4 · Functions of Matrices

Throughout these notes we have encountered a number of *functions of matrices* without even pausing to give that general concept much thought. Matrix powers provide the easiest example: we can think of $\mathbf{A}^2 = \mathbf{A}\mathbf{A}$ as the evaluation of the scalar-valued function $f(z) = z^2$ at the matrix argument $\mathbf{A}$. Similarly, the matrix inverse $\mathbf{A}^{-1}$ is the scalar function $f(z) = 1/z$ evaluated at $\mathbf{A}$. (The resolvent $\mathbf{R}(z) = (zI - \mathbf{A})^{-1}$ is a touch more complicated, for now we have $f(z, \alpha) = 1/(z - \alpha)$ evaluated at $\alpha = \mathbf{A}$.) In the special case of Hermitian positive definite matrices, we have computed $\sqrt{\mathbf{A}}$ in Section 2.4.2. But what might it mean to take more complicated functions, like $\mathrm{e}^{\mathbf{A}}$ or $\log(\mathbf{A})$ or $\mathrm{sign}(\mathbf{A})$? This question is not idle speculation; such functions have important applications in dynamical systems.

Once we have defined a function of matrix, we might naturally wish to know what properties of the scalar function $f(z)$ are inherited by $f(\mathbf{A})$. For example, a fundamental property of the scalar exponential $\mathrm{e}^{t\alpha}$ is that

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{e}^{t\alpha} = \alpha \mathrm{e}^{t\alpha}. \tag{4.1}$$

We would like the matrix-valued version to mimic this property:

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{e}^{t\mathbf{A}} = \mathbf{A}\mathrm{e}^{t\mathbf{A}}.$$

Yet, we will see that the convenient scalar identity

$$\mathrm{e}^{\alpha+\beta} = \mathrm{e}^{\alpha}\mathrm{e}^{\beta}$$

does not generalize to the matrix case for all $\mathbf{A}$ and $\mathbf{B}$.

We need not content ourselves by trying to recover properties of scalar-valued functions. We can ask richer questions, such as how the entries in $f(\mathbf{A}+\mathbf{E})$ compare to those of $f(\mathbf{A})$ for small perturbations $\mathbf{E}$. This will lead us to the notion of the FRÉCHET *derivative* of a function of a matrix.

In these notes we shall but scratch the surface of this interesting and vital topic. For many more details, see HIGHAM's monograph [Hig08], as well as [HJ91, chap. 6].

4.1 Defining the Function of a Matrix

Given some scalar function $f : \mathbb{C} \to \mathbb{C}$ and a square matrix $\mathbf{A} \in \mathbb{C}^{n\times n}$, we seek to define $f(\mathbf{A})$ in such a way that is both general and useful. We shall work from two extremes, and view the general case as an assemblage of the two ideas.

4.1.1 Defining $f(\mathbf{A})$ for Hermitian and Diagonalizable $\mathbf{A}$

First let $\mathbf{A} \in \mathbb{C}^{n\times n}$ be Hermitian, so there exist unitary $\mathbf{U}$ and diagonal $\mathbf{\Lambda}$ such that

$$\mathbf{A} = \mathbf{U}\mathbf{\Lambda}\mathbf{U}^*,$$

which we can also write as the spectral decomposition (1.16)

$$\mathbf{A} = \sum_{j=1}^{n} \lambda_j \mathbf{u}_j \mathbf{u}_j^*.$$

Notice that

$$\mathbf{A}^* = \mathbf{U}\mathbf{\Lambda}\mathbf{U}^*\mathbf{U}\mathbf{\Lambda}\mathbf{U}^* = \mathbf{U}\mathbf{\Lambda}^2\mathbf{U}^*,$$

and similarly, for any positive integer p,

$$\mathbf{A}^p = \mathbf{U}\mathbf{\Lambda}^p\mathbf{U}^* = \sum_{j=1}^{n} \lambda_j^p \mathbf{u}_j \mathbf{u}_j^*.$$

Since a polynomial $\phi(z) = c_0 + c_1 z + c_2 z^2 + \cdots + c_m z^m$ is just a linear combination of powers, we can build

$$\phi(\mathbf{A}) = \mathbf{U}\phi(\mathbf{\Lambda})\mathbf{U}^* = \sum_{j=1}^{n} \phi(\lambda_j) \mathbf{u}_j \mathbf{u}_j^*. \tag{4.2}$$

The same pattern follows for negative powers, since one can also show that

$$\mathbf{A}^{-1} = (\mathbf{U}\mathbf{\Lambda}\mathbf{U}^*)^{-1}\mathbf{U}\mathbf{\Lambda}^{-1}\mathbf{U} = \sum_{j=1}^{n} \frac{1}{\lambda_j} \mathbf{u}_j \mathbf{u}_j^*.$$

Apply this idea to the polynomial $\phi(\mathbf{A})$ in (4.2) to get

$$\phi(\mathbf{A})^{-1} = \mathbf{U}\phi(\mathbf{\Lambda})^{-1}\mathbf{U}^* = \sum_{j=1}^{n} \frac{1}{\phi(\lambda_j)} \mathbf{u}_j \mathbf{u}_j^*. \tag{4.3}$$

