## Appendix C

## Eigenvalues and Inner-Product Norms

The analysis of differential equations and of finite difference methods for their solution relies heavily on "spectral analysis," based on the eigenvalues and eigenfunctions of differential operators or the eigenvalues and eigenvectors of matrices approximating these operators. In particular, knowledge of the spectrum of a matrix (the set of eigenvalues) gives critical information about the behavior of powers or exponentials of the matrix, as reviewed in Appendix D. An understanding of this is crucial in order to analyze the behavior and stability properties of differential or finite difference equations, as discussed in Section D.2.1 and at length in the main text.

This appendix contains a review of basic spectral theory and also some additional results on inner-product norms and the relation between these norms and spectra.

Let $A \in \mathbb{C}^{m \times m}$ be an $m \times m$ matrix with possibly complex components. We will mostly be working with real matrices, but many of the results carry over directly to the complex case or are most easily presented in this generality. Moreover, even real matrices can have complex eigenvalues and eigenvectors, so we must work in the complex plane.

The matrix $A$ has $m$ eigenvalues $\lambda_{1}, \lambda_{2}, \ldots, \lambda_{m}$ that are the roots of the characteristic polynomial,

$$
p_{A}(z)=\operatorname{det}(A-z I)=\left(z-\lambda_{1}\right)\left(z-\lambda_{2}\right) \cdots\left(z-\lambda_{m}\right)
$$

This polynomial of degree $m$ always has $m$ roots, although some may be multiple roots. If no two are equal, then we say the roots are distinct. The set of $m$ eigenvalues is called the spectrum of the matrix, and the spectral radius of $A$, denoted by $\rho(A)$, is the maximum magnitude of any eigenvalue,

$$
\rho(A)=\max _{1 \leq p \leq m}\left|\lambda_{p}\right| .
$$

If the characteristic polynomial $p_{A}(z)$ has a factor $(z-\lambda)^{s}$, then the eigenvalue $\lambda$ is said to have algebraic multiplicity $m_{a}(\lambda)=s$. If $\lambda$ is an eigenvalue, then $A-\lambda I$ is a singular matrix and the null space of this matrix is the eigenspace of $A$ corresponding to this eigenvalue,

$$
\mathcal{N}(A-\lambda I)=\left\{u \in \mathbb{C}^{m}:(A-\lambda I) u=0\right\}=\left\{u \in \mathbb{C}^{m}: A u=\lambda u\right\}
$$

Any vector $u$ in the eigenspace satisfies $A u=\lambda u$. The dimension of this eigenspace is called the geometric multiplicity $m_{g}(\lambda)$ of the eigenvalue $\lambda$. We always have

$$
\begin{equation*}
1 \leq m_{g}(\lambda) \leq m_{a}(\lambda) \tag{C.1}
\end{equation*}
$$

If $m_{g}(\lambda)=m_{a}(\lambda)$, then $A$ has a complete set of eigenvectors for this eigenvalue. Otherwise this eigenvalue is said to be defective. If $A$ has one or more defective eigenvalues, then $A$ is a defective matrix.

Example C.1. If the eigenvalues of $A$ are all distinct, then $m_{g}=m_{a}=1$ for every eigenvalue and the matrix is not defective.

Example C.2. A diagonal matrix cannot be defective. The eigenvalues are simply the diagonal elements, and the unit vectors $e_{j}$ (the vector with a 1 in the $j$ th element, zeros elsewhere) form a complete set of eigenvectors. For example,

$$
A=\left[\begin{array}{lll}
3 & 0 & 0 \\
0 & 3 & 0 \\
0 & 0 & 5
\end{array}\right]
$$

has $\lambda_{1}=\lambda_{2}=3$ and $\lambda_{3}=5$. The two-dimensional eigenspace for $\lambda=3$ is spanned by $e_{1}=(1,0,0)^{T}$ and $e_{2}=(0,1,0)^{T}$. The one-dimensional eigenspace for $\lambda=5$ is spanned by $e_{3}=(0,0,1)^{T}$.

Example C.3. Any upper triangular matrix has eigenvalues equal to its diagonal elements $d_{i}$ since the characteristic polynomial is simply $p_{A}(z)=\left(z-d_{1}\right) \cdots\left(z-d_{m}\right)$. The matrix may be defective if there are repeated roots. For example,

$$
A=\left[\begin{array}{llll}
3 & 1 & 0 & 0 \\
0 & 3 & 0 & 0 \\
0 & 0 & 3 & 0 \\
0 & 0 & 0 & 5
\end{array}\right]
$$

has $\lambda_{1}=\lambda_{2}=\lambda_{3}=3$ and $\lambda_{4}=5$. The eigenvalue $\lambda=3$ has algebraic multiplicity $m_{a}=3$ but there is only a two-dimensional space of eigenvectors associated with $\lambda=3$, spanned by $e_{1}$ and $e_{3}$, so $m_{g}=2$.

## C. 1 Similarity transformations

Let $S$ be any nonsingular matrix and set

$$
\begin{equation*}
B=S^{-1} A S \tag{C.2}
\end{equation*}
$$

Then $B$ has the same eigenvalues as $A$. To see this, suppose

$$
\begin{equation*}
A r=\lambda r \tag{C.3}
\end{equation*}
$$

for some vector $r$ and scalar $\lambda$. Let $w=S^{-1} r$ and multiply (C.3) by $S^{-1}$ to obtain

$$
\left(S^{-1} A S\right)\left(S^{-1} r\right)=\lambda\left(S^{-1} r\right) \quad \Longrightarrow \quad B w=\lambda w
$$

so $\lambda$ is also an eigenvalue of $B$ with eigenvector $S^{-1} r$. Conversely, if $\lambda$ is any eigenvalue of $B$ with eigenvector $w$, then similar manipulations in reverse show that $\lambda$ is also an eigenvalue of $A$ with eigenvector $S w$.

