Methods of Applied Mathematics
Lecture Notes

William G. Faris

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Chapter 1

Linear Algebra

1.1 Matrices

1.1.1 Matrix algebra

An m by n matrix A is an array of complex numbers A_{ij} for $1 \leq i \leq m$ and $1 \leq j \leq n$.

The vector space operations are the sum $A + B$ and the scalar multiple cA. Let A and B have the same dimensions. The operations are defined by

$$(A + B)_{ij} = A_{ij} + B_{ij} \tag{1.1}$$

and

$$(cA)_{ij} = cA_{ij}. \tag{1.2}$$

The m by n zero matrix is defined by

$$0_{ij} = 0. \tag{1.3}$$

A matrix is a linear combination of other matrices if it is obtained from those matrices by adding scalar multiples of those matrices.

Let A be an m by n matrix and B be an n by p matrix. Then the product AB is defined by

$$(AB)_{ik} = \sum_{j=1}^{n} A_{ij} B_{jk}. \tag{1.4}$$

The n by n identity matrix is defined by

$$I_{ij} = \delta_{ij}. \tag{1.5}$$

Here δ_{ij} is the Kronecker delta that is equal to 1 when $i = j$ and to 0 when $i \neq j$.

Matrix algebra satisfies the usual properties of addition and many of the usual properties of multiplication. In particular, we have the associative law

$$(AB)C = A(BC) \tag{1.6}$$

and the unit law

$$AI = IA = A. \tag{1.7}$$

Even more important, we have the distributive laws

$$\begin{aligned} A(B+C) &= AB + AC \\ (B+C)A &= BA + CA. \end{aligned} \tag{1.8}$$

However multiplication is not commutative; in general $AB \neq BA$.

An n by n matrix A is invertible if there is another n by n matrix B with $AB = I$ and $BA = I$. In this case we write $B = A^{-1}$. (It turns out that if $BA = I$, then also $AB = I$, but this is not obvious at first.) The inverse operation has several nice properties, including $(A^{-1})^{-1} = A$ and $(AB)^{-1} = B^{-1}A^{-1}$.

The notion of division is ambiguous. Suppose B is invertible. Then both AB^{-1} and $B^{-1}A$ exist, but they are usually not equal.

Let A be an n by n square matrix. The trace of A is the sum of the diagonal entries. It is easy to check that $\mathrm{tr}(AB) = \mathrm{tr}(BA)$ for all such matrices. Although matrices do not commute, their traces do.

1.1.2 Reduced row echelon form

An m component vector is an m by 1 matrix. The ith standard basis vector is the vector with 1 in the ith row and zeros everywhere else.

An m by n matrix R is in reduced row echelon form (rref) if each column is either the next unit basis vector, or a a linear combination of the previous unit basis vectors. The columns where unit basis vectors occur are called pivot columns. The rank r of R is the number of pivot columns.

Theorem. If A is an m by n matrix, then there is an m by m matrix E that is invertible and such that

$$EA = R, \tag{1.9}$$

where R is in reduced row echelon form. The matrix R is uniquely determined by A.

This theorem allows us to speak of the pivot columns of A and the rank of A. Notice that if A is n by n and had rank n, then R is the identity matrix and E is the inverse of A.

Example. Let

$$A = \begin{bmatrix} 4 & 12 & 2 & 16 & 1 \\ 0 & 0 & 3 & 12 & -2 \\ -1 & -3 & 0 & -2 & -3 \end{bmatrix}. \tag{1.10}$$

Then the rref of A is

$$R = \begin{bmatrix} 1 & 3 & 0 & 2 & 0 \\ 0 & 0 & 1 & 4 & 0 \\ 0 & 0 & 0 & 0 & 1 \end{bmatrix}. \tag{1.11}$$

Corollary. Let A have reduced row echelon form R. The null space of A is the null space of R. That is, the solutions of the homogeneous equation $A\mathbf{x} = 0$ are the same as the solutions of the homogeneous equation $R\mathbf{x} = 0$.

Introduce a definition: A matrix is flipped rref if when flipped left-right (fliplr) and flipped up-down (flipud) it is rref.

The way reduced row echelon form is usually defined, one works from left to right and from top to bottom. If you try to define a corresponding concept where you work from right to left and from bottom to top, a perhaps sensible name for this is flipped reduced row echelon form.

Theorem. Let A be an m by n matrix with rank r. Then there is a unique n by $n-r$ matrix N such that the transpose of N is flipped rref and such that the transpose has pivot columns that are the non pivot columns of A and such that

$$AN = 0 \tag{1.12}$$

The columns of N are called the rational basis for the null space of A. It is easy to find N by solving $RN = 0$. The rational null space matrix N has the property that its transpose is in flipped reduced row echelon form.

Example: In the above example the null space matrix of A is

$$N = \begin{bmatrix} -3 & -2 \\ 1 & 0 \\ 0 & -4 \\ 0 & 1 \\ 0 & 0 \end{bmatrix}. \tag{1.13}$$

That is, the solutions of $A\mathbf{x} = \mathbf{0}$ are the vectors of the form $\mathbf{x} = N\mathbf{z}$. In other words, the columns of N span the null space of A.

One can also use the technique to solve inhomogeneous equations $A\mathbf{x} = \mathbf{b}$. One simply applies the theory to the augmented matrix $[A \ -\mathbf{b}]$. There is a solution when the last column of A is not a pivot column. A particular solution may be read off from the last column of the rational basis.

Example. Solve $A\mathbf{x} = \mathbf{b}$, where

$$\mathbf{b} = \begin{bmatrix} 4 \\ -19 \\ -9 \end{bmatrix}. \tag{1.14}$$

To accomplish this, let

$$A_1 = \begin{bmatrix} 4 & 12 & 2 & 16 & 1 & -4 \\ 0 & 0 & 3 & 12 & -2 & 19 \\ -1 & -3 & 0 & -2 & -3 & 9 \end{bmatrix}. \tag{1.15}$$

Then the rref of A_1 is

$$R = \begin{bmatrix} 1 & 3 & 0 & 2 & 0 & -3 \\ 0 & 0 & 1 & 4 & 0 & 5 \\ 0 & 0 & 0 & 0 & 1 & -2 \end{bmatrix}. \tag{1.16}$$

The null space matrix of A_1 is

$$N_1 = \begin{bmatrix} -3 & -2 & 3 \\ 1 & 0 & 0 \\ 0 & -4 & -5 \\ 0 & 1 & 0 \\ 0 & 0 & 2 \\ 0 & 0 & 1 \end{bmatrix}. \tag{1.17}$$

Thus the solution of $A\mathbf{x} = \mathbf{b}$ is

$$\mathbf{x} = \begin{bmatrix} 3 \\ 0 \\ -5 \\ 0 \\ 2 \end{bmatrix}. \tag{1.18}$$

1.1.3 Problems

Recall that the columns of a matrix A are linearly dependent if and only if the homogeneous equation $A\mathbf{x} = 0$ has a non-trivial solution. Also, a vector $\mathbf{y}$ is in the span of the columns if and only if the inhomogeneous equation $A\mathbf{x} = \mathbf{y}$ has a solution.

1. Show that if $\mathbf{p}$ is a particular solution of the equation $A\mathbf{x} = \mathbf{b}$, then every other solution is of the form $\mathbf{x} = \mathbf{p} + \mathbf{z}$, where $A\mathbf{z} = 0$.

2. Consider the matrix

$$A = \begin{bmatrix} 2 & 4 & 5 & 19 & -3 \\ 2 & 4 & 3 & 9 & -2 \\ -4 & -8 & 1 & 17 & 2 \\ 3 & 6 & 1 & -4 & -2 \\ 4 & 8 & 1 & -7 & -3 \\ 2 & 4 & -3 & -21 & 0 \end{bmatrix}.$$

   Use Matlab to find the reduced row echelon form of the matrix. Use this to find the rational basis for the solution of the homogeneous equation $A\mathbf{z} = 0$. Check this with the Matlab solution. Write the general solution of the homogeneous equation.

3. Let A be the matrix given above. Use Matlab to find an invertible matrix E such that $EA = R$ is in reduced echelon form. Find the determinant of E.

4. Consider the system $A\mathbf{x} = \mathbf{b}$, where A is as above, and

$$\mathbf{b} = \begin{bmatrix} 36 \\ 21 \\ 9 \\ 6 \\ 6 \\ -23 \end{bmatrix}.$$

Find the reduced echelon form of the matrix A augmented by the column $-\mathbf{b}$ on the right. Use this to find the rational basis for the solution of the homogeneous equation involving the augmented matrix. Use this to find the general solution of the original inhomogeneous equation.

5. Consider a system of 6 linear equations in 5 unknowns. It could be overdetermined, that is, have no solutions. Or it could have special properties and be under determined, that is, have many solutions. Could it be neither, that is, have exactly one solution? Is there such an example? Answer this question, and prove that your answer is correct.

6. Consider a system of 5 linear equations in 6 unknowns. Could it have exactly one solution? Is there such an example? Answer this question, and prove that your answer is correct.

7. Consider the five vectors in $\mathbf{R}^6$ formed by the columns of A. Show that the vector $\mathbf{b}$ is in the span of these five vectors. Find explicit weights that give it as a linear combination.

8. Is every vector $\mathbf{y}$ in $\mathbf{R}^6$ in the span of these five vectors? If so, prove it. If not, give an explicit example of a vector that is not in the span, and prove that it is not in the span.

9. Are these five vectors linearly independent? Prove that your answer is correct.

   The vectors in A that are pivot columns of A have the same span as the columns of A, yet are linearly independent. Find these vectors. How many are they? Prove that they are linearly independent.

1.1.4 The Jordan form

Two matrices A, B are said to be similar if there is an invertible matrix P with $P^{-1}AP = B$. Notice that if A and B are similar, then $\mathrm{tr}(A) = \mathrm{tr}(B)$.

Theorem. Let A be an n by n matrix. Then there is an invertible matrix P such that

$$P^{-1}AP = D + N, \tag{1.19}$$

where D is diagonal with diagonal entries $D_{kk} = \lambda_k$. Each entry of N is zero, except if $\lambda_k = \lambda_{k-1}$, then it is allowed that $N_{k-1\,k} = 1$.

Important note: Even if the matrix A is real, it may be that the matrices P and D are complex.

The equation may also be written $AP = PD + PN$. If we let $D_{kk} = \lambda_k$, then this is

$$\sum_{j=1}^{n} A_{ij}P_{jk} = P_{ik}\lambda_k + P_{i\,k-1}N_{k-1\,k}. \tag{1.20}$$

The $N_{k-1\,k}$ factor is zero, except in cases where $\lambda_k = \lambda_{k-1}$, when it is allowed to be 1. We can also write this in vector form. It is the eigenvalue equation

$$A\mathbf{u}_k = \lambda_k \mathbf{u}_k \tag{1.21}$$

except when $\lambda_k = \lambda_{k-1}$, when it may take the form

$$A\mathbf{u}_k = \lambda_k \mathbf{u}_k + \mathbf{u}_{k-1}. \tag{1.22}$$

The hard thing is to actually find the eigenvalues λ_k that form the diagonal elements of the matrix D. This is a nonlinear problem. One way to see this is the following. For each $k = 1, \ldots, n$ the matrix power A^k is similar to a matrix $(D + N)^k$ with the same diagonal entries as D^k. Thus we have the identity

$$\mathrm{tr}(A^k) = \lambda_1^k + \cdots + \lambda_n^k. \tag{1.23}$$

This is a system of n nonlinear polynomial equations in n unknowns $\lambda_1, \ldots, \lambda_k$. As is well known, there is another way of writing these equations in terms of the characteristic polynomial. This gives a single nth order polynomial equation in one unknown λ. This single equation has the same n solutions. For $n = 2$ the equation is quite easy to deal with by hand. For larger n one is often driven to computer algorithms.

Example: Let

$$A = \begin{bmatrix} 1 & 2 \\ -15 & 12 \end{bmatrix}. \tag{1.24}$$

The eigenvalues are 7, 6. The eigenvectors are the columns of

$$P = \begin{bmatrix} 1 & 2 \\ 3 & 5 \end{bmatrix}. \tag{1.25}$$

Let

$$D = \begin{bmatrix} 7 & 0 \\ 0 & 6 \end{bmatrix}. \tag{1.26}$$

Then $AP = PD$.