Thus, if we have a *rational function* $r(z) = \phi(z)/\psi(z)$, we can put together the ideas from (4.2) and (4.3) to get

$$r(\mathbf{A}) = \mathbf{U}\phi(\mathbf{\Lambda})\psi(\mathbf{\Lambda})^{-1}\mathbf{U}^* = \sum_{j=1}^{n} \frac{\phi(\lambda_j)}{\psi(\lambda_j)} \mathbf{u}_j \mathbf{u}_j^* = \sum_{j=1}^{n} r(z) \mathbf{u}_j \mathbf{u}_j^*.$$

No doubt you have seen a consistent pattern emerge: to compute $f(\mathbf{A})$ for Hermitian $\mathbf{A}$, simply replace λ_j by $f(\lambda_j)$ in the spectral decomposition. We can extrapolate this observation to obtain a definition for $f(\mathbf{A})$ for general functions $\mathbf{A}$.

Definition of $f(\mathbf{A})$ for Hermitian $\mathbf{A}$

Theorem 4.1. *Let $\mathbf{A} \in \mathbb{C}^{n \times n}$ be Hermitian with spectral decomposition*

$$\mathbf{A} = \sum_{j=1}^{n} \lambda_j \mathbf{u}_j \mathbf{u}_j^*,$$

and suppose $f : \mathbb{C} \to \mathbb{C}$ is defined for all $z \in \sigma(\mathbf{A}) \subset \mathbb{R}$. Then

$$f(\mathbf{A}) = \sum_{j=1}^{n} f(\lambda_j) \mathbf{u}_j \mathbf{u}_j^*.$$

We shall take a particular interest in the function $f(z) = \mathrm{e}^{tz}$, where t is a real number. Apply Definition 4.1 to this f to get

$$\mathrm{e}^{t\mathbf{A}} = \sum_{j=1}^{n} \mathrm{e}^{t\lambda_j} \mathbf{u}_j \mathbf{u}_j^*.$$

Does this function inherit the fundamental property (4.1)? We compute

$$\begin{aligned}\frac{\mathrm{d}}{\mathrm{d}t}\, \mathrm{e}^{t\mathbf{A}} = \frac{\mathrm{d}}{\mathrm{d}t} \sum_{j=1}^{n} \mathrm{e}^{t\lambda_j} \mathbf{u}_j \mathbf{u}_j^* &= \sum_{j=1}^{n} \lambda_j \mathrm{e}^{t\lambda_j} \mathbf{u}_j \mathbf{u}_j^* \\ &= \left(\sum_{j=1}^{n} \lambda_j \mathbf{u}_j \mathbf{u}_j^* \right) \left(\sum_{k=1}^{n} \mathrm{e}^{t\lambda_k} \mathbf{u}_k \mathbf{u}_k^* \right) = \mathbf{A}\mathrm{e}^{t\mathbf{A}},\end{aligned}$$

as desired. For Hermitian matrices, Definition 4.1 appears to provide a good working definition. How can we handle non-Hermitian $\mathbf{A}$? When $\mathbf{A}$ is diagonalizable, recall that Theorem 1.15 gives the spectral representation

$$\mathbf{A} = \mathbf{V}\boldsymbol{\Lambda}\mathbf{V}^{-1} = \sum_{j=1}^{n} \lambda_j \mathbf{v}_j \widehat{\mathbf{v}}_j^*,$$

where

$$\mathbf{v}_j^* \widehat{\mathbf{v}}_k = \begin{cases} 1, & j = k; \\ 0, & j \neq k. \end{cases}$$

Apply the same arguments we have had on the preceding pages, *mutatis mutandis*, to define $f(\mathbf{A})$ for diagonalizable matrices. (Since Hermitian matrices are diagonalizable, this new definition subsumes Definition 4.1.)

Definition of $f(\mathbf{A})$ for Diagonalizable $\mathbf{A}$

Definition 4.2. *Let $\mathbf{A} \in \mathbb{C}^{n\times n}$ be diagonalizable with spectral decomposition*

$$\mathbf{A} = \sum_{j=1}^{n} \lambda_j \mathbf{v}_j \widehat{\mathbf{v}}_j^*,$$

and suppose $f : \mathbb{C} \to \mathbb{C}$ is defined for all $z \in \sigma(\mathbf{A}) \subset \mathbb{C}$. Then

$$f(\mathbf{A}) = \sum_{j=1}^{n} f(\lambda_j) \mathbf{v}_j \widehat{\mathbf{v}}_j^*.$$

Keep in mind how to interpret Definition 4.2 in terms of the diagonalization $\mathbf{A} = \mathbf{V}\boldsymbol{\Lambda}\mathbf{V}^{-1}$:

$$f(\mathbf{A}) = \mathbf{V} \begin{bmatrix} f(\lambda_1) & & & \\ & f(\lambda_2) & & \\ & & \ddots & \\ & & & f(\lambda_n) \end{bmatrix} \mathbf{V}^{-1},$$

with zeros off the diagonal of that central factor.