The transformation (C.2) from $A$ to $B$ is called a similarity transformation and we say that the matrices $A$ and $B$ are similar if such a relation holds. The fact that similar matrices have the same eigenvalues is exploited in most numerical methods for computing eigenvalues of a matrix - a sequence of similarity transformations is performed to approximately reduce $A$ to a simpler form from which it is easy to determine the eigenvalues, such as a diagonal or upper triangular matrix. See, for example, [35] for introductory discussions of such algorithms.

## C. 2 Diagonalizable matrices

If $A$ is not defective (i.e., if every eigenvalue has a complete set of eigenvectors), then it is diagonalizable. In this case we can choose a set of $m$ linearly independent right eigenvectors $r_{j}$ spanning all of $\mathbb{C}^{m}$ such that $A r_{j}=\lambda_{j} r_{j}$ for $j=1,2, \ldots, m$. Let $R$ be the matrix of right eigenvectors

$$
\begin{equation*}
R=\left[r_{1}\left|r_{2}\right| \cdots \mid r_{m}\right] \tag{C.4}
\end{equation*}
$$

Then

$$
\begin{equation*}
A R=R \Lambda \tag{C.5}
\end{equation*}
$$

where

$$
\begin{equation*}
\Lambda=\operatorname{diag}\left(\lambda_{1}, \lambda_{2}, \ldots, \lambda_{m}\right) \tag{C.6}
\end{equation*}
$$

This follows by viewing the matrix multiplication columnwise. Since the vectors $r_{j}$ are linearly independent, the matrix $R$ is invertible and so from (C.5) we obtain

$$
\begin{equation*}
R^{-1} A R=\Lambda, \tag{C.7}
\end{equation*}
$$

and hence we can diagonalize $A$ by a similarity transformation. We can also write

$$
\begin{equation*}
A=R \Lambda R^{-1} \tag{C.8}
\end{equation*}
$$

which is sometimes called the eigendecomposition of $A$. This is a special case of the Jordan canonical form discussed in the next section.

Let $\ell_{j}^{T}$ be the $j$ th row of $R^{-1}$. We can also write the above expressions as

$$
R^{-1} A=\Lambda R^{-1}
$$

and when these multiplications are viewed rowwise we obtain $\ell_{j}^{T} A=\lambda_{j} \ell_{j}^{T}$, which shows that the rows of $R^{-1}$ are the left eigenvectors of $A$.

## C. 3 The Jordan canonical form

If $A$ is diagonalizable, we have just seen in (C.8) that we can decompose $A$ as $A=$ $R \wedge R^{-1}$. If $A$ is defective, then it cannot be written in this form; $A$ is not similar to a
diagonal matrix. The closest we can come is to write it in the form $A=R J R^{-1}$, where the matrix $J$ is block diagonal. Each block has nonzeros everywhere except perhaps on its diagonal and superdiagonal, and is a Jordan block of some order. The Jordan blocks of orders 1, 2, and 3 are

$$
J(\lambda, 1)=\lambda, \quad J(\lambda, 2)=\left[\begin{array}{cc}
\lambda & 1 \\
0 & \lambda
\end{array}\right], \quad J(\lambda, 3)=\left[\begin{array}{ccc}
\lambda & 1 & 0 \\
0 & \lambda & 1 \\
0 & 0 & \lambda
\end{array}\right] .
$$

In general a Jordan block of order $k$ has the form

$$
\begin{equation*}
J(\lambda, k)=\lambda I_{k}+S_{k}, \tag{C.9}
\end{equation*}
$$

where $I_{k}$ is the $k \times k$ identity matrix and $S_{k}$ is the $k \times k$ shift matrix

$$
S_{k}=\left[\begin{array}{cccccc}
0 & 1 & 0 & 0 & \cdots & 0  \tag{C.10}\\
0 & 0 & 1 & 0 & \cdots & 0 \\
\vdots & \vdots & & & & \vdots \\
0 & 0 & 0 & 0 & \cdots & 1 \\
0 & 0 & 0 & 0 & \cdots & 0
\end{array}\right] \quad \text { for } k>1 \quad \text { (with } S_{1}=0 \text { ), }
$$

so called because $S_{k}\left(u_{1}, u_{2}, \ldots, u_{k-1}, u_{k}\right)^{T}=\left(u_{2}, u_{3}, \ldots, u_{k}, 0\right)^{T}$. A Jordan block of order $k$ has eigenvalues $\lambda$ with algebraic multiplicity $m_{a}=k$ and geometric multiplicity $m_{g}=1$. The unit vector $e_{1}=(1,0, \ldots, 0)^{T} \in \mathbb{C}^{k}$ is a basis for the one-dimensional eigenspace of this block.

Theorem C.1. Every $m \times m$ matrix $A \in \mathbb{C}^{m \times m}$ can be transformed into the form

$$
\begin{equation*}
A=R J R^{-1}, \tag{C.11}
\end{equation*}
$$

where $J$ is a block diagonal matrix of the form

$$
J=\left[\begin{array}{cccc}
J\left(\lambda_{1}, k_{1}\right) & & &  \tag{C.12}\\
& J\left(\lambda_{2}, k_{2}\right) & & \\
& & \ddots & \\
& & & J\left(\lambda_{s}, k_{s}\right)
\end{array}\right]
$$

Each $J\left(\lambda_{i}, k_{i}\right)$ is a Jordan block of some order $k_{i}$ and $\sum_{i=1}^{s} k_{i}=m$. If $\lambda$ is an eigenvalue of $A$ with algebraic multiplicity $m_{a}$ and geometric multiplicity $m_{g}$, then $\lambda$ appears in $m_{g}$ blocks and the sum of the orders of these blocks is $m_{a}$.

The nonsingular matrix $R$ contains eigenvectors of $A$. In the defective case, $R$ must also contain other vectors since there is not a complete set of eigenvectors in this case. These other vectors are called principal vectors.

