm

Now let us consider how the HZ iteration can be implemented implicitly, as a bulge-chasing algorithm. For simplicity consider first an iteration of degree m=1. The iteration begins by computing a vector x as in (6.3.5). In this special case x is proportional to $(T - \rho D)e_1$, where ρ is the single shift. The first transformation matrix H_1 will satisfy $H_1e_1 = \beta_1 x$ for some convenient nonzero scalar β_1 . Only the first two entries of x are nonzero, so the first transformation acts only on rows 1 and 2. The step

$$T_{1/2} = H_1^{-1}T, \qquad D_{1/2} = H_1^{-1}D$$

creates a bulge in $D_{1/2}$. From the description of the generic bulge-chasing algorithm we know that the next transformation (Z_1) is supposed to remove the bulge from $D_{1/2}$. On the other hand, (6.4.2) suggests that Z_1 should be H_1^{-T} , giving

$$T_1 = H_1^{-1}TH_1^{-T}, \qquad D_1 = H_1^{-1}DH_1^{-T}.$$

At this point the bulge should be removed from D_1 . Moreover, in the end we want \hat{D} to be a signature matrix, so it is only reasonable that we should require D_1 to be a signature matrix. Indeed, at each step of the bulge-chase we should defend the signature matrix form of the "D" matrix. Then, in the end, \hat{D} will be a signature matrix.

This determines the form of H_1 (and all subsequent transformation matrices). If d_{11} and d_{22} have the same sign, then H_1 should be an orthogonal matrix, for example, a rotator. Then $D_1 = D$ is automatically satisfied. If d_{11} and d_{22} have opposite sign, H_1 should be a hyperbolic transformation of type 1 (3.1.3) or type 2. In the former case we have $D_1 = D$; in the latter case D_1 is the signature matrix obtained from D by swapping the (1, 1) and (2, 2) entries.

After the first step, T_1 is symmetric but not tridiagonal. It has a bulge in position (3, 1) and a symmetric bulge at (1, 3). The bulge at (3, 1) is removed by a transformation H_2^{-1} , applied on the left, that acts on rows 2 and 3. The form of H_2 is determined by the signs of the (2, 2) and (3, 3) entries of D_1 . If they have the same sign, H_2 should be orthogonal; if they have opposite sign, H_2 should be hyperbolic. Either way, $D_2 = H_2^{-1}D_1H_2^{-T}$ is a signature matrix. $T_2 = H_2^{-1}T_1H_2^{-T}$ is a symmetric, nearly tridiagonal, matrix with a bulge in position (4, 2). The next transformation is set up in an entirely analogous manner and pushes the bulge from (4, 2) to (5, 3), and so on. After n-1 transformations, the bulge-chase is complete. An HZ iteration has been completed.

An implicit HZ iteration of higher degree can be arranged similarly. At each step, more than one entry has to be eliminated. This can be done by a transformation of the type guaranteed by Theorem 3.1.5. The method of constructing such transformations is outlined in the proof of the theorem. Their use guarantees that the "D" matrix remains a signature matrix, and an HZ iteration is effected.

We should not neglect to mention that the HZ bulge-chasing process can sometimes break down. If we wish to use a hyperbolic transformation on the vector $\begin{bmatrix} \alpha \\ \beta \end{bmatrix}$ to zero out β , the desired transformation does not exist if $\alpha^2 = \beta^2$.

There is one situation when we know we will never have a breakdown. If all the entries of D have the same sign, $D=\pm I$, all of the transformations will be orthogonal. Then the HZ algorithm reduces to the QR algorithm on the symmetric matrix T.

Exercises

6.4.1.

- (a) Suppose $\hat{D} = H^T D H$, where D and \hat{D} are signature matrices. Let $\tilde{H} = H^{-T}$. Show that $\tilde{H} = D H \hat{D}$ and $\tilde{H}^T D \tilde{H} = \hat{D}$.
- (b) Show that $p(D^{-1}T) = D^{-1}p(TD^{-1})D$ for every polynomial p.
- **6.4.2.** Write an algorithm that does an HZ iteration of degree m.

6.5 Infinite Eigenvalues

Consider once again a pair (A, B) with no special structure. So far we have made the assumption that B is nonsingular, which implies that all eigenvalues of (A, B) are finite.

Now let us consider briefly what happens if B is singular. If we do not know beforehand whether B is singular or not, it will usually be evident once (A, B) is in Hessenberg-triangular form. Singularity will be signaled by one or more zeros on the main diagonal of the triangular matrix B. This signals either an infinite eigenvalue or a singular pair.

Pushing the Zeros to the Top

We begin by showing that if B is singular, then the reduction to Hessenberg-triangular form tends to push the main-diagonal zeros to the top of B [220]. Consider the reduction to Hessenberg-triangular form outlined in the proof of Theorem 6.2.1. This begins by reducing B to upper-triangular form, at which point there will already be zeros on the main diagonal of B. We will show that the rest of the algorithm, which reduces A to upper Hessenberg form, tends to push the zeros to the top of B.

After the initial transformation of B to triangular form, b_{11} remains untouched by the algorithm. If it happens to be zero, it stays zero. Now suppose $b_{kk} = 0$ for some k > 1, and let us consider what happens to that zero subsequently.

Recall that the algorithm applies elimination matrices (e.g., rotators) to adjacent pairs of rows to transform $a_{n1}, a_{n-1,1}, \ldots, a_{31}$ successively to zero. Each of these transformations is applied to the B matrix as well and is immediately followed by a transformation on two adjacent columns to return B to triangular form. Once these transformations have been done, the first column of A is in Hessenberg form. A similar process transforms the second column of A to Hessenberg form, and so on.