Example: Let

$$A = \begin{bmatrix} 10 & -1 \\ 9 & 4 \end{bmatrix}. \tag{1.27}$$

The only eigenvalue is 7. The eigenvector is the first column of

$$P = \begin{bmatrix} 1 & 2 \\ 3 & 5 \end{bmatrix}. \tag{1.28}$$

Let

$$D + N = \begin{bmatrix} 7 & 1 \\ 0 & 7 \end{bmatrix}. \tag{1.29}$$

Then $AP = P(D + N)$.

1.1.5 Problems

1. If A is a square matrix and f is a function defined by a convergent power series, then $f(A)$ is defined. Show that if A is similar to B, then $f(A)$ is similar to $f(B)$.

2. By the Jordan form theorem, A is similar to $D+N$, where D is diagonal, N is nilpotent, and D, N commute. To say that N is nilpotent is to say that for some $p \geq 1$ the power $N^p = 0$. Show that

$$f(D+N) = \sum_{m=0}^{p-1} \frac{1}{m!} f^{(m)}(D) N^m \tag{1.30}$$

3. Show that

$$\exp(t(D+N)) = \exp(tD) \sum_{m=0}^{p-1} \frac{1}{m!} N^m t^m. \tag{1.31}$$

Use this to describe the set of all solutions $\mathbf{x} = \exp(tA)\mathbf{z}$ to the differential equation

$$\frac{d\mathbf{x}}{dt} = A\mathbf{x}. \tag{1.32}$$

with initial condition $\mathbf{x} = \mathbf{z}$ when $t = 0$.

4. Take

$$A = \begin{bmatrix} 0 & 1 \\ -k & -2c \end{bmatrix}, \tag{1.33}$$

where $k \geq 0$ and $c \geq 0$. The differential equation describes an oscillator with spring constant k and friction coefficient $2c$. Find the eigenvalues and sketch a typical solution in the x_1, x_2 plane in each of the following cases: over damped $c^2 > k > 0$; critically damped $c^2 = k > 0$; under damped $0 < c^2 < k$; undamped $0 = c^2 < k$; free motion $0 = c^2 = k$.

5. Consider the critically damped case. Find the Jordan form of the matrix A, and find a similarity transformation that transforms A to its Jordan form.

6. If $A = PDP^{-1}$, where the diagonal matrix D has diagonal entries λ_i, then $f(A)$ may be defined for an arbitrary function f by $f(A) = Pf(D)P^{-1}$, where $f(D)$ is the diagonal matrix with entries $f(\lambda_i)$. Thus, for instance, if each $\lambda_i \geq 0$, then $\sqrt{A}$ is defined. Find the square root of

$$A = \begin{bmatrix} 20 & 40 \\ -8 & -16 \end{bmatrix}. \tag{1.34}$$

7. Give an example of a matrix A with each eigenvalue $\lambda_i \geq 0$, but for which no square root $\sqrt{A}$ can be defined? Why does the formula in the second problem not work?

1.1.6 Quadratic forms

Given an m by n matrix A, its adjoint is an n by n matrix A^* defined by

$$A^*_{ij} = \bar{A}_{ji}. \tag{1.35}$$

If we are dealing with real numbers, then the adjoint is just the transpose. The adjoint operator has several nice properties, including $A^{**} = A$ and $(AB)^* = B^*A^*$.

Two matrices A, B are said to be congruent if there is an invertible matrix P with $P^*AP = B$.

Theorem. Let A be an n by n matrix with $A = A^*$. Then there is an invertible matrix P such that

$$P^*AP = D, \tag{1.36}$$

where D is diagonal with entries 1, -1, and 0.

Define the quadratic form $Q(\mathbf{x}) = \mathbf{x}^*A\mathbf{x}$. Then the equation says that one may make a change of variables $\mathbf{x} = P\mathbf{y}$ so that $Q(\mathbf{x}) = \mathbf{y}^*D\mathbf{y}$.

1.1.7 Spectral theorem

A matrix U is said to be unitary if $U^{-1} = U^*$. In the real case this is the same as being an orthogonal matrix.

Theorem. Let A be an n by n matrix with $A = A^*$. Then there is a unitary matrix U such that

$$U^{-1}AU = D, \tag{1.37}$$

where D is diagonal with real entries.

Example: Let

$$A = \begin{bmatrix} 1 & 2 \\ 2 & 1 \end{bmatrix}. \tag{1.38}$$

The eigenvalues are given by

$$D = \begin{bmatrix} 3 & 0 \\ 0 & -1 \end{bmatrix}. \tag{1.39}$$

A suitable orthogonal matrix P is

$$P = \frac{1}{\sqrt{2}} \begin{bmatrix} 1 & -1 \\ 1 & 1 \end{bmatrix}. \tag{1.40}$$

Then $AP = PD$.

A matrix A is said to be normal if $AA^* = A^*A$. A self-adjoint matrix ($A^* = A$) is normal. A skew-adjoint matrix ($A^* = -A$) is normal. A unitary matrix ($A^* = A^{-1}$) is normal.

Theorem. Let A be an n by n matrix that is normal. Then there is a unitary matrix U such that

$$U^{-1}AU = D, \tag{1.41}$$

where D is diagonal.

Notice that this is the eigenvalue equation $AU = UD$. The columns of U are the eigenvectors, and the diagonal entries of D are the eigenvalues.

Example: Let

$$P = \frac{1}{\sqrt{2}} \begin{bmatrix} 1 & -1 \\ 1 & 1 \end{bmatrix}. \tag{1.42}$$

Then P is a rotation by $\pi/4$. The eigenvalues are on the diagonal of

$$F = \frac{1}{\sqrt{2}} \begin{bmatrix} 1+i & 0 \\ 0 & 1-i \end{bmatrix}. \tag{1.43}$$

A suitable unitary matrix Q is

$$Q = \frac{1}{\sqrt{2}} \begin{bmatrix} 1 & i \\ -i & -1 \end{bmatrix}. \tag{1.44}$$

Then $PQ = QF$.

1.1.8 Circulant (convolution) matrices

If A is normal, then there are unitary U and diagonal D with $AU = UD$. But they are difficult to compute. Here is one special but important situation where everything is explicit.

A circulant (convolution) matrix is an n by n matrix such that there is a function a with $A_{pq} = a(p-q)$, where the difference is computed modulo n. [For instance, a 4 by 4 matrix would have the same entry $a(3)$ in the 12, 23, 34, and 41 positions.]

The DFT (discrete Fourier transform) matrix is an n by n unitary matrix given by

$$U_{qk} = \frac{1}{\sqrt{n}} e^{\frac{2\pi i q k}{n}}. \tag{1.45}$$

Theorem. Let A be a circulant matrix. If U is the DFT matrix, then

$$U^{-1} A U = D, \tag{1.46}$$

where D is a diagonal matrix with

$$D_{kk} = \hat{a}(k) = \sum_r a(r) e^{-\frac{2\pi i r k}{n}}. \tag{1.47}$$

1.1.9 Problems

1. Let

$$A = \begin{bmatrix} 5 & 1 & 4 & 2 & 3 \\ 1 & 2 & 6 & 3 & 1 \\ 4 & 6 & 3 & 0 & 4 \\ 2 & 3 & 0 & 1 & 2 \\ 3 & 1 & 4 & 2 & 3 \end{bmatrix}. \tag{1.48}$$

Use Matlab to find orthogonal P and diagonal D so that $P^{-1}AP = D$.

2. Find unitary Q and diagonal F so that $Q^{-1}PQ = F$.

3. The orthogonal matrix P is made of rotations in two planes and possibly a reflection. What are the two angles of rotations? Is there a reflection present as well? Explain.

4. Find an invertible matrix R such that $R^*AR = G$, where G is diagonal with all entries ± 1 or 0.

5. In the following problems the matrix A need not be square. Let A be a matrix with trivial null space. Show that A^*A is invertible.

6. Let $E = A(A^*A)^{-1}A^*$. Show that $E^* = E$ and $E^2 = E$.

7. Define the pseudo-inverse $A^+ = (A^*A)^{-1}A^*$. Show that $AA^+ = E$ and $A^+A = I$.

8. Let
$$A = \begin{bmatrix} 1 & 1 & 1 \\ 1 & 2 & 4 \\ 1 & 3 & 9 \\ 1 & 4 & 16 \\ 1 & 5 & 25 \\ 1 & 6 & 36 \\ 1 & 7 & 49 \end{bmatrix}. \tag{1.49}$$
Calculate E and check the identities above. Find the eigenvalues of E. Explain the geometric meaning of E.

9. Find the parameter values $\mathbf{x}$ such that $A\mathbf{x}$ best approximates
$$\mathbf{y} = \begin{bmatrix} 7 \\ 5 \\ 6 \\ -1 \\ -3 \\ -7 \\ -24 \end{bmatrix}. \tag{1.50}$$
(Hint: Let $\mathbf{x} = A^+\mathbf{y}$.) What is the geometric interpretation of $A\mathbf{x}$?

1.2 Vector spaces

1.2.1 Vector spaces

A vector space is a collection V of objects that may be combined with vector addition and scalar multiplication. There will be two possibilities for the scalars. They may be elements of the field $\mathbf{R}$ of real numbers. Or they may be elements of the field $\mathbf{C}$ of complex numbers. To handle both cases together, we shall consider the scalars as belonging to a field $\mathbf{F}$.

The vector space addition axioms say that the sum of each two vectors $\mathbf{u}, \mathbf{v}$ in V is another vector in the space called $\mathbf{u} + \mathbf{v}$ in V. Addition must satisfy the following axioms: associative law

$$(\mathbf{u} + \mathbf{v}) + \mathbf{w} = \mathbf{u} + (\mathbf{v} + \mathbf{w}) \tag{1.51}$$

additive identity law

$$\mathbf{u} + \mathbf{0} = \mathbf{0} + \mathbf{u} = \mathbf{u} \tag{1.52}$$

additive inverse law

$$\mathbf{u} + (-\mathbf{u}) = (-\mathbf{u}) + \mathbf{u} = \mathbf{0} \tag{1.53}$$

and commutative law

$$\mathbf{u} + \mathbf{v} = \mathbf{v} + \mathbf{u}. \tag{1.54}$$

The vector space axioms also require that for each scalar c in $\mathbf{F}$ and each $\mathbf{u}$ in V there is a vector $c\mathbf{u}$ in V. Scalar multiplication must satisfy the following axioms: distributive law for vector addition

$$c(\mathbf{u} + \mathbf{v}) = c\mathbf{u} + c\mathbf{v} \tag{1.55}$$

distributive law for scalar addition

$$(c + d)\mathbf{u} = c\mathbf{u} + c\mathbf{u} \tag{1.56}$$

associative law for scalar multiplication

$$(cd)\mathbf{u} = c(d\mathbf{u}) \tag{1.57}$$

identity law for scalar multiplication

$$1\mathbf{u} = \mathbf{u}. \tag{1.58}$$

The elements of a vector space are pictured as arrows starting at a fixed origin. The vector sum is pictured in terms of the parallelogram law. The sum of two arrows starting at the origin is the diagonal of the parallelogram formed by the two arrows.

A subspace of a vector space is a subset that is itself a vector space. The smallest possible subspace consists of the zero vector at the origin. A one dimensional vector subspace is pictured as a line through the origin. A two dimensional vector subspace is pictured as a plane through the origin, and so on.

1.2.2 Linear transformations

Let V and W be vector spaces. A linear transformation $T : V \to W$ is a function from V to W that preserves the vector space operations. Thus

$$T(\mathbf{u} + \mathbf{v}) = T\mathbf{u} + T\mathbf{v} \tag{1.59}$$

and

$$T(c\mathbf{u}) = cT\mathbf{u}. \tag{1.60}$$

The null space of a linear transformation $T : V \to W$ is the set of all vectors $\mathbf{u}$ in V such that $T\mathbf{u} = \mathbf{0}$. The null space is sometimes called the kernel.