Definition 4.2 will enable you to handle the vast majority of situations in which you seek to evaluate a function of a matrix. As with the Jordan decomposition, one expends substantially more energy to pin down those special cases of nondiagonalizable $\mathbf{A}$.

4.1.2 Defining $f(\mathbf{A})$ for a Jordan block

To construction a definition for the function of a nondiagonalizable matrix, start with the single Jordan block

$$\mathbf{J} = \begin{bmatrix} \lambda & 1 & & \\ & \lambda & \ddots & \\ & & \ddots & 1 \\ & & & \lambda \end{bmatrix} \in \mathbb{C}^{n\times n} \tag{4.4}$$

for some fixed value of $\lambda \in \mathbb{C}$.

The following Lemma (which can be proved as a homework exercise) gives a helpful starting point.

Lemma 4.3. *Let $\mathbf{J} \in \mathbb{C}^{n\times n}$ be the Jordan block 4.11. The for any nonnegative integer p, and $j, k \in \{1, \ldots, n\}$, the (j,k) entry of $\mathbf{J}^p$ is given by*

$$(\mathbf{J}^p)_{j,k} = \binom{p}{k-j}\lambda^{p-k+j} = \frac{p!}{(k-j)!\,(p-k+j)!}\lambda^{p-k+j}. \tag{4.5}$$

If $j > k$, then the (j,k) entry is below the main diagonal. In this case $k - j < 0$, so $\binom{p}{k-j} = 0$, consistent with the fact that $\mathbf{J}^p$ is upper triangular. It helps to see a few 5×5 examples:

$$\mathbf{J} = \begin{bmatrix} \lambda & 1 & & & \\ & \lambda & 1 & & \\ & & \lambda & 1 & \\ & & & \lambda & 1 \\ & & & & \lambda \end{bmatrix}, \quad \mathbf{J}^2 = \begin{bmatrix} \lambda^2 & 2\lambda & 1 & & \\ & \lambda^2 & 2\lambda & 1 & \\ & & \lambda^2 & 2\lambda & 1 \\ & & & \lambda^2 & 2\lambda \\ & & & & \lambda^2 \end{bmatrix},$$

$$\mathbf{J}^3 = \begin{bmatrix} \lambda^3 & 3\lambda^2 & 3\lambda & 1 & \\ & \lambda^3 & 3\lambda^2 & 3\lambda & 1 \\ & & \lambda^3 & 3\lambda^2 & 3\lambda \\ & & & \lambda^3 & 3\lambda^2 \\ & & & & \lambda^3 \end{bmatrix}, \quad \mathbf{J}^4 = \begin{bmatrix} \lambda^4 & 4\lambda^3 & 6\lambda^2 & 4\lambda & 1 \\ & \lambda^4 & 4\lambda^3 & 6\lambda^2 & 4\lambda \\ & & \lambda^4 & 4\lambda^3 & 6\lambda^2 \\ & & & \lambda^4 & 4\lambda^3 \\ & & & & \lambda^4 \end{bmatrix}.$$

(Yes indeed, the coefficients of each first row do come from a row of Pascal's triangle, due to the binomial coefficient in the formula (4.5).)

Lemma 4.3 gives an explicit formula for powers of $\mathbf{J}$. When $f(z) = z^p$, any definition of $f(\mathbf{J})$ that we construct should certainly agree with the formula (4.5) for $\mathbf{J}^p$. Consider derivatives of such an f:

$$\begin{aligned} f(\lambda) &= \lambda^p \\ f'(\lambda) &= p\lambda^{p-1} \\ f''(\lambda) &= p(p-1)\lambda^{p-2} \\ &\vdots \\ f^{(\ell)}(\lambda) &= p(p-1)\cdots(p-\ell+1)\lambda^{p-\ell} \end{aligned}$$

for any $\ell \in \{1,\ldots,p\}$. Deduce the general formula

$$f^{(\ell)}(\lambda) = \frac{p!}{(p-\ell)!}\lambda^{p-\ell}. \tag{4.6}$$

so that when $\ell = k-j$,

$$f^{(k-j)}(\lambda) = \frac{p!}{(p-k+j)!}\lambda^{p-k+j}. \tag{4.7}$$

Compare (4.5) to (4.7) and notice that

$$(\mathbf{J}^p)_{j,k} = \frac{p!}{(k-j)!\,(p-k+j)!}\lambda^{p-k+j} = \frac{f^{(k-j)}(\lambda)}{(k-j)!}. \tag{4.8}$$

Thus, the (j,k) entry of $f(\mathbf{J}) = \mathbf{J}^p$ is given by the $(k-j)$th derivative of $f(z) = z^p$, scaled by $1/(k-j)!$. This inspires a definition for *all* f (that are sufficiently differentiable).