Example C.4. For illustration, consider a $3 \times 3$ matrix $A$ with a single eigenvalue $\lambda$ with $m_{a}(\lambda)=3$ but $m_{g}(\lambda)=1$. Then we wish to find a $3 \times 3$ invertible matrix $R$ such that

$$
A R=R J=\left[r_{1}\left|r_{2}\right| r_{3}\right]\left[\begin{array}{ccc}
\lambda & 1 & 0 \\
0 & \lambda & 1 \\
0 & 0 & \lambda
\end{array}\right]
$$

From this we obtain

$$
\begin{align*}
A r_{1}=\lambda r_{1} & \Longrightarrow \quad(A-\lambda I) r_{1}=0, \\
A r_{2}=r_{1}+\lambda r_{2} & \Longrightarrow \quad(A-\lambda I) r_{2}=r_{1} \quad \Longrightarrow \quad(A-\lambda I)^{2} r_{2}=0,  \tag{C.13}\\
A r_{3}=r_{2}+\lambda r_{3} \quad & \Longrightarrow \quad(A-\lambda I) r_{3}=r_{2} \quad \Longrightarrow \quad(A-\lambda I)^{3} r_{3}=0 .
\end{align*}
$$

The vector $r_{1}$ forms a basis for the one-dimensional eigenspace. The vectors $r_{2}$ and $r_{3}$ are principal vectors. They are linearly independent vectors in the null space of $(A-\lambda I)^{2}$ and the null space of $(A-\lambda I)^{3}$ that are not in the null space of $A-\lambda I$.

The choice of the value 1 on the superdiagonal of the nontrivial Jordan blocks is the standard convention, but this can be replaced with any nonzero value $\delta$ by modifying the matrix $R$ appropriately. This is easy to verify by applying the following similarity transformation to a Jordan block $J(\lambda, k)$. Choose $\delta \neq 0$ and set

$$
D=\left[\begin{array}{lllll}
1 & & & &  \tag{C.14}\\
& \delta & & & \\
& & \delta^{2} & & \\
& & & \ddots & \\
& & & & \delta^{k-1}
\end{array}\right], \quad D^{-1}=\left[\begin{array}{ccccc}
1 & & & & \\
& \delta^{-1} & & & \\
& & \delta^{-2} & & \\
& & & \ddots & \\
& & & & \delta^{-(k-1)}
\end{array}\right]
$$

Then

$$
D^{-1} J(\lambda, k) D=\lambda I_{k}+\delta S_{k} .
$$

Note that left multiplying by $D^{-1}$ multiplies the $i$ th row by $\delta^{-(i-1)}$, while right multiplying by $D$ multiplies the $j$ th column by $\delta^{j-1}$. On the diagonal the two effects cancel, while on the superdiagonal the net effect is to multiply each element by $\delta$.

Similarity transformations of this nature are useful in other contexts as well. If this transformation is applied to an arbitrary matrix, then all elements on the $p$ th diagonal will be multiplied by $\delta^{p}$ (with $p$ positive for superdiagonals and negative for subdiagonals).

By applying this idea to each block in the Jordan canonical form with $\delta \ll 1$, we can find a matrix $R$ so that $R^{-1} A R$ is close to diagonal with the 0 or $\delta$ at each location on the superdiagonal. This is done, for example, in the proof of Theorem C.4. But note that for $\delta<1$ the condition number is $\kappa(D)=\delta^{1-k}$ and this blows up as $\delta \rightarrow 0$ if $k>1$, so bringing a defective matrix to nearly diagonal form requires an increasingly illconditioned matrix $R$ as the off-diagonals vanish. There is no nonsingular matrix $R$ that will diagonalize $A$ in the defective case.

## C. 4 Symmetric and Hermitian matrices

If $A \in \mathbb{R}^{m \times m}$ and $A=A^{T}$, then $A$ is a symmetric matrix. Symmetric matrices arise naturally in many applications, in particular when discretizing "self-adjoint" differential equations. The complex analogue of the transpose is the complex conjugate transpose or adjoint matrix $A^{H}=\bar{A}^{T}$, in which the matrix is transposed and then the complex conjugate of each element taken. If $A$ is a real matrix, then $A^{H}=A^{T}$. If $A=A^{H}$, then $A$ is said to be Hermitian (so in particular a real symmetric matrix is Hermitian).

Hermitian matrices always have real eigenvalues and are always diagonalizable. Moreover, the eigenvectors $r_{1}, \ldots, r_{m}$ can be chosen to be mutually orthogonal, and normalized to have $r_{j}^{H} r_{j}=1$, so that the eigenvector matrix $R$ is a unitary matrix, $R^{H} R=I$, and hence $R^{-1}=R^{H}$. (If $R$ is real and Hermitian, then $R^{-1}=R^{T}$ and $R$ is called an orthogonal matrix.)

If $R=R^{T}$ and the eigenvalues of $A$ are all positive, then $A$ is said to be symmetric positive definite (SPD), or Hermitian positive definite in the complex case, or often simply "positive definite." In this case

$$
\begin{equation*}
u^{H} A u>0 \tag{C.15}
\end{equation*}
$$

for any vector $u \neq 0$.
This concept is generalized to the following: $A$ is

$$
\begin{array}{ll}
\text { positive definite } & \Longleftrightarrow u^{H} A u>0 \text { for all } u \neq 0 \Longleftrightarrow \lambda_{p}>0 \text { for all } p, \\
\text { positive semidefinite } & \Longleftrightarrow u^{H} A u \geq 0 \text { for all } u \neq 0 \Longleftrightarrow \lambda_{p} \geq 0 \text { for all } p, \\
\text { negative definite } & \Longleftrightarrow u^{H} A u<0 \text { for all } u \neq 0 \Longleftrightarrow \lambda_{p}<0 \text { for all } p, \\
\text { negative semidefinite } & \Longleftrightarrow u^{H} A u \leq 0 \text { for all } u \neq 0 \Longleftrightarrow \lambda_{p} \leq 0 \text { for all } p, \\
\text { indefinite } & \Longleftrightarrow u^{H} A u \text { indefinite } \Longleftrightarrow \lambda_{p}<0<\lambda_{q} \\
&
\end{array}
$$

The proofs follow directly from the observation that

$$
u^{H} A u=u^{H} R \Lambda R^{H} u=w^{H} \Lambda w=\sum_{i=1}^{m} \lambda^{i}\left|w_{i}\right|^{2},
$$

where $w=R^{H} u$.