If $b_{kk} = 0$, then it will remain zero until one of the elimination matrices touches the kth row or column. The first one to do so acts on rows k and k+1. This one leaves b_{kk} at zero, since it recombines the zeros in positions (k,k) and (k+1,k) to create new zeros in those positions. The next transformation acts on rows k-1 and k, and this one normally does make b_{kk} nonzero. Let us focus on the 2×2 submatrix consisting of rows and columns k-1 and k. Before the transformation it has the form

$$\begin{bmatrix} b_{k-1,k-1} & b_{k-1,k} \\ 0 & 0 \end{bmatrix}. \tag{6.5.1}$$

Its rank is obviously one. When the transformation is applied, it disturbs both of the zeros. The submatrix now looks like

$$\begin{bmatrix} \tilde{b}_{k-1,k-1} & \tilde{b}_{k-1,k} \\ \tilde{b}_{k,k-1} & \tilde{b}_{k,k} \end{bmatrix}, \tag{6.5.2}$$

but its rank is still one. The next step in the reduction is to apply an elimination matrix to columns k-1 and k that annihilates $\tilde{b}_{k,k-1}$, returning B to upper triangular form. Application of this elimination matrix transforms the submatrix to

$$\begin{bmatrix} 0 & \hat{b}_{k-1,k} \\ 0 & \hat{b}_{kk} \end{bmatrix}. \tag{6.5.3}$$

³In practice there may not be any exact zeros, but any number that is on the order of the unit roundoff, relative to other matrix entries, can be considered to be a zero. However, we must caution that it can happen that a triangular matrix is nearly singular without any of its main-diagonal entries being tiny.

Since the rank is still one, $\hat{b}_{k-1,k-1}$ is forced to be zero. The zero has been moved from position (k, k) to position (k - 1, k - 1).

The next pair of transformations acts on rows and columns k-2 and k-1 and pushes the zero up to position (k-2, k-2) by the same process. The zero thus normally continues upward until it either arrives at position (2, 2) or collides with another zero. The only way the upward movement can be stopped is if a trivial elimination transformation is applied on the left at some point. This happens when and only when the entry of A that is to be eliminated is already zero to begin with. In this event the zero in B stops and remains where it is until the next upward wave of rotators (corresponding to elimination of the next column of A) passes through.

Collision of Two Zeros

Suppose that B has two or more zeros on the main diagonal. Note that the number of zeros on the main diagonal is not necessarily equal to the number of infinite eigenvalues of the pair (A, B). We will see examples below in which B is strictly upper triangular, having nothing but zeros on its main-diagonal, and yet the pair (A, B) has only one infinite eigenvalue. During the reduction to Hessenberg-triangular form, the number of zeros on the main diagonal of B need not remain constant. Consider what happens when a zero that is moving upward on the main diagonal of B runs into another zero. Then we have the configuration

$$\left[\begin{array}{cc} 0 & b_{k-1,k} \\ 0 & 0 \end{array}\right]. \tag{6.5.4}$$

The left transformation of rows k-1 and k then gives

$$\begin{bmatrix} 0 & \tilde{b}_{k-1,k} \\ 0 & \tilde{b}_{k,k} \end{bmatrix}, \tag{6.5.5}$$

in which \tilde{b}_{kk} is normally nonzero. Once it becomes nonzero, it stays nonzero. The next transformation acts on columns k-1 and k to annihilate $\tilde{b}_{k,k-1}$, but this transformation is trivial because $\tilde{b}_{k,k-1}$ is already zero. We conclude that in a collision of two zeros, the lower zero is normally destroyed. This can be prevented by two things: (i) $b_{k-1,k}$ could also be zero, and (ii) the transformation on rows k-1 and k could be trivial. The conclusion is that when two zeros collide, the upper one survives but the lower one is normally (but not necessarily) destroyed.

The number of zeros on the main diagonal of B can decrease, but it cannot increase. If the matrix

$$\left[\begin{array}{cc}b_{k-1,k-1}&b_{k-1,k}\\0&b_{kk}\end{array}\right]$$

has rank two before the transformations on rows and columns k-1 and k, then it must still have rank two afterward. Thus zeros cannot spontaneously appear. The same is true during the GZ iterations, as we will see. It follows that the number of zeros on the main diagonal of B can never be less than the number of infinite eigenvalues, since the generalized Schur form at which we arrive in the end must have one zero on the main diagonal for each infinite eigenvalue.

Preliminary Removal of Infinite Eigenvalues

Once the pair (A, B) is in Hessenberg-triangular form, it is easy to remove the infinite eigenvalues at the outset if one wishes to. If the Hessenberg-triangular form was reached by the algorithm described above, the zeros on the main diagonal of B will tend to be near the top. Suppose first that $b_{11} = 0$. Then a rotator or other elimination matrix that acts on rows 1 and 2 can be applied (on the left) to transform a_{21} to 0. When this same transformation is applied to B, it leaves $b_{11} = 0$ and does not disturb the upper triangular form. The resulting pair has a form exemplified by

$$\begin{bmatrix} a_{11} & a_{12} & a_{13} & a_{14} \\ 0 & a_{22} & a_{23} & a_{24} \\ 0 & a_{32} & a_{33} & a_{34} \\ 0 & 0 & a_{43} & a_{44} \end{bmatrix}, \begin{bmatrix} 0 & b_{12} & b_{13} & b_{14} \\ 0 & b_{22} & b_{23} & b_{24} \\ 0 & 0 & b_{33} & b_{34} \\ 0 & 0 & 0 & b_{44} \end{bmatrix}.$$
(6.5.6)

Now we deflate an infinite eigenvalue by deleting the first row and column.⁴ Now suppose $b_{11} \neq 0$ but $b_{22} = 0$. Then the deflation begins with a rotator acting on columns 1 and 2, transforming b_{11} to zero. This leaves b_{22} at zero. When the same transformation is applied to A, it creates a bulge at a_{31} . Now a transformation on the left, acting on rows 2 and 3, can eliminate a_{31} , returning A to Hessenberg form. When the same transformation is applied to B, it does not disturb the triangular form of B because $b_{22} = 0$. Now a left transformation on rows 1 and 2 transforms a_{21} to zero. When this transformation is applied to B, it destroys the zero at b_{22} but leaves $b_{11} = 0$. Now we are in the situation exemplified by (6.5.6), and we can deflate an infinite eigenvalue (or discover that the pair is singular). This process can be generalized to remove a zero from any position on the main diagonal of B (Exercise 6.5.1). A sequence of rotators moves the zero to the (1, 1) position, from which it can be deflated. An analogous algorithm can be used to drive a zero to the bottom of B for deflation at the bottom (Exercise 6.5.1). That variant is obviously more economical for zeros that are near the bottom to begin with.

Nonremoval of the Infinite Eigenvalues

We show next that it is not strictly necessary to remove the infinite eigenvalues beforehand. However experiments of Kågström and Kressner [123] suggest that the following material should be viewed as theoretical rather than practical. If infinite eigenvalues are not extracted immediately, they might never be detected, as they will be masked by subsequent roundoff errors.