The range of a linear transformation $T : V \to W$ is the set of all vectors $T\mathbf{u}$ in W, where $\mathbf{u}$ is in V. The range is sometimes called the image.

Theorem. The null space of a linear transformation $T : V \to W$ is a subspace of V.

Theorem. The range of a linear transformation $T : V \to W$ is a subspace of W.

Theorem. A linear transformation $T : V \to W$ is one-to-one if and only if its null space is the zero subspace.

Theorem. A linear transformation $T : V \to W$ is onto W if and only if its range is W.

Theorem. A linear transformation $T : V \to W$ has an inverse $T^{-1} : W \to V$ if and only if its null space is the zero subspace and its range is W.

An invertible linear transformation will also be called a vector space isomorphism.

Consider a list of vectors $\mathbf{p}_1, \ldots, \mathbf{p}_n$. They define a linear transformation $P : \mathbf{F}^n \to V$, by taking the vector in $\mathbf{F}^n$ to be the weights of a linear combination of the $\mathbf{p}_1, \ldots, \mathbf{p}_n$.

Theorem. A list of vectors is linearly independent if and only if the corresponding linear transformation has zero null space.

Theorem. A list of vectors spans the vector space V if and only if the corresponding linear transformation has range V.

Theorem. A list of vectors is a basis for V if and only if the corresponding linear transformation $P : \mathbf{F}^n \to V$ is a vector space isomorphism. In that case the inverse transformation $P^{-1} : V \to \mathbf{F}^n$ is the transformation that carries a vector to its coordinates with respect to the basis.

In case there is a basis transformation $P : \mathbf{F}^n \to V$, the vector space V is said to be n dimensional.

1.2.3 Reduced row echelon form

Theorem Let $\mathbf{p}_1, \ldots, \mathbf{p}_n$ be a list of vectors in an m dimensional vector space V. Let $P : \mathbf{F}^n \to V$ be the corresponding transformation. Then there is an isomorphism $E : V \to \mathbf{F}^m$ such that

$$EP = R, \tag{1.61}$$

where R is in reduced row echelon form. The m by n matrix R is uniquely determined by the list of vectors.

Thus for an arbitrary list of vectors, there are certain vectors that are pivot vectors. These vectors are those that are not linear combinations of previous vectors in the list. The reduced row echelon form of a list of vectors expresses the extent to which each vector in the list is a linear combination of previous pivot vectors in the list.

1.2.4 Jordan form

Theorem. Let $T : V \to V$ be a linear transformation of an n dimensional vector space to itself. Then there is an invertible matrix $P : \mathbf{R}^n \to V$ such that

$$P^{-1}TP = D + N, \tag{1.62}$$

where D is diagonal with diagonal entries $D_{kk} = \lambda_k$. Each entry of N is zero, except if $\lambda_k = \lambda_{k-1}$, then it is allowed that $N_{k-1\,k} = 1$.

We can also write this in vector form. The equation $TP = P(D + N)$ is equivalent to the eigenvalue equation

$$T\mathbf{p}_k = \lambda_k \mathbf{p}_k \tag{1.63}$$

except when $\lambda_k = \lambda_{k-1}$, when it may take the form

$$T\mathbf{p}_k = \lambda_k \mathbf{p}_k + \mathbf{p}_{k-1}. \tag{1.64}$$

It is difficult to picture such a linear transformation, even for a real vector space. One way to do it works especially well in the case when the dimension of V is 2. Then the linear transformation T maps each vector $\mathbf{u}$ in V to another vector $T\mathbf{u}$ in V. Think of each $\mathbf{u}$ as determining a point in the plane. Draw the vector $T\mathbf{u}$ as a vector starting at the point $\mathbf{u}$. Then this gives a picture of the linear transformation as a vector field. The qualitative features of this vector field depend on whether the eigenvalues are real or occur as a complex conjugate pair. In the real case, they can be both positive, both negative, or of mixed sign. These give repelling, attracting, and hyperbolic fixed points. In the complex case the real part can be either positive or negative. In the first case the rotation has magnitude less than $\pi/2$, and the vector field is a repelling spiral. In the second case the rotation has magnitude greater than $\pi/2$ and the vector field is an attracting spiral. The case of complex eigenvalues with real part equal to zero is special but important. The transformation is similar to a rotation that has magnitude $\pm\pi/2$, and so the vector field goes around in closed elliptical paths.

1.2.5 Forms and dual spaces

The dual space V^* of a vector space V consists of all linear transformations from V to the field of scalars $\mathbf{F}$. If ω is in V^*, then the value of ω on $\mathbf{u}$ in V is written $\langle \omega, \mathbf{u} \rangle$.

We think of the elements of $\mathbf{F}^n$ as column vectors. The elements of the dual space of $\mathbf{F}^n$ are row vectors. The value of a row vector on a column vector is given by taking the row vector on the left and the column vector on the right and using matrix multiplication.

The way to picture an element of V^* is via its contour lines. These are straight lines at regularly spaced intervals. The value of ω on $\mathbf{u}$ is obtained by taking the vector $\mathbf{u}$ and seeing how many contour lines it crosses.

Sometimes vectors in the original space V are called contravariant vectors, while forms in the dual space V^* are called covariant vectors.

1.2.6 Quadratic forms

A sesquilinear form is a function that assigns to each ordered pair of vectors $\mathbf{u}$, $\mathbf{v}$ in V a scalar $a(\mathbf{u}, \mathbf{v})$. It is required that it be linear in the second variable. Thus

$$a(\mathbf{u}, \mathbf{v} + \mathbf{w}) = a(\mathbf{u}, \mathbf{v}) + a(\mathbf{u}, \mathbf{w}) \tag{1.65}$$

and

$$a(\mathbf{u}, c\mathbf{v}) = ca(\mathbf{u}, \mathbf{v}). \tag{1.66}$$

Furthermore, it is required to be conjugate linear in the first variable. this says that

$$a(\mathbf{u} + \mathbf{v}, \mathbf{w}) = a(\mathbf{u}, \mathbf{w}) + a(\mathbf{v}, \mathbf{w}) \tag{1.67}$$

and

$$a(c\mathbf{u}, \mathbf{v}) = \bar{c}a(\mathbf{u}, \mathbf{v}). \tag{1.68}$$

In the real case one does not need the complex conjugates on the scalars. In this case this is called a bilinear form.

A sesquilinear form defines a linear transformation from V to V^*. (Actually, in the complex case it is a conjugate linear transformation.) This linear transformation takes the vector $\mathbf{u}$ to the form $a(\mathbf{u}, \cdot)$. So a sesquilinear form may be viewed as a special kind of linear transformation, but not one from a space to itself.

A sesquilinear form is sometimes regarded as a covariant tensor. By contrast, a linear transformation a mixed tensor.

A sesquilinear form is Hermitian if

$$a(\mathbf{u}, \mathbf{v}) = \overline{a(\mathbf{v}, \mathbf{u})}. \tag{1.69}$$

In the real case the complex conjugate does not occur. In this case the bilinear form is called symmetric.

A Hermitian form defines a quadratic form $a(\mathbf{u}, \mathbf{u})$ that is real. The quadratic form determines the Hermitian form. In fact,

$$4\Re a(\mathbf{u}, \mathbf{v}) = a(\mathbf{u} + \mathbf{v}, \mathbf{u} + \mathbf{v}) + a(\mathbf{u} - \mathbf{v}, \mathbf{u} - \mathbf{v}) \tag{1.70}$$

determines the real part. Then $\Im a(\mathbf{u}, \mathbf{v}) = \Re a(i\mathbf{u}, \mathbf{v})$ determines the imaginary part.

Theorem. Let a be a Hermitian form defined for vectors in an n dimensional vector space V. Then there exists an invertible linear transformation $P : \mathbf{F}^n \to V$ such that

$$a(P\mathbf{x}, P\mathbf{x}) = \mathbf{x}^* D\mathbf{x}, \tag{1.71}$$

where D is diagonal with entries 1, -1, and 0.

It is sometimes possible to get a good picture of a quadratic form. In the real case when V is two dimensional a quadratic form may be pictured by its contour lines. There are different cases depending on whether one has $+1$s or -1s or a $+1$, -1 combination.

1.2.7 Special relativity

In special relativity V is the four dimensional real vector space of displacements in space-time. Thus a vector $\mathbf{u}$ takes one event in space-time into another event in space-time. It represents a separation between these space-time events.

There is a quadratic form g with signature $+1$, -1, -1, -1. The vector $\mathbf{u}$ is said to be time-like, light-like, or space-like according to whether $g(\mathbf{u}, \mathbf{u}) > 0$, $g(\mathbf{u}, \mathbf{u}) = 0$, or $g(\mathbf{u}, \mathbf{u}) < 0$. The time (perhaps in seconds) between time-like separated events is $\sqrt{g(\mathbf{u}, \mathbf{u})}$. The distance (perhaps in light-seconds) between space-like separated events is $\sqrt{-g(\mathbf{u}, \mathbf{u})}$.

The light cone is the set of light-like vectors. The rest of the vector space consists of three parts: forward time-like vectors, backward time-like vectors, and space-like vectors.

Lemma. If two forward time-like vectors $\mathbf{u}, \mathbf{v}$ have unit length $\sqrt{g(\mathbf{u}, \mathbf{u})} = \sqrt{g(\mathbf{v}, \mathbf{v})} = 1$, then their difference $\mathbf{u} - \mathbf{v}$ is space-like.

Proof: This lemma is at least geometrically plausible. It may be proved by using the diagonal form D of the quadratic form.

Lemma If $\mathbf{u}, \mathbf{v}$ are forward time-like vectors with unit length, then $g(\mathbf{u}, \mathbf{v}) > 1$.

Proof: This follows immediately from the previous lemma.

Anti-Schwarz inequality. If $\mathbf{u}, \mathbf{v}$ are forward time-like vectors, then $g(\mathbf{u}, \mathbf{v}) > \sqrt{g(\mathbf{u}, \mathbf{u})}\sqrt{g(\mathbf{v}, \mathbf{v})}$.

Proof: This follows immediately from the previous lemma.

Anti-triangle inequality. If $\mathbf{u}, \mathbf{v}$ are forward time-like vectors, and $\mathbf{u}+\mathbf{v} = \mathbf{w}$, then

$$\sqrt{g(\mathbf{w}, \mathbf{w})} > \sqrt{g(\mathbf{u}, \mathbf{u})} + \sqrt{g(\mathbf{v}, \mathbf{v})}. \tag{1.72}$$

Proof: This follows immediately from the anti-Schwarz inequality.

The anti-triangle inequality is the basis of the twin paradox. In this case the lengths of the vectors are measured in time units. One twin undergoes no acceleration; the total displacement in space time is given by $\mathbf{w}$. The other twin begins a journey according to vector $\mathbf{u}$, then changes course and returns to a meeting event according to vector $\mathbf{v}$. At this meeting the more adventurous twin is younger.

The anti-triangle inequality is also the basis of the famous conversion of mass to energy. In this case $\mathbf{w}$ is the energy-momentum vector of a particle,

and $\sqrt{g(\mathbf{w},\mathbf{w})}$ is its rest mass. (Consider energy, momentum, and mass as all measured in energy units.) The particle splits into two particles that fly apart from each other. The energy-momentum vectors of the two particles are $\mathbf{u}$ and $\mathbf{v}$. By conservation of energy-momentum, $\mathbf{w} = \mathbf{u} + \mathbf{v}$. The total rest mass $\sqrt{g(\mathbf{u},\mathbf{u})} + \sqrt{g(\mathbf{v},\mathbf{v}}$ of the two particles is smaller than the original rest mass. This has released the energy that allows the particles to fly apart.

1.2.8 Scalar products and adjoint

A Hermitian form $g(\mathbf{u},\mathbf{v})$ is an inner product (or scalar product) if $g(\mathbf{u},\mathbf{u}) > 0$ except when $\mathbf{u} = \mathbf{0}$. Often when there is just one scalar product in consideration it is written $g(\mathbf{u},\mathbf{v}) = (\mathbf{u},\mathbf{v})$. However we shall continue to use the more explicit notation for a while, since it is important to realize that to use these notions there must be some mechanism that chooses an inner product. In the simplest cases the inner product arises from elementary geometry, but there can be other sources for a definition of a natural inner product.