Definition of $f(\mathbf{J})$ for a Jordan block $\mathbf{J}$

Definition 4.4. *Let $\mathbf{J} \in \mathbb{C}^{n\times n}$ be* Jordan *block of the form (4.11), and suppose $f : \mathbb{C} \to \mathbb{C}$ and the derivatives $f', f'', \ldots, f^{(n-1)}$ exist at λ. Then for $j,k \in \{1,\ldots,n\}$*

$$f(\mathbf{J})_{j,k} = \begin{cases} \dfrac{f^{(k-j)}(\lambda)}{(k-j)!}, & j \le k; \\ 0, & j > k. \end{cases} \tag{4.9}$$

It helps to see this definition in matrix form, again with $n = 5$:

$$f(\mathbf{J}) = \begin{bmatrix} f(\lambda) & f'(\lambda) & \frac{1}{2}f''(\lambda) & \frac{1}{3!}f'''(\lambda) & \frac{1}{4!}f^{(iv)}(\lambda) \\ & f(\lambda) & f'(\lambda) & \frac{1}{2}f''(\lambda) & \frac{1}{3!}f'''(\lambda) \\ & & f(\lambda) & f'(\lambda) & \frac{1}{2}f''(\lambda) \\ & & & f(\lambda) & f'(\lambda) \\ & & & & f(\lambda) \end{bmatrix}.$$

Notice that these terms are simply the coefficients that appear in the TAYLOR series for f at λ.

We have constructed this definition of $f(\mathbf{A})$ to give the expected result when $f(z) = z^p$. Does it make sense for other functions? For example, when $\lambda \neq 0$, $\mathbf{J}$ is invertible. The derivatives of $f(z) = z^{-1}$ are $f^{(k)}(z) = k!(-1)^k z^{-k-1}$. Thus the formula in Definition 4.4 gives

$$f(z) = z^{-1} \quad \Longrightarrow \quad f(\mathbf{J}) = \begin{bmatrix} 1/\lambda & -1/\lambda^2 & 1/\lambda^3 & -1/\lambda^4 & 1/\lambda^5 \\ & 1/\lambda & -1/\lambda^2 & 1/\lambda^3 & -1/\lambda^4 \\ & & 1/\lambda & -1/\lambda^2 & 1/\lambda^3 \\ & & & 1/\lambda & -1/\lambda^2 \\ & & & & 1/\lambda \end{bmatrix},$$

from which one can readily spot the pattern for general n. The alternating signs in $f(\mathbf{J})$ give, for general n, $\mathbf{J}f(\mathbf{J}) = \mathbf{I}$, and so Definition 4.4 applied to $f(z) = 1/z$ indeed gives $f(\mathbf{J}) = \mathbf{J}^{-1}$.

Now apply Definition 4.4 to $f(z) = \mathrm{e}^{tz}$. Since $f^{(k)}(z) = t^k\mathrm{e}^{tz}$, for $n = 5$,

$$f(z) = \mathrm{e}^{tz} \quad \Longrightarrow \quad f(\mathbf{J}) = \mathrm{e}^{t\mathbf{J}} = \mathrm{e}^{t\lambda} \begin{bmatrix} 1 & t & t^2/2 & t^3/3! & t^4/4! \\ & 1 & t & t^2/2 & t^3/3! \\ & & 1 & t & t^2/2 \\ & & & 1 & t \\ & & & & 1 \end{bmatrix}. \tag{4.10}$$

We wish to test that this definition for $\mathrm{e}^{t\mathbf{J}}$ satisfies the important property (4.1),

$$\frac{\mathrm{d}}{\mathrm{d}t}\,\mathrm{e}^{t\mathbf{J}} = \mathbf{J}\mathrm{e}^{t\mathbf{J}},$$

just as we verified for Hermitian matrices earlier. For $n = 5$, apply the product rule to (4.10) to get

$$\frac{\mathrm{d}}{\mathrm{d}t}\,\mathrm{e}^{t\mathbf{J}} = \lambda \mathrm{e}^{t\lambda}\begin{bmatrix} 1 & t & t^2/2 & t^3/3! & t^4/4! \\ & 1 & t & t^2/2 & t^3/3! \\ & & 1 & t & t^2/2 \\ & & & 1 & t \\ & & & & 1 \end{bmatrix} + \mathrm{e}^{t\lambda}\begin{bmatrix} 0 & 1 & t & t^2/2! & t^3/3! \\ & 0 & 1 & t & t^2/2! \\ & & 0 & 1 & t \\ & & & 0 & 1 \\ & & & & 0 \end{bmatrix}.$$

Notice how the matrix on the right is just $\mathrm{e}^{t\mathbf{J}}$*, but shifted up one diagonal.* For general n and $k > j$ we have

$$\left[\frac{\mathrm{d}}{\mathrm{d}t}\,\mathrm{e}^{t\mathbf{J}}\right]_{j,k} = \lambda\left[\mathrm{e}^{t\mathbf{J}}\right]_{j,k} + \left[\mathrm{e}^{t\mathbf{J}}\right]_{j,k-1} = \left[\mathbf{J}\mathrm{e}^{t\mathbf{J}}\right]_{j,k},$$

and the same identity holds more trivially for $k \le j$. We thus conclude that this definition of $\mathrm{e}^{t\mathbf{J}}$ indeed recovers the desired scalar property:

$$\frac{\mathrm{d}}{\mathrm{d}t}\,\mathrm{e}^{t\mathbf{J}} = \mathbf{J}\mathrm{e}^{t\mathbf{J}}.$$

We have thus seen how to define functions of a matrix for diagonalizable matrices (n Jordan blocks of size 1×1) and a single Jordan block (one Jordan block of size $n \times n$). It only remains to treat the general case.

