

SEMINAR ON JACOBI MATRICES

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CHAPTER 1

Introduction

1.1. Motivation

The laws of nature are encoded in differential equations.

It is no coincidence that modern science and the calculus of derivatives and integrals were invented at the same time and by the same people. Physics attempts to describe the evolution of a system of physical objects. The objects are represented by certain quantities (things which can be measured quantitatively) and these quantities are allowed to change (evolve) over time thus bringing derivatives into the game. One of the first and most important of these laws is Newton's law of motion $F = ma$ where a is the second derivative of the position function of a particle of mass m and F is the force acting on the particle. This force might involve the position or the velocity of the particle so that $F = ma$ becomes a differential equation.

The differential equations describing physical systems are very often of the second order. In mechanical systems (and hence in quantum mechanical systems) this is, in fact, due to Newton's law. Maxwell's equations which describe electric and magnetic phenomena are of the first order but certain important second order equations may be deduced from them. The equations of general relativity, geometric in nature, are also of the second order.

Sometimes the basic differential equations of physics are linear and sometimes they may be approximated by linear equations if one is satisfied with describing only small effects. In any case, as linear differential equations can already be very difficult, their thorough understanding is the first and fundamental step in the study of mathematical physics.

Among the linear second order differential equations there are three prototypes, hyperbolic, parabolic and elliptic.¹

- The wave equation

$$u_{tt} = \Delta u$$

is the prototypical hyperbolic equation. It describes the propagation of electromagnetic waves and can be easily deduced from Maxwell's equations. It also describes the propagation of sound and water waves (for small waves at least).

- The heat or diffusion equation

$$u_t = \Delta u$$

is the prototypical parabolic equation. It describes the diffusion of heat or particles in an ambient medium.

- Laplace's equation

$$\Delta u = 0$$

¹These names are related to the ancient classification of the conic sections, but we won't have to worry about that.

is the prototypical elliptic equation. It describes the strength of a conservative field (e.g., electric or gravitational) in a space devoid of charges or masses.²

Here Δ is the so called Laplace operator, an abbreviation for

$$\Delta = \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}$$

when one uses cartesian coordinates.

One of the most important tools in studying partial differential equations is separation of the variables. Let's assume we want to solve the heat equation in one space variable, i.e., our PDE is $u_t = u_{xx}$. One assumes now that the solution of the equation is not just any function of the two variables t and x but is a product of a function T of t and a function X of x , i.e., $u(x, t) = T(t)X(x)$. Then one obtains $XT' = TX''$, or after division by XT

$$\frac{T'}{T} = \frac{X''}{X}.$$

The left hand side of this equation is now a function of t only and independent of x . The right hand side, however, is a function of x only and independent of t . For them to be equal it is necessary that both sides are actually independent of both x and t , i.e., they are equal to a constant, say λ . This implies that

$$T' = \lambda T \quad \text{and} \quad X'' = \lambda X.$$

Now we have obtained ODEs and that is a big step forward. Note that the ODEs are still linear and second order (at most). However, they do involve the new parameter λ as a multiplier of the dependent variable. For historical reasons such parameters are often called spectral parameters.

Formally, the most general second order linear differential equation involving a spectral parameter is the equation

$$(1) \quad py'' + ry' + qy = \lambda wy$$

where p, r, q and w are functions of the independent variable. By a change of variables this may be transformed into the equation

$$(2) \quad - (py')' + qy = \lambda wy$$

and this equation is known as the Sturm-Liouville equation in honor of Charles-François Sturm (1803–1855) and Joseph Liouville (1809–1882).

The next simplification, which will be discussed in the next section and is often numerically motivated, is to look at discretized differential (i.e., difference) equations. Another motivation for considering difference equations is the construction of so called toy models. These are models which may capture an important facet of a (physical) system in order to gain some basic understanding but are not designed to obtain quantitative information on a real system. Discrete models like the ones we will study in this seminar can often serve as such toy models.

Historically, the need for creating a mathematical theory of equations like (1) or (2) can be considered as one of the most important reasons for the development of the mathematical fields of Operator Theory and, serving as its foundation, Functional Analysis. It is one of the main goals of this seminar to use linear differential and difference equations to give an example driven introduction to these fields.

²In the presence of charges or masses of density ρ Laplace's equation is replaced by Poisson's equation $\Delta u = 4\pi\rho$.

The starting point for this is to view the left hand sides of (1) or (2) as "operators acting on functions". For example, we introduce the *linear differential expression*

$$L = p(x) \left(\frac{d}{dx} \right)^2 + r(x) \frac{d}{dx} + q(x).$$

We think of L as acting on twice differentiable functions u by differentiation, multiplication and summing, and thus recover the left of (1) as Lu . It is easily seen that L defines a linear mapping of the vector space of twice differentiable functions on \mathbb{R} into the vector space of all functions on \mathbb{R} . After the domain of a linear mapping such as L is fixed (which of course is always a required part of defining a mapping in mathematics) we refer to L as a linear operator, here a linear differential operator. The term "linear differential expression" is used in a more vague sense, when one doesn't want to decide on a specific domain right away.

Let us now also assume that $w = 1$ in (1). If w has no roots, then this can be achieved by dividing by w and redefining p, q, r . Then (1) takes the form

$$(3) \quad Lu = \lambda u.$$

This looks very similar to the eigenvalue equation $Av = \lambda v$ for square matrices A , or, in linear algebra language, for linear mappings in finite dimensional vector spaces. The main difference between this and (3) is that the function spaces on which (3) will have to be studied are rarely finite dimensional. As a result it becomes necessary to develop a theory of linear mappings on infinite dimensional vector spaces. This is exactly the content of operator theory, while functional analysis is the theory of infinite dimensional vector spaces.

1.2. Discretization of Differential Expressions

Instead of directly starting the investigation of linear differential expressions and linear differential operators, in particular Sturm-Liouville operators, we will first study *finite difference expressions* and the operators associated with them. This allows for a number of simplifications and, in particular, can be done with more elementary operator theoretic background than in the case of differential operators. At the same time many of the most important concepts, questions and results from the theory of linear differential operators can already be introduced and studied with finite difference operators.

Linear finite difference equations quite frequently appear in mathematics and, even more so, in physical models for their own sake. But for now we will take the point of view that they arise through *discretization* of linear differential equations. The most important use of this idea is made in numerical mathematics. By its very nature a computer can not handle the continuum processes which are described by differential equations (where, for example, physical space is considered as a continuum). Thus almost every numerical algorithm for solving differential equations starts with discretizing the equations and thereby reducing it to a finite difference equation, which the computer can solve in finitely many steps.

Our approach here is not the one from numerical mathematics, in the sense that we will not solve finite difference equations on the computer, but instead study them with theoretical tools. But we can still think of them as motivated through discretization.

The most basic differential expression is

$$L = \frac{d}{dx}.$$

It acts on functions $u \in C^1(\mathbb{R})$, the complex-valued continuously differentiable functions on the real line, by differentiation:

$$(4) \quad Lu = u'.$$

We will discretize L and u separately: A function u is discretized by restricting it to a discrete subset of \mathbb{R} . A simple choice for this set are the integers \mathbb{Z} . Thus we discretize u by replacing it with its restriction to \mathbb{Z} ,

$$u : \mathbb{R} \rightarrow \mathbb{C} \quad \rightsquigarrow \quad u : \mathbb{Z} \rightarrow \mathbb{C}.$$

To discretize L we have to prescribe how its discrete counterpart acts on $u : \mathbb{Z} \rightarrow \mathbb{C}$, i.e. we have to say how a function on \mathbb{Z} is transformed into another function on \mathbb{Z} . There are a number of natural choices here. One of them is the so-called *right difference operator* D_r , which is defined through

$$(5) \quad (D_r u)(n) = u(n+1) - u(n) \quad \text{for all } n \in \mathbb{Z}.$$

This means that we have replaced the “differential quotient” $u' = du/dx$ with the difference quotient $u(x+1) - u(x)$ and restricted it to the integers. Note that the difference quotient doesn’t have a denominator as $(x+1) - x = 1$. We could also use the *left difference operator* D_l defined by

$$(6) \quad (D_l u)(n) = u(n) - u(n-1) \quad \text{for all } n \in \mathbb{Z},$$

or the *central difference operator*

$$(7) \quad (D_c u)(n) = \frac{u(n+1) - u(n-1)}{2} \quad \text{for all } n \in \mathbb{Z}.$$

One can write $u : \mathbb{Z} \rightarrow \mathbb{C}$ as an infinite (column) vector,

$$(8) \quad u = \begin{pmatrix} \vdots \\ u(-1) \\ u(0) \\ u(1) \\ \vdots \end{pmatrix},$$

and the difference operators as infinite matrices, for example

$$(9) \quad D_r = \begin{pmatrix} \ddots & \ddots & & & & \\ & \ddots & -1 & 1 & & \\ & & 0 & -1 & 1 & \\ & & & 0 & -1 & \ddots \\ & & & & & \ddots & \ddots \end{pmatrix},$$

where all the (infinitely many) missing entries are filled in with zeros if not indicated otherwise by dots. Using the rules of matrix multiplication, the infinitely many equations (5) can then be thought of as the single equation

$$D_r u = \begin{pmatrix} \vdots \\ u(0) - u(-1) \\ u(1) - u(0) \\ u(2) - u(1) \\ \vdots \end{pmatrix}.$$

In a similar way one can write D_l and D_c as infinite matrices and then think of (6) and (7) as matrix equations.

Let us now consider the second order differential expression

$$(10) \quad \Delta = \left(\frac{d}{dx} \right)^2,$$

which to twice differentiable functions assigns their second derivative: $Lu = \frac{d}{dx} \left(\frac{d}{dx} u \right) = u''$. Δ is called the (one-dimensional) *Laplace operator*. One way to discretize it would be to displace both expressions d/dx with D_r . The resulting difference expression D_r^2 would act on functions $u : \mathbb{N} \rightarrow \mathbb{C}$ as

$$\begin{aligned} (D_r^2 u)(n) &= (D_r(D_r u))(n) \\ &= (D_r u)(n+1) - (D_r u)(n) \\ &= (u(n+2) - u(n+1)) - (u(n+1) - u(n)) \\ &= u(n+2) - 2u(n+1) + u(n). \end{aligned}$$

The result is not very satisfying as it approximates the second derivative at n by an expression which only depends on values of u to the right of n . A more symmetric expression is found if we replace one d/dx with D_r and the other one with D_l (check this):

$$(11) \quad (D_l(D_r u))(n) = u(n+1) - 2u(n) + u(n-1).$$

The same expression is found for $(D_r(D_l u))(n)$. The difference expression $\Delta_d := D_l D_r = D_r D_l$ is the most widely used discretization of the Laplacian and frequently denoted as the *discrete Laplacian*. The matrix form of Δ_d can be read off (11) or, alternatively, found by multiplying the infinite matrices representing D_l and D_r (which is possible since the formally appearing infinite sums have only finitely many non-zero terms). One gets

$$(12) \quad \Delta_d = \begin{pmatrix} \ddots & \ddots & & & & & \\ & \ddots & -2 & 1 & & & \\ & & 1 & -2 & 1 & & \\ & & & 1 & -2 & \ddots & \\ & & & & \ddots & \ddots & \\ & & & & & \ddots & \ddots \end{pmatrix}.$$