Remark. An inner product gives a linear transformation from a vector space to its dual space. Let V be a vector space with inner product g. Let $\mathbf{u}$ be in V. Then there is a corresponding linear form $\mathbf{u}^*$ in the dual space of V defined by

$$\langle \mathbf{u}^*, \mathbf{v} \rangle = g(\mathbf{u},\mathbf{v}) \tag{1.73}$$

for all $\mathbf{v}$ in V. This form could also be denoted $\mathbf{u}^* = g\mathbf{u}$.

The picture associated with this construction is that given a vector $\mathbf{u}$ represented by an arrow, the $\mathbf{u}^* = g\mathbf{u}$ is a form with contour lines perpendicular to the arrow. The longer the vector, the more closely spaced the contour lines.

Theorem. (Riesz representation theorem) An inner product not only gives a transformation from a vector space to its dual space, but this is an isomorphism. Let V be a finite dimensional vector space with inner product g. Let $\omega : V \to \mathbf{F}$ be a linear form in the dual space of V. Then there is a unique vector ω^* in V such that

$$g(\omega^*, \mathbf{v}) = \langle \omega, \mathbf{v} \rangle \tag{1.74}$$

for all $\mathbf{v}$ in V. This vector could also be denoted $\omega^* = g^{-1}\omega$.

The picture associated with this construction is that given a form ω represented by contour lines, the $\omega^* = g^{-1}\omega$ is a vector perpendicular to the lines. The more closely spaced the contour lines, the longer the vector.

Theorem: Let V_1 and V_2 be two finite dimensional vector spaces with inner products g_1 and g_2. Let $A : V_1 \to V_2$ be a linear transformation. Then there is another operator $A^* : V_2 \to V_1$ such that

$$g_1(A^*\mathbf{u},\mathbf{v}) = \overline{g_2(A\mathbf{v},\mathbf{u})} \tag{1.75}$$

for every $\mathbf{u}$ in V_2 and $\mathbf{v}$ in V_1. Equivalently,

$$g_1(A^*\mathbf{u},\mathbf{v}) = g_2(\mathbf{u},A\mathbf{v}) \tag{1.76}$$

for every $\mathbf{u}$ in V_2 and $\mathbf{v}$ in V_1.

The outline of the proof of this theorem is the following. If $\mathbf{u}$ is given, then the map $g_2(\mathbf{u}, A\cdot)$ is an element of the dual space V_1^*. It follows from the previous theorem that it is represented by a vector. This vector is $A^*\mathbf{u}$.

A linear transformation $A : V_1 \to V_2$ is unitary if $A^* = A^{-1}$.

There are more possibilities when the two spaces are the same. A linear transformation $A : V \to V$ is self-adjoint if $A^* = A$. It is skew-adjoint if $A^* = -A$. It is unitary if $A^* = A^{-1}$.

A linear transformation $A : V \to V$ is normal if $AA^* = A^*A$. Every operator that is self-adjoint, skew-adjoint, or unitary is normal.

Remark 1. Here is a special case of the definition of adjoint. Fix a vector $\mathbf{u}$ in V. Let $A : \mathbf{F} \to V$ be defined by $Ac = c\mathbf{u}$. Then $A^* : V \to \mathbf{F}$ is a form $\mathbf{u}^*$ such that $\overline{\langle \mathbf{u}^*, \mathbf{z}\rangle} c = g(\mathbf{z}, c\mathbf{u})$. Thus justifies the definition $\langle \mathbf{u}^*, \mathbf{z}\rangle = g(\mathbf{u}, \mathbf{z})$.

Remark 2. Here is another special case of the definition of adjoint. Let $A : V \to \mathbf{F}$ be given by a form ω. Then the adjoint $A^* : \mathbf{F} \to V$ applied to c is the vector $c\omega^*$ such that $g(c\omega^*, \mathbf{v}) = \bar{c}\langle \omega, \mathbf{v}\rangle$. This justifies the definition $g(\omega^*, \mathbf{v}) = \langle \omega, \mathbf{v}\rangle$.

There are standard equalities and inequalities for inner products. Two vectors $\mathbf{u}, \mathbf{v}$ are said to be orthogonal (or perpendicular) if $g(\mathbf{u}, \mathbf{v}) = 0$.

Theorem. (Pythagorus) If $\mathbf{u}, \mathbf{v}$ are orthogonal and $\mathbf{w} = \mathbf{u} + \mathbf{v}$, then

$$g(\mathbf{w}, \mathbf{w}) = g(\mathbf{u}, \mathbf{u}) + g(\mathbf{v}, \mathbf{v}). \tag{1.77}$$

Lemma. If $\mathbf{u}, \mathbf{v}$ are vectors with unit length, then $\Re g(\mathbf{u}, \mathbf{v}) \leq 1$.

Proof: Compute $0 \leq g(\mathbf{u} - \mathbf{v}, \mathbf{u} - \mathbf{v}) = 2 - 2\Re g(\mathbf{u}, \mathbf{v})$.

Lemma. If $\mathbf{u}, \mathbf{v}$ are vectors with unit length, then $|g(\mathbf{u}, \mathbf{v})| \leq 1$.

Proof: This follows easily from the previous lemma.

Notice that in the real case this says that $-1 \leq g(\mathbf{u}, \mathbf{v}) \leq 1$. This allows us to define the angle between two unit vectors $\mathbf{u}, \mathbf{v}$ to be the number θ with $0 \leq \theta \leq \pi$ and $\cos(\theta) = g(\mathbf{u}, \mathbf{v})$.

Schwarz inequality. We have the inequality $|g(\mathbf{u}, \mathbf{v})| \leq \sqrt{g(\mathbf{u}, \mathbf{u})}\sqrt{g(\mathbf{v}, \mathbf{v})}$.

Proof: This follows immediately from the previous lemma.

Triangle inequality. If $\mathbf{u} + \mathbf{v} = \mathbf{w}$, then

$$\sqrt{g(\mathbf{w}, \mathbf{w})} \leq \sqrt{g(\mathbf{u}, \mathbf{u})} + \sqrt{g(\mathbf{v}, \mathbf{v})}. \tag{1.78}$$

Proof: This follows immediately from the Schwarz inequality.

1.2.9 Spectral theorem

Theorem. Let V be an n dimensional vector space with an inner product g. Let $T : V \to V$ be a linear transformation that is normal. Then there is a unitary transformation $U : \mathbf{F}^n \to V$ such that

$$U^{-1}TU = D, \tag{1.79}$$

where D is diagonal.

We can also write this in vector form. The transformation U defines an orthonormal basis of vectors. The equation is equivalent to the eigenvalue equation $TU = UD$, or, explicitly,

$$T\mathbf{u}_k = \lambda_k \mathbf{u}_k. \tag{1.80}$$

The distinction between linear transformations and quadratic forms sometimes shows up even in the context of matrix theory. Let A be a self-adjoint matrix, regarded as defining a quadratic form. Let B be a self-adjoint matrix that has all eigenvalues strictly positive. Then B defines a quadratic form that is in fact a scalar product. The natural linear transformation to consider is then $T = B^{-1}A$. The eigenvalue problem for this linear transformation then takes the form

$$A\mathbf{u} = \lambda B\mathbf{u}. \tag{1.81}$$

Indeed, this version is often encountered in concrete problems. The linear transformation $B^{-1}A$ is a self-adjoint linear transformation relative to the quadratic form defined by B. Therefore the eigenvalues λ are automatically real.

Example: Consider a system of linear spring oscillators. The equation of motion is

$$M\frac{d^2\mathbf{x}}{dt^2} = -A\mathbf{x}. \tag{1.82}$$

Here M is the matrix of mass coefficients (a diagonal matrix with strictly positive entries). The matrix A is real and symmetric, and it is assumed to have positive eigenvalues. If we try a solution of the form $\mathbf{x} = \mathbf{z}\cos(\sqrt{\lambda}t)$, we get the condition

$$A\mathbf{z} = \lambda M\mathbf{z}. \tag{1.83}$$

The λ should be real and positive, so the $\sqrt{\lambda}$ indeed make sense as resonant angular frequencies.

In this example the inner product is defined by the mass matrix M. The matrix $M^{-1}A$ is a self-adjoint operator relative to the inner product defined by M. That is why the eigenvalues of $M^{-1}A$ are real. In fact, the eigenvalues of the linear transformation $M^{-1}A$ are also positive. This is because the associated quadratic form is defined by A, which is positive.

1.3 Vector fields and differential forms

1.3.1 Coordinate systems

In mathematical modeling it is important to be flexible in the choice of coordinate system. For this reason we shall consider what one can do with arbitrary coordinate systems. We consider systems whose state can be described by two coordinates. However the same ideas work for higher dimensional systems.

Say some part of the system can be described by coordinates u, v. Let α, β be another coordinate system for that part of the system. Then the scalars α and β may be expressed as functions of the u and v. Furthermore, the matrix

$$J = \begin{bmatrix} \frac{\partial \alpha}{\partial u} & \frac{\partial \alpha}{\partial v} \\ \frac{\partial \beta}{\partial u} & \frac{\partial \beta}{\partial v} \end{bmatrix} \tag{1.84}$$

is invertible at each point, and the scalars u and v may be expressed as functions of the α and β.

Consider the partial derivative $\partial/\partial u$ as the derivative holding the coordinate v constant. Similarly, the partial derivative $\partial/\partial v$ is the derivative holding u constant. Then the chain rule says that

$$\frac{\partial}{\partial u} = \frac{\partial \alpha}{\partial u}\frac{\partial}{\partial \alpha} + \frac{\partial \beta}{\partial u}\frac{\partial}{\partial \beta}. \tag{1.85}$$

Similarly,

$$\frac{\partial}{\partial v} = \frac{\partial \alpha}{\partial v}\frac{\partial}{\partial \alpha} + \frac{\partial \beta}{\partial v}\frac{\partial}{\partial \beta}. \tag{1.86}$$

These formulas are true when applied to an arbitrary scalar. Notice that these formulas amount to the application of the transpose of the matrix J to the partial derivatives.

One must be careful to note that an expression such as $\partial/\partial u$ makes no sense without reference to a coordinate system u, v. For instance, say that we were interested in coordinate system u, β. Then $\partial/\partial u$ would be computed as a derivative along a curve where β is constant. This would be something quite different. Thus we would have, for instance, by taking $u = \alpha$, the relation

$$\frac{\partial}{\partial u} = \frac{\partial}{\partial u} + \frac{\partial \beta}{\partial u}\frac{\partial}{\partial \beta}. \tag{1.87}$$

This seems like complete nonsense, until one realizes that the first $\partial/\partial u$ is taken holding v constant, while the second $\partial/\partial u$ is taken holding β constant.

One way out of this kind of puzzle is to be very careful to specify the entire coordinate system whenever a partial derivative is taken. Alternatively, one can do as the chemists do and use notation that explicitly specifies what is being held constant.

One can do similar computations with differentials of the coordinates. Thus, for instance,

$$du = \frac{\partial u}{\partial \alpha}\, d\alpha + \frac{\partial u}{\partial \beta}\, d\beta \tag{1.88}$$

and

$$dv = \frac{\partial v}{\partial \alpha}\, d\alpha + \frac{\partial v}{\partial \beta}\, d\beta \tag{1.89}$$

Differentials such as these occur in line integrals. Notice that the relations are quite different: they involve the inverse of the matrix J.

Here it is important to note that expressions such as du are defined quite independently of the other members of the coordinate system. In fact, let h be an arbitrary scalar. Then dh is defined and may be expressed in terms of an arbitrary coordinate system. For instance

$$dh = \frac{\partial h}{\partial u}\, du + \frac{\partial h}{\partial v}\, dv \tag{1.90}$$

and also

$$dh = \frac{\partial h}{\partial \alpha}\, d\alpha + \frac{\partial h}{\partial \beta}\, d\beta. \tag{1.91}$$

1.3.2 Vector fields

For each point P in the space being studied, there is a vector space $V(P)$, called the tangent space at the point P. The elements of $V(P)$ are pictured as arrows starting at the point P. There are of course infinitely many vectors in each $V(P)$. One can pick a linearly independent list that spans $V(P)$ as basis vectors for $V(P)$.