## C. 5 Skew-symmetric and skew-Hermitian matrices

If $A=-A^{T}$, then $A$ is said to be skew-symmetric (or skew-Hermitian in the complex case if $A=-A^{H}$ ). Matrices of this form also arise in discretizing certain types of differential equations (e.g., the advection equation as discussed in Chapter 10). Skew-Hermitian matrices are diagonalizable and have eigenvalues that are pure imaginary. This is a generalization of the fact that for a scalar $\lambda$, if $\bar{\lambda}=-\lambda$, then $\lambda$ is pure imaginary. As in the Hermitian case, the eigenvectors of a skew-Hermitian matrix can be chosen so that the matrix $R$ is unitary, $R^{H} R=I$.

## C. 6 Normal matrices

If $A$ commutes with its adjoint, $A A^{H}=A^{H} A$, then $A$ is said to be a normal matrix. In particular, Hermitian and skew-Hermitian matrices are normal. Any normal matrix is diagonalizable and $R$ can be chosen to be unitary. Conversely, if $A$ can be decomposed as

$$
A=R \Lambda R^{H}
$$

with $R^{H}=R^{-1}$ and $\Lambda$ diagonal, then $A$ is normal since $\Lambda \Lambda^{H}=\Lambda^{H} \Lambda$ for any diagonal matrix.

Eigenvalue analysis is particularly useful for normal matrices, since they can be diagonalized by a unitary matrix. A unitary matrix $R$ satisfies $\|R\|_{2}=\left\|R^{-1}\right\|_{2}=1$, and hence the behavior of powers of $A$ is very closely related to the powers of the eigenvalues, for example. Nonnormal matrices can be harder to analyze, and in this case studying only the eigenvalues of $A$ can be misleading. See Section D. 4 for more discussion of this.

## C. 7 Toeplitz and circulant matrices

A matrix is said to be Toeplitz if the value along each diagonal is constant, e.g.,

$$
A=\left[\begin{array}{cccc}
d_{0} & d_{1} & d_{2} & d_{3} \\
d_{-1} & d_{0} & d_{1} & d_{2} \\
d_{-2} & d_{-1} & d_{0} & d_{1} \\
d_{-3} & d_{-2} & d_{-1} & d_{0}
\end{array}\right]
$$

is a $4 \times 4$ example. Here we use $d_{i}$ to denote the constant element along the $i$ th diagonal.
If $d_{1}=d_{-3}, d_{2}=d_{-2}$, and $d_{3}=d_{-1}$ in the above example, or more generally if $d_{i}=d_{i-m}$ for $i=1,2, \ldots, m-1$ in the $m \times m$ case, then the matrix is said to be circulant.

Toeplitz matrices naturally arise in the study of finite difference methods (see, e.g., Section 2.4) and it is useful to have closed-form expressions for their eigenvalues and eigenvectors. This is often possible because of their simple structure.

First consider a "tridiagonal" circulant matrix (which also has nonzero corner terms) of the form

$$
A=\left[\begin{array}{cccccc}
d_{0} & d_{1} & & & & d_{-1}  \tag{C.16}\\
d_{-1} & d_{0} & d_{1} & & & \\
& d_{-1} & d_{0} & & & \\
& & & \ddots & & \\
& & & & & d_{1} \\
d_{1} & & & & d_{-1} & d_{0}
\end{array}\right] \in \mathbb{R}^{(m+1) \times(m+1)}
$$

Alternatively we could use the symbol $d_{m}$ in place of $d_{-1}$. We take the dimension to be $m+$ 1 to be consistent with notation used in Chapter 2, since such matrices arise in studying 3point difference equations on the unit interval with periodic boundary conditions. Then $h=$ $1 /(m+1)$ is the mesh spacing between grid points and the unknowns are $U_{1}, \ldots, U_{m+1}$.

The $p$ th eigenvalue of the matrix (C.16) is given by

$$
\begin{equation*}
\lambda_{p}=d_{-1} e^{-2 \pi i p h}+d_{0}+d_{1} e^{2 \pi i p h} \tag{C.17}
\end{equation*}
$$

where $i=\sqrt{-1}$, and the $j$ th element of the corresponding eigenvector $r_{p}$ is given by

$$
\begin{equation*}
r_{j p}=e^{2 \pi i p j h} \tag{C.18}
\end{equation*}
$$

This is the $(j, p)$ element of the matrix $R$ that diagonalizes $A$. Once the form of the eigenvector has been "guessed," it is easy to compute the corresponding eigenvalue $\lambda_{p}$ by computing the $j$ th component of $A r_{p}$ and using the fact that

$$
\begin{equation*}
e^{2 \pi i p(j \pm 1) h}=e^{ \pm 2 \pi i p h} e^{2 \pi i p j h} \tag{C.19}
\end{equation*}
$$

to obtain

$$
\left(A r_{p}\right)_{j}=\left(d_{-1} e^{-2 \pi i p h}+d_{0}+d_{1} e^{2 \pi i p h}\right) r_{j p}
$$

The circulant structure is needed to verify that this formula also holds for $j=1$ and $j=m+1$, using $e^{2 \pi i(m+1) h}=1$.

The same vectors $r_{p}$ with components (C.18) are the eigenvectors of any $(m+1) \times$ $(m+1)$ circulant matrix with diagonals $d_{0}, d_{1}, \ldots, d_{m}$. It can be verified, as in the computation above, that the corresponding eigenvalue is

$$
\begin{equation*}
\lambda_{p}=\sum_{k=0}^{m} d_{k} e^{2 \pi i p k h} \tag{C.20}
\end{equation*}
$$

In the "tridiagonal" example above we used the label $d_{-1}$ instead of $d_{m}$, but note that $e^{-2 \pi i h}=e^{2 \pi i m h}$, so the expression (C.20) is invariant under this change of notation.