It is now clear how to get discretizations of higher order differential expressions $\left(\frac{d}{dx} \right)^n$, or, more generally, arbitrary general linear differential expressions of n -th order with constant coefficients:

$$(13) \quad L = a_n \left(\frac{d}{dx} \right)^n + \dots + a_1 \frac{d}{dx} + a_0, \quad a_n, \dots, a_0 \in \mathbb{C}.$$

The resulting finite difference expression will have a matrix representation of the form

$$(14) \quad C = \begin{pmatrix} \ddots & \ddots & \ddots & & & & \\ & \ddots & c_0 & \ddots & c_k & & \\ & \ddots & \ddots & c_0 & \ddots & c_k & \\ & & c_{-m} & \ddots & c_0 & \ddots & c_k \\ & & & c_{-m} & \ddots & c_0 & \ddots \\ & & & & c_{-m} & \ddots & c_0 \\ & & & & & \ddots & \ddots \\ & & & & & \ddots & \ddots \end{pmatrix},$$

Second Order Finite Difference Equations

2.1. Difference Equations and Initial Value Problems

2.1.1. Vector spaces of sequences. Suppose Z is a subset of \mathbb{Z} . Let $s(Z)$ denote the set of all complex-valued functions on Z . We define an addition and a scalar multiplication on $s(Z)$ by letting

$$(u + v)(n) = u(n) + v(n)$$

and

$$(\alpha u)(n) = \alpha u(n)$$

whenever $n \in Z$, $u, v \in s(Z)$, and $\alpha \in \mathbb{C}$. One can then show immediately that $s(Z)$ is a complex vector space. We will mostly be interested in the cases where $Z = \mathbb{Z}$ (i.e., the set of all doubly infinite sequences) or where $Z = \mathbb{N}$ (i.e., the set of all infinite sequences). If Z is a set with m elements then $s(Z)$ is isomorphic to \mathbb{C}^m .

As usual for sequences, we will sometimes write u_n instead of $u(n)$.

2.1.2. Second order finite difference expressions. For three given doubly infinite sequences a, b and c such that $a_n \in \mathbb{C} \setminus \{0\}$, $b_n \in \mathbb{C}$ and $c_n \in \mathbb{C} \setminus \{0\}$ for all $n \in \mathbb{Z}$, we define a second order finite difference expression J as the mapping $J : s(\mathbb{Z}) \rightarrow s(\mathbb{Z})$ given by

$$(18) \quad (Ju)(n) = a_n u(n-1) + b_n u(n) + c_{n+1} u(n+1)$$

for each $n \in \mathbb{Z}$. It is easily checked that the mapping $J : s(\mathbb{Z}) \rightarrow s(\mathbb{Z})$ is linear.

2.1.3. Jacobi matrices. We will frequently write J in the form of an infinite matrix

$$(19) \quad J = \begin{pmatrix} \ddots & \ddots & & & & & \\ & \ddots & b_{-1} & c_0 & & & \\ & & a_0 & b_0 & c_1 & & \\ & & & a_1 & b_1 & \ddots & \\ & & & & \ddots & \ddots & \\ & & & & & \ddots & \ddots \end{pmatrix}$$

and refer to J as a (two-sided) **Jacobi matrix**. If $u \in s(\mathbb{Z})$ is written as an infinite column vector,

$$(20) \quad u = \begin{pmatrix} \vdots \\ u(-1) \\ u(0) \\ u(1) \\ \vdots \end{pmatrix},$$

then Ju in (18) can be interpreted as the matrix product of J and u . Note that some care is needed here in correctly identifying the “0-th” column of J with the 0-th component of u .

2.1.4. Finite difference equations. Let J be a second order finite difference expression. The system of equations

$$(21) \quad (Ju)(n) = 0, \quad n \in \mathbb{Z},$$

or, in equivalent vector notation,

$$(22) \quad Ju = 0,$$

is called the homogeneous second order finite difference equation associated with J .

For given $f \in s(\mathbb{Z})$ the system of equations

$$(23) \quad (Ju)(n) = f(n), \quad n \in \mathbb{Z},$$

or

$$(24) \quad Ju = f,$$

is called the inhomogeneous second order finite difference equation associated with J .

A sequence $u \in s(\mathbb{Z})$ such that $Ju = 0$ ($Ju = f$) is called a solution of the homogeneous (inhomogeneous) finite difference equation.

2.1.5. Initial value problems. For a given Jacobi matrix J , $f \in s(\mathbb{Z})$, $n_0 \in \mathbb{Z}$ and $a, b \in \mathbb{C}$, the system of equations

$$(25) \quad Ju = f, \quad u(n_0) = a, \quad u(n_0 + 1) = b,$$

is referred to as the initial value problem for J and f at n_0 . A sequence $u \in s(\mathbb{Z})$ which satisfies all of (25) is a solution of the initial value problem.

2.1.6. Existence and uniqueness. The initial value problem (25) has a unique solution.

Proof: For fixed n consider the equation $(Ju)(n) = f(n)$, that is

$$a_n u(n-1) + b_n u(n) + c_{n+1} u(n+1) = f(n).$$

As $c_{n+1} \neq 0$, $u(n+1)$ is uniquely determined by $u(n-1)$ and $u(n)$ through

$$u(n+1) = \frac{1}{c_{n+1}} (f(n) - a_n u(n-1) - b_n u(n)).$$

Similarly, as $a_n \neq 0$, $u(n)$ and $u(n+1)$ uniquely determine $u(n-1)$. From this one gets inductively that $u(n_0) = a$ and $u(n_0 + 1) = b$ uniquely determine a solution of $Ju = f$. \square

2.1.7. Transfer matrices. Let J be a Jacobi matrix given by (18) or (19), respectively. The transfer matrices associated with J are given by

$$(26) \quad A_n := \begin{pmatrix} 0 & 1 \\ -\frac{a_n}{c_{n+1}} & -\frac{b_n}{c_{n+1}} \end{pmatrix}.$$

The significance of transfer matrices (and reason for the term “transfer”) lies in the following fact:

The sequence $u \in s(\mathbb{Z})$ solves the homogeneous difference equation $Ju = 0$ if and only if

$$(27) \quad \begin{pmatrix} u(n) \\ u(n+1) \end{pmatrix} = A_n \begin{pmatrix} u(n-1) \\ u(n) \end{pmatrix}$$

for all $n \in \mathbb{Z}$.

Proof: This follows easily by using the expression (18) for the right hand side of $Ju = 0$. \square

Note that $\det A_n = a_n/c_{n+1} \neq 0$. Thus A_n is invertible,

$$A_n^{-1} = \begin{pmatrix} -\frac{b_n}{a_n} & -\frac{c_{n+1}}{a_n} \\ 1 & 0 \end{pmatrix},$$

and we have

$$\begin{pmatrix} u(n-1) \\ u(n) \end{pmatrix} = A_n^{-1} \begin{pmatrix} u(n) \\ u(n+1) \end{pmatrix},$$

which can also be seen directly from (18).

If one defines the matrices

$$(28) \quad T_n := \begin{cases} A_n \dots A_1 & \text{for } n > 0, \\ I_2 & \text{for } n = 0, \\ A_{n+1}^{-1} \dots A_0^{-1} & \text{for } n < 0, \end{cases}$$

where I_2 denotes the 2×2 identity matrix, then we see that $Ju = 0$ if and only if

$$(29) \quad \begin{pmatrix} u(n) \\ u(n+1) \end{pmatrix} = T_n \begin{pmatrix} u(0) \\ u(1) \end{pmatrix} \quad \text{for all } n \in \mathbb{Z}.$$

2.1.8. Nullspace of J . The null space $N_0(J) := \{u : Ju = 0\}$ of the linear mapping J is a two-dimensional subspace of $s(\mathbb{Z})$.

Sketch of proof: Define the mapping $L : \mathbb{C}^2 \rightarrow s(\mathbb{Z})$ by $L((a, b)) = u$ where u is the unique solution of $Ju = 0$ with $u(0) = a$ and $u(1) = b$. One can show that L is linear, one-to-one and that $\text{ran}(L) = N_0(J)$. Thus $N_0(J)$ is a subspace of dimension 2. \square

2.1.9. Eigenspaces of J . For $\lambda \in \mathbb{C}$ let $N_\lambda(J) = \{u : Ju = \lambda u\}$.

In other words, $N_\lambda(J)$ is the eigenspace to the eigenvalue λ for the linear mapping J . Denoting by I the identity mapping in $s(\mathbb{Z})$, we have $Ju = \lambda u$ if and only if $(J - \lambda I)u = 0$. As $J - \lambda I$ again is a Jacobi matrix, we see from Section 2.1.8 that $\dim N_\lambda(J) = 2$ for every $\lambda \in \mathbb{C}$. In particular, every complex number is an eigenvalue of J with geometric multiplicity 2.

By $A_n(\lambda)$ and $T_n(\lambda)$ we denote the transfer matrices for $J - \lambda I$, defined as in (26) and (28), respectively. In particular,

$$(30) \quad A_n(\lambda) := \begin{pmatrix} 0 & 1 \\ -\frac{a_n}{c_{n+1}} & -\frac{b_n - \lambda}{c_{n+1}} \end{pmatrix}.$$

2.1.10. Fundamental systems. A basis of $N_\lambda(J)$ will be called a fundamental system of $Ju = \lambda u$.

2.2. The Free Jacobi Matrix

We now introduce a specific example of a Jacobi matrix J_0 , which, inspired by related concepts from Quantum Mechanics, will be called the “free Jacobi matrix”. J_0 provides us with an “exactly solvable model”, where explicit formulas for fundamental systems of $J_0 u = \lambda u$ can be found.

2.2.1. The free Jacobi matrix. The free Jacobi matrix J_0 is the Jacobi matrix such that

$$(31) \quad (J_0 u)(n) = u(n-1) + u(n+1) \quad \text{for all } n \in \mathbb{Z}.$$

In matrix notation, J_0 is given by

$$(32) \quad J_0 = \begin{pmatrix} \ddots & \ddots & & & & & \\ & \ddots & 0 & 1 & & & \\ & & 1 & 0 & 1 & & \\ & & & & & \ddots & \\ & & & & 1 & 0 & \ddots \\ & & & & & \ddots & \ddots \end{pmatrix}.$$

J_0 is structurally simpler but closely related to the finite difference approximation Δ_d for d^2/dx^2 found in Section 1.2. In fact, $J_0 = \Delta_d + 2I$ and thus $J_0 u = \lambda u$ if and only if $\Delta_d u = (\lambda - 2)u$. Thus finding all eigenvectors for J_0 is equivalent to finding all eigenvectors for Δ_d (with eigenvalues shifted by 2).

The corresponding transfer matrices are

$$(33) \quad A_n(\lambda) = A(\lambda) := \begin{pmatrix} 0 & 1 \\ -1 & \lambda \end{pmatrix}$$

and $T_n(\lambda) = A(\lambda)^n$ for all $n \in \mathbb{Z}$ (here we define $A^0 = I_2$ and $A^{-n} = (A^{-1})^n$ for $n \in \mathbb{N}$).