We consider arbitrary coordinates x, y in the plane. These are not necessarily Cartesian coordinates. Then there is a corresponding basis at each point given by the partial derivatives $\partial/\partial x$ and $\partial/\partial y$. This kind of basis is called a coordinate basis.

A vector field assigns to each point a vector in the tangent space at that point. (The vector should depend on the point in a smooth way.) Thus a vector field is a first order linear partial differential operator of the form

$$L = a\frac{\partial}{\partial x} + b\frac{\partial}{\partial y} \tag{1.92}$$

where a and b are functions of x and y. It is sometimes called a contravariant vector field.

With each vector field L there is an associated ordinary differential equation

$$\frac{dx}{dt} = a = f(x, y) \tag{1.93}$$

$$\frac{dy}{dt} = b = g(x, y). \tag{1.94}$$

Theorem. Let h be a scalar function of x and y. Then along each solution of the differential equation

$$\frac{dh}{dt} = Lh. \tag{1.95}$$

The vector field determines the differential equation. Furthermore, the differential equation determines the vector field. They are the same thing, expressed in somewhat different language. The vector field or the differential equation may be expressed in an arbitrary coordinate system.

A solution of the differential equation is a parameterized curve such that the tangent velocity vector at each point of the curve is the value of the vector field at that point.

Theorem. (straightening out theorem) Consider a point where $L \neq 0$. Then near that point there is a new coordinate system u and v such that

$$L = \frac{\partial}{\partial u}. \tag{1.96}$$

1.3.3 Differential forms

A differential form assigns to each point a linear form on the tangent space at that point. (Again the assignment should be smooth.) Thus it is an expression of the form

$$\omega = p\,dx + q\,dy \tag{1.97}$$

where p and q are functions of x and y. It is sometimes called a covariant vector field.

The value of the differential form on the vector field is the scalar function

$$\langle \omega, L \rangle = pa + qb. \tag{1.98}$$

It is a scalar function of x and y. Again, a differential form may be expressed in an arbitrary coordinate system.

A differential form may be pictured in a rough way by indicating a bunch of parallel lines near each point of the space. However, as we shall see, these lines fit together in a nice way only in a special situation (for an exact form).

A differential form is said to be exact in a region if there is a smooth scalar function h defined on the region such that

$$\omega = dh. \tag{1.99}$$

Explicitly, this says that

$$p\,dx + q\,dy = \frac{\partial h}{\partial x}\,dx + \frac{\partial h}{\partial y}\,dy. \tag{1.100}$$

In this case the contour lines of the differential form at each tangent space fit together on a small scale as pieces of the contour curves of the function h.

A differential form is said to be closed in a region if it satisfies the integrability condition

$$\frac{\partial p}{\partial y} = \frac{\partial q}{\partial x} \tag{1.101}$$

in the region.

Theorem. If a form is exact, then it is closed.

Theorem. (Poincaré lemma) If a form is closed, then it is locally exact.

It is not true that if a form is closed in a region, then it is exact in the region. Thus, for example, the form $(-y\,dx + x\,dy)/(x^2 + y^2)$ is closed in the plane minus the origin, but it is not exact in this region. On the other hand, it is locally exact, by the Poincaré lemma. In fact, consider any smaller region, obtained by removing a line from the origin to infinity. In this smaller region this form may be represented as $d\theta$, where the angle θ has a discontinuity only on the line.

When a differential form is exact it is easy to picture. Then it is of the form dh. The contour lines of h are curves. The differential at any point is obtained by zooming in at the point so close that the contour lines look straight.

A differential form is what occurs as the integrand of a line integral. Let C be an oriented curve. Then the line integral

$$\int_C \omega = \int_C p\,dx + q\,dy \tag{1.102}$$

may be computed with an arbitrary coordinate system and with an arbitrary parameterization of the oriented curve. The numerical answer is always the same.

If a form is exact in a region, so that $\omega = dh$, and if the curve C goes from point P to point Q, then the integral

$$\int_C \omega = h(Q) - h(P). \tag{1.103}$$

Thus the value of the line integral depends only on the end points. It turns out that the form is exact in the region if and only if the value of the line integral along each curve in the region depends only on the end points. Another way to formulate this is to say that a form is exact in a region if and only if the line integral around each closed curve is zero.

1.3.4 Linearization of a vector field near a zero

The situation is more complicated at a point where $L = 0$. At such a point, there is a linearization of the vector field. Thus u, v are coordinates that vanish at the point, and the linearization is given by

$$\frac{du}{dt} = \frac{\partial a}{\partial x}u + \frac{\partial a}{\partial y}v \tag{1.104}$$

$$\frac{dy}{dt} = \frac{\partial b}{\partial x}u + \frac{\partial b}{\partial y}v. \tag{1.105}$$

The partial derivatives are evaluated at the point. Thus this equation has the matrix form

$$\frac{d}{dt}\begin{bmatrix} u \\ v \end{bmatrix} = \begin{bmatrix} a_x & a_y \\ b_x & b_y \end{bmatrix}\begin{bmatrix} u \\ v \end{bmatrix}. \tag{1.106}$$

The idea is that the vector field is somehow approximated by this linear vector field. The u and v represent deviations of the x and y from their values at this point. This linear differential equation can be analyzed using the Jordan form of the matrix.

It is natural to ask whether at an isolated zero of the vector field coordinates can be chosen so that the linear equation is exactly equivalent to the original non-linear equation. The answer is: usually, but not always. In particular, there is a problem when the eigenvalues satisfy certain linear equations with integer coefficients, such as $\lambda_1 + \lambda_2 = 0$. This situation includes some of the most interesting cases, such as that of conjugate pure imaginary eigenvalues.

The precise statement of the eigenvalue condition is in terms of integer linear combinations $m_1\lambda_1 + m_2\lambda_2$ with $m_1 \geq 0$, $m_2 \geq 0$, and $m_1 + m_2 \geq 2$. The condition is that neither λ_1 nor λ_2 may be expressed in this form.

How can this condition be violated? One possibility is to have $\lambda_1 = 2\lambda_1$, which says $\lambda_1 = 0$. Another is to have $\lambda_1 = 2\lambda_2$. More interesting is $\lambda_1 = 2\lambda_1 + \lambda_2$, which gives $\lambda_1 + \lambda_2 = 0$. This includes the case of conjugate pure imaginary eigenvalues.

Theorem. (Sternberg linearization theorem). Suppose that a vector field satisfies the eigenvalue condition at a zero. Then there is a new coordinate system near that zero in which the vector field is a linear vector field.

For the straightening out theorem and the Sternberg linearization theorem, see E. Nelson, Topics in Dynamics I: Flows, Princeton University Press, Princeton, NJ, 1969.

1.3.5 Quadratic approximation to a function at a critical point

The useful way to picture a function h is by its contour lines.

Consider a function h such that at a particular point we have $dh = 0$. Then there is a naturally defined quadratic form

$$d^2h = h_{xx}(dx)^2 + 2h_{xy}dxdy + h_{yy}(dy)^2. \tag{1.107}$$

The partial derivatives are evaluated at the point. This quadratic form is called the Hessian. It is determined by a symmetric matrix

$$H = \begin{bmatrix} h_{xx} & h_{xy} \\ h_{xy} & h_{yy} \end{bmatrix}. \tag{1.108}$$

Its value on a tangent vector L at the point is

$$d^2h(L, L) = h_{xx}a^2 + 2h_{xy}ab + h_{yy}b^2. \tag{1.109}$$

Theorem (Morse lemma) Let h be such that dh vanishes at a point. Let h_0 be the value of h at this point. Suppose that the Hessian is non-degenerate at the point. Then there is a coordinate system u, v such that near the point

$$h - h_0 = \epsilon_1 u^2 + \epsilon_2 v^2, \tag{1.110}$$

where ϵ_1 and ϵ_2 are constants that are each equal to ± 1.

For the Morse lemma, see J. Milnor, Morse Theory, Princeton University Press, Princeton, NJ, 1969.

1.3.6 Differential, gradient, and divergence

It is important to distinguish between differential and gradient. The differential of a scalar function h is given in an arbitrary coordinate system by

$$dh = \frac{\partial h}{\partial u}\, du + \frac{\partial h}{\partial v}\, dv. \tag{1.111}$$

On the other hand, the definition of the gradient depends on the quadratic form that defines the metric:

$$g = E(du)^2 + 2F\, du\, dv + G(dv)^2. \tag{1.112}$$

It is obtained by applying the inverse g^{-1} of the quadratic form to the differential to obtain the corresponding vector field. The inverse of the matrix

$$g = \begin{bmatrix} E & F \\ F & G \end{bmatrix} \tag{1.113}$$

is

$$g^{-1} = \frac{1}{|g|} \begin{bmatrix} G & -F \\ -F & E \end{bmatrix}, \tag{1.114}$$

where $|g| = EG - F^2$ is the determinant of the matrix g. Thus

$$\nabla h = \frac{1}{|g|} \left(G \frac{\partial h}{\partial u} - F \frac{\partial h}{\partial v} \right) \frac{\partial}{\partial u} + \frac{1}{|g|} \left(-F \frac{\partial h}{\partial u} + E \frac{\partial h}{\partial v} \right) \frac{\partial}{\partial v} \tag{1.115}$$

For orthogonal coordinates, when $F = 0$, the metric has the form $g = E(du)^2 + F(dv)^2$. In this case, the expression is simpler:

$$\nabla h = \frac{1}{E} \left(\frac{\partial h}{\partial u} \right) \frac{\partial}{\partial u} + \frac{1}{G} \left(\frac{\partial h}{\partial v} \right) \frac{\partial}{\partial v} \tag{1.116}$$

Example: In polar coordinates

$$g = (dr)^2 + r^2 (d\theta)^2 \tag{1.117}$$

with determinant $|g| = r^2$. So

$$\nabla h = \frac{\partial h}{\partial r} \frac{\partial}{\partial r} + \frac{1}{r^2} \frac{\partial h}{\partial \theta} \frac{\partial}{\partial \theta}. \tag{1.118}$$

Another useful operation is the divergence of a vector field. For a vector field

$$\mathbf{v} = a \frac{\partial}{\partial u} + b \frac{\partial}{\partial v} \tag{1.119}$$

the divergence is

$$\nabla \cdot \mathbf{v} = \frac{1}{\sqrt{g}} \frac{\partial \sqrt{g} a}{\partial u} + \frac{1}{\sqrt{g}} \frac{\partial \sqrt{g} b}{\partial v}. \tag{1.120}$$

In this formula $\sqrt{g}$ denotes the square root of the determinant of the metric form in this coordinate system. It is not immediately clear why this is the correct quantity. However it may ultimately be traced back to the fact that the volume element in an arbitrary coordinate system is $\sqrt{g}\, du\, dv$. For instance, in polar coordinates it is $r\, dr\, d\theta$.

Thus, for example, in polar coordinates the divergence of

$$\mathbf{v} = a \frac{\partial}{\partial r} + b \frac{\partial}{\partial \theta} \tag{1.121}$$

is

$$\nabla \cdot \mathbf{v} = \frac{1}{r} \frac{\partial r a}{\partial r} + \frac{1}{r} \frac{\partial r b}{\partial \theta} = \frac{1}{r} \frac{\partial r a}{\partial r} + \frac{\partial b}{\partial \theta}. \tag{1.122}$$

The Laplace operator is the divergence of the gradient. Thus

$$\nabla \cdot \nabla h = \frac{1}{\sqrt{g}} \frac{\partial}{\partial u} \frac{1}{\sqrt{g}} \left(G \frac{\partial h}{\partial u} - F \frac{\partial h}{\partial v} \right) + \frac{1}{\sqrt{g}} \frac{\partial}{\partial v} \frac{1}{\sqrt{g}} \left(-F \frac{\partial h}{\partial u} + E \frac{\partial h}{\partial v} \right). \tag{1.123}$$

Again this simplifies in orthogonal coordinates:

$$\nabla \cdot \nabla h = \frac{1}{\sqrt{g}} \frac{\partial}{\partial u} \frac{\sqrt{g}}{E} \frac{\partial h}{\partial u} + \frac{1}{\sqrt{g}} \frac{\partial}{\partial v} \frac{\sqrt{g}}{G} \frac{\partial h}{\partial v}. \tag{1.124}$$

In polar coordinates this is

$$\nabla \cdot \nabla h = \frac{1}{r} \frac{\partial}{\partial r} \left(r \frac{\partial h}{\partial r} \right) + \frac{1}{r^2} \frac{\partial^2 h}{\partial \theta^2}. \tag{1.125}$$

There are similar definitions in higher definitions. The important thing to emphasize is that vector fields are very different from differential forms, and this difference is highly visible once one leaves Cartesian coordinates. These objects play different roles. A differential form is the sort of object that fits naturally into a line integral. On the other hand, a vector field is something that defines a flow, via the solution of a system of ordinary differential equations.