4.1.3 Definition of $f(\mathbf{A})$ for general $\mathbf{A}$

Recall the Jordan canonical form derived in Section 1.8. Suppose $\mathbf{A} \in \mathbb{C}^{n\times n}$ has distinct eigenvalues $\lambda_1, \ldots, \lambda_p$ with algebraic multiplicities $a_1, \ldots, a_p$, geometric multiplicities $g_1, \ldots, g_p$, and indices $i_1, \ldots, i_p$. Then Theorem 1.22 gives $\mathbf{J} \in \mathbb{C}^{n\times n}$ and invertible $\mathbf{X} \in \mathbb{C}^{n\times n}$ such that

$$\mathbf{A} = \mathbf{X}\mathbf{J}\mathbf{X}^{-1},$$

which can be partitioned in the form

$$\mathbf{X} = [\,\mathbf{X}_1 \quad \cdots \quad \mathbf{X}_p\,], \quad \mathbf{J} = \begin{bmatrix} \mathbf{J}_1 & & \\ & \ddots & \\ & & \mathbf{J}_p \end{bmatrix}, \quad \mathbf{X}^{-1} = \begin{bmatrix} \widehat{\mathbf{X}}_1^* \\ \vdots \\ \widehat{\mathbf{X}}_p^* \end{bmatrix}$$

with $\mathbf{X}_j \in \mathbb{C}^{n\times a_j}$, $\mathbf{J}_j \in \mathbb{C}^{a_j\times a_j}$. Each matrix $\mathbf{J}_j$ has the form

$$\mathbf{J}_j = \begin{bmatrix} \mathbf{J}_{j,1} & & \\ & \ddots & \\ & & \mathbf{J}_{j,g_j} \end{bmatrix}$$

with submatrices $\mathbf{J}_{j,k}$ that are JORDAN blocks

$$\mathbf{J}_{j,k} = \begin{bmatrix} \lambda_j & 1 & & \\ & \lambda_j & \ddots & \\ & & \ddots & 1 \\ & & & \lambda_j \end{bmatrix}. \tag{4.11}$$

Now the definition of $f(\mathbf{A})$ is simple: Just apply Definition 4.4 for the single JORDAN block to each of the $\mathbf{J}_{j,k}$ JORDAN blocks.

Definition of $f(\mathbf{A})$ for general matrix $\mathbf{A} \in \mathbb{C}^{n\times n}$

Theorem 4.5. *Let $\mathbf{A} \in \mathbb{C}^{n\times n}$ have the JORDAN form just described, and suppose $f : \mathbb{C} \to \mathbb{C}$ and its first $i_j - 1$ derivatives are all defined at the eigenvalue λ_j for $j = 1, \ldots, p$. (Recall that i_j denotes the index of λ_j, i.e., the size of the largest JORDAN block associated with λ_j.) Then*

$$f(\mathbf{A}) = \mathbf{X} f(\mathbf{J}) \mathbf{X}^{-1},$$

where

$$f(\mathbf{J}) = \begin{bmatrix} f(\mathbf{J}_1) & & \\ & \ddots & \\ & & f(\mathbf{J}_p) \end{bmatrix}$$

and

$$f(\mathbf{J}_j) = \begin{bmatrix} f(\mathbf{J}_{j,1}) & & \\ & \ddots & \\ & & f(\mathbf{J}_{j,g_j}) \end{bmatrix}.$$

Since $\mathbf{J}_{j,k}$ is a JORDAN block of the form (4.11), $f(\mathbf{J}_{j,k})$ is given by Definition 4.4.

4.1.4 Equivalent polynomials

Definition 4.5 gives a formula for $f(\mathbf{A})$ that only depends on the value of f and its derivatives at the eigenvalues of $\mathbf{A}$. A natural question arises: Does this $f(\mathbf{A})$ commute with $\mathbf{A}$? For diagonalizable $\mathbf{A}$, Definition 4.2 gives a quick affirmative answer, since diagonal matrices commute:

$$\begin{aligned}\mathbf{A}f(\mathbf{A}) &= \mathbf{V}\mathbf{\Lambda}\mathbf{V}^{-1}\mathbf{V}f(\mathbf{\Lambda})\mathbf{V}^{-1}\\ &= \mathbf{V}\mathbf{\Lambda}f(\mathbf{\Lambda})\mathbf{V}^{-1} = \mathbf{V}f(\mathbf{\Lambda})\mathbf{\Lambda}\mathbf{V}^{-1}\\ &\qquad\qquad = \mathbf{V}f(\mathbf{\Lambda})\mathbf{V}^{-1}\mathbf{V}\mathbf{\Lambda}\mathbf{V}^{-1} = f(\mathbf{A})\mathbf{A}.\end{aligned}$$

Making the same conclusion for matrices with nontrivial Jordan structure would be a little more complicated. Instead we will make a helpful observation that gives additional insight into functions of matrices and trivializes the proof of commutativity.