Below, we will find simple explicit fundamental systems for $J_0 u = \lambda u$ by diagonalizing $A(\lambda)$. If $\lambda \neq \pm 2$, then this is possible as we will see that $A(\lambda)$ has two distinct eigenvalues. The case $\lambda = \pm 2$ will be considered separately as the corresponding transfer matrices turn out to have non-trivial Jordan form.

2.2.2. Square roots of complex numbers. We define the principal square root \sqrt{z} of a complex number z through the polar representation of z as follows: If $z = re^{i\theta}$ with $r \geq 0$ and $-\pi < \theta \leq \pi$, then $\sqrt{z} = \sqrt{r}e^{i\theta/2}$. Note that every non-zero complex number has exactly two square roots $a_{\pm} = \pm\sqrt{z}$ with the property $a_{\pm}^2 = z$.

2.2.3. Eigenvalues for $\lambda \neq \pm 2$. We will prove the

Proposition. (a) If $\lambda \in \mathbb{C} \setminus \{\pm 2\}$, then $A(\lambda)$ has two distinct eigenvalues $z_+(\lambda)$ and $z_-(\lambda)$ such that $z_-(\lambda)z_+(\lambda) = 1$. The corresponding eigenvectors are

$$v_+(\lambda) = \begin{pmatrix} 1 \\ z_+(\lambda) \end{pmatrix} \quad \text{and} \quad v_-(\lambda) = \begin{pmatrix} 1 \\ z_-(\lambda) \end{pmatrix}.$$

(b) If $\lambda \in \mathbb{C} \setminus [-2, 2]$, then $|z_{\pm}(\lambda)| \neq 1$ and, in particular, we can choose $z_{\pm}(\lambda)$ such that $|z_+(\lambda)| < 1$ and $|z_-(\lambda)| > 1$.

(c) If λ is real and $-2 < \lambda < 2$, then $|z_{\pm}(\lambda)| = 1$ and $z_-(\lambda) = \overline{z_+(\lambda)}$.

Proof: The characteristic equation for $A(\lambda)$ is

$$(34) \quad \det(A(\lambda) - zI_2) = z^2 - \lambda z + 1 = 0,$$

which is solved by

$$(35) \quad z_{\pm}(\lambda) = \frac{1}{2}(\lambda \pm \sqrt{\lambda^2 - 4}).$$

If $\lambda \neq \pm 2$ and thus $\sqrt{\lambda^2 - 4} \neq 0$, then $z_+(\lambda)$ and $z_-(\lambda)$ are distinct eigenvalues of $A(\lambda)$. One checks that $(1, z_{\pm}(\lambda))^t$ are corresponding eigenvectors. We have $z_+(\lambda)z_-(\lambda) = \det A(\lambda) = 1$.

This shows (a) and, in particular, that $|z_{\pm}(\lambda)|$ are either both 1 or both different from 1 (in which case one of them is strictly larger and one strictly smaller than one).

To prove (b), assume that $|z_{\pm}(\lambda)| = 1$. Then $z_-(\lambda) = 1/z_+(\lambda) = \overline{z_+(\lambda)}$ and

$$\lambda = \operatorname{tr} A(\lambda) = z_+(\lambda) + z_-(\lambda) = 2 \operatorname{Re} z_+(\lambda).$$

Thus λ is real and $-2 \leq \lambda \leq 2$. We conclude that if $\lambda \in \mathbb{C} \setminus [-2, 2]$, then $|z_{\pm}(\lambda)| \neq 1$. Thus we may label the eigenvalues of $A(\lambda)$ such that $|z_+(\lambda)| < 1$ and $|z_-(\lambda)| > 1$ (which may involve changing the choice made in (35)).

If, on the other hand, $-2 < \lambda < 2$, then (35) implies $z_{\pm}(\lambda) = \frac{1}{2}(\lambda \pm i\sqrt{4 - \lambda^2})$, which yields (c). \square

2.2.4. The case $\lambda = \pm 2$. If $\lambda = \pm 2$ then the characteristic equation (34) has only one root ± 1 and the corresponding (geometric) eigenspaces are one-dimensional. Thus we construct a Jordan chain consisting of an eigenvector and a generalized eigenvector:

Proposition. (a) $A(2)$ has a single eigenvalue 1 of geometric multiplicity 1 with eigenvector

$$v(2) = \begin{pmatrix} 1 \\ 1 \end{pmatrix}.$$

A generalized eigenvector $w(2)$ with $(A(2) - I_2)w(2) = v(2)$ is given by

$$w(2) = \begin{pmatrix} 0 \\ 1 \end{pmatrix}.$$

(b) $A(-2)$ has a single eigenvalue -1 of geometric multiplicity 1 with eigenvector

$$v(-2) = \begin{pmatrix} 1 \\ -1 \end{pmatrix}.$$

A generalized eigenvector $w(-2)$ with $(A(-2) + I_2)w(-2) = v(-2)$ is given by

$$w(-2) = \begin{pmatrix} 0 \\ 1 \end{pmatrix}.$$

Proof: All this follows from straightforward calculations. \square

2.2.5. Fundamental systems for $J_0 u = \lambda u$. Based on the previous two propositions we now find fundamental systems for $J_0 u = \lambda u$:

Theorem. (a) If $\lambda \in \mathbb{C} \setminus \{\pm 2\}$, then $J_0 u = \lambda u$ has a fundamental system of solutions $\{u_+, u_-\}$ given by $u_{\pm}(n) = z_{\pm}(\lambda)^n$ for all $n \in \mathbb{Z}$.

If $z \in \mathbb{C} \setminus [-2, 2]$, then $|u_{\pm}(n)|$ decays exponentially as $n \rightarrow \pm\infty$ and grows exponentially as $n \rightarrow \mp\infty$.

If λ is real with $-2 < \lambda < 2$, then all solutions of $J_0 u = \lambda u$ are bounded on \mathbb{Z} .

(b) A fundamental system of solutions of $J_0 u = 2u$ is given by $\{u_1, u_2\}$, where $u_1(n) = 1$, $u_2(n) = n$ for all $n \in \mathbb{Z}$.

A fundamental system of solutions of $J_0 u = -2u$ is given by $\{u_1, u_2\}$, where $u_1(n) = (-1)^n$, $u_2(n) = (-1)^n n$ for all $n \in \mathbb{Z}$.

In each case no solution grows faster than linear in n .

Proof: If $\lambda \in \mathbb{C} \setminus \{-2, 2\}$, then $v_{\pm}(\lambda) = (1, z_{\pm}(\lambda))^t$ are linearly independent. As the mapping L from the proof the existence and uniqueness proof in Section 2.1.6 preserves

linear independence, the solutions u_{\pm} with $(u_{\pm}(0), u_{\pm}(1)) = (1, z_{\pm}(\lambda))$ are a fundamental system for $J_0 u = \lambda u$. It follows from (29) that

$$\begin{pmatrix} u_{\pm}(n) \\ u_{\pm}(n+1) \end{pmatrix} = A(\lambda)^n \begin{pmatrix} 1 \\ z_{\pm}(\lambda) \end{pmatrix} = z_{\pm}(\lambda)^n \begin{pmatrix} 1 \\ z_{\pm}(\lambda) \end{pmatrix}$$

and thus $u_{\pm}(n) = z_{\pm}(\lambda)^n$. This and Lemma 2.2.3 show the claims about exponential growth and decay made in (a). If $-2 < \lambda < 2$, then u_{\pm} are bounded on \mathbb{Z} by Lemma 2.2.3(c), yielding boundedness of all solutions on \mathbb{Z} .

Using the eigenvectors and generalized eigenvectors found in Lemma 2.2.4 as initial conditions to solve $J_0 u = \pm 2u$ via (29), one finds the solutions given in (b). The linear growth follows from this. \square

2.2.6. Remark. We could have determined fundamental systems for $J_0 u = \lambda u$ by a simple “guess and verify” approach. This is based on the observation that for every solution z of the characteristic equation (34) it holds that

$$\lambda = z + \frac{1}{z}.$$

If we let $u(n) = z^n$ for all $n \in \mathbb{Z}$, then we can verify easily that $u(n-1) + u(n+1) = \lambda u(n)$ for all n , i.e. $J_0 u = \lambda u$. If (34) has two different roots (as for $\lambda \neq \pm 2$), then one also sees easily that the corresponding u 's are linearly independent and thus form a fundamental system for $J_0 u = \lambda u$. If $\lambda = \pm 2$, then we find only the solution u_1 from part (b) of the above Theorem in this way. That u_2 is a second linearly independent solution has to be checked separately, which also is done with little effort.

The reason for providing the more systematic constructions in Sections 2.2.3, 2.2.4 and 2.2.5 is that this method generalizes to finding fundamental systems of homogeneous finite difference equations with constant coefficients of arbitrary order. Instead of J_0 one works with one of the constant coefficient finite difference expressions discussed in Section 1.2. One can generalize most of the above theory to this case, including transfer matrices (which are now of a bigger size). Using the Jordan form of the transfer matrix of a constant coefficient expression one can construct a fundamental system. This procedure is the “discrete version” of solving constant coefficient linear ordinary differential equations by the exponential ansatz.

2.3. Solving Inhomogeneous Difference Equations

2.3.1. The general solution of $(J - \lambda I)u = f$. Let J be a Jacobi matrix, $\lambda \in \mathbb{C}$, $f \in s(\mathbb{Z})$ and u_1, u_2 a fundamental system for the homogeneous equation $(J - \lambda I)u = 0$. Also, let $w \in s(\mathbb{Z})$ be a particular solution of $(J - \lambda I)w = f$. Then $u \in s(\mathbb{Z})$ is a solution of $(J - \lambda I)u = f$ if and only if there exist a_1 and a_2 such that

$$(36) \quad u = a_1 u_1 + a_2 u_2 + w.$$

Proof: If u has the form (36), then it easily follows from linearity that $(J - \lambda I)u = f$.

If, on the other hand, $(J - \lambda I)u = f$, then

$$(J - \lambda I)(u - w) = (J - \lambda I)u - (J - \lambda I)w = f - f = 0.$$

As u_1, u_2 is a fundamental system of the homogeneous equation there must be $a_1, a_2 \in \mathbb{C}$ such that $u - w = a_1 u_1 + a_2 u_2$. \square

In the rest of this section we will provide an explicit formula for a particular solution w of the inhomogeneous equation, assuming that a fundamental system of the homogeneous

define the step function $G : \mathbb{R} \rightarrow \mathbb{C}$ by $G(x) = g(n)$ for arbitrary $n \in \mathbb{Z}$ and $x \in [n, n+1)$. One checks that $\int_n^m g = \int_n^m G(x) dx$. The above properties of sums are now an immediate consequence of the corresponding properties of Riemann integrals.