If the Hessenberg-triangular pair was not obtained by a reduction process, the zeros can be anywhere in B. We have seen that it is possible to remove the infinite eigenvalues in advance. We now wish to show that there is no immediate need to do so, unless the zeros are very near the top or the bottom of B. The reason for removing zeros from the bottom is that we do not want them to get in the way of the shift computation. Every shift strategy gets its information from the lower right corner of the matrix. A common strategy is as

 $^{^4}$ If $a_{11} = 0$, the pair is singular. In that case one can, optionally, determine the fine structure (Kronecker canonical form) of the pair by the staircase algorithm [206, 73], which we choose not to discuss.

follows. If m shifts are needed, consider the pair (A, B) in the partitioned form

$$\left[\begin{array}{cc} A_{11} & A_{12} \\ A_{21} & A_{22} \end{array}\right], \qquad \left[\begin{array}{cc} B_{11} & B_{12} \\ 0 & B_{22} \end{array}\right],$$

where A_{22} and B_{22} are $m \times m$. Take the m shifts to be the eigenvalues of the pair (A_{22}, B_{22}) . Since we would like all of the shifts to be finite numbers, we cannot tolerate zeros on the main diagonal of B_{22} . Therefore, if there are any such zeros, they should be pushed to the bottom and deflated out by the algorithm of part (b) of Exercise 6.5.1.

The reason for removing zeros from the top of B is that they will interfere with the computation of $p(AB^{-1})e_1$ in (6.3.5). Exercise 6.3.1 makes it clear that successful completion of (6.3.5) does not actually depend on the existence of B^{-1} . The step $y \leftarrow B^{-1}x$ is effected by solving By = x by back substitution. Since only the first few entries of x are nonzero, the process involves only the upper left-hand corner of B. To be precise, one easily checks that (6.3.5) requires only that b_{11}, \ldots, b_{mm} be nonzero. If any of those entries is zero, it should be pushed to the top by the algorithm of part (a) of Exercise 6.5.1 and deflated before the bulge-chase is begun.

We now consider what happens to zeros on the main diagonal of B in the course of a bulge-chase. This was studied in the QZ case (with m=1 or 2) by Ward [211] and much later but in greater generality in [220], which was written in ignorance of [211]. Since the GZ iteration consists of an initial transformation followed by a reduction to Hessenberg-triangular form, we expect the GZ iteration to have the effect of moving the zeros upward. However, the bulge-chase is a very special reduction to Hessenberg-triangular form in which most of the entries to be zeroed out are already zero to begin with. Thus most of the transformations in the reduction are trivial and therefore skipped. Thus we expect the GZ iteration to have a much weaker upward-moving effect on the zeros on the main diagonal of B.

First consider the case m=1. The bulge is 1×1 , and it is chased back and forth between B and A. Let's suppose $b_{kk}=0$ and see what happens as the bulge passes through that part of the matrix. When the bulge is at $a_{k,k-2}$, a transformation acting on rows k-1 and k is used to set that entry to zero. Just before that transformation is applied to B, the submatrix consisting of rows and columns k-1 and k has the form

$$\left[\begin{array}{cc}b_{k-1,k-1}&b_{k-1,k}\\0&0\end{array}\right],$$

since $b_{kk} = 0$. This matrix definitely has rank one. After the transformation, which hits rows k - 1 and k, the submatrix looks like

$$\left[\begin{array}{ccc} \tilde{b}_{k-1,k-1} & \tilde{b}_{k-1,k} \\ \tilde{b}_{k,k-1} & \tilde{b}_{kk} \end{array}\right].$$

The entry $\tilde{b}_{k,k-1}$, which is the new bulge, is definitely nonzero by Exercise 6.5.3. Furthermore, the submatrix has rank one, since the transformation did not alter the rank. The next transformation acts on columns k-1 and k, annihilating the bulge. The submatrix looks like

$$\left[\begin{array}{cc} \hat{b}_{k-1,k-1} & \hat{b}_{k-1,k} \\ 0 & \hat{b}_{kk} \end{array}\right],\,$$

it still has rank one, and \hat{b}_{kk} is definitely nonzero by Exercise 6.5.3. Therefore $\hat{b}_{k-1,k-1}$ must be zero. The bulge-chase is now past this point, so this entry will not undergo any further changes. At the end of the bulge-chase we will have $\hat{b}_{k-1,k-1} = 0$. We conclude that the bulge-chase moves each zero on the main diagonal of B up by one position. After k-1 bulge-chases, a zero that was originally in position (k,k) will have moved up to position (1,1), and an infinite eigenvalue can be deflated. A bulge-chase neither creates nor destroys zeros. However, a zero can be destroyed in the deflation process (Exercise 6.5.4).

Since a GZ iteration of degree m is equivalent to m GZ iterations of degree 1, we might hope that each bulge-chase of degree m moves a zero up m positions. It turns out that that is what normally happens. Let us suppose $b_{kk} = 0$ and that a bulge of degree m is about to reach the kth row of B. Consider the submatrix consisting of rows and columns k - m through k. This is the part of B that contains the bulge, and just before the step that returns column k - m - 1 of A to Hessenberg form it has the form

$$\check{B} = \begin{bmatrix} \check{b}_{k-m,k-m} & \cdots & \check{b}_{k-m,k-1} & \check{b}_{k-m,k} \\ \vdots & & \vdots & \vdots \\ \check{b}_{k-1,k-m} & \cdots & \check{b}_{k-1,k-1} & \check{b}_{k-1,k} \\ \hline 0 & \cdots & 0 & 0 \end{bmatrix},$$

because $b_{kk} = 0$, and the bulge-chase has not yet touched the kth row. Let S denote the space spanned by the rows of \check{B} , and let r denote its dimension. Then clearly $r = \operatorname{rank}(\check{B}) \leq m$.