Start with a thought experiment. Suppose I have two functions $f, g : \mathbb{C} \to \mathbb{C}$ that behave identically at the eigenvalues of $\mathbf{A}$, including all the appropriate derivatives that factor into $f(\mathbf{A})$ and $g(\mathbf{A})$. That is (using the notation from the Jordan form surrounding Definition 4.5),

$$f(\lambda_j) = g(\lambda_j), \quad \ldots, \quad f^{(i_j-1)}(\lambda_j) = g^{(i_j-1)}(\lambda_j) \tag{4.12}$$

for $j = 1, \ldots, p$. In this case, Definition 4.5 gives an identical result for $f(\mathbf{A})$ and $g(\mathbf{A})$, *regardless of how different f and g might be at other points in the complex plane.*

In particular, given any f, we can always choose that matching function g to be a *polynomial*. Since the conditions (4.12) gives at most n conditions that g must satisfy, we can always take g to be a polynomial of degree $n-1$ (which has n coefficients, including the constant term). One can find g by expressing it as

$$g(z) = c_0 + c_1 z + \cdots + c_{n-1}z^{n-1}$$

and then writing out each of the n interpolation conditions. Each condition gives another equation that is *linear* in the unknown coefficients $c_0, \ldots, c_{n-1}$. Together, the n conditions give a linear system of n equations for the n unknown coefficients. (When $\mathbf{A}$ is diagonalizable, one would typically prefer to express g in the Lagrange form of the interpolating polynomial, a mainstay of any basic numerical analysis course.)

A few concrete examples will illuminate the interpolation idea and illustrate the procedure for finding g.

Example 1: Diagonalizable A. Consider $f(z) = 1/z$ with

$$\mathbf{A} = \begin{bmatrix} 1/2 & & \\ & 2 & \\ & & 4 \end{bmatrix}, \qquad f(\mathbf{A}) = \mathbf{A}^{-1} = \begin{bmatrix} 2 & & \\ & 1/2 & \\ & & 1/4 \end{bmatrix}.$$

We seek a degree $n-1=2$ (quadratic) polynomial that *interpolates* f at the eigenvalues $\lambda_1 = 1/2$, $\lambda_2 = 2$, and $\lambda_3 = 4$. In particular, we seek to find c_0, c_1, and c_2 that specify $g(z) = c_0 + c_1 z + c_2 z$ such that

$$\begin{aligned} 2 = f(\lambda_1) &= g(\lambda_1) = c_0 + (1/2)c_1 + (1/4)c_2 \\ 1/2 = f(\lambda_2) &= g(\lambda_2) = c_0 + 2c_1 + 4c_2 \\ 1/4 = f(\lambda_3) &= g(\lambda_3) = c_0 + 4c_1 + 16c_2. \end{aligned}$$

These conditions give a linear system three equations in three unknowns:

$$\begin{bmatrix} 1 & 1/2 & 1/4 \\ 1 & 2 & 4 \\ 1 & 4 & 16 \end{bmatrix} \begin{bmatrix} c_0 \\ c_1 \\ c_2 \end{bmatrix} = \begin{bmatrix} 2 \\ 1/2 \\ 1/4 \end{bmatrix},$$

which has the solution

$$c_0 = \frac{11}{4}, \qquad c_1 = -\frac{13}{8}, \qquad c_2 = \frac{1}{4}.$$

One can verify:

$$\begin{aligned} g(\mathbf{A}) &= c_0\mathbf{I} + c_1\mathbf{A} + c_2\mathbf{A}^2 \\ &= \frac{11}{4}\begin{bmatrix} 1 & & \\ & 1 & \\ & & 1 \end{bmatrix} - \frac{13}{8}\begin{bmatrix} 1/2 & & \\ & 2 & \\ & & 4 \end{bmatrix} + \frac{1}{4}\begin{bmatrix} 1/4 & & \\ & 4 & \\ & & 16 \end{bmatrix} \\ &= \begin{bmatrix} 2 & & \\ & 1/2 & \\ & & 1/4 \end{bmatrix} = \mathbf{A}^{-1} = f(\mathbf{A}). \end{aligned}$$

Figure 4.1 compares f and g: these two functions are very different, yet they look the same as far as $\mathbf{A}$ is concerned.

Example 2: Nondiagonalizable A. Enlarge the previous example slightly, to make $\lambda_3 = 4$ a double eigenvalue ($a_3 = 2$) with a 2×2 JORDAN block ($i_3 = 2$):

$$\mathbf{A} = \begin{bmatrix} 1/2 & & & \\ & 2 & & \\ & & 4 & 1 \\ & & & 4 \end{bmatrix}, \qquad f(\mathbf{A}) = \mathbf{A}^{-1} = \begin{bmatrix} 2 & & & \\ & 1/2 & & \\ & & 1/4 & -1/16 \\ & & & 1/4 \end{bmatrix}.$$