2.3.5. Summation by parts.

$$\int_{m=r}^s (a(m+1) - a(m))b(m+1) = a(s)b(s) - a(r)b(r) - \int_{m=r}^s a(m)(b(m+1) - b(m))$$

Sketch of proof: The statement is true for $s = r$. If $s > r$ one can prove it easily by induction. For $s < r$ it follows then from (41). \square

2.3.6. Variation of parameters. The following Theorem provides a discrete version of the variation of parameters formula for the solution of inhomogeneous linear differential equations.

Theorem. Let J be a discrete Schrödinger operator, $\lambda \in \mathbb{C}$, u_1, u_2 a fundamental system for $(J - \lambda I)u = 0$, $f \in s(\mathbb{Z})$ and $n_0 \in \mathbb{Z}$. Then a particular solution w of $(J - \lambda I)w = f$ is given by

$$(42) \quad w(n) = \frac{1}{W(u_1, u_2)} \left(u_2(n) \int_{n_0}^n u_1 f - u_1(n) \int_{n_0}^n u_2 f \right).$$

Proof: That w is a solution of the inhomogeneous equation follows from a calculation, which uses the definition of J , the definition of w , the properties of the modified Σ -notation and that u_1 and u_2 solve $(J - \lambda I)u = 0$:

$$((J - \lambda I)w)(n) = w(n-1) + (q_n - \lambda)w(n) + w(n+1) = f(n).$$

\square

Based on (2.3.1) we therefore have that the most general solution of $(J - \lambda I)u = f$ is of the form $u = a_1 u_1 + a_2 u_2 + w$. In particular, we can combine this with the results of Section 2.2 to find explicit expressions for all solutions of $(J_0 - \lambda I)u = f$.

2.4. Floquet Theory for Periodic Jacobi Matrices

2.4.1. Periodic discrete Schrödinger operators. For $L \in \mathbb{N}$ a discrete Schrödinger operator J is called L -periodic if the potential q is L -periodic, i.e., $q_{n+L} = q_n$ for all $n \in \mathbb{Z}$.

Given a solution u of $Ju = \lambda u$ define v by $v(n) = u(n+L)$. The periodicity of q implies immediately that v is also a solution of the difference equation, i.e., $Jv = \lambda v$. The operator M which assigns u to v is therefore a function from $N_\lambda(J)$ to itself. It is called the monodromy or Floquet operator.

2.4.2. Floquet multipliers and Floquet solutions. The eigenvalues of the monodromy operator are called Floquet multipliers and its eigenfunction are called Floquet solutions. We know from linear algebra that M has at least one eigenvalue z_1 and eigenvector u_1 , i.e., a solution of $Ju = \lambda u$ such $Mu_1 = z_1 u_1$. Moreover, there is either a second eigenvector u_2 so that $\{u_1, u_2\}$ is linearly independent or else there is a generalized eigenvector u_2 satisfying $Ju_2 = \lambda u_2$ and $Mu_2 = z_1 u_2 + u_1$. In either case we have $Mu_2 = z_2 u_2 + \alpha u_1$ where $\alpha \in \{0, 1\}$ and $z_2 = z_1$ if $\alpha = 1$. Now one computes

$$\begin{aligned} W(u_1, u_2)(n+L) &= (Mu_1)(n)(Mu_2)(n+1) - (Mu_2)(n)(Mu_1)(n+1) \\ &= z_1 z_2 W(u_1, u_2)(n) + z_1 \alpha W(u_1, u_1)(n). \end{aligned}$$

Since $W(u_1, u_1)(n) = 0$ and since, according to Section 2.3.3, $W(u_1, u_2)(n)$ does not depend on n we obtain that $z_1 z_2 = 1$. In particular, if $z_1 = z_2$ then $z_1 = \pm 1$. Note that $\det M = 1$ since the determinant is, by definition, the product of its eigenvalues.

The monodromy operator can be represented by a 2×2 -matrix by choosing a basis in $N_\lambda(J)$. The most convenient basis is $\{c, s\}$ where c and s are the unique solutions of $Ju = \lambda u$ satisfying $c(0) = s(1) = 1$ and $c(1) = s(0) = 0$. The matrix then obtained is

$$\begin{pmatrix} c(L) & s(L) \\ c(L+1) & s(L+1) \end{pmatrix}$$

which coincides with the transfer matrix T_L . For this reason T_L is called monodromy matrix.

Note that all quantities considered here actually depend on λ .

2.4.3. Discriminant and stability set. The function

$$(43) \quad D(\lambda) := \operatorname{tr} T_L(\lambda) = z(\lambda) + \frac{1}{z(\lambda)}$$

is called the discriminant of J . The set

$$(44) \quad S := \{\lambda \in \mathbb{C} : |z(\lambda)| = 1\}$$

is called the stability set of J .

Proposition. $\lambda \in S$ if and only if $D(\lambda) \in [-2, 2]$.

Proof: If $|z(\lambda)| = 1$, then $1/z(\lambda) = \overline{z(\lambda)}$ and thus $D(\lambda) = z(\lambda) + \overline{z(\lambda)} = 2\operatorname{Re} z(\lambda) \in [-2, 2]$.

If, on the other hand, $D(\lambda) \in [-2, 2]$, then there is a $\theta \in [0, \pi]$ such that (for $z = z(\lambda)$) $z + 1/z = 2 \cos \theta$. Therefore $z^2 - 2z \cos \theta + 1 = 0$ and

$$z = \cos \theta \pm \sqrt{\cos^2 \theta - 1} = \cos \theta \pm i \sin \theta.$$

Thus $|z| = 1$. □

2.4.4. Fundamental systems for periodic Jacobi matrices.

Theorem. (a) If $D(\lambda) \in \mathbb{C} \setminus [-2, 2]$, then there is a fundamental system u_+ , u_- for $Ju = \lambda u$ such that u_\pm decays exponentially as $n \rightarrow \pm\infty$.

(b) Let either $D(\lambda) \in (-2, 2)$ or let $D(\lambda) = \pm 2$ such that $z(\lambda)$ has geometric multiplicity 2. Then all solutions of $Ju = \lambda u$ are bounded on \mathbb{Z} .

(c) Suppose that $D(\lambda) = \pm 2$ and $z(\lambda)$ has geometric multiplicity 1. Then there is a fundamental system u_1, u_2 of $Ju = \lambda u$ such that u_1 is bounded and u_2 is unbounded with $|u_2(n)| \leq C(|n| + 1)$ for some C and all $n \in \mathbb{Z}$.

Sketch of Proof: Based on (2.4.2) and (2.4.3) the proof of these results is very similar to the arguments provided for the case of the free Jacobi matrix J_0 in Section 2.2.5. In case (c), where $z(\lambda) = \pm 1$, there exists a Jordan chain $\{v, w\}$ for $T_L(\lambda)$, i.e. $T_L(\lambda)v = \pm v$ and $(T_L(\lambda) \mp I)w = v$. With v and w as initial conditions we get one bounded and one linearly growing solution of $Ju = \lambda u$. □

Note that if $D(\lambda) = \pm 2$, then the geometric multiplicity of $z(\lambda)$ may be either one or two. Examples with geometric multiplicity one are given by the numbers $\lambda = \pm 2$ for the free Jacobi matrix, see Section 2.2.4. An example with geometric multiplicity two will be found in Section 2.4.7 below.

2.4.5. Real potentials.

Theorem. If q is real-valued, then $S \subset \mathbb{R}$.

Proof: Let $\lambda \in S$ and z the corresponding Floquet multiplier with $|z| = 1$. By Section 2.4.2 there is a non-zero solution of $Ju = \lambda u$ with $u(n+L) = zu(n)$ for all $n \in \mathbb{Z}$. Using this for $n = 0$ and $n = 1$ in $u(n-1) + q_n u(n) + u(n+1) = \lambda u(n)$ we see that

$$q(1)u(1) + u(2) + \frac{1}{z}u(L) = \lambda u(1)$$

and

$$zu(1) + u(L-1) + q(L)u(L) = \lambda u(L).$$

This implies that

$$(45) \quad \begin{pmatrix} q_1 & 1 & & & 1/z \\ 1 & q_2 & \ddots & & \\ & \ddots & \ddots & \ddots & \\ & & \ddots & \ddots & 1 \\ z & & & 1 & q_L \end{pmatrix} \begin{pmatrix} u(1) \\ u(2) \\ \\ \\ u(L) \end{pmatrix} = \lambda \begin{pmatrix} u(1) \\ u(2) \\ \\ \\ u(L) \end{pmatrix}.$$

As $1/z = \bar{z}$, the matrix on the left of (45) is hermitean. Thus its eigenvalue λ is real. \square

2.4.6. Example. Find the discriminant and stability set for the 3-periodic potential q with $q_1 = 1$, $q_2 = 0$ and $q_3 = -1$.

2.4.7. Example. Let $a \in \mathbb{C}$ and the 2-periodic potential q be given by

$$q_n := \left\{ \begin{array}{ll} a & \text{if } n \text{ odd,} \\ -a & \text{if } n \text{ even.} \end{array} \right\}$$

Find the discriminant $D(\lambda) = D_a(\lambda)$ for every $a \in \mathbb{C}$. Find the stability set $S = S_a$ for (i) all $a \in \mathbb{R}$, (ii) $a = i$, and (iii) $a = 3i$.

Functional Analysis

We have seen that Jacobi matrices can be thought of as linear operators acting in the form of infinite-dimensional matrices on the vector space of sequences $s(\mathbb{Z})$. In order to do analysis with Jacobi matrices we will need to be able to measure the “size” of a Jacobi matrix and also the “distance” between two of them. Recall that this is done for finite matrices through the introduction of norms. A particularly useful way of defining a norm on, say, the complex $N \times N$ -matrices is by first choosing a norm $\|\cdot\|$ on \mathbb{C}^N and then setting

$$(46) \quad \|A\| = \sup \frac{\|Ax\|}{\|x\|},$$

where the supremum is taken over all non-zero vectors x in \mathbb{C}^N .

In the following we will try to do the same for linear operators on infinite dimensional vector spaces such as $s(\mathbb{Z})$. This will come with a number of substantial difficulties:

First of all we will have to find norms on spaces of sequences (which replace \mathbb{C}^N). It turns out that there are no useful norms on the space of *all* sequences $s(\mathbb{Z})$. However, we will find that some of the familiar ways of introducing norms on \mathbb{C}^N can be extended to certain naturally chosen subspaces of $s(\mathbb{Z})$. In at least one of these cases the norm will be induced by an inner product, a fact which will have tremendous implications for the theory of linear operators to be built up later.

Once we have norms on sequence spaces, we can try to use (46) to define a norm for linear operators such as Jacobi matrices on these spaces. Here we run into two more difficulties: Due to having been forced into working with subspaces of $s(\mathbb{Z})$ in the definition of norms, it will not be automatic that $\|Ax\|$ is even defined. Also, even if $\|Ax\|/\|x\|$ makes sense for every x , the supremum in (46) may become infinite.

All these difficulties can be overcome, but their presence demonstrates that the theory of infinite dimensional matrices (or, more generally, linear operators in infinite dimensional vector spaces) is much richer than the finite dimensional counterpart. It is exactly at this point where Linear Algebra turns into Functional Analysis and Operator Theory.