The operation that returns row k-m-1 of A to Hessenberg form acts on rows k-m through k. When it is applied to B, it recombines the rows of \check{B} , filling in the zeros in the bottom row. The result, $\check{B} = G^{-1}\check{B}$, has the form

$$ilde{B} = \left[egin{array}{cccccc} ilde{b}_{k-m,k-m} & \cdots & ilde{b}_{k-m,k-1} & ilde{b}_{k-m,k} \\ dots & & dots & dots \\ ilde{b}_{k-1,k-m} & \cdots & ilde{b}_{k-1,k-1} & ilde{b}_{k-1,k} \\ ilde{b}_{k,k-m} & \cdots & ilde{b}_{k,k-1} & ilde{b}_{kk} \end{array}
ight].$$

Although the zeros have been filled in, the rank is still r. The rows of \tilde{B} span S. The next step applies a right transformation to columns k-m through k to return the (k-m)th column of B (the first column of \tilde{B}) to triangular form. The result, $\hat{B} = \tilde{B}H^*$,

$$\hat{B} = \begin{bmatrix} \hat{b}_{k-m,k-m} & \hat{b}_{k-m,k-m+1} & \cdots & \hat{b}_{k-m,k} \\ 0 & \hat{b}_{k-m+1,k-m+1} & \cdots & \hat{b}_{k-m+1,k} \\ \vdots & \vdots & & \vdots \\ 0 & \hat{b}_{k,k-m+1} & \cdots & \hat{b}_{kk} \end{bmatrix}.$$

The zeros appear because rows 2 through m+1 of \tilde{B} are orthogonal to the first row of the transforming matrix H. Recall that the rows of \tilde{B} are linearly dependent. It is possible to throw out one row of \tilde{B} , and the remaining m rows will still span S. Sometimes it matters which row is thrown out, but in most cases (almost always) it does not. If the vectors are in generic position, you can throw out any row, and the remaining rows will still span S.

We would like to throw out the first row and keep the others. We hope that rows 2 through m+1 span S. Whether or not this is so depends upon the transforming matrix G^{-1} . Since this matrix has no special relationship with \check{B} or \tilde{B} , we expect that rows 2 through m+1 of \tilde{B} will span S.

Let us now suppose that rows 2 through m+1 of \tilde{B} span S. The first row of H is orthogonal to all of these rows, so it is orthogonal to S. But the first row of \tilde{B} also lies in S, so the first row of H must be orthogonal to it. This implies that $\hat{b}_{k-m,k-m}=0$. That entry will not be touched by any subsequent operations of the bulge-chase, so at the end of the iteration we have $\hat{b}_{k-m,k-m}=0$. The zero has moved up m positions. In conclusion, we expect each bulge-chase of degree m to move the zero up m positions. After a number of bulge-chases, the zero will have been moved up to one of the top m positions on the main diagonal of B, at which point it must be removed by the algorithm of part (a) of Exercise 6.5.1.

This argument proves nothing, because we cannot say for sure that our assumption that rows 2 through m+1 of \tilde{B} span S is correct. Therefore we did some experiments to see what happens in practice. Our experiments confirmed that the bulge-chase does normally move the zero up m positions.⁵

We have now seen how zeros on the main diagonal of B move during a GZ iteration. Before we are satisfied, we must ask one additional question. Do the zeros impede the convergence of the GZ iterations in any way? Numerical experiments [220] show that they do not; the good quadratic convergence is maintained. This is so because the infinite eigenvalues do not interfere with the process by which shifts are transmitted through the matrix during the bulge-chase. This topic is discussed thoroughly in Chapter 7.

Exercises

- **6.5.1.** Let (A, B) be a Hessenberg-triangular pair with $b_{ii} = 0$. This exercise develops two algorithms for removing the zero.
 - (a) Describe an algorithm that pushes the zero up to the upper left-hand corner of B for deflation there. The first step acts on columns i-1 and i to transform $b_{i-i,i-1}$ to zero. This creates a bulge in A. Then a transformation from the left is used to return A to Hessenberg form. The next transformation sets $b_{i-2,i-2}$ to zero, and so on.
 - (b) Describe an algorithm that pushes the zero downward to the bottom right-hand corner of B for deflation there. The first transformation acts on rows i and i + 1 of B and transforms $b_{i+1,i+1}$ to zero.
- **6.5.2.** Let (A, B) be a pair in Hessenberg-triangular form, and suppose that B has k zeros on its main diagonal.
 - (a) Show that k is an upper bound on the number of infinite eigenvalues of (A, B) (algebraic multiplicity).

⁵The experiments were QZ iterations of degrees 2, 3, 4, and 5. We did sometimes find that after a large number of iterations, the zero would not have moved up as far as it should have. In other words, after k iterations of degree k, the zero might have moved up only km-1 or km-2 positions, instead of the expected km. We suspect that this was caused by roundoff errors rather than any rank-deficiency problems. We believe it would not have happened if the arithmetic had been exact.

- (b) Give a simple example that shows that the number of infinite eigenvalues of (A, B) can be less than k.
- **6.5.3.** Consider a bulge-chase of degree m = 1 on a pair (A, B) for which A is properly upper Hessenberg and B is upper triangular with $b_{11} \neq 0$.
 - (a) The vector x that determines the initial transformation is generated by (6.3.5) with m=1. This has only two nonzero entries. Show that the nonzero part of x is proportional to $\begin{bmatrix} a_{11} \rho \\ a_{21} \end{bmatrix}$. Deduce that $x_2 \neq 0$. Show that after the initial transformation, the bulge at position b_{21} is definitely nonzero, given that $b_{11} \neq 0$.
 - (b) Show that the transformation that transforms the bulge at b_{21} to zero creates a bulge at a_{31} that is definitely nonzero. Also, show that the new entry at position b_{22} is definitely nonzero (even if the original b_{22} was zero).
 - (c) Prove by induction that every bulge that appears in the bulge-chase with m=1 is certainly nonzero. (In other words, the bulge cannot suddenly become zero by accident.)
- **6.5.4.** Suppose that (A, B) is a Hessenberg-triangular pair, A is properly upper Hessenberg, and $b_{11} = b_{22} = 0$. Show that in the process of deflating an infinite eigenvalue corresponding to $b_{11} = 0$, the entry in position (2, 2) becomes nonzero, unless b_{12} is zero as well. Thus two adjacent zeros can correspond to only one infinite eigenvalue.

6.6 Deflating Subspaces

We observed early on that the concept of an invariant subspace is central to the theory and practice of the standard eigenvalue problem. For the generalized eigenvalue problem the analogous concept is that of a *deflating pair* of subspaces. This is an important idea, and we would have introduced it sooner if we had been taking a more theoretical approach. In most of this chapter we have restricted our attention to pairs (A, B) for which B is nonsingular, in which case the concept of a deflating pair reduces to that of invariant subspaces (of AB^{-1} and $B^{-1}A$). Material developed in this section will be used in Section 7.3.