1.3.7 Spherical polar coordinates

These ideas have analogs in higher dimensions. The differential has the same form in any coordinate system. On the other hand, the gradient depends on the inner product.

Example: Consider spherical polar coordinates, where θ is co-latitude and ϕ is longitude. Then the metric form is

$$g = (dr)^2 + r^2 (d\theta)^2 + r^2 \sin^2(\theta) (d\phi)^2. \tag{1.126}$$

In this case the gradient is

$$\nabla h = \frac{\partial h}{\partial r}\frac{\partial}{\partial r} + \frac{1}{r^2}\frac{\partial h}{\partial \theta}\frac{\partial}{\partial \theta} + \frac{1}{r^2\sin^2(\theta)}\frac{\partial h}{\partial \phi}\frac{\partial}{\partial \phi}. \tag{1.127}$$

The divergence of a vector field makes sense in any number of dimensions. For spherical polar coordinates the volume element is $r^2\sin(\theta)\,dr\,d\theta\,d\phi$. The divergence of

$$\mathbf{v} = a\frac{\partial}{\partial r} + b\frac{\partial}{\partial \theta} + c\frac{\partial}{\partial \phi} \tag{1.128}$$

is

$$\nabla\cdot\mathbf{v} = \frac{1}{r^2\sin(\theta)}\frac{\partial r^2\sin(\theta)a}{\partial r} + \frac{1}{r^2\sin(\theta)}\frac{\partial r^2\sin(\theta)b}{\partial \theta} + \frac{1}{r^2\sin(\theta)}\frac{\partial r^2\sin(\theta)c}{\partial \phi}. \tag{1.129}$$

This can be written more simply as

$$\nabla\cdot\mathbf{v} = \frac{1}{r^2}\frac{\partial r^2 a}{\partial r} + \frac{1}{\sin(\theta)}\frac{\partial \sin(\theta)b}{\partial \theta} + \frac{\partial c}{\partial \phi}. \tag{1.130}$$

The Laplace operator is the divergence of the gradient. In spherical polar coordinates this is

$$\nabla\cdot\nabla h = \frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial h}{\partial r}\right) + \frac{1}{r^2\sin(\theta)}\frac{\partial}{\partial \theta}\sin(\theta)\frac{\partial h}{\partial \theta} + \frac{1}{r^2\sin^2(\theta)}\frac{\partial^2 h}{\partial \phi^2}. \tag{1.131}$$

1.3.8 Gradient systems

Now we use Cartesian coordinates x, y and the usual inner product. This inner product maps a form to a corresponding vector field. Thus the differential form

$$dh = \frac{\partial h}{\partial x}\,dx + \frac{\partial h}{\partial y}\,dy \tag{1.132}$$

determines a gradient vector field

$$\nabla h = \frac{\partial h}{\partial x}\frac{\partial}{\partial x} + \frac{\partial h}{\partial y}\frac{\partial}{\partial y}. \tag{1.133}$$

The corresponding differential equation is

$$\frac{dx}{dt} = h_x \tag{1.134}$$

$$\frac{dy}{dt} = h_y. \tag{1.135}$$

Theorem. Along a solution of a gradient system

$$\frac{dh}{dt} = h_x^2 + h_y^2 \geq 0. \tag{1.136}$$

This is hill climbing. The picture is that at each point, the gradient vector field points uphill in the steepest direction.

Consider a point where $dh = 0$. Then the linearization of the equation is given by

$$\frac{du}{dt} = h_{xx}u + h_{xy}v \tag{1.137}$$

$$\frac{dv}{dt} = h_{xy}u + h_{yy}v. \tag{1.138}$$

where the partial derivatives are evaluated at the point. This is a real symmetric matrix, and therefore its eigenvalues are real.

1.3.9 Hamiltonian systems

Now we use Cartesian coordinates x, y, but now instead of a symmetric inner product we use a skew-symmetric form to map a form to a corresponding vector. Thus the differential form

$$dH = \frac{\partial H}{\partial x}\,dx + \frac{\partial H}{\partial y}\,dy \tag{1.139}$$

determines a Hamiltonian vector field

$$\check{\nabla} H = \frac{\partial H}{\partial y}\frac{\partial}{\partial x} - \frac{\partial H}{\partial x}\frac{\partial}{\partial y}. \tag{1.140}$$

The corresponding differential equation is

$$\frac{dx}{dt} = H_y \tag{1.141}$$

$$\frac{dy}{dt} = -H_x. \tag{1.142}$$

Theorem. (Conservation of Energy) Along a solution of a Hamiltonian system.

$$\frac{dH}{dt} = H_y H_x - H_x H_y = 0. \tag{1.143}$$

This is conservation of energy. The picture is that at each point the vector field points along one of the contour lines of H.

Consider a point where $dH = 0$. Then the linearization of the equation is given by

$$\frac{du}{dt} = H_{xy}u + H_{yy}v \tag{1.144}$$

$$\frac{dv}{dt} = -H_{xx}u - H_{xy}v. \tag{1.145}$$

where the partial derivatives are evaluated at the point. This is a special kind of matrix. The eigenvalues λ satisfy the equation

$$\lambda^2 = H_{xy}^2 - H_{xx}H_{yy}. \tag{1.146}$$

So they are either real with opposite sign, or they are complex conjugate pure imaginary. In the real case solutions linger near the equilibrium point. In the complex case solutions oscillate near the equilibrium point.

1.3.10 Contravariant and covariant

Here is a summary that may be useful. Contravariant objects include points and vectors (arrows). These are objects that live in the space. They also include oriented curves (whose tangent vectors are arrows). Thus a vector field (contravariant) determines solution curves of the associated system of differential equations (contravariant).

Covariant objects associate numbers to objects that live in the space. They include scalars, linear forms (elements of the dual space), and bilinear forms. They also include scalar functions and differential forms. Often covariant objects are described by their contours. The differential of a scalar function (covariant) is a differential form (covariant). The integral of a differential form (a covariant object) along an oriented curve (a contravariant object) is a number.

There are also mixed objects. A linear transformation is a mixed object, since it takes vectors as inputs (covariant), but it gives vectors as outputs (contravariant).

A bilinear form may be used to move from the contravariant world to the covariant world. The input is a vector, and the output is a linear form. If the bilinear form is non-degenerate, then there is an inverse that can take a linear form as an input and give a vector as an output. This occurs for instance when we take the differential of a scalar function (covariant) and use a symmetric bilinear form to get a gradient vector field (contravariant). It also occurs when we take the differential of a scalar function (covariant) and use an anti-symmetric bilinear form to get a Hamiltonian vector field (contravariant).

1.3.11 Problems

1. A vector field that is non-zero at a point can be transformed into a constant vector field near that point. Pick a point away from the origin and find coordinates u and v near there so that

$$-y\frac{\partial}{\partial x} + x\frac{\partial}{\partial y} = \frac{\partial}{\partial u}. \tag{1.147}$$

2. A vector field that is non-zero at a point can be transformed into a constant vector field near that point. Pick a point away from the origin and find coordinates u and v so that

$$-\frac{y}{x^2+y^2}\frac{\partial}{\partial x} + \frac{x}{x^2+y^2}\frac{\partial}{\partial y} = \frac{\partial}{\partial u}. \tag{1.148}$$

3. A differential form usually cannot be transformed into a constant differential form, but there special circumstances when that can occur. Is it

possible to find coordinates u and v near a given point (not the origin) so that

$$-y\,dx + x\,dy = du? \tag{1.149}$$

4. A differential form usually cannot be transformed into a constant differential form, but there special circumstances when that can occur. Is it possible to find coordinates u and v near a given point (not the origin) so that

$$-\frac{y}{x^2+y^2}\,dx + \frac{x}{x^2+y^2}\,dy = du? \tag{1.150}$$

5. Consider the vector field

$$L = x(4-x-y)\frac{\partial}{\partial x} + (x-2)y\frac{\partial}{\partial y}. \tag{1.151}$$

Find its zeros. At each zero, find the linearization. For each linearization, find the eigenvalues. Use this information to sketch the vector field.

6. Let h be a smooth function. Its gradient expressed with respect to Cartesian basis vectors $\partial/\partial x$ and $\partial/\partial y$ is

$$\nabla h = \frac{\partial h}{\partial x}\frac{\partial}{\partial x} + \frac{\partial h}{\partial y}\frac{\partial}{\partial y}. \tag{1.152}$$

Find the gradient ∇h expressed with respect to polar basis vectors $\partial/\partial r$ and $\partial/\partial\theta$.

7. Let H be a smooth function. Its Hamiltonian vector field expressed with respect to Cartesian basis vectors $\partial/\partial x$ and $\partial/\partial y$ is

$$\check{\nabla} H = \frac{\partial H}{\partial y}\frac{\partial}{\partial x} - \frac{\partial H}{\partial x}\frac{\partial}{\partial y}. \tag{1.153}$$

Find this same vector field expressed with respect to polar basis vectors $\partial/\partial r$ and $\partial/\partial\theta$.

8. Consider the vector field

$$L = (1+x^2+y^2)y\frac{\partial}{\partial x} - (1+x^2+y^2)x\frac{\partial}{\partial y}. \tag{1.154}$$

Find its linearization at 0. Show that there is no coordinate system near 0 in which the vector field L is expressed by its linearization. Hint: Solve the associated system of ordinary differential equations, both for L and for its linearization. Find the period of a solution in both cases.

9. Here is an example of a fixed point where the linear stability analysis gives an elliptic fixed point but changing to polar coordinates shows the unstable nature of the fixed point:

$$\frac{dx}{dt} = -y + x(x^2+y^2) \tag{1.155}$$

$$\frac{dy}{dt} = x + y(x^2+y^2). \tag{1.156}$$

Change the vector field to the polar coordinate representation and solve the corresponding system of ordinary differential equations.

Chapter 2

Fourier series

2.1 Orthonormal families

Let T be the circle parameterized by $[0, 2\pi)$ or by $[-\pi, \pi)$. Let f be a complex function on T that is integrable. The nth Fourier coefficient is

$$c_n = \frac{1}{2\pi} \int_0^{2\pi} e^{-inx} f(x)\, dx. \tag{2.1}$$

The goal is to show that f has a representation as a Fourier series

$$f(x) = \sum_{n=-\infty}^{\infty} c_n e^{inx}. \tag{2.2}$$

There are two problems. One is to interpret the sense in which the series converges. The second is to show that it actually converges to f.

This is a huge subject. However the simplest and most useful theory is in the context of Hilbert space. Let $L^2(T)$ be the space of all (Borel measurable) functions such that

$$\|f\|^2 = \frac{1}{2\pi} \int_0^{2\pi} |f(x)|^2\, dx < \infty. \tag{2.3}$$

Then $L^2(T)$ is a Hilbert space with inner product

$$(f, g) = \frac{1}{2\pi} \int_0^{2\pi} \overline{f(x)} g(x)\, dx. \tag{2.4}$$

Let

$$\phi_n(x) = \exp(inx). \tag{2.5}$$

Then the ϕ_n form an orthogonal family in $L^2(T)$. Furthermore, we have the identity

$$\|f\|^2 = \sum_{|n| \le N} |c_n|^2 + \|f - \sum_{|n| \le N} c_n \phi_n\|^2. \tag{2.6}$$

In particular, we have Bessel's inequality

$$\|f\|^2 \geq \sum_{|n|\leq N} |c_n|^2. \tag{2.7}$$

This shows that

$$\sum_{n=-\infty}^{\infty} |c_n|^2 < \infty. \tag{2.8}$$

The space of sequences satisfying this identity is called ℓ^2. Thus we have proved the following theorem.