3.1. Vector Spaces of Sequences

3.1.1. Norms and inner products. Let V be a vector space. A function $\|\cdot\| : V \rightarrow \mathbb{R}$ is called a norm on V if it satisfies the following conditions:

- (a) $\|x\| \geq 0$ for all $x \in V$,
- (b) $\|x\| = 0$ if and only if $x = 0$,
- (c) $\|\alpha x\| = |\alpha| \|x\|$ for all $\alpha \in \mathbb{C}$ and all $x \in V$,
- (d) $\|x + y\| \leq \|x\| + \|y\|$ for all $x, y \in V$. (This inequality is called the triangle inequality.)

A function $(\cdot, \cdot) : V \times V \rightarrow \mathbb{C}$ is called an *inner product* or a *scalar product* if it satisfies the following conditions:

- (a) $(x, x) \geq 0$ for all $x \in V$,
- (b) $(x, x) = 0$ if and only if $x = 0$,

- (c) $(x, \alpha y + \beta z) = \alpha(x, y) + \beta(x, z)$, for all $\alpha, \beta \in \mathbb{C}$ and all $x, y, z \in V$,
 (d) $(x, y) = \overline{(y, x)}$ for all $x, y \in V$.

A complete normed vector space is called a Banach space and a complete inner product space is called a Hilbert space.

3.1.2. Schwarz's inequality. An inner product satisfies Schwarz's inequality¹, i.e.,

$$|(x, y)| \leq (x, x)^{1/2}(y, y)^{1/2}.$$

Sketch of proof: Note that $(x, y) = 0$ for all $x \in V$ if and only if $y = 0$. Assume now that $(x, y) \neq 0$ (otherwise there is nothing to prove). Let $s = |(x, y)|/(x, y)$. Then, for any real r ,

$$0 \leq (x - rsy, x - rsy) = (x, x) - 2r|(x, y)| + r^2(y, y).$$

Schwarz's inequality follows now from choosing $r = |(x, y)|/(y, y)$. \square

Because of Schwarz' inequality one sees immediately that every inner product space is a normed vector space under the norm $x \mapsto \|x\| = (x, x)^{1/2}$.

3.1.3. Continuity of norm and inner product. Since, by the triangle inequality, $|\|x\| - \|x_0\|| \leq \|x - x_0\|$ we have that the norm is a continuous function.

The inner product is jointly continuous in its arguments. More precisely, if x tends to x_0 and y tends to y_0 , i.e., if $\|x - x_0\|$ and $\|y - y_0\|$ tend to zero, then

$$\lim_{\substack{x \rightarrow x_0 \\ y \rightarrow y_0}} (x, y) = (x_0, y_0).$$

In particular,

$$\lim_{x \rightarrow x_0} (x, y_0) = \lim_{y \rightarrow y_0} (x_0, y) = (x_0, y_0).$$

For the proof show, using Schwarz's inequality, that $|(x, y) - (x_0, y_0)| \leq c(\|x - x_0\| + \|y - y_0\|)$ for some constant c .

3.1.4. The ℓ^p spaces. Let $p \geq 1$ be a real number. Recall that one can uniquely define the p -th power and the p -th root of a nonnegative real number. We define

$$\ell^p(Z) = \{f \in s(Z) : \sum_{n \in Z} |f(n)|^p < \infty\}.$$

We also define

$$\ell^\infty(Z) = \{f \in s(Z) : \sup\{|f(n)| : n \in Z\} < \infty\}.$$

For $1 \leq p < \infty$ we also define

$$\|f\|_p = \left(\sum_{n \in Z} |f(n)|^p \right)^{1/p}$$

if $f \in \ell^p(Z)$. If $f \notin \ell^p(Z)$ we set $\|f\|_p = \infty$. Similarly, $\|f\|_\infty = \sup\{|f(n)| : n \in Z\}$ if $f \in \ell^\infty(Z)$ and $\|f\|_\infty = \infty$ if $f \notin \ell^\infty(Z)$. We will later show that the $\|\cdot\|$ -notation is justified.

¹For finite sums the inequality was first discovered by Augustin-Louis Cauchy (1789-1857). Victor Ya. Bunyakovskii (1804-1889) wrote it first down for integrals in 1859. Hermann A. Schwarz (1843-1921) published it again 1885 and the inequality carries his name since Bunyakovskii's paper was not widely known.

3.1.5. Hölder's inequality. If $1 < p < \infty$ then the number q satisfying $1/p + 1/q = 1$ is called the *conjugate exponent* for p . One defines also that ∞ is the conjugate exponent to 1 and vice versa. (Note that the equation $1/p + 1/q = 1$ is still satisfied in a sense.)

Theorem. If $p, q \in [1, \infty]$ and $1/p + 1/q = 1$ then

$$\sum_{n \in Z} |f(n)g(n)| \leq \|f\|_p \|g\|_q.$$

This fundamental inequality is called Hölder's inequality.

Sketch of proof: The claim is evident if $p = 1$ and $q = \infty$ or if $p = \infty$ and $q = 1$. Also there is nothing to show if $\|f\|_p$ or $\|g\|_q$ equals zero or infinity. Assume therefore that $p, q \in (1, \infty)$ and that $\|f\|_p$ and $\|g\|_q$ are positive finite numbers. One sees from the graph of the exponential function, due to its convexity, that

$$\exp\left(\frac{s}{p} + \frac{t}{q}\right) \leq \frac{\exp(s)}{p} + \frac{\exp(t)}{q}$$

for any real numbers s and t which implies that

$$ab \leq \frac{a^p}{p} + \frac{b^q}{q}$$

whenever a and b are nonnegative real numbers. Hölder's inequality follows now easily by choosing $a = |f(n)|/\|f\|_p$ and $b = |g(n)|/\|g\|_q$ and then summing over n . \square

3.1.6. Minkowski's inequality. If $p \in [1, \infty]$ and $f, g \in \ell^p(Z)$ then

$$\|f + g\|_p \leq \|f\|_p + \|g\|_p.$$

This is the triangle inequality which, in the present context, is often called Minkowski's inequality.

Sketch of proof: The cases $p = 1$ and $p = \infty$ are trivial. If $\|f + g\|_p = \infty$ one shows that at least one of $\|f\|_p$ and $\|g\|_p$ is infinite (note that $(a+b)^p \leq (2a)^p + (2b)^p$ for $a, b \geq 0$). Assume therefore now that $1 < p < \infty$ and $\|f + g\|_p < \infty$. From Hölder's inequality we obtain

$$\sum_{n \in Z} |f(n)| |f(n) + g(n)|^{p-1} \leq \|f\|_p \|f + g\|_p^{p/q}$$

where $q = p/(p-1)$. Similarly

$$\sum_{n \in Z} |g(n)| |f(n) + g(n)|^{p-1} \leq \|g\|_p \|f + g\|_p^{p/q}$$

Adding these two inequalities and using the triangle inequality we get

$$\|f + g\|_p^p \leq (\|f\|_p + \|g\|_p) \|f + g\|_p^{p-1}.$$

which is the desired result since $\|f + g\|_p < \infty$. \square

3.1.7. $\ell^p(Z)$ is a Banach space. If $p \in [1, \infty]$ then $\ell^p(Z)$ is a vector space and $\|\cdot\|_p$ is a norm on $\ell^p(Z)$. $\ell^p(Z)$ is complete.

Sketch of proof: The triangle inequality is just Minkowski's inequality.

Let $n \mapsto f_n$ be a Cauchy sequence in $\ell^p(Z)$. One can show quickly that, for any fixed $k \in Z$ the sequence $n \mapsto f_n(k)$ is also Cauchy and hence convergent (we know that \mathbb{C} is complete). Denote the limit by $f(k)$. Thus, given $\varepsilon > 0$ there is an $m(k)$ such that

$|f_n(k) - f(k)| < \varepsilon$ for all $n \geq m(k)$. Since $n \mapsto f_n$ is Cauchy the sequence $n \mapsto \|f_n\|_p$ is also Cauchy and hence bounded by some constant C . Introduce the sequence $f_n^{(N)}$ by letting

$$f_n^{(N)}(k) = \begin{cases} f_n(k) & \text{if } |k| \leq N \\ 0 & \text{otherwise} \end{cases}$$

and similarly the sequence $f^{(N)}$. Then we have

$$\|f_n^{(N)}\|_p \leq \|f_n\|_p \leq C$$

and

$$\|f^{(N)}\|_p - \|f_n^{(N)}\|_p \leq \|f^{(N)} - f_n^{(N)}\|_p \leq (2N + 1)^{1/p} \varepsilon$$

for all $n \geq \max\{m(k) : |k| \leq N\}$. This implies that $\|f^{(N)}\|_p \leq C$ regardless of N and hence $\|f\|_p \leq C$. \square

3.1.8. $\ell^2(Z)$ is a Hilbert space. If $f, g \in \ell^2(Z)$ we let

$$(f, g) = \sum_{n \in Z} \overline{f(n)} g(n).$$

This defines an inner product on $\ell^2(Z)$.

Sketch of proof: The main task is to show that (f, g) is finite, but this follows immediately from Hölder's inequality. \square

$\ell^2(Z)$ is a Hilbert space since we proved before that it is complete.

3.1.9. A basis of $\ell^p(Z)$. By e_k , $k \in Z$, we denote the vectors for which $e_k(k) = 1$ but $e_k(n) = 0$ when $n \neq k$. All of these vectors are in $\ell^p(Z)$ for any $p \in [1, \infty]$. It is clear that, unless Z is a finite set, the collection $B = \{e_k : k \in Z\}$ does not form an algebraic basis of $\ell^p(Z)$ since the span $\langle B \rangle$ of B contains only sequences which are zero for all but finitely many arguments.

However, defining

$$f_N = \sum_{\substack{k \in Z \\ |k| \leq N}} f(k) e_k \in \langle B \rangle$$

we see that

$$\|f - f_N\|_p^p = \sum_{\substack{\ell \in Z \\ |\ell| > N}} |f(\ell)|^p$$

tends to zero as N tends to infinity provided that $p < \infty$. Hence $\ell^p(Z)$, for $p < \infty$ is the closure of the span of B .

We will therefore henceforth use a different definition of basis than is commonly used in algebra. A subset of a normed vector space V is called a *basis* of V if it is linearly independent and if its span is dense in V .

In this sense B is a basis of $\ell^p(Z)$ when $p < \infty$. It is called the canonical basis.

When $p = 2$ then the vectors in B are normalized (i.e., have norm one) and any two different ones are orthogonal (i.e., their inner product is zero). The canonical basis is therefore an orthonormal basis.

3.2. The Geometry of Hilbert Space

3.2.1. Orthogonality. Two elements x and y of an inner product space are called orthogonal if $(x, y) = 0$. In this case we write $x \perp y$. If $(x, y) = 0$ for all $y \in M$, some subset of the inner product space, we write $x \perp M$.

If x and y are orthogonal, then the Pythagorean identity

$$\|x + y\|^2 = \|x\|^2 + \|y\|^2$$

is satisfied.