Let (A, B) be a regular pair, and let (S, \mathcal{U}) be a pair of subspaces of \mathbb{C}^n of the same dimension k. Then (S, \mathcal{U}) is called a *deflating pair* for (A, B) if $AS \subseteq \mathcal{U}$ and $BS \subseteq \mathcal{U}$. When B is nonsingular, the situation is as follows (Exercise 6.6.1).

Proposition 6.6.1. *Suppose that B is nonsingular.*

- (a) If (S, U) is a deflating pair of (A, B), then U = BS, $S = B^{-1}U$, S is invariant under $B^{-1}A$, and U is invariant under AB^{-1} .
- (b) Conversely, if S is invariant under $B^{-1}A$ and U = BS, then U is invariant under AB^{-1} , and (S, U) is a deflating pair for (A, B).

The next proposition gives a useful matrix characterization of deflating pairs.

Proposition 6.6.2. Let S_1 , $U_1 \in \mathbb{C}^{n \times k}$ be matrices whose columns form bases for S and U, respectively; $S = \mathcal{R}(S_1)$ and $U = \mathcal{R}(U_1)$.

(a) Then (S, U) is a deflating pair for (A, B) if and only if there exist matrices E_{11} and F_{11} such that

$$AS_1 = U_1 E_{11}$$
 and $BS_1 = U_1 F_{11}$. (6.6.1)

- (b) If (S, U) is a deflating pair, then every eigenvalue of the pair (E_{11}, F_{11}) is an eigenvalue of (A, B). If x is an eigenvector of (E_{11}, F_{11}) with eigenvalue λ , then S_1x is an eigenvector of (A, B) with eigenvalue λ .
- (c) If (S, U) is a deflating pair, then if $v \in S$ is an eigenvector of (A, B) with eigenvalue λ , and $v = S_1 x$, then x is an eigenvector of (E_{11}, F_{11}) with eigenvalue λ .

If (S, U) is a deflating pair for (A, B), then the eigenvalues of (E_{11}, F_{11}) in Proposition 6.6.2 are called the *eigenvalues of* (A, B) *associated with* (S, U).

Proposition 6.6.3. *Let* (S, U) *be a deflating pair for* (A, B).

- (a) Then BS = U if and only if all of the eigenvalues of (A, B) associated with (S, U) are finite.
- (b) If BS = U and we take $U_1 = BS_1$, then the equations (6.6.1) simplify to the single equation

$$AS_1 = BS_1E_{11}.$$

The eigenvalues of E_{11} are the eigenvalues of (A, B) associated with (S, U).

Knowledge of deflating subspaces allows us to transform a matrix pair to block triangular form.

Proposition 6.6.4. Let (S, U) be a k-dimensional deflating pair for (A, B), and let S_1 , $U_1 \in \mathbb{C}^{n \times k}$ be matrices such that $S = \mathcal{R}(S_1)$ and $U = \mathcal{R}(U_1)$. Let S_2 , $U_2 \in \mathbb{C}^{n \times (n-k)}$ be such that the matrices $S = \begin{bmatrix} S_1 & S_2 \end{bmatrix}$ and $U = \begin{bmatrix} U_1 & U_2 \end{bmatrix}$ are nonsingular. Let $E = U^{-1}AS$ and $F = U^{-1}BS$. Then

$$E - \lambda F = \begin{bmatrix} E_{11} & E_{12} \\ 0 & E_{22} \end{bmatrix} - \lambda \begin{bmatrix} F_{11} & F_{12} \\ 0 & F_{22} \end{bmatrix}.$$

 E_{11} and F_{11} are $k \times k$ and satisfy (6.6.1).

A pair that is in the block triangular form of (E, F) in Proposition 6.6.4 has $(\mathcal{E}_k, \mathcal{E}_k)$ as a deflating pair, where $\mathcal{E}_k = \text{span}\{e_1, \dots, e_k\}$.

Deflating pairs are also known as *right deflating pairs*. A *left deflating pair* of subspaces for (A, B) is a pair that is right deflating for (A^*, B^*) . The next proposition gives the matrix characterization of left deflating pairs.

Proposition 6.6.5. Let \hat{S}_1 , $\hat{U}_1 \in \mathbb{C}^{n \times k}$ be matrices whose columns form bases for \hat{S} and \hat{U} , respectively.

(a) Then (\hat{S}, \hat{U}) is a left deflating pair for (A, B) if and only if there exist matrices \hat{E}_{11} and \hat{F}_{11} such that

$$\hat{S}_{1}^{*}A = \hat{E}_{11}\hat{U}_{1}^{*} \quad and \quad \hat{S}_{1}^{*}B = \hat{F}_{11}\hat{U}_{1}^{*}.$$
 (6.6.2)

- (b) If (\hat{S}, \hat{U}) is a left deflating pair, then every eigenvalue of the pair $(\hat{E}_{11}, \hat{F}_{11})$ is an eigenvalue of (A, B). If x^* is a left eigenvector of $(\hat{E}_{11}, \hat{F}_{11})$ with eigenvalue λ , then $x^*\hat{S}_1^*$ in a left eigenvector of (A, B) with eigenvalue λ .
- (c) If (\hat{S}, \hat{U}) is a left deflating pair, then if $v \in \hat{S}$, v^* is a left eigenvector of (A, B) with eigenvalue λ , and $v = S_1 x$, then x^* is a left eigenvector of $(\hat{E}_{11}, \hat{F}_{11})$ with eigenvalue λ .

If (\hat{S}, \hat{U}) is a left deflating pair for (A, B), then the eigenvalues of $(\hat{E}_{11}, \hat{F}_{11})$ in Proposition 6.6.5 are called the *eigenvalues of* (A, B) *associated with* (\hat{S}, \hat{U}) .

Proposition 6.6.6. The pair (S, \mathcal{U}) is a right deflating pair for (A, B) if and only if $(\mathcal{U}^{\perp}, S^{\perp})$ is a left deflating pair. If (S, \mathcal{U}) is a deflating pair, then the sets of eigenvalues associated with (S, \mathcal{U}) and $(\mathcal{U}^{\perp}, S^{\perp})$ are complementary subsets of the spectrum of (A, B), counting multiplicity.