Any constant coefficient difference equation with periodic boundary conditions gives rise to a circulant matrix of this form and has eigenvectors with components (C.18). Note that the $j$ th component of $r_{p}$ can be rewritten as

$$
r_{j p}=e^{2 \pi i p x_{j}}=\phi_{p}\left(x_{j}\right),
$$

where $x_{j}=j h$ is the $j$ th grid point and $\phi_{p}(x)=e^{2 \pi i p x}$. The function $\phi_{p}(x)$ is the $p$ th eigenfunction of the differentiation operator $\partial_{x}$ on the unit interval with periodic boundary conditions,

$$
\partial_{x} \phi_{p}(x)=(2 \pi i p) \phi_{p}(x)
$$

It is also the eigenfunction of any higher order derivative $\partial_{x}^{s}$, with eigenvalue $(2 \pi i p)^{s}$. This is the basis of Fourier analysis of linear differential equations, and the fact that difference equations have eigenvectors that are discretized versions of $\phi_{p}(x)$ means that discrete Fourier analysis can be used to analyze finite difference methods for constant coefficient problems, as is done in von Neumann analysis; see Sections 9.6 and 10.5.

Now consider the symmetric tridiagonal Toeplitz matrix (now truly tridiagonal)

$$
A=\left[\begin{array}{cccccc}
d_{0} & d_{1} & & & &  \tag{C.21}\\
d_{1} & d_{0} & d_{1} & & & \\
& d_{1} & d_{0} & d_{1} & & \\
& & & \ddots & & \\
& & & & & d_{1} \\
& & & & d_{1} & d_{0}
\end{array}\right] \in \mathbb{R}^{m \times m}
$$

Such matrices arise in 3-point discretizations of $u_{x x}$ with Dirichlet boundary conditions, for example; see Section 2.4. The eigenvalues of $A$ are now

$$
\begin{equation*}
\lambda_{p}=d_{0}+2 d_{1} \cos (p \pi h), \quad p=1,2, \ldots, m \tag{C.22}
\end{equation*}
$$

where again $h=1 /(m+1)$ and now $A$ has dimension $m$ since boundary values are not included in the solution vector. The eigenvector now has components

$$
\begin{equation*}
r_{j p}=\sin (p \pi j h), \quad j=1,2, \ldots, m \tag{C.23}
\end{equation*}
$$

Again it is easy to verify that (C.22) gives the eigenvalue once the form of the eigenvector is known. In this case we use the fact that, for any $p$,

$$
\sin (p \pi j h)=0 \quad \text { for } j=0 \text { and } j=m+1
$$

to verify that $\left(A r_{p}\right)_{j}=\lambda_{p} r_{j p}$ for $j=0$ and $j=m+1$ as well as in the interior. Now consider a nonsymmetric tridiagonal Toeplitz matrix,

$$
A=\left[\begin{array}{cccccc}
d_{0} & d_{1} & & & &  \tag{C.24}\\
d_{-1} & d_{0} & d_{1} & & & \\
& d_{-1} & d_{0} & d_{1} & & \\
& & & \ddots & & \\
& & & & & d_{1} \\
& & & & d_{-1} & d_{0}
\end{array}\right] \in \mathbb{R}^{m \times m}
$$

If $d_{1}=d_{-1}=0$, then the matrix is diagonal with all eigenvalues equal to $d_{0}$. Otherwise, if one of $d_{1}$ or $d_{-1}$ is zero the eigenvalues are all equal to $d_{0}$ but the matrix is a single Jordan block, a defective matrix with a one-dimensional eigenspace.

In the general case where both $d_{1}$ and $d_{-1}$ are nonzero, the eigenvalues are

$$
\begin{equation*}
\lambda_{p}=d_{0}+2 d_{1} \sqrt{d_{-1} / d_{1}} \cos (p \pi h), \quad p=1,2, \ldots, m, \tag{C.25}
\end{equation*}
$$

and the corresponding eigenvector $r_{p}$ has $j$ th component

$$
\begin{equation*}
r_{j p}=\left(\sqrt{d_{-1} / d_{1}}\right)^{j} \sin (p \pi j h), \quad j=1,2, \ldots, m \tag{C.26}
\end{equation*}
$$

These formulas hold also if $d_{-1} / d_{1}$ is negative, in which case the eigenvalues are complex. For example, the skew-symmetric centered difference matrix with $d_{-1}=-1, d_{0}=0$, and $d_{1}=1$ has eigenvalues

$$
\begin{equation*}
\lambda_{p}=2 i \cos (p \pi h) . \tag{C.27}
\end{equation*}
$$

## C. 8 The Gershgorin theorem

If $A$ is diagonal, then its eigenvalues are simply the diagonal elements. If $A$ is "nearly diagonal," in the sense that the off-diagonal elements are small compared to the diagonal, then we might expect the diagonal elements to be good approximations to the eigenvalues. The Gerschgorin theorem quantifies this and also provides bounds on the eigenvalues in terms of the diagonal and off-diagonal elements. These bounds are valid in general and often very useful even when $A$ is far from diagonal.

Theorem C.2. Let $A \in \mathbb{C}^{m \times m}$ and let $D_{i}$ be the closed disk in the complex plane centered at $a_{i i}$ with radius $r_{i}=\sum_{j \neq i}\left|a_{i j}\right|$, the sum of the magnitude of all the off-diagonal elements in the ith row of $A$,

$$
D_{i}=\left\{z \in \mathbb{C}:\left|z-a_{i i}\right| \leq r_{i}\right\} .
$$

Then,

1. all the eigenvalues of $A$ lie in the union of the disks $D_{i}$ for $i=1,2, \ldots, m$.
2. if some set of $k$ overlapping disks is disjoint from all the other disks, then exactly $k$ eigenvalues lie in the union of these $k$ disks.

Note the following:

- If a disk $D_{i}$ is disjoint from all other disks, then it contains exactly one eigenvalue of $A$.
- If a disk $D_{i}$ overlaps other disks, then it need not contain any eigenvalues (although the union of the overlapping disks contains the appropriate number).
- If $A$ is real, then $A^{T}$ has the same eigenvalues as $A$. Then the theorem can also be applied to $A^{T}$ (or equivalently the disk radii can be defined by summing elements of columns rather than rows).