3.2.2. The parallelogram identity. For arbitrary elements x, y of an inner product space one has the parallelogram identity

$$\|x + y\|^2 + \|x - y\|^2 = 2\|x\|^2 + 2\|y\|^2.$$

3.2.3. Convex sets. A subset C of a vector space is called convex if with every pair x, y of points in C the line segment $[x, y] = \{tx + (1 - t)y : t \in [0, 1]\}$ joining x and y is also contained in C .

Theorem. Let C be a closed convex set in the Hilbert space \mathcal{H} and $x_0 \in \mathcal{H}$. Then there exists a unique $x_C \in C$ such that

$$\|x_0 - x_C\| = \inf\{\|x_0 - y\| : y \in C\}.$$

For a proof see, for instance, W. Rudin, Real and Complex Analysis, Theorem 4.10. Note that subspaces of vector spaces are convex.

3.2.4. Orthogonal complements. Let M be a subset of the Hilbert space \mathcal{H} . Then

$$M^\perp := \{x \in \mathcal{H} : x \perp M\},$$

called the orthogonal complement of M in \mathcal{H} , is a closed subspace of \mathcal{H} .

Theorem. If M is a closed subspace of the Hilbert space \mathcal{H} , then

$$\mathcal{H} = M \oplus M^\perp.$$

Sketch of proof: Assume $x \in M \cap M^\perp$. Then $(x, x) = 0$, i.e., $x = 0$. Now choose $x \in H$ and let a be the unique element of M closest to x (as found in (3.2.3)). Then $b = x - a \perp M$ (and thus $x = b + a \in M + M^\perp$). To see that $b \in M^\perp$ note that $\|b\|^2 \leq \|b - ty\|^2$ for any $y \in M$ of norm one and any complex number t . Choosing $t = (y, b)$ gives then $0 \leq -|(y, b)|^2$. Thus $x - a = b \perp y$. \square

Corollary. If M is a closed subspace of a Hilbert space \mathcal{H} , then $M = M^{\perp\perp}$. $M^\perp = \{0\}$ if and only if $M = \mathcal{H}$.

3.3. Bounded Linear Operators

3.3.1. Linear operators. Let X and Y be vector space. A function (or operator) A from X to Y is called *linear* if $A(rx + sx') = rAx + sAx'$ whenever $r, s \in \mathbb{C}$ and $x, x' \in X$. The set of all linear operators from X to Y is denoted by $\mathcal{L}(X, Y)$. It is itself a complex vector space.

3.3.2. Bounded linear operators. Let A be a linear transformation from a normed vector space X to a normed vector space Y . Define

$$\|A\| = \sup\left\{\frac{\|Ax\|}{\|x\|} : 0 \neq x \in X\right\}.$$

Note that the symbol $\|\cdot\|$ is used here for two different functions. However, a confusion can not arise.

The linear operator A is called *bounded* if $\|A\| < \infty$. Other wise it is called *unbounded*. The set of all bounded linear operators from X to Y is denoted by $\mathcal{B}(X, Y)$. It is a subspace of $\mathcal{L}(X, Y)$.

The function $A \mapsto \|A\|$ is a norm on $\mathcal{B}(X, Y)$.

One may show that

$$\|A\| = \sup\{\|Ax\| : x \in X, \|x\| \leq 1\} = \sup\{\|Ax\| : x \in X, \|x\| = 1\}$$

and

$$\|A\| = \inf\{C : \forall x \in X : \|Ax\| \leq C\|x\|\}.$$

Moreover,

$$\|AB\| \leq \|A\| \|B\|.$$

When Y is an inner product space, one also has

$$\|A\| = \sup\{|(Ax, y)| : x \in X, y \in Y, \|x\| = 1, \|y\| = 1\}.$$

This is due to the fact that $\|y\| = \sup\{|(z, y)| : z \in Y, \|z\| = 1\}$ in the inner product space Y .

3.3.3. Bounded operators are continuous. Let A be a bounded linear transformation from a normed vector space X to a normed vector space Y and suppose that $n \mapsto x_n$ is a convergent sequence in X . Then

$$\|Ax_n - Ax\| = \|A(x_n - x)\| \leq \|A\| \|x_n - x\|$$

tends to zero and hence the sequence $n \mapsto Ax_n$ tends to Ax . This shows (by definition) that A is a continuous function at x . Since x was arbitrary we have that A is continuous.

The converse of this statement is also true.

3.3.4. The Neumann series for an operator of small norm. Suppose A be a bounded linear transformation from a Hilbert space H to itself such that $\|A\| < 1$. Choose any $x \in H$. Then $\|A^k x\| \leq \|A\|^k \|x\|$ so that the sequence $n \mapsto \sum_{k=0}^n A^k x$ is Cauchy and hence convergent. Therefore one may define the transformation $B : H \rightarrow H : x \mapsto \sum_{k=0}^{\infty} A^k x$. The transformation B is linear and bounded. Moreover, $(I - A)B = B(I - A) = I$ so that

$$(I - A)^{-1} = \sum_{k=0}^{\infty} A^k.$$

3.3.5. Matrix representation of bounded operators. Just as in the case of linear transformations between finite-dimensional vector spaces one may associate a matrix with a bounded linear operator A from $\ell^p(Z)$ to $\ell^{\tilde{p}}(\tilde{Z})$ when p and \tilde{p} are finite. Not surprisingly the matrix will in general be infinite in size. When $j \in Z$ consider Ae_j as an (infinite) column. One collects these columns in a matrix M so that $M_{k,j} = (Ae_j)(k)$ for $j \in Z$ and $k \in \tilde{Z}$.

One now wants to interpret the application of the map A to the sequence f as a matrix multiplication of the matrix M and the column f , i.e., one wants that, for each fixed k ,

$$(Af)(k) = \sum_{j \in Z} M_{k,j} f_j.$$

But this, including the convergence of the series on the right follows from the continuity and linearity of A . In particular, $\sum_{j \in Z} |M_{k,j}|^q < \infty$ when q is exponent conjugate to p .

Conversely, given a matrix M , matrix multiplication defines a bounded linear transformation A at least from $\ell^p(Z)$ to $\ell^\infty(\tilde{Z})$ when $\sup_{k \in \tilde{Z}} \sum_{j \in Z} |M_{k,j}|^q < \infty$. In this case

$$\|A\| \leq \sup_{k \in \tilde{Z}} \|M_{k,\cdot}\|_q.$$

A sufficient (but not necessary) condition for M to provide a linear transformation from $\ell^p(Z)$ to $\ell^{\tilde{p}}(\tilde{Z})$ is that

$$\sum_{k \in \tilde{Z}} \|M_{k,\cdot}\|_q^{\tilde{p}} < \infty.$$

3.3.6. Shift operators. We now define so called shift operators S_+ and S_- from $\ell^p(Z)$ to $\ell^p(Z)$ for $Z = \mathbb{Z}$ and for $Z = \mathbb{N}$. In the first case we let $(S_+f)(n) = f(n-1)$ and $(S_-f)(n) = f(n+1)$. In the second case we let $(S_+f)(1) = 0$ while all other assignments remain unchanged. Obviously S_+ is a shift to the right while S_- is a shift to the left. The entries in the matrices associated with shift operators are all zeros except for ones in the superdiagonal (for S_-) or the subdiagonal (for S_+).

When defined on \mathbb{Z} we have $S_\pm = S_\mp^{-1}$, while on \mathbb{N} we have $S_-S_+ = I$ and $S_+S_- \neq I$. Thus, in this case, S_+ is the right-inverse but not the left-inverse of S_- .

Note that both S_+ and S_- are linear operators of norm one.

The operator $J_0 = S_+ + S_- : \ell^p(Z) \rightarrow \ell^p(Z)$ is the free Jacobi matrix introduced in (31). It is also a bounded linear operator. Its norm is less than two by the triangle inequality. By choosing an appropriate sequence of vectors in $\ell^p(Z)$ one can show that, in fact, $\|J_0\| = 2$ regardless of $p \in [1, \infty]$.

3.3.7. Multiplication operators. Let $Z \subset \mathbb{Z}$ and $1 \leq p \leq \infty$. Let $a : Z \mapsto \mathbb{C}$ be a bounded function, that is, $\|a\|_\infty = \sup\{|a(n)| : n \in Z\} < \infty$. Then $A : \ell^p(Z) \mapsto \ell^p(Z)$ defined through

$$(47) \quad (Af)(n) = a(n)f(n), \quad n \in Z,$$

is a bounded linear operator with $\|A\| = \|a\|_\infty$.

If a is unbounded, then one does not get a bounded operator on $\ell^p(Z)$ in this way. In fact, in this case the operator $A : V \mapsto \ell^p(Z)$ defined through (47), where

$$V = \{f \in \ell^p(Z) : f(n) = 0 \text{ for all but finitely many } n \in Z\},$$

is an unbounded linear operator.

3.3.8. Bounded Jacobi matrices. Let J be a Jacobi matrix as given by (19) with bounded sequences a , b and c . Then J defines a bounded linear operator on $\ell^p(\mathbb{Z})$ through (18) for every $1 \leq p \leq \infty$. One has $\|J\| \leq \|a\|_\infty + \|b\|_\infty + \|c\|_\infty$.

Sketch of proof: If A , B and C are the multiplication operators defined by the sequences a , b and c , then $J = AS_+ + B + S_-C$.

Note that a similar result holds for more general matrices of the form (14). Is it possible to find conditions under which this result can be generalized to hold for matrices with infinitely many non-zero diagonals?

3.4. Dual Spaces and Adjoint Operators

While much of the theory of dual spaces and adjoint operators can be carried out in the more general setting of normed spaces (and, particularly nicely, for the Banach spaces $\ell^p(Z)$, $1 < p < \infty$), we will for simplicity mostly consider the case of Hilbert spaces.

3.4.1. Dual spaces. A linear operator from a normed linear space X to the field of complex numbers is called a linear functional. The set $\mathcal{B}(X, \mathbb{C})$ of all bounded linear functionals on X is a vector space. This space is called the *dual space* of X and is denoted by X^* . Note that X^* is a normed vector space (in fact a Banach space) under the operator norm.

3.4.2. The Riesz representation theorem.

Theorem. Let \mathcal{H} be a Hilbert space and $\phi \in \mathcal{H}^*$. Then there exists a unique $x_\phi \in \mathcal{H}$ such that

$$(48) \quad \phi x = (x_\phi, x)$$

for all $x \in \mathcal{H}$. One has $\|\phi\| = \|x_\phi\|$.

For a proof see, for instance, W. Rudin, Real and Complex Analysis, Theorem 4.12.

A bijective linear map is called an *isomorphism*. A map Φ for which $\|\Phi x\| = \|x\|$ for all x is called an *isometry*. Hence the map $\phi \mapsto x_\phi$ described in the theorem is an isometric isomorphism from \mathcal{H}^* to \mathcal{H} (“onto” is seen easily, the rest follows from the theorem). In this sense Hilbert spaces are “self-dual”, a property not shared by general Banach spaces.

3.4.3. Adjoint operators.

Theorem. Let \mathcal{H}_1 and \mathcal{H}_2 be Hilbert spaces with inner products $(\cdot, \cdot)_1$ and $(\cdot, \cdot)_2$. To $A \in B(\mathcal{H}_1, \mathcal{H}_2)$ there exists a unique $A^* \in B(\mathcal{H}_2, \mathcal{H}_1)$ such that

$$(49) \quad (A^*y, x)_1 = (y, Ax)_2$$

for all $x \in \mathcal{H}_1$ and $y \in \mathcal{H}_2$. A^* is called the adjoint of A . One has $\|A^*\| = \|A\|$.