Theorem. If f is in $L^2(T)$, then its sequence of Fourier coefficients is in ℓ^2.

2.2 L^2 convergence

It is easy to see that $\sum_{|n|\leq N} c_n \phi_n$ is a Cauchy sequence in $L^2(T)$ as $N \to \infty$. It follows from the completeness of $L^2(T)$ that it converges in the L^2 sense to a sum g in $L^2(T)$. That is, we have

$$\lim_{N\to\infty} \|g - \sum_{|n|\leq N} c_n \phi_n\|^2 = 0. \tag{2.9}$$

The only remaining thing to show is that $g = f$. This, however, requires some additional ideas.

One way to do it is to take r with $0 < r < 1$ and look at the sum

$$\sum_{n=-\infty}^{\infty} r^{|n|} c_n e^{inx} = \frac{1}{2\pi} \int_0^{2\pi} P_r(x-y) f(y)\, dy. \tag{2.10}$$

Here

$$P_r(x) = \sum_{n=-\infty}^{\infty} r^{|n|} e^{inx} = \frac{1-r^2}{1-2r\cos(x)+r^2}. \tag{2.11}$$

The functions $\frac{1}{2\pi} P_r(x)$ have the properties of an approximate delta function. Each such function is positive and has integral 1 over the periodic interval. Furthermore,

$$P_r(x) \leq \frac{1-r^2}{2r(1-\cos(x))}, \tag{2.12}$$

which approaches zero as $r \to 1$ away from points where $\cos(x) = 1$.

Theorem. If f is continuous on T, then

$$f(x) = \lim_{r\uparrow 1} \sum_{n=-\infty}^{\infty} r^{|n|} c_n e^{inx}, \tag{2.13}$$

and the convergence is uniform.

Proof: It is easy to compute that

$$\sum_{n=-\infty}^{\infty} r^{|n|} c_n e^{inx} = \frac{1}{2\pi}\int_0^{2\pi} P_r(x-y) f(y)\, dy = \frac{1}{2\pi}\int_0^{2\pi} P_r(z) f(x-z)\, dz. \quad (2.14)$$

Hence

$$f(x) - \sum_{n=-\infty}^{\infty} r^{|n|} c_n e^{inx} = \frac{1}{2\pi}\int_0^{2\pi} P_r(z)(f(x) - f(x-z))\, dz. \quad (2.15)$$

Thus

$$|f(x) - \sum_{n=-\infty}^{\infty} r^{|n|} c_n e^{inx}| = |\frac{1}{2\pi}\int_0^{2\pi} P_r(z)(f(x)-f(x-z))\, dz| \leq \frac{1}{2\pi}\int_0^{2\pi} P_r(z)|f(x)-f(x-z)|\, dz. \quad (2.16)$$

Since f is continuous on T, its absolute value is bounded by some constant M. Furthermore, since f is continuous on T, it is uniformly continuous on T. Consider arbitrary $\epsilon > 0$. It follows from the uniform continuity that there exists $\delta > 0$ such that for all x and all z with $|z| < \delta$ we have $|f(x) - f(x-z)| < \epsilon/2$. Thus the right hand side is bounded by

$$\frac{1}{2\pi}\int_{|z|<\delta} P_r(z)|f(x)-f(x-z)|\, dz + \frac{1}{2\pi}\int_{|z|\geq\delta} P_r(z)|f(x)-f(x-z)|\, dx \leq \epsilon/2 + \frac{1-r^2}{2r(1-\cos(\delta))} 2M. \quad (2.17)$$

Take r so close to 1 that the second term is also less than $\epsilon/2$. Then the difference that is being estimated is less than ϵ for such r. This proves the result.

Theorem. If f is in $L^2(T)$, then

$$f = \sum_{n=-\infty}^{\infty} c_n \phi_n \quad (2.18)$$

in the sense that

$$\lim_{N\to\infty} \|f - \sum_{|n|\leq N} c_n \phi_n\|^2 = 0. \quad (2.19)$$

Proof: Let f have Fourier coefficients c_n and $g = \sum_n c_n \phi_n$. Let $\epsilon > 0$ be arbitrary. Let h be in $C(T)$ with

$$\|f - h\|_2 < \epsilon/2. \quad (2.20)$$

Suppose h has Fourier coefficients d_n. Then there exists $r < 1$ such that

$$\|h - \sum_n r^n d_n e^{inx}\|_\infty < \epsilon/2. \quad (2.21)$$

It follows that

$$\|h - \sum_n r^n d_n e^{inx}\|_2 < \epsilon/2. \quad (2.22)$$

Thus

$$\|f - \sum_n r^n d_n e^{inx}\|_2 < \epsilon. \tag{2.23}$$

However since g is the orthogonal projection of f onto the span of the ϕ_n, it is also the best approximation of f in the span of the ϕ_n. Thus

$$\|f - g\|_2 < \epsilon. \tag{2.24}$$

Since $\epsilon > 0$ is arbitrary, we can only conclude that $f = g$.

Theorem. If f is in $L^2(T)$, then

$$\|f\|^2 = \sum_{n=-\infty}^{\infty} |c_n|^2. \tag{2.25}$$

2.3 Absolute convergence

Define the function spaces

$$C(T) \subset L^\infty(T) \subset L^2(T) \subset L^1(T). \tag{2.26}$$

The norms $\|f\|_\infty$ on the first two spaces are the same, the smallest number M such that $|f(x)| \le M$ (with the possible exception of a set of x of measure zero). The space $C(T)$ consists of continuous functions; the space $L^\infty(T)$ consists of all bounded functions. The norm on $L^2(T)$ is given by $\|f\|_2^2 = \frac{1}{2\pi}\int_0^{2\pi} |f(x)|^2\, dx$. The norm on $L^1(T)$ is given by $\|f\|_1 = \frac{1}{2\pi}\int_0^{2\pi} |f(x)|\, dx$. Since the integral is a probability average, their relation is

$$\|f\|_1 \le \|f\|_2 \le \|f\|_\infty. \tag{2.27}$$

Also define the sequence spaces

$$\ell^1 \subset \ell^2 \subset c_0 \subset \ell^\infty. \tag{2.28}$$

The norm on ℓ^1 is $\|c\|_1 = \sum_n |c_n|$. Then norm on ℓ^2 is given by $\|c\|_2^2 = \sum_n |c_n|^2$. The norms on the last two spaces are the same, that is, $\|c\|_\infty$ is the smallest M such that $|c_n| \le M$. The space c_0 consists of all sequences with limit 0 at infinity. The relation between these norms is

$$\|c\|_\infty \le \|c\|_2 \le \|c\|_1. \tag{2.29}$$

We have seen that the Fourier series theorem gives a perfect correspondence between $L^2(T)$ and ℓ^2. For the other spaces the situation is more complex.

Riemann-Lebesgue Lemma. If f is in $L^1(T)$, then the Fourier coefficients of f are in c_0, that is, they approaches 0 at infinity.

Proof: Each function in $L^2(T)$ has Fourier coefficients in ℓ^2, so each function in $L^2(T)$ has Fourier coefficients that vanish at infinity. The map from a function to its Fourier coefficients gives a continuous map from $L^1(T)$ to ℓ^∞. However

every function in $L^1(T)$ may be approximated arbitrarily closely in $L^1(T)$ norm by a function in $L^2(T)$. Hence its coefficients may be approximated arbitrarily well in ℓ^∞ norm by coefficients that vanish at infinity. Therefore the coefficients vanish at infinity.

In summary, the map from a function to its Fourier coefficients gives a continuous map from $L^1(T)$ to c_0. That is, the Fourier coefficients of an integrable function are bounded (this is obvious) and approach zero (Riemann-Lebesgue lemma). Furthermore, the Fourier coefficients determine the function.

The map from Fourier coefficients to functions gives a continuous map from ℓ^1 to $C(T)$. An sequence that is absolutely summable defines a Fourier series that converges absolutely and uniformly to a continuous function.

Theorem. If f is in $L^2(T)$ and if f' exists (in the sense that f is an integral of f) and if f' is also in $L^2(T)$, then the Fourier coefficients are in ℓ^1.

2.4 Pointwise convergence

This gives a very satisfactory picture of Fourier series. However there is one slightly unsatisfying point. The convergence in the L^2 sense does not imply convergence at a particular point. Of course, if the derivative is in L^2 then we have uniform convergence, and in particular convergence at each point. But what if the function is differentiable at one point but has discontinuities at other points? What can we say about convergence at that one point? Fortunately, we can find something about that case by a closer examination of the partial sums.

One looks at the partial sum

$$\sum_{|n|\le N} c_n e^{inx} = \frac{1}{2\pi}\int_0^{2\pi} D_N(x-y) f(y)\, dy. \tag{2.30}$$

Here

$$D_N(x) = \sum_{|n|\le N} e^{inx} = \frac{\sin((N+\frac{1}{2})x)}{\sin(\frac{1}{2}x)}. \tag{2.31}$$

This Dirichlet kernel $D_N(x)$ has at least some of the properties of an approximate delta function. Unfortunately, it is not positive; instead it oscillates wildly for large N at points away from where $\sin(x/2) = 0$. However the function $1/(2\pi)D_N(x)$ does have integral 1.

Theorem. If for some x the function

$$d_x(z) = \frac{f(x+z) - f(x)}{2\sin(z/2)} \tag{2.32}$$

is in $L^1(T)$, then at that point

$$f(x) = \sum_{n=-\infty}^{\infty} c_n \phi_n(x). \tag{2.33}$$

Note that if $d_x(z)$ is continuous at $z = 0$, then its value at $z = 0$ is $d_x(0) = f'(x)$. So the hypothesis of the theorem is a condition related to differentiability of f at the point x. The conclusion of the theorem is pointwise convergence of the Fourier series at that point. Since f may be discontinuous at other points, it is possible that this Fourier series is not absolutely convergent.

Proof: We have

$$f(x) - \sum_{|n|\le N} c_n e^{inx} = \frac{1}{2\pi}\int_0^{2\pi} D_N(z)(f(x) - f(x-z))\,dz. \tag{2.34}$$

We can write this as

$$f(x) - \sum_{|n|\le N} c_n e^{inx} = \frac{1}{2\pi}\int_0^{2\pi} 2\sin((N+\frac{1}{2})z)d_x(-z)\,dz. \tag{2.35}$$

This goes to zero as $N \to \infty$, by the Riemann-Lebesgue lemma.

2.5 Problems

1. Let $f(x) = x$ defined for $-\pi \le x < \pi$. Find the $L^1(T)$, $L^2(T)$, and $L^\infty(T)$ norms of f, and compare them.

2. Find the Fourier coefficients c_n of f for all n in Z.

3. Find the ℓ^∞, ℓ^2, and ℓ^1 norms of these Fourier coefficients, and compare them.

4. Use the equality of L^2 and ℓ^2 norms to compute

$$\zeta(2) = \sum_{n=1}^{\infty} \frac{1}{n^2}.$$

5. Compare the ℓ^∞ and L^1 norms for this problem. Compare the L^∞ and ℓ^1 norms for this problem.

6. Use the pointwise convergence at $x = \pi/2$ to evaluate the infinite sum

$$\sum_{k=0}^{\infty} (-1)^k \frac{1}{2k+1},$$

regarded as a limit of partial sums. Does this sum converge absolutely?