For a proof of this theorem see Wilkinson [103], for example.
Example C.5. Let

$$
A=\left[\begin{array}{ccc}
5 & 0.6 & 0.1 \\
-1 & 6 & -0.1 \\
1 & 0 & 2
\end{array}\right]
$$

Applying the Gershgorin theorem to $A$, we have

$$
D_{1}=\{z:|z-5| \leq 0.7\}, \quad D_{2}=\{z:|z-6| \leq 1.1\}, \quad D_{3}=\{z:|z-2| \leq 1.0\}
$$

as shown in Figure C.1(a). From the theorem we can conclude that there is exactly one eigenvalue in $D_{3}$ and two eigenvalues in $D_{1} \cup D_{2}$. We can also conclude that all eigenvalues have real parts between 1 and 7.7 (and hence positive real parts, in particular). The eigenvalue in $D_{3}$ must be real, since complex eigenvalues must appear in conjugate pairs (since $A$ is real). The eigenvalues in $D_{1} \cup D_{2}$ could be real or imaginary, but the imaginary part must be bounded by 1.1. The actual eigenvalues of $A$ are also shown in Figure C.1(a), and are

$$
\lambda \approx 1.9639,5.518 \pm 0.6142 i .
$$

Applying the theorem to $A^{T}$ would give

$$
D_{1}=\{z:|z-5| \leq 2.0\}, \quad D_{2}=\{z:|z-6| \leq 0.6\}, \quad D_{3}=\{z:|z-2| \leq 0.2\}
$$

as shown in Figure C.1(b). Note that this gives a tighter bound on the eigenvalue near 2 but a larger region around the complex pair.

A matrix is said to be reducible if it is possible to reorder the rows and columns in such a way that the eigenvalue problem is decoupled into simpler problem, specifically if there exists a permutation matrix $P$ so that

$$
P A P^{-1}=\left[\begin{array}{cc}
A_{11} & 0 \\
A_{12} & A_{22}
\end{array}\right],
$$



Figure C.1. Gerschgorin circles containing the eigenvalues of $A$ for Example C.5.
where $A_{11}$ and $A_{22}$ are square matrices of size at least $1 \times 1$. In this case the eigenvalues of $A$ consist of the eigenvalues of $A_{11}$ together with those of $A_{22}$. If no such $P$ exists, then $A$ is irreducible. The matrix of Example C. 5 is irreducible, for example.

For irreducible matrices, a more refined version of the Gerschgorin theorem states also that a point on the boundary of a set of Gerschgorin disks can be an eigenvalue only if it is on the boundary of all disks.

Example C.6. The tridiagonal matrix $A$ of (2.10) arises from discretizing the second derivative. Since this matrix is symmetric all its eigenvalues are real. By the Gerschgorin theorem they must lie in the circle of radius $2 / h^{2}$ centered at $-2 / h^{2}$. In fact, they must lie in the interior of this disk since the matrix is irreducible and the first and last row of $A$ give disks with radius $1 / h^{2}$. Hence $-4 / h^{2}<\lambda_{p}<0$ for all eigenvalues $\lambda_{p}$. In particular this shows that all the eigenvalues are negative and hence the matrix $A$ is nonsingular and negative definite. Showing nonsingularity is one use of the Gerschgorin theorem.

For the tridiagonal matrix (2.10) the eigenvalues can be explicitly computed and are given by the formula (2.23),

$$
\lambda_{p}=\frac{2}{h^{2}}(\cos (p \pi h)-1) \text { for } p=1,2, \ldots, m
$$

where $h=1 /(m+1)$. They are distributed all along the interval $-4 / h^{2}<\lambda_{p}<0$. For related matrices that arise from discretizing variable coefficient elliptic equations the matrices cannot be explicitly computed, but the Gerschgorin theorem can still be used to show nonsingularity.

Example C.7. Consider the matrix (2.73) with all $\kappa>0$. The Gerschgorin disks all lie in the left half-plane and the disks $D_{1}$ and $D_{m}$ are bounded away from the origin. The matrix is irreducible and hence must be negative definite (and in particular nonsingular).

## C. 9 Inner-product norms

Some standard vector norms and the corresponding matrix norms were introduced in Section A.3. Here we further investigate the 2 -norm and its relation to the spectral radius of
a matrix. We will also see how new inner-product norms can be defined that are closely related to a particular matrix.

Let $A \in \mathbb{C}^{m \times m}$ and $u \in \mathbb{C}^{m}$. The 2-norm of of $u$ is defined by

$$
\begin{equation*}
\|u\|_{2}^{2}=u^{H} u=\sum_{i=1}^{m}\left|u_{i}\right|^{2}=\langle u, u\rangle \tag{C.28}
\end{equation*}
$$

where $\langle\cdot, \cdot\rangle$ is the standard inner product,

$$
\begin{equation*}
\langle u, v\rangle=u^{H} v=\sum_{i=1}^{m} \bar{u}_{i} v_{i} . \tag{C.29}
\end{equation*}
$$

The 2-norm of the matrix $A$ is defined by the formula (A.9) as

$$
\|A\|_{2}=\sup _{\|u\|_{2}=1}\|A u\|_{2}=\sup _{\|u\|_{2}=1}\left(u^{H} A^{H} A u\right)^{1 / 2}
$$