Sketch of proof: Let $y \in \mathcal{H}_2$ and define $\phi_y x := (y, Ax)_2$. Thus $\phi_y \in \mathcal{H}_1^*$ and by Riesz there is a unique $y^* \in \mathcal{H}_1$ such that $(y^*, x)_1 = \phi_y x = (y, Ax)_2$. One defines $A^*y := y^*$ and checks that $A^* \in B(\mathcal{H}_2, \mathcal{H}_1)$ with $\|A^*\| = \|A\|$. \square

Note that $(A^*)^* = A$, $(A + B)^* = A^* + B^*$ and $(AB)^* = B^*A^*$ whenever A and B are bounded linear operators between appropriate Hilbert spaces.

3.4.4. Matrix of the adjoint operators. If $\mathcal{H}_1 = \ell^2(Z)$ and $\mathcal{H}_2 = \ell^2(\tilde{Z})$ and if M is the matrix associated with A , then the conjugate transpose M^* of M (defined through $M^*(j, k) = \overline{M(k, j)}$) is the matrix associated with A^* . This follows by applying (49) to the basis vectors e_j and e_k .

3.4.5. Adjoints of shift operators. With the aid of (49) one computes immediately that $S_+^* = S_-$ and that $S_-^* = S_+$.

It is now obvious that the free Jacobi matrix $J_0 = S_+ + S_-$ is its own adjoint.

3.4.6. Selfadjoint linear operators. An operator $T \in B(\mathcal{H}, \mathcal{H})$ is called selfadjoint if $T = T^*$.

3.5.7. The spectrum of a selfadjoint linear operator.

Theorem. If T is a bounded self-adjoint operator from a Hilbert space H to itself then its spectrum is a subset of the real line. Moreover, the residual spectrum of T is empty.

Sketch of proof: Let $\lambda = s + it$ where $s, t \in \mathbb{R}$. Then

$$\|(T - \lambda)x\|^2 = \|(T - s)x\|^2 + t^2\|x\|^2.$$

If t is different from zero, then $T - \lambda$ is injective as a proof by contradiction shows. Hence the point spectrum of T is real.

Now assume that the sequence $y_n = (T - \lambda)x_n$ in the image of $T - \lambda$ converges to a point $y \in H$. If $t \neq 0$ then

$$\|x_n - x_m\|^2 \leq \frac{1}{t^2} \|(T - \lambda)(x_n - x_m)\|^2 = \frac{\|y_n - y_m\|^2}{t^2}.$$

Hence x_n is a Cauchy sequence which converges since H is complete. Denote its limit by x . Then

$$\|y - (T - \lambda)x\| = \lim_{n \rightarrow \infty} \|(T - \lambda)(x_n - x)\| \leq \|T - \lambda\| \lim_{n \rightarrow \infty} \|x_n - x\| = 0,$$

i.e., the image of $T - \lambda$ is closed. This proves that the continuous spectrum of T is real.

Finally assume that $T - \lambda$ is injective and that the image of $T - \lambda$ is a proper subset of H . Then there is a nonzero vector $x' \in H$ which is orthogonal to the image of $T - \lambda$ (cf. Theorem 3.2.4). Hence $0 = (x', (T - s - it)x) = ((T - s + it)x', x)$ for all $x \in H$, which implies that $\bar{\lambda} = s - it$ is an eigenvalue of T . But this is impossible. \square

3.5.8. Spectrum and resolvent of J_0 .

Theorem. The spectrum of the free Jacobi matrix J_0 is purely continuous and consists of the interval $[-2, 2]$. The resolvent of J_0 is the “integral” operator \mathcal{G} defined by

$$(\mathcal{G}f)(n) = \sum_{m=-\infty}^{\infty} \frac{z^{1+|m-n|}}{z^2 - 1} f(m)$$

where z is the root of the equation $\lambda = z + 1/z$ which is located inside the unit disk.

Sketch of proof: Suppose $|z| < 1$. First note that

$$\sum_{m=-\infty}^{\infty} |z|^{|m-n|} = \sum_{n=-\infty}^{\infty} |z|^{|m-n|} = \frac{2}{1 - |z|}.$$

By Schwarz’s inequality, assuming that $f \in \ell^2(\mathbb{Z})$, one obtains

$$\left(\sum_{m=-\infty}^{\infty} |z|^{|m-n|} |f(m)| \right)^2 \leq \frac{2}{1 - |z|} \sum_{m=-\infty}^{\infty} |z|^{|m-n|} |f(m)|^2.$$

Therefore

$$\begin{aligned} \|\mathcal{G}f\|^2 &= \sum_{n=-\infty}^{\infty} |(\mathcal{G}f)(n)|^2 \leq \frac{|z|^2}{(1 - |z|^2)^2} \sum_{n=-\infty}^{\infty} \left(\sum_{m=-\infty}^{\infty} |z|^{|m-n|} |f(m)| \right)^2 \\ &\leq \frac{|z|^2}{(1 - |z|^2)^2} \frac{2}{1 - |z|} \sum_{n=-\infty}^{\infty} \sum_{m=-\infty}^{\infty} |z|^{|m-n|} |f(m)|^2. \end{aligned}$$

Interchanging the summations² over n and m yields

$$\|\mathcal{G}f\|^2 \leq \frac{|z|^2}{(1-|z|^2)^2} \frac{4}{(1-|z|)^2} \|f\|_2^2.$$

Hence $\mathcal{G}f$ is in $\ell^2(\mathbb{Z})$ and \mathcal{G} is a bounded operator with norm at most $2/(1-|z|)^2$.

Since $J_0 - \lambda$ is continuous and linear one finds next that $((J_0 - \lambda) \circ \mathcal{G})f = f$. Also, after shifting summation indices, one shows that $(\mathcal{G} \circ (J_0 - \lambda))f = f$. Therefore $\mathcal{G} = (J_0 - \lambda)^{-1}$.

We have now proved that $J_0 - \lambda$ is a bijection from $\ell^2(\mathbb{Z})$ to itself when $|z| < 1$, i.e., when $\lambda \notin [-2, 2]$. This shows that the spectrum of J_0 is contained in $[-2, 2]$.

Next we prove that we actually have equality here. Assume first that $\lambda \in (-2, 2)$. Then the general solution of $J_0 f = \lambda f$ is $f = \alpha z^n + \beta z^{-n}$ where $|z| = 1$ (cf. 2.2.5). From this one sees quickly that λ can not be an eigenvalue. Hence both the point spectrum and, by 3.5.7, the residual spectrum of J_0 are empty. To show that λ is in the continuous spectrum we only have to show that $J_0 - \lambda$ is not onto. We will now show that the sequence e_0 is not in the image of $J_0 - \lambda$. According to the variation of constants formula (42) (or by direct computation) a particular solution of $(J_0 - \lambda)f = e_0$ is given by

$$f(n) = \frac{z}{z^2 - 1} \begin{cases} 0 & \text{if } n \geq 0 \\ z^n - z^{-n} & \text{if } n \leq 0 \end{cases}.$$

This implies that no solution of $(J_0 - \lambda)f = e_0$ can be square summable. Hence $(-2, 2)$ is in the continuous spectrum of J_0 . A similar argument can be made to prove that both -2 and 2 are also in the continuous spectrum. This fact also follows since the spectrum is closed but point and residual spectrum are empty. \square

This proof can be adapted in a straightforward manner to show that the spectrum of a periodic Jacobi matrix is purely continuous and coincides with its stability set.

²This does not come for free as interchanging limit processes is generally not allowed. In the present case where the summands are all positive, however, this is justifiable.

In particular for Dirichlet boundary conditions on both sides the matrix is obtained by suitably truncating an infinite Jacobi matrix.

The system of equations $(L\check{y})(n) = \lambda\check{y}(n)$, $n = 1, \dots, N$ is represented by $Jy = f$ where $y = \psi^{-1}(\check{y}) \in s(Z)$ and $y(k) = \check{y}(k)$, $k = 1, \dots, N$. In the future we will make no more notational distinctions between y and \check{y} since their meaning will be clear from the context.

J is called the Jacobi matrix associated with L and the boundary conditions $y(0) - h_\ell y(1) = 0$ and $y(N+1) - h_r y(N) = 0$.

One can also make sense of the cases where h_ℓ and/or h_r becomes infinite.

4.1.2. First results in inverse problems for Jacobi matrices. The characteristic polynomial of a matrix A is $\det(\lambda - A)$. The trace of A , written as $\text{tr}(A)$ is the negative of the next to leading coefficient of the characteristic polynomial. Given an $n \times n$ -matrix A we denote by

$$P_k(\lambda) = \lambda^k + a_k \lambda^{k-1} + b_k \lambda^{k-2} + \dots$$

the characteristic polynomial of the upper left $k \times k$ block of A .

Theorem. Let A be an $n \times n$ -matrix such that $A_{j,k} = 0$ if $|j - k| \geq 2$ and $A_{j,k} \neq 0$ if $|j - k| = 1$. Let B be the $(n-1) \times (n-1)$ -matrix obtained from A by deleting the last row and column. If all eigenvalues of A and B (including their algebraic multiplicities) are known then so are the $2n-1$ quantities $A_{1,1}, \dots, A_{n,n}, A_{2,1}A_{1,2}, \dots, A_{n,n-1}A_{n-1,n}$.

PROOF. The proof is by induction on n . The statement is true for $n = 1$. Assume therefore that the statement holds for $n-1$.

Since knowing the eigenvalues of a matrix, including their algebraic multiplicities, is equivalent to knowing its characteristic polynomial we may assume that the polynomials P_n and P_{n-1} and hence the numbers a_n, a_{n-1}, b_n , and b_{n-1} are given. Compute P_n by expansion with respect to the last column. This gives

$$(51) \quad P_n(\lambda) = (\lambda - A_{n,n})P_{n-1}(\lambda) - A_{n-1,n}A_{n,n-1}P_{n-2}(\lambda)$$

Comparing here the coefficients of λ^{n-1} gives that $A_{n,n} = a_{n-1} - a_n$ is known. Next, comparing the coefficients of λ^{n-2} yields

$$A_{n-1,n}A_{n,n-1} = b_{n-1} - b_n + A_{n,n}a_{n-1}.$$

Since $A_{n-1,n}A_{n,n-1} \neq 0$ we may solve equation (51) for P_{n-2} , which therefore is uniquely determined. Induction completes now the proof. \square

It is not possible to retrieve the quantities $A_{k,k-1}$ and $A_{k-1,k}$ themselves. This is shown by the following proposition.

Proposition. Let A be an $n \times n$ -matrix such that $A_{j,k} = 0$ if $|j - k| \geq 2$. Then the coefficients of the characteristic polynomial of A are polynomials in the $2n-1$ variables $A_{1,1}, \dots, A_{n,n}, A_{2,1}A_{1,2}, \dots, A_{n,n-1}A_{n-1,n}$.