Proof: We outline a proof here. (Some details are worked out in Exercise 6.6.6.) $AS \subseteq \mathcal{U}$ if and only if $A^*\mathcal{U}^{\perp} \subseteq S^{\perp}$. Since this is true for any matrix, it is true for B as well. This establishes the first part of the proposition.

The second part is perhaps most easily seen using matrices. If (S, \mathcal{U}) is a deflating pair, then there is an equivalence transformation to block triangular form

$$U^{-1}(A - \lambda B)S = E - \lambda F = \begin{bmatrix} E_{11} & E_{12} \\ 0 & E_{22} \end{bmatrix} - \lambda \begin{bmatrix} F_{11} & F_{12} \\ 0 & F_{22} \end{bmatrix}, \tag{6.6.3}$$

where $S = \begin{bmatrix} S_1 & S_2 \end{bmatrix}$ and $U = \begin{bmatrix} U_1 & U_2 \end{bmatrix}$, as described in Proposition 6.6.4. The eigenvalues of (E_{11}, F_{11}) are the eigenvalues of (A, B) associated with (S, U). The transformation (6.6.3) can be rewritten as

$$U^{-1}(A - \lambda B) = (E - \lambda F)S^{-1}.$$
 (6.6.4)

Define matrices $V = \begin{bmatrix} V_1 & V_2 \end{bmatrix}$ and $W = \begin{bmatrix} W_1 & W_2 \end{bmatrix}$ by $V^* = S^{-1}$ and $W^* = U^{-1}$. Then $V^*S = I$, which implies that $\mathcal{R}(V_2) = \mathcal{S}^{\perp}$. Similarly $\mathcal{R}(W_2) = \mathcal{U}^{\perp}$. Equation (6.6.4) can be written in block form as

$$\left[\begin{array}{c}W_1^*\\W_2^*\end{array}\right](A-\lambda B)=\left[\begin{array}{cc}E_{11}-\lambda F_{11}&E_{12}-\lambda F_{12}\\0&E_{22}-\lambda F_{22}\end{array}\right]\left[\begin{array}{c}V_1^*\\V_2^*\end{array}\right],$$

the second equation of which implies

$$W_2^*A = E_{22}V_2^*$$
 and $W_2^*B = F_{22}V_2^*$.

Since $\mathcal{R}(W_2) = \mathcal{U}^{\perp}$ and $\mathcal{R}(V_2) = \mathcal{S}^{\perp}$, these equations show, by Proposition 6.6.5, that $(\mathcal{U}^{\perp}, \mathcal{S}^{\perp})$ is a left deflating pair for (A, B) (reproving part one), and the associated eigenvalues are the eigenvalues of (E_{22}, F_{22}) . Since the eigenvalues of (E_{11}, F_{11}) and (E_{22}, F_{22}) are complementary subsets of the spectrum of (A, B), the proof is complete. \square

Finally we have the following very compact characterization.

Proposition 6.6.7. Let $S_1 \in \mathbb{C}^{n \times k}$ and $W_2 \in \mathbb{C}^{n \times (n-k)}$ be matrices such that $S = \mathcal{R}(S_1)$ and $U^{\perp} = \mathcal{R}(W_2)$. Then (S, \mathcal{U}) is a deflating pair for (A, B) if and only if

$$W_2^* A S_1 = 0$$
 and $W_2^* B S_1 = 0$.

Swapping Blocks

At this point we find it convenient to use the pencil notation. Whether we speak of a matrix pair (E, F) or a matrix pencil $E - \lambda F$, we are speaking of the same thing. Consider the following swapping problem. A block triangular matrix pencil

$$E - \lambda F = \begin{bmatrix} E_{11} & E_{12} \\ 0 & E_{22} \end{bmatrix} - \lambda \begin{bmatrix} F_{11} & F_{12} \\ 0 & F_{22} \end{bmatrix}$$
 (6.6.5)

is given. Suppose that F is nonsingular, so that all of the eigenvalues are finite. Suppose further that the eigenvalues of $E_{11} - \lambda F_{11}$ are ρ_1, \ldots, ρ_m , the eigenvalues of $E_{22} - \lambda F_{22}$ are τ_1, \ldots, τ_k , and $\rho_i \neq \tau_j$ for all i and j. The problem is to make a unitary equivalence that transforms (6.6.5) to

$$\hat{E} - \lambda \hat{F} = \begin{bmatrix} \hat{E}_{11} & \hat{E}_{12} \\ 0 & \hat{E}_{22} \end{bmatrix} - \lambda \begin{bmatrix} \hat{F}_{11} & \hat{F}_{12} \\ 0 & \hat{F}_{22} \end{bmatrix}, \tag{6.6.6}$$

where $\hat{E}_{11} - \lambda \hat{F}_{11}$ has eigenvalues τ_1, \ldots, τ_k , and $\hat{E}_{22} - \lambda \hat{F}_{22}$ has eigenvalues ρ_1, \ldots, ρ_m . We considered a problem like this in connection with standard eigenvalue problems in Section 4.8. There we discussed the interchange of blocks in a block triangular matrix in order to compute an invariant subspace associated with specified eigenvalues. We found that we could do this if we could solve a Sylvester equation (2.4.4). The block swapping problem that we are studying here can be useful in a similar context. Once we have transformed a pair to triangular or quasi-triangular form by the QZ algorithm, if we wish to compute a deflating pair of subspaces associated with a specified set of eigenvalues, we must move those eigenvalues or the blocks containing those eigenvalues to the upper left-hand corner of the pair. This requires swapping small blocks. The need to swap blocks will also arise in a different context in Section 7.3. As we shall see, this sort of swap requires solving a generalized Sylvester equation.