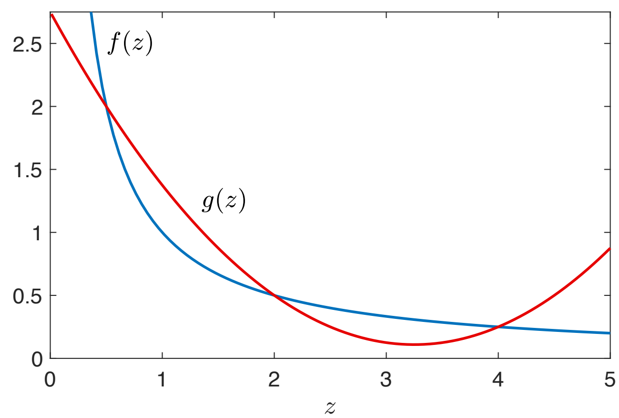

Figure 4.1. For Example 1, the quadratic polynomial $g(z)$ matches the function $f(z) = 1/z$ (but none of its derivatives) at the eigenvalues $\lambda_1 = 1$, $\lambda_2 = 2$, and $\lambda_3 = 4$ of the diagonalizable matrix $\mathbf{A}$.

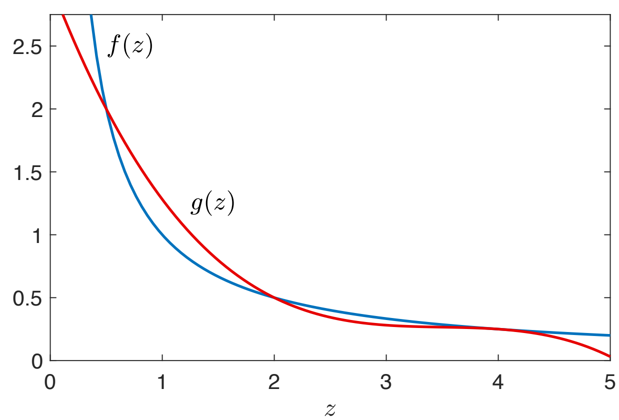

Figure 4.2. For Example 2, the cubic polynomial $g(z)$ matches the function $f(z) = 1/z$ at the eigenvalues $\lambda_1 = 1$, $\lambda_2 = 2$, and $\lambda_3 = 4$ of $\mathbf{A}$. Since $\lambda_3 = 4$ has a 2×2 Jordan block, $g'(\lambda_3) = f'(\lambda_3)$, reflected in the figure by the matching slope of f and g at $\lambda_3 = 4$.

Now we seek a degree $n - 1 = 3$ (cubic) polynomial that interpolates f at the three eigenvalues, *but also interpolates f' at λ_3, the double eigenvalue.* Now $g(z) = c_0 + c_1 z + c_2 z^2 + c_3 z^3$ with

$$\begin{aligned} 2 = f(\lambda_1) &= g(\lambda_1) = c_0 + (1/2)c_1 + (1/4)c_2 + (1/8)c_3 \\ 1/2 = f(\lambda_2) &= g(\lambda_2) = c_0 + 2c_1 + 4c_2 + 8c_3 \\ 1/4 = f(\lambda_3) &= g(\lambda_3) = c_0 + 4c_1 + 16c_2 + 64c_3 \end{aligned}$$

$$-1/16 = f'(\lambda_3) \;=\; g'(\lambda_3) = c_1 + 8c_2 + 48c_3.$$

with the last equation using $g'(z) = c_1 + 2c_2z + 3c_3z^2$. Now we solve

$$\begin{bmatrix} 1 & 1/2 & 1/4 & 1/8 \\ 1 & 2 & 4 & 8 \\ 1 & 4 & 16 & 64 \\ 0 & 1 & 8 & 48 \end{bmatrix} \begin{bmatrix} c_0 \\ c_1 \\ c_2 \\ c_3 \end{bmatrix} = \begin{bmatrix} 2 \\ 1/2 \\ 1/4 \\ -1/16 \end{bmatrix},$$

which has the solution

$$c_0 = 3, \qquad c_1 = -\frac{37}{16}, \qquad c_2 = \frac{21}{32}, \qquad c_3 = -\frac{1}{16}.$$

4.1.5 Approach 3: Contour integration

We briefly mention a third approach to defining the function of a matrix based on contour integrals. Suppose $f : \mathbb{C} \to \mathbb{C}$ is an analytic function defined on the Jordan curve Γ and its interior. Then for any point $a \in \mathbb{C}$ in the interior of Γ, the Cauchy integral formula gives

$$f(a) = \frac{1}{2\pi \mathrm{i}} \int_\Gamma \frac{f(z)}{z-a}\,\mathrm{d}z, \tag{4.13}$$

a central result in a complex analysis course.