PROOF. The proof is again by induction on n . The statement is true for $n = 1$. Assume it is true for $k \times k$ -matrices of the type described when $k < n$. Equation (51) and induction complete the proof. \square

If one assumes additionally that $A_{k,k-1}$ and $A_{k-1,k}$ are equal then they are, of course, determined up to a sign.

While it might appear intriguing that the $2n+1$ eigenvalues of A and B determine the $2n+1$ quantities $A_{1,1}, \dots, A_{n,n}, A_{2,1}A_{1,2}, \dots, A_{n,n-1}A_{n-1,n}$ it should be remarked that in general such a count is too naive. To see this, consider the inverse problem for a matrix A

where $A_{j,k} = 0$ if $|j - k| \geq 2$ and $A_{j,k} = 1$ if $|j - k| = 1$. In this case one has n quantities to determine, namely the diagonal elements. One might therefore think that the n eigenvalues of A determine the matrix. However, the matrices

$$\begin{pmatrix} b_1 & 1 \\ 1 & b_2 \end{pmatrix} \quad \text{and} \quad \begin{pmatrix} b_2 & 1 \\ 1 & b_1 \end{pmatrix}$$

have the same eigenvalues even when they are different.

4.1.3. Borg's theorem for finite Jacobi matrices. The following theorem was first proved by G. Borg in the context of one-dimensional Schrödinger equations.

Theorem. Consider a Jacobi expression L on $\{0, \dots, N + 1\}$. Suppose the following data are given:

- (1) Two distinct numbers h_1 and h_2 .
- (2) The eigenvalues associated with the boundary conditions

$$y(0) = y(N + 1) - h_1 y(N) = 0.$$

- (3) The eigenvalues associated with the boundary conditions

$$y(0) = y(N + 1) - h_2 y(N) = 0.$$

Then the quantities b_1, \dots, b_N and the quantities $a_1 c_1, \dots, a_{N-1} c_{N-1}$ as well as c_N are uniquely determined.

PROOF. Let J_k , $k = 1, 2$, be given by

$$\begin{pmatrix} b_1 & c_1 & & & & \\ a_1 & b_2 & c_2 & & & \\ & \ddots & \ddots & \ddots & & \\ & & a_{N-2} & b_{N-1} & c_{N-1} & \\ & & & a_{N-1} & b_N + h_k c_N & \end{pmatrix}.$$

Our assumptions mean that the characteristic polynomials of J_1 and J_2 are given. First note that $c_N = \text{tr}(J_1 - J_2)/(h_1 - h_2)$.

Next let P_k denote the characteristic polynomial of the upper left $k \times k$ block of J_1 and let Q be the characteristic polynomial of J_2 . Then

$$P_N(\lambda) = (b_N + h_1 c_N - \lambda)P_{N-1}(\lambda) - c_{N-1} a_{N-1} P_{N-2}(\lambda)$$

and

$$Q(\lambda) = (b_N + h_2 c_N - \lambda)P_{N-1}(\lambda) - c_{N-1} a_{N-1} P_{N-2}(\lambda)$$

so that

$$P_{N-1}(\lambda) = \frac{P_N(\lambda) - Q(\lambda)}{(h_1 - h_2)c_N}.$$

Now apply Theorem 4.1.2. □

4.1.4. The Titchmarsh-Weyl m -function. We denote by $C(\lambda, \cdot)$ and $S(\lambda, \cdot)$ the solutions of $Ly = \lambda y$ satisfying initial conditions

$$C(\lambda, 0) = 1, \quad C(\lambda, 1) = 1, \quad S(\lambda, 0) = 0, \quad S(\lambda, 1) = 1.$$

Note that $S(\cdot, n)$ and $C(\cdot, n)$ are polynomials of degree $n - 1$ each with leading coefficient $c_1 \dots c_{n-1}$ when $2 \leq n \leq N + 1$.

For every boundary condition on the right, characterized by the parameter h , we define the so called Weyl-Titchmarsh m -function by $\lambda \mapsto m_h(\lambda)$ where $m_h(\lambda)$ is chosen so that the function

$$C(\lambda, \cdot) + m_h(\lambda)S(\lambda, \cdot)$$

satisfies the given boundary condition. (Why is m_h well defined?) One computes immediately that

$$m_h(\lambda) = -\frac{C(\lambda, N+1) - hC(\lambda, N)}{S(\lambda, N+1) - hS(\lambda, N)}.$$

Hence m_h is a rational function which tends to -1 as its argument tends to infinity. Its poles are the eigenvalues of the problem defined by the boundary conditions $y(0) = y(N+1) - hy(N) = 0$. Its zeros are the eigenvalues of the problem defined by the boundary conditions $y(0) - y(1) = y(N+1) - hy(N) = 0$.

Denote the unique solution of the initial value problem $Ly = \lambda y$, $y(N+1) = h$, $y(N) = 1$ by $\psi_h(\lambda, \cdot)$. This solution (or its constant multiples) is called the Weyl solution associated with h . Any solution which satisfies the boundary condition on the right is a multiple of $\psi_h(\lambda, \cdot)$. In particular, this is the case for $C(\lambda, \cdot) + m_h(\lambda)S(\lambda, \cdot)$. Therefore

$$m_h(\lambda) = \frac{\psi_h(\lambda, 1) - \psi_h(\lambda, 0)}{\psi_h(\lambda, 0)}.$$

4.1.5. The m -function determines uniquely its Jacobi matrix. Let L be a difference expression defined on $\{0, \dots, N+1\}$ and h a fixed complex number. Let m_h be the associated Titchmarsh-Weyl m -function. Given m_h we know that its zeros and poles are two sets of eigenvalues (see 4.1.4), which, by Borg's theorem determine the quantities $a_j c_j$ and b_j for $j = 1, \dots, N-1$ as well as the numbers a_0 and $b_N + hc_N$.

It should be noted that, conversely, m_h can be immediately computed from the spectra associated with two sets of appropriate boundary conditions. More precisely, if $\lambda_1, \dots, \lambda_N$ are the eigenvalues for the boundary conditions $y(0) = y(N+1) - hy(N) = 0$ and μ_1, \dots, μ_N are the eigenvalues for the boundary conditions $y(0) - y(1) = y(N+1) - hy(N) = 0$, then

$$m_h(\lambda) = -\frac{\prod_{k=1}^N (\lambda - \mu_k)}{\prod_{k=1}^N (\lambda - \lambda_k)}.$$

Mathematical Background

A.1. Linear Algebra

A.1.1. Vector spaces. Let V be a set and suppose there is an associative and commutative binary operation (called an addition and denoted by $+$) on V . If V has an identity and every element of V has an inverse then V is called a commutative group. Suppose there is also a function from $\mathbb{C} \times V$ to V (called a scalar multiplication and denoted by juxtaposition) such that, for all $r, s \in \mathbb{C}$ and all $x, y \in V$, the following properties are satisfied

- (a) $(rs)x = r(sx)$,
- (b) $(r + s)x = rx + sx$,
- (c) $r(x + y) = rx + ry$, and
- (d) $1x = x$.

Then V is called a complex vector space.

A.1.2. Linear independence and span. If x_1, \dots, x_n are elements of a vector space V and if $\alpha_1, \dots, \alpha_n$ are scalars then the vector

$$\alpha_1 x_1 + \dots + \alpha_n x_n$$

is called a *linear combination* of x_1, \dots, x_n .

The vectors $x_1, \dots, x_n \in V$ are called *linearly independent* if $\alpha_1 x_1 + \dots + \alpha_n x_n = 0$ implies that $\alpha_1 = \dots = \alpha_n = 0$. Otherwise they are called linearly dependent. A set $M \subset V$ is called linearly independent if any finite number of distinct elements of M are linearly independent. Otherwise M is called linearly dependent.

If A is a subset of V then the set of all linear combinations of elements of A is called the *span* of A . We denote it by $\langle A \rangle$.

A.2. Topology

A.2.1. Metric spaces. Let M be a set. A function $d : M \times M \rightarrow \mathbb{R}$ is called a *distance* or *metric* on M if it satisfies the following conditions:

- (a) $d(x, y) \geq 0$ for all $x, y \in M$,
- (b) $d(x, y) = 0$ if and only if $x = y$,
- (c) $d(x, y) = d(y, x)$ for all $x, y, z \in M$,
- (d) $d(x, y) \leq d(x, z) + d(z, y)$ for all $x, y, z \in M$. (This inequality is called the triangle inequality.)

If there is a metric on M then (M, d) is called a metric space.

We say that a sequence $n \mapsto x_n \in M$ converges to $a \in M$ if $d(a, x_n)$ tends to zero as n tends to infinity. The sequence is then called *convergent* and the point a is called the *limit* of the sequence.

The important example of a metric space is the real line where the distance function is $d(x, y) = |x - y|$.

It was only in 1906 that Maurice Frechet (1878-1973) realized that the above properties are the essential features of $|x - y|$ which allow to do analysis.

A.2.2. Open and closed sets. Let (M, d) be a metric space. The set $B_r(x_0) = \{x \in M : d(x, x_0) < r\}$ is called the *ball* of radius r centered at x_0 .

A subset U of M is called *open* if for every $x_0 \in U$ there is a positive number r such that $B_r(x_0) \subset U$.

A subset F of M is called *closed* if for every convergent sequence $n \mapsto x_n \in F$ the limit is an element of F .

The complement of a closed set is open and vice versa.

The closure \bar{U} of a subset U of M is the set of all limit points of sequence in U . Note that $U \subset \bar{U}$.

A subset S of a metric space M is called *dense* in M if its closure equals M .

A.2.3. Cauchy sequences and completeness. Let (M, d) be a metric space. A sequence $n \mapsto x_n \in M$ is called a Cauchy sequence if for every positive ε there is a natural number N such that $d(x_n, x_m) < \varepsilon$ whenever n and m are at least as large as N .

A metric space is called *complete* if every Cauchy sequence converges to a limit in the space.

The set of real numbers and the set of complex numbers are complete metric spaces with the distance function $d(x, y) = |x - y|$.

A.3. Functional Analysis

There are two fundamental theorems in Functional Analysis which we use but which we do not want to prove, the open mapping theorem and a theorem on the geometry of Hilbert space.

A.3.1. The open mapping theorem. Let X and Y be Banach spaces and suppose $T : X \rightarrow Y$ is a bounded linear surjection. Then the image of every open set in X is an open set in Y . In particular, there is $\delta > 0$ unit ball in Y

This theorem has the following corollary.

Corollary. Let X and Y be Banach spaces and suppose $T : X \rightarrow Y$ is a bounded linear bijection. Then T^{-1} is bounded.

Sketch of proof: Since the image of the unit ball U in X is open and since the zero vector of Y is in $T(U)$ we know that there is a positive δ such that the ball of radius δ centered at zero is contained in $T(U)$. Since T is one-to-one we have that $\|Tx\| < \delta$ implies $\|x\| < 1$ or, equivalently, $\|Tx\| < 1$ implies $\|x\| < 1/\delta$. Since $x = T^{-1}y$ this means that $\|T^{-1}\| \leq 1/\delta$. \square

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