Proceeding as in Section 4.8, we begin by transforming by

$$\left[\begin{array}{cc} 0 & I \\ I & 0 \end{array}\right]$$

on left and right to transform (6.6.5) to

$$\left[\begin{array}{cc} E_{22} & 0 \\ E_{12} & E_{11} \end{array}\right] - \lambda \left[\begin{array}{cc} F_{22} & 0 \\ F_{12} & F_{11} \end{array}\right].$$

Now the main-diagonal blocks are in the right place at least, but the off-diagonal blocks are not. In Section 4.8 (standard eigenvalue problem) we were able to make a similarity

⁶Another use for generalized Sylvester equations is the study of the sensitivity of deflating subspaces [195, 196].

transformation (2.4.3) to eliminate the off-diagonal block. This required solving a Sylvester equation (2.4.4); see Theorem 2.4.2 and Exercise 2.4.5. In our present situation we have two blocks to annihilate, but we have greater flexibility, as we are not restricted to similarity transformations. Using (2.4.3) as a guide, it seems reasonable to seek $X, Y \in \mathbb{C}^{m \times k}$ such that

$$\begin{bmatrix} I & 0 \\ Y & I \end{bmatrix} \begin{bmatrix} E_{22} - \lambda F_{22} & 0 \\ E_{12} - \lambda F_{12} & E_{11} - \lambda F_{11} \end{bmatrix} \begin{bmatrix} I & 0 \\ X & I \end{bmatrix}$$

$$= \begin{bmatrix} E_{22} - \lambda F_{22} & 0 \\ 0 & E_{11} - \lambda F_{11} \end{bmatrix}. \tag{6.6.7}$$

One easily checks that X and Y achieve this if and only if

$$E_{11}X + YE_{22} = -E_{12}$$
 and $F_{11}X + YF_{22} = -F_{12}$. (6.6.8)

These are the *generalized Sylvester equations*. This is a system of 2mk linear equations in 2mk unknowns.

Theorem 6.6.8. The generalized Sylvester equations (6.6.8) have a unique solution if and only if the pairs (E_{11}, F_{11}) and (E_{22}, F_{22}) have disjoint spectra.

The proof (Exercise 6.6.9) is similar to that for the standard Sylvester equation (Exercises 2.4.4 and 2.4.5); the ideas are exactly the same, but the details are a bit more complicated. Exercise 6.6.9 also sketches a method for solving generalized Sylvester equations efficiently in practice. A number of variants have appeared in the literature [58, 82, 122, 124, 125]. All use generalizations of the Bartels–Stewart algorithm to triangularize the system and render the subsequent solution process trivial.

Once we have X and Y, we can perform the transformation (6.6.7). However, we prefer not to do this literally because the transforming matrices could be ill conditioned. Instead we make two decompositions,

$$\begin{bmatrix} I & 0 \\ X & I \end{bmatrix} = QR = \begin{bmatrix} Q_{11} & Q_{12} \\ Q_{21} & Q_{22} \end{bmatrix} \begin{bmatrix} R_{11} & R_{12} \\ 0 & R_{22} \end{bmatrix}$$
(6.6.9)

and

$$\begin{bmatrix} I & 0 \\ Y & I \end{bmatrix} = SZ = \begin{bmatrix} S_{11} & S_{12} \\ 0 & S_{22} \end{bmatrix} \begin{bmatrix} Z_{11} & Z_{12} \\ Z_{21} & Z_{22} \end{bmatrix}, \tag{6.6.10}$$

where Q and Z are unitary and R and S are upper triangular. Then, letting

$$\begin{bmatrix} \hat{E}_{11} - \lambda \hat{F}_{11} & \hat{E}_{12} - \lambda \hat{F}_{12} \\ \hat{E}_{21} - \lambda \hat{F}_{21} & \hat{E}_{22} - \lambda \hat{F}_{22} \end{bmatrix}$$

$$= \begin{bmatrix} Z_{11} & Z_{12} \\ Z_{21} & Z_{22} \end{bmatrix} \begin{bmatrix} E_{22} - \lambda F_{22} & 0 \\ E_{12} - \lambda F_{12} & E_{11} - \lambda F_{11} \end{bmatrix} \begin{bmatrix} Q_{11} & Q_{12} \\ Q_{21} & Q_{22} \end{bmatrix}, \quad (6.6.11)$$

we have $\hat{E}_{21} = \hat{F}_{21} = 0$; the eigenvalues of $(\hat{E}_{11}, \hat{F}_{11})$ are those of (E_{22}, F_{22}) , i.e., τ_1, \ldots, τ_k , and the eigenvalues of $(\hat{E}_{22}, \hat{F}_{22})$ are those of (E_{11}, F_{11}) , i.e., ρ_1, \ldots, ρ_m . These facts are verified in Exercise 6.6.10. The desired exchange, from (6.6.5) to (6.6.6), has been accomplished.

This is a theoretical result. In practice roundoff errors cause \hat{E}_{21} and \hat{F}_{21} to be nonzero, and if they are too far from zero we must reject the swap. To improve performance an additional QR or RQ decomposition can be applied to \hat{F} to enforce block triangularity. Then the same transformation can be applied to \hat{E} [122]. Finally, $\|\hat{E}_{21}\|$ is checked as a stability check. If this is small enough, we set it to zero. If it is not small enough, we must reject the exchange.

Relationship to Deflating Subspaces

The important part of (6.6.7) is the (2,1) block, which can be written as

$$\begin{bmatrix} Y & I \end{bmatrix} \begin{bmatrix} E_{22} & 0 \\ E_{12} & E_{11} \end{bmatrix} \begin{bmatrix} I \\ X \end{bmatrix} = 0, \qquad \begin{bmatrix} Y & I \end{bmatrix} \begin{bmatrix} F_{22} & 0 \\ F_{12} & F_{11} \end{bmatrix} \begin{bmatrix} I \\ X \end{bmatrix} = 0,$$
(6.6.12)

and is equivalent to the generalized Sylvester equations (6.6.8). If we let $S_1 = \begin{bmatrix} I \\ X \end{bmatrix}$,

 $S = \mathcal{R}(S_1)$, $W_2 = \begin{bmatrix} Y^* \\ I \end{bmatrix}$, and $\mathcal{U} = \mathcal{R}(W_2)^{\perp}$ and compare with Proposition 6.6.7, we see that (S, \mathcal{U}) is a deflating pair for the pencil

$$\begin{bmatrix} E_{22} & 0 \\ E_{12} & E_{11} \end{bmatrix} - \lambda \begin{bmatrix} F_{22} & 0 \\ F_{12} & F_{11} \end{bmatrix}. \tag{6.6.13}$$

Thus solving the generalized Sylvester equation amounts to computing a deflating pair of subspaces. Exercise 6.6.11 shows that the eigenvalues associated with (S, U) are the eigenvalues of (E_{22}, F_{22}) , while the eigenvalues associated with (U^{\perp}, S^{\perp}) are those of (E_{11}, F_{11}) . The decompositions (6.6.9) and (6.6.10) guarantee that the columns of $\begin{bmatrix} Q_{11} \\ Q_{21} \end{bmatrix}$ span the same space as the columns of $\begin{bmatrix} I \\ X \end{bmatrix}$, and the rows of $\begin{bmatrix} Z_{21} & Z_{22} \end{bmatrix}$ span the same space as the rows of $\begin{bmatrix} Y & I \end{bmatrix}$. These equalities guarantee that the transformation (6.6.11) has the desired effect (cf. Proposition 6.6.4).