Note that if we choose $u$ to be an eigenvector of $A$, with $A u=\lambda u$, then

$$
\left(u^{H} A^{H} A u\right)^{1 / 2}=|\lambda|,
$$

and so $\|A\|_{2} \geq \max _{1 \leq p \leq m}\left|\lambda_{p}\right|=\rho(A)$. The 2-norm of $A$ is always at least as large as the spectral radius. Note that the matrix $B=A^{H} A$ is always Hermitian ( $B^{H}=B$ ) and so it is diagonalizable with a unitary eigenvector matrix,

$$
B=R M R^{H} \quad\left(R^{H}=R^{-1}\right),
$$

where $M$ is the diagonal matrix of eigenvectors $\mu_{j} \geq 0$ of $B$. Any vector $u$ can be written as $u=R w$ where $w=R^{H} u$. Note that $\|u\|_{2}=\|w\|_{2}$ since

$$
u^{H} u=w^{H} R^{H} R w=w^{H} w,
$$

i.e., multiplication by a unitary matrix preserves the 2 -norm. It follows that

$$
\begin{align*}
\|A\|_{2} & =\sup _{\|u\|_{2}=1}\left(u^{H} B u\right)^{1 / 2} \\
& =\sup _{\|w\|_{2}=1}\left(w^{H} R^{H} B R w\right)^{1 / 2} \\
& =\sup _{\|w\|_{2}=1}\left(w^{H} M w\right)^{1 / 2}  \tag{C.30}\\
& =\max _{p=1,2, \ldots, m}\left|\mu_{p}\right|^{1 / 2}=\sqrt{\rho\left(A^{H} A\right)} .
\end{align*}
$$

If $A^{H}=A$, then $\rho\left(A^{H} A\right)=(\rho(A))^{2}$ and $\|A\|_{2}=\rho(A)$. More generally this is true for any normal matrix $A$ (as defined in Section C.6). If $A$ is normal, then $A$ and $A^{H}$ have the same eigenvector matrix $R$ and so

$$
A^{H} A=\left(R \Lambda^{H} R\right)\left(R \Lambda R^{H}\right)=R \Lambda^{H} \Lambda R^{H} .
$$

It follows that $\rho\left(A^{H} A\right)=\max _{p=1,2, \ldots, m}\left|\lambda_{p}\right|^{2}$.

If $A$ is not normal, then typically $\|A\|_{2}>\rho(A)$. If $A$ is diagonalizable, then an upper bound on $\|A\|_{2}$ can be obtained from

$$
\begin{align*}
\|A\|_{2} & =\left\|R \Lambda R^{-1}\right\|_{2} \\
& \leq\|R\|_{2}\left\|R^{-1}\right\|_{2} \max _{p=1,2, \ldots, m}\left|\lambda_{p}\right|=\kappa_{2}(R) \rho(A), \tag{C.31}
\end{align*}
$$

where $\kappa_{2}(R)=\|R\|_{2}\left\|R^{-1}\right\|_{2}$ is the 2 -norm condition number of the eigenvector matrix $R$. We thus have the general relation

$$
\begin{equation*}
\rho(A) \leq\|A\|_{2} \leq \kappa_{2}(R) \rho(A), \tag{C.32}
\end{equation*}
$$

which holds for any diagonalizable matrix $A$. If $A$ is normal, then $R$ is unitary and $\kappa_{2}(R)=1$.

This relation between the norm and spectral radius is important in studying iterations of the form $U^{n+1}=A U^{n}$, which leads to $U^{n}=A^{n} U^{0}$ (where the superscript on $U$ is an index and the superscript on $A$ is a power). Such iterations arise both in time-stepping algorithms for solving differential equations and in iterative methods for solving linear systems. We often wish to investigate the behavior of $\left\|U^{n}\right\|$ as $n \rightarrow \infty$, or the related question of the behavior of powers of the matrix $A$. For diagonalizable $A$ we have $A^{n}=$ $R \Lambda^{n} R^{-1}$, so that

$$
\begin{equation*}
\left\|A^{n}\right\|_{2} \leq \kappa_{2}(R)(\rho(A))^{n} \tag{C.33}
\end{equation*}
$$

From this we see that $\left\|A^{n}\right\|_{2} \rightarrow 0$ as $n \rightarrow \infty$ if $\rho(A)<1$. In fact this is true for any $A$, not just diagonalizable matrices, as can be seen by using the Jordan canonical form. See Appendix D for more about bounding powers of a matrix.

This spectral analysis is particularly useful when $A$ is normal, in which case $\kappa_{2}(R)=$ 1. In this case $\left\|A^{n}\right\|_{2} \leq(\rho(A))^{n}$ and if $\rho(A)<1$, then we have a strictly decreasing upper bound on the norm. The asymptotic behavior is still the same if $A$ is not normal, but convergence is not necessarily monotone and this spectral analysis can be quite misleading if $A$ is far from normal. This topic is discussed in more detail in Appendix D along with a discussion of the nondiagonalizable (defective) case.

## C. 10 Other inner-product norms

If $T$ is any nonsingular matrix, then we can define an inner product based on $T$ in terms of the standard inner product (C.29) by

$$
\begin{equation*}
\langle u, v\rangle_{T}=\left\langle T^{-1} u, T^{-1} v\right\rangle=u^{H} G v, \tag{C.34}
\end{equation*}
$$

where $G=T^{-H} T^{-1}$. The matrix $G$ is always Hermitian positive definite (SPD if $T$ is real). We can define a corresponding norm (the $T$-norm of $u$ ) by

$$
\begin{equation*}
\|u\|_{T}=\langle u, u\rangle_{T}=\left\|T^{-1} u\right\|_{2}=\left(u^{H} G u\right)^{1 / 2}=\langle u, G u\rangle . \tag{C.35}
\end{equation*}
$$

This satisfies the requirements of a norm summarized in Section A.3.
Inner-product norms of this type naturally arise in the study of conjugate gradient methods for solving linear system $A u=f$ when $A$ is SPD. In this case $G=A$ is used
(see Section 4.3.4) and $T$ could be defined as a "square root" of $A$, e.g., $T=R \Lambda^{1 / 2} R^{-1}$ if $A=R \Lambda R^{-1}$.

In studying iterations of the form $U^{n+1}=A U^{n}$, and variants such as $U^{n+1}=$ $A_{n} U^{n}$ (where the matrix $A_{n}$ changes in each iteration), it is often useful to choose norms that are adapted to the matrix or matrices in question in order to obtain more insight into the asymptotic behavior of $U^{n}$. A few results are summarized below that are used elsewhere.