Now if $\mathbf{A} \in \mathbb{C}^{n\times n}$ has all its eigenvalues contained within Γ, one can *define*

$$f(\mathbf{A}) = \frac{1}{2\pi \mathrm{i}} \int_\Gamma f(z)(z\mathbf{I} - \mathbf{A})^{-1}\,\mathrm{d}z, \tag{4.14}$$

which is sometimes called the Dunford–Taylor integral. The integral of a matrix is defined *entrywise*, so for

$$\mathbf{A} = \begin{bmatrix} 1 & 1 \\ 0 & 2 \end{bmatrix}, \qquad (z\mathbf{I} - \mathbf{A})^{-1} = \begin{bmatrix} \dfrac{1}{z-1} & \dfrac{1}{(z-1)(z-2)} \\ 0 & \dfrac{1}{z-2} \end{bmatrix},$$

equation (**??**) gives

$$f(\mathbf{A}) = \begin{bmatrix} \dfrac{1}{2\pi \mathrm{i}} \displaystyle\int_\Gamma \frac{f(z)}{z-1}\,\mathrm{d}z & \dfrac{1}{2\pi \mathrm{i}} \displaystyle\int_\Gamma \frac{f(z)}{(z-1)(z-2)}\,\mathrm{d}z \\ 0 & \dfrac{1}{2\pi \mathrm{i}} \displaystyle\int_\Gamma \frac{f(z)}{z-2}\,\mathrm{d}z \end{bmatrix}.$$

One can evaluate each of these entries using the Cauchy integral formula,

$$\frac{1}{2\pi \mathrm{i}}\int_\Gamma \frac{f(z)}{z-1}\,\mathrm{d}z = f(1), \qquad \frac{1}{2\pi \mathrm{i}}\int_\Gamma \frac{f(z)}{z-2}\,\mathrm{d}z = f(2)$$

$$\frac{1}{2\pi \mathrm{i}}\int_\Gamma \frac{f(z)}{(z-1)(z-2)}\,\mathrm{d}z = \frac{f(z)}{z-2}\bigg|_{z=1} + \frac{f(z)}{z-1}\bigg|_{z=2} = -f(1)+f(2),$$

giving

$$f(\mathbf{A}) = \begin{bmatrix} f(1) & f(2)-f(1) \\ 0 & f(2) \end{bmatrix}.$$

Since we can diagonalize

$$\mathbf{A} = \mathbf{V}\mathbf{\Lambda}\mathbf{V}^{-1} = \begin{bmatrix} 1 & 1 \\ 0 & 1 \end{bmatrix}\begin{bmatrix} 1 & 0 \\ 0 & 2 \end{bmatrix}\begin{bmatrix} 1 & -1 \\ 0 & 1 \end{bmatrix}$$

Definition 4.2 of $f(\mathbf{A})$ for diagonalizable $\mathbf{A}$ gives

$$\begin{aligned} f(\mathbf{A}) = \mathbf{V}f(\mathbf{\Lambda})\mathbf{V}^{-1} &= \begin{bmatrix} 1 & 1 \\ 0 & 1 \end{bmatrix}\begin{bmatrix} f(1) & 0 \\ 0 & f(2) \end{bmatrix}\begin{bmatrix} 1 & -1 \\ 0 & 1 \end{bmatrix} \\ &= \begin{bmatrix} f(1) & f(2)-f(1) \\ 0 & f(2) \end{bmatrix}, \end{aligned}$$

in perfect agreement with the integral definition (4.14).

Diagonalizable $\mathbf{A}$

The last example showed that Definition 4.2 agrees with the integral formulation (4.14) for a small example, but the general case of diagonalizable $\mathbf{A}$ is easy to tackle directly. Writing $\mathbf{A} = \mathbf{V}\mathbf{\Lambda}\mathbf{V}^{-1}$, the integral (4.14) gives

$$\begin{aligned} f(\mathbf{A}) = \frac{1}{2\pi \mathrm{i}}\int_\Gamma f(z)(z\mathbf{I}-\mathbf{A})^{-1}\,\mathrm{d}z &= \frac{1}{2\pi \mathrm{i}}\int_\Gamma f(z)\mathbf{V}(z\mathbf{I}-\mathbf{\Lambda})^{-1}\mathbf{V}^{-1}\,\mathrm{d}z \\ &= \mathbf{V}\bigg(\frac{1}{2\pi \mathrm{i}}\int_\Gamma f(z)(z\mathbf{I}-\mathbf{\Lambda})^{-1}\,\mathrm{d}z\bigg)\mathbf{V}^{-1}. \end{aligned}$$

The integrand on the right-hand side is a diagonal matrix whose (j,j) entry is simply

$$\frac{1}{2\pi \mathrm{i}}\int_\Gamma f(z)(z-\lambda_j)^{-1}\,\mathrm{d}z = f(\lambda_j),$$

and whose off-diagonal entries are integrals of zero, and hence are zero. Thus, the integral definition (4.14) reduces to

$$f(\mathbf{A}) = \mathbf{V} \begin{bmatrix} f(\lambda_1) & & \\ & \ddots & \\ & & f(\lambda_n) \end{bmatrix} \mathbf{V}^{-1} = \sum_{j=1}^{n} f(\lambda_j)\mathbf{v}_j \widehat{\mathbf{v}}_j^*,$$

and given by Definition 4.2.

Jordan blocks

At the other extreme, one can apply the integral definition (4.14) to a Jordan block

$$\mathbf{J} = \begin{bmatrix} \lambda & 1 & & \\ & \lambda & \ddots & \\ & & \ddots & 1 \\ & & & \lambda \end{bmatrix} \in \mathbb{C}^{n\times n},$$

and show agreement with Definition 4.4.

4.2 The Exponential of a Matrix

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