Exercises

- **6.6.1.** Prove Proposition 6.6.1.
- **6.6.2.** Prove Proposition 6.6.2.
- **6.6.3.** Prove Proposition 6.6.3.
- **6.6.4.** Prove Proposition 6.6.4. (Rewrite the equation $E = U^{-1}AS$ as AS = UE. Partition S, U, and E appropriately, and show that $E_{21} = 0$. Do the same for the equation $F = U^{-1}BS$.)
- **6.6.5.** Prove Proposition 6.6.5.
- **6.6.6.** This exercise works out some details of the proof of Proposition 6.6.6.
 - (a) Use Proposition 1.2.2 to show that $AS \subseteq \mathcal{U}$ if and only if $A^*\mathcal{U}^{\perp} \subseteq S^{\perp}$.
 - (b) Show that $V^*S = I$, $V_2^*S_1 = 0$, and prove that $\mathcal{R}(V_2) = \mathcal{S}^{\perp}$. Similarly prove $\mathcal{R}(W_2) = \mathcal{U}^{\perp}$.

- **6.6.7.** Prove Proposition 6.6.7.
- **6.6.8.** Verify that (6.6.7) holds if and only if the generalized Sylvester equations (6.6.8) hold.
- **6.6.9.** This exercise proves Theorem 6.6.8.
 - (a) Apply the generalized Schur theorem (Theorem 6.1.2) to the pairs (E_{11}^T, F_{11}^T) and (E_{22}, F_{22}) to show that the generalized Sylvester equations (6.6.8) can be replaced by an equivalent system in which E_{11} and F_{11} are lower triangular and E_{22} and F_{22} are upper triangular.
 - (b) Using properties of Kronecker products (Exercises 2.4.3 and 2.4.4), show that the generalized Sylvester equations (6.6.8) can be rewritten as

$$\begin{bmatrix} I \otimes E_{11} & E_{22}^T \otimes I \\ I \otimes F_{11} & F_{22}^T \otimes I \end{bmatrix} \begin{bmatrix} \operatorname{vec}(X) \\ \operatorname{vec}(Y) \end{bmatrix} = - \begin{bmatrix} \operatorname{vec}(E_{12}) \\ \operatorname{vec}(F_{12}) \end{bmatrix}. \tag{6.6.14}$$

- (c) From part (a) we can assume that E_{11} , F_{11} , E_{22}^T , and F_{22}^T are all lower triangular in (6.6.14). Assume this for the remainder of the exercise. Show that each of the four blocks in the coefficient matrix of (6.6.14) is lower triangular.
- (d) Transform (6.6.14) to an equivalent system by doing a perfect shuffle of the rows and the columns. Thus rows (or columns) that were ordered $1, 2, \ldots, 2n$ get reordered as $1, n+1, 2, n+2, \ldots, n, 2n$. Show that the resulting system is block lower triangular with 2×2 blocks. Show that each main-diagonal block has the form

$$\left[\begin{array}{cc} e_1 & e_2 \\ f_1 & f_2 \end{array}\right],$$

where e_i/f_i is an eigenvalue of the pair (E_{ii}, F_{ii}) for i = 1, 2. Deduce that the coefficient matrix is nonsingular if and only if (E_{11}, F_{11}) and (E_{22}, F_{22}) have no eigenvalues in common. This completes the proof of Theorem 6.6.8.

- (e) Describe an algorithm to solve the block triangular generalized Sylvester equations. (You will probably find it easier to work with the unshuffled version.) This is a generalization of the (complex version of the) Bartels–Stewart algorithm.
- **6.6.10.** Suppose $\hat{E} \lambda \hat{F}$ is given by (6.6.11).
 - (a) Show that

$$\begin{bmatrix} \hat{E}_{11} - \lambda \hat{F}_{11} & \hat{E}_{12} - \lambda \hat{F}_{12} \\ \hat{E}_{21} - \lambda \hat{F}_{21} & \hat{E}_{22} - \lambda \hat{F}_{22} \end{bmatrix}$$

$$= \begin{bmatrix} S_{11} & S_{12} \\ 0 & S_{22} \end{bmatrix}^{-1} \begin{bmatrix} E_{22} - \lambda F_{22} & 0 \\ 0 & E_{11} - \lambda F_{11} \end{bmatrix} \begin{bmatrix} R_{11} & R_{12} \\ 0 & R_{22} \end{bmatrix}^{-1}.$$

- (b) Deduce that $\hat{E}_{21} \lambda \hat{F}_{21} = 0$.
- (c) Show that $\hat{E}_{11} \lambda \hat{F}_{11} = S_{11}^{-1}(E_{22} \lambda F_{22})R_{11}^{-1}$. Deduce that the eigenvalues of $\hat{E}_{11} \lambda \hat{F}_{11}$ are τ_1, \ldots, τ_k .

(d) Show that $\hat{E}_{22} - \lambda \hat{F}_{22} = S_{22}^{-1} (E_{11} - \lambda F_{11}) R_{22}^{-1}$. Deduce that the eigenvalues of $\hat{E}_{22} - \lambda \hat{F}_{22}$ are ρ_1, \ldots, ρ_m .

6.6.11.

- (a) Show that if the columns of $\begin{bmatrix} I \\ X \end{bmatrix}$ span a deflating subspace $\mathcal S$ of the pencil (6.6.13), then the eigenvalues associated with $\mathcal S$ are the eigenvalues of (E_{22}, F_{22}) .
- (b) Show that if the columns of $\begin{bmatrix} Y^* \\ I \end{bmatrix}$ span a left deflating subspace \mathcal{U}^{\perp} of the pencil (6.6.13), then the eigenvalues associated with \mathcal{U}^{\perp} are the eigenvalues of (E_{11}, F_{11}) .