Note that $w=T^{-1} u$ can be viewed as the vector of coefficients obtained if $u$ is written as a linear combination of the columns of $T, u=T w$. Hence $\|u\|_{T}=\|w\|_{2}$ can be viewed as a measure of $u$ based on its representation in the coordinate system defined by $T$ rather than in the standard basis vectors. A particularly useful coordinate system is the coordinates defined by the eigenvectors, as we will see below.

We can compute the matrix $T$-norm of a matrix $A$ using the standard definition of a matrix norm from (A.9):

$$
\begin{align*}
\|A\|_{T} & =\sup _{u \neq 0} \frac{\|A u\|_{T}}{\|u\|_{T}}=\sup _{w \neq 0} \frac{\|A T w\|_{T}}{\|T w\|_{T}} \\
& =\sup _{w \neq 0} \frac{\left\|T^{-1} A T w\right\|_{2}}{\|w\|_{2}}  \tag{C.36}\\
& =\left\|T^{-1} A T\right\|_{2}
\end{align*}
$$

Now suppose $A$ is a diagonalizable matrix with $R^{-1} A R=\Lambda$. Then choosing $T=$ $R$ yields $\|A\|_{R}=\left\|R^{-1} A R\right\|_{2}=\rho(A)$. Recall that $\|A\| \geq \rho(A)$ in any matrix norm subordinate to a vector norm. We have just shown that equality can be achieved by an appropriate choice of norm in the case when $A$ is diagonalizable. We have proved the following theorem.

Theorem C.3. Suppose $A \in \mathbb{C}^{m \times m}$ is diagonalizable. Then there exists a norm $\|\cdot\|$ in which $\|A\|=\rho(A)$. The norm is given by the $R$-norm based on the eigenvector matrix.

This theorem will be generalized to the defective case in Theorem C. 4 below.
Note that in general the $T$-norm, for any nonsingular $T$, is "equivalent" to the 2-norm in the sense of Section A.3.1 with the equivalence inequalities

$$
\begin{equation*}
\|T\|_{2}^{-1}\|u\|_{2} \leq\|u\|_{T} \leq\left\|T^{-1}\right\|_{2}\|u\|_{2} \tag{C.37}
\end{equation*}
$$

for the vector norm and

$$
\begin{equation*}
\kappa_{2}(T)^{-1}\|A\|_{2} \leq\|A\|_{T} \leq \kappa_{2}(T)\|A\|_{2} \tag{C.38}
\end{equation*}
$$

for the matrix norm, where $\kappa_{2}(T)$ is the 2-norm condition number of $T$. Applying this last inequality in conjunction with Theorem C. 3 gives

$$
\begin{equation*}
\rho(A)=\|A\|_{R} \leq \kappa_{2}(R)\|A\|_{2} \tag{C.39}
\end{equation*}
$$

which agrees with the bound (C.31) obtained earlier.
For general matrices $A \in \mathbb{C}^{m \times m}$ that are not necessarily diagonalizable, Theorem C. 3 can be generalized to the following.

Theorem C.4. (a) If $A \in \mathbb{C}^{m \times m}$ has no defective eigenvalues with modulus $\rho(A)$, then there exists a nonsingular matrix $T$ such that

$$
\|A\|_{T}=\rho(A) .
$$

(b) If $A$ has defective eigenvalue(s) of modulus $\rho(A)$, then for every $\epsilon>0$ there exists a matrix $T(\epsilon)$ such that

$$
\begin{equation*}
\|A\|_{T(\epsilon)}<\rho(A)+\epsilon \tag{C.40}
\end{equation*}
$$

In the latter case we can find a norm in which $\|A\|$ is arbitrarily close to $\rho(A)$, but $T(\epsilon)$ becomes increasingly ill conditioned as $\epsilon \rightarrow 0$. The proof of this theorem is based on a modification of the Jordan canonical form in which the superdiagonal elements are made sufficiently small by the transformation discussed in Section C.3. Let $R^{-1} A R=J$ have the form (C.12), and let $Z=\left\{i:\left|\lambda_{i}\right|=\rho(A)\right\}$, the set of indices of the maximal eigenvalues. To prove part (a), if $i \in Z$, then $k_{i}=1$ and $J_{i}=\lambda_{i}$ with $\left|\lambda_{i}\right|=\rho(A)$. In this case set $D_{i}=1$. If $i \notin Z$, let $\delta_{i}=\rho(A)-\left|\lambda_{i}\right|>0$ and set

$$
D_{i}=\operatorname{diag}\left(1, \delta_{i}, \ldots, \delta_{i}^{k_{i}-1}\right)
$$

Let $D$ be the block diagonal matrix formed by these blocks. Then $\tilde{J}=D^{-1} J D$ has Jordan blocks $\lambda_{i} I+\delta_{i} S_{k_{i}}$ and so

$$
\left\|\tilde{J}_{i}\right\|_{2} \leq\left|\lambda_{i}\right|+\delta_{i} \leq \rho(A) \quad \text { for } i \notin Z
$$

It follows that $\|A\|_{T}=\|\tilde{J}\|_{2}=\rho(A)$, where the matrix $A$ is given by $T=R D$.
To prove part (b), let $\epsilon>0$ be given and choose

$$
\delta_{i}= \begin{cases}\epsilon & \text { if } i \in Z, \\ \rho(A)-\left|\lambda_{i}\right|>0 & \text { if } i \notin Z .\end{cases}
$$

Define $D_{i}$ and $D$ as before and we will achieve

$$
\begin{aligned}
& \left\|\tilde{J}_{i}\right\| \leq \rho(A) \text { for } i \notin Z, \\
& \left\|\tilde{J}_{i}\right\| \leq \rho(A)+\epsilon \text { for } i \in Z,
\end{aligned}
$$

and so taking $T(\epsilon)=R D(\epsilon)$ gives $\|A\|_{T(\epsilon)} \leq \rho(A)+\epsilon$. Recall that $\kappa_{2}(D(\epsilon)) \rightarrow \infty$ as $\epsilon \rightarrow 0$ and so $\kappa_{2}(T(\epsilon)) \rightarrow \infty$ as $\epsilon \rightarrow 0$ in case (b).