7. Let $F(x) = \frac{1}{2}x^2$ defined for $-\pi \le x < \pi$. Find the Fourier coefficients of this function.

8. Use the equality of L^2 and ℓ^2 norms to compute

$$\zeta(4) = \sum_{n=1}^{\infty} \frac{1}{n^4}.$$

9. Compare the ℓ^∞ and L^1 norms for this problem. Compare the L^∞ and ℓ^1 norms for this problem.

10. At which points x of T is $F(x)$ continuous? Differentiable? At which points x of T is $f(x)$ continuous? Differentiable? At which x does $F'(x) = f(x)$? Can the Fourier series of $f(x)$ be obtained by differentiating the Fourier series of $F(x)$ pointwise? (This last question can be answered by inspecting the explicit form of the Fourier series for the two problems.)

Chapter 3

Fourier transforms

3.1 Introduction

Let R be the line parameterized by x. Let f be a complex function on R that is integrable. The Fourier transform $\hat{f} = Ff$ is

$$\hat{f}(k) = \int_{-\infty}^{\infty} e^{-ikx} f(x)\, dx. \tag{3.1}$$

It is a function on the (dual) real line R' parameterized by k. The goal is to show that f has a representation as an inverse Fourier transform

$$f(x) = \int_{-\infty}^{\infty} e^{ikx} \hat{f}(k)\, \frac{dk}{2\pi}. \tag{3.2}$$

There are two problems. One is to interpret the sense in which these integrals converge. The second is to show that the inversion formula actually holds.

The simplest and most useful theory is in the context of Hilbert space. Let $L^2(R)$ be the space of all (Borel measurable) complex functions such that

$$\|f\|_2^2 = \int_{-\infty}^{\infty} |f(x)|^2\, dx < \infty. \tag{3.3}$$

Then $L^2(R)$ is a Hilbert space with inner product

$$(f, g) = \int \overline{f(x)} g(x)\, dx. \tag{3.4}$$

Let $L^2(R')$ be the space of all (Borel measurable) complex functions such that

$$\|h\|_2^2 = \int_{-\infty}^{\infty} |h(k))|^2\, \frac{dk}{2\pi} < \infty. \tag{3.5}$$

Then $L^2(R')$ is a Hilbert space with inner product

$$(h, u) = \int_{-\infty}^{\infty} \overline{h(k)} u(k)\, \frac{dk}{2\pi}. \tag{3.6}$$

We shall see that the correspondence between f and $\hat{f}$ is a unitary map from $L^2(R)$ onto $L^2(R')$. So this theory is simple and powerful.

3.2 L^1 theory

First, we need to develop the L^1 theory. The space L^1 is a Banach space. Its dual space is L^∞, the space of essentially bounded functions. An example of a function in the dual space is the exponential function $\phi_k(x) = e^{ikx}$. The Fourier transform is then

$$\hat{f}(k) = \langle \phi_k, f \rangle = \int_{-\infty}^{\infty} \overline{\phi_k(x)} f(x)\, dx, \tag{3.7}$$

where ϕ_k is in L^∞ and f is in L^1.

Theorem. If f, g are in $L^1(R)$, then the convolution $f * g$ is another function in $L^1(R)$ defined by

$$(f * g)(x) = \int_{-\infty}^{\infty} f(x-y) g(y)\, dy. \tag{3.8}$$

Theorem. If f, g are in $L^1(R)$, then the Fourier transform of the convolution is the product of the Fourier transforms:

$$\widehat{(f * g)}(k) = \hat{f}(k)\hat{g}(k). \tag{3.9}$$

Theorem. Let $f^*(x) = \overline{f(-x)}$. Then the Fourier transform of f^* is the complex conjugate of $\hat{f}$.

Theorem. If f is in $L^1(R)$, then its Fourier transform $\hat{f}$ is in $L^\infty(R')$ and satisfies $\|\hat{f}\|_\infty \leq \|f\|_1$. Furthermore, $\hat{f}$ is in $C_0(R')$, the space of bounded continuous functions that vanish at infinity.

Theorem. If f is in L^1 and is also continuous and bounded, we have the inversion formula in the form

$$f(x) = \lim_{\epsilon \downarrow 0} \int_{-\infty}^{\infty} e^{ikx} \hat{\delta}_\epsilon(k) \hat{f}(k)\, \frac{dk}{2\pi}, \tag{3.10}$$

where

$$\hat{\delta}_\epsilon(k) = \exp(-\epsilon |k|). \tag{3.11}$$

Proof: The inverse Fourier transform of this is

$$\delta_\epsilon(x) = \frac{1}{\pi} \frac{\epsilon}{x^2 + \epsilon^2}. \tag{3.12}$$

It is easy to calculate that

$$\int_{-\infty}^{\infty} e^{ikx} \hat{\delta}_\epsilon(k) \hat{f}(k)\, \frac{dk}{2\pi} = (\delta_\epsilon * f)(x). \tag{3.13}$$

However δ_ϵ is an approximate delta function. The result follows by taking $\epsilon \to 0$.

3.3 L^2 theory

The space L^2 is its own dual space, and it is a Hilbert space. It is the setting for the most elegant and simple theory of the Fourier transform.

Lemma. If f is in $L^1(R)$ and in $L^2(R)$, then $\hat{f}$ is in $L^2(R')$, and $\|f\|_2^2 = \|\hat{f}\|_2^2$.

Proof. Let $g = f^* * f$. Then g is in L^1 and is continuous and bounded. Furthermore, the Fourier transform of g is $|\hat{f}(k)|^2$. Thus

$$\|f\|_2^2 = g(0) = \lim_{\epsilon \downarrow 0} \int_{-\infty}^{\infty} \hat{\delta}_\epsilon(k) |\hat{f}(k)|^2 \, \frac{dk}{2\pi} = \int_{-\infty}^{\infty} |\hat{f}(k)|^2 \, \frac{dk}{2\pi}. \tag{3.14}$$

Theorem. Let f be in $L^2(R)$. For each a, let $f_a = 1_{[-a,a]} f$. Then f_a is in $L^1(R)$ and in $L^2(R)$, and $f_a \to f$ in $L^2(R)$ as $a \to \infty$. Furthermore, there exists $\hat{f}$ in $L^2(R')$ such that $\hat{f}_a \to \hat{f}$ as $a \to \infty$.

Explicitly, this says that the Fourier transform $\hat{f}(k)$ is characterized by

$$\int_{-\infty}^{\infty} |\hat{f}(k) - \int_{-a}^{a} e^{-ikx} f(x) \, dx|^2 \frac{dk}{2\pi} \to 0 \tag{3.15}$$

as $a \to \infty$.

These arguments show that the Fourier transformation $F : L^2(R) \to L^2(R')$ defined by $Ff = \hat{f}$ is well-defined and preserves norm. It is easy to see from the fact that it preserves norm that it also preserves inner product: $(Ff, Fg) = (f, g)$.

Define the inverse Fourier transform F^* in the same way, so that if h is in $L^1(R')$ and in $L^2(R')$, then F^*h is in $L^2(R)$ and is given by the usual inverse Fourier transform formula. Again we can extend the inverse transformation to $F^* : L^2(R') \to L^2(R)$ so that it preserves norm and inner product.

Now it is easy to check that $(F^*h, f) = (h, Ff)$. Take $h = Fg$. Then $(F^*Fg, f) = (Fg, Ff) = (g, f)$. That is $F^*Fg = g$. Similarly, one may show that $FF^*u = u$. These equations show that F is unitary and that $F^* = F^{-1}$ is the inverse of F. This proves the following result.

Theorem. The Fourier transform F initially defined on $L^1(R) \cap L^2(R)$ extends by continuity to $F : L^2(R) \to L^2(R')$. The inverse Fourier transform F^* initially defined on $L^1(R') \cap L^2(R')$ extends by continuity to $F^* : L^2(R') \to L^2(R)$. These are unitary operators that preserve L^2 norm and preserve inner product. Furthermore, F^* is the inverse of F.

3.4 Absolute convergence

We have seen that the Fourier transform gives a perfect correspondence between $L^2(R)$ and $L^2(R')$. For the other spaces the situation is more complex.

The map from a function to its Fourier transform gives a continuous map from $L^1(R)$ to part of $C_0(R')$. That is, the Fourier transform of an integrable function is continuous and bounded (this is obvious) and approach zero

(Riemann-Lebesgue lemma). Furthermore, this map is one-to-one. That is, the Fourier transform determines the function.

The inverse Fourier transform gives a continuous map from $L^1(R')$ to $C_0(R)$. This is also a one-to-one transformation.

One useful fact is that if f is in $L^1(R)$ and g is in $L^2(R)$, then the convolution $f * g$ is in $L^2(R)$. Furthermore, $\widehat{f * g}(k) = \hat{f}(k)\hat{g}(k)$ is the product of a bounded function with an $L^2(R')$ function, and therefore is in $L^2(R')$.

However the same pattern of the product of a bounded function with an L^2 function can arise in other ways. For instance, consider the translate f_a of a function f in $L^2(R)$ defined by $f_a(x) = f(x-a)$. Then $\widehat{f_a}(k) = \exp(-ika)\hat{f}(k)$. This is also the product of a bounded function with an $L^2(R')$ function.

One can think of this last example as a limiting case of a convolution. Let δ_ϵ be an approximate δ function. Then $(\delta_\epsilon)_a * f$ has Fourier transform $\exp(-ika)\hat{\delta}_\epsilon(k)\hat{f}(k)$. Now let $\epsilon \to 0$. Then $(\delta_\epsilon)_a * f \to f_a$, while $\exp(-ika)\hat{\delta}_\epsilon(k)\hat{f}(k) \to \exp(-ika)\hat{f}(k)$.

Theorem. If f is in $L^2(R)$ and if f' exists (in the sense that f is an integral of f) and if f' is also in $L^2(R)$, then the Fourier transform is in $L^1(R')$. As a consequence f is is $C_0(R)$.

Proof: $\hat{f}(k) = (1/\sqrt{1+k^2}) \cdot \sqrt{1+k^2}\hat{f}(k)$. Since f is in $L^2(R)$, it follows that $\hat{f}(k)$ is in $L^2(R)$. Since f' is in $L^2(R)$, it follows that $k\hat{f}(k)$ is in $L^2(R')$. Hence $\sqrt{1+k^2}\hat{f}(k)$ is in $L^2(R')$. Since $1/\sqrt{1+k^2}$ is also in $L^2(R')$, it follows from the Schwarz inequality that $\hat{f}(k)$ is in $L^1(R')$.

3.5 Fourier transform pairs

There are some famous Fourier transforms.

Fix $\sigma > 0$. Consider the Gaussian

$$g_\sigma(x) = \frac{1}{\sqrt{2\pi\sigma^2}} \exp(-\frac{x^2}{2\sigma^2}). \tag{3.16}$$

Its Fourier transform is

$$\hat{g}_\sigma(k) = \exp(-\frac{\sigma^2 k^2}{2}). \tag{3.17}$$

Proof: Define the Fourier transform $\hat{g}_\sigma(k)$ by the usual formula. Check that

$$\left(\frac{d}{dk} + \sigma^2 k\right) \hat{g}_\sigma(k) = 0. \tag{3.18}$$

This proves that

$$\hat{g}_\sigma(k) = C \exp(-\frac{\sigma^2 k^2}{2}). \tag{3.19}$$

Now apply the equality of L^2 norms. This implies that $C^2 = 1$. By looking at the case $k = 0$ it becomes obvious that $C = 1$.

Let $\epsilon > 0$. Introduce the Heaviside function $H(k)$ that is 1 for $k > 0$ and 0 for $k < 0$. The two basic Fourier transform pairs are

$$f_\epsilon(x) = \frac{1}{x - i\epsilon} \tag{3.20}$$

with Fourier transform

$$\hat{f}_\epsilon(k) = 2\pi i H(-k) e^{\epsilon k}. \tag{3.21}$$

and its complex conjugate

$$\overline{f_\epsilon(x)} = \frac{1}{x + i\epsilon} \tag{3.22}$$

with Fourier transform

$$\overline{\hat{f}_\epsilon(-k)} = -2\pi i H(k) e^{-\epsilon k}. \tag{3.23}$$

These may be checked by computing the inverse Fourier transform. Notice that f_ϵ and its conjugate are not in $L^1(R)$.

Take $1/\pi$ times the imaginary part. This gives the approximate delta function

$$\delta_\epsilon(x) = \frac{1}{\pi} \frac{\epsilon}{x^2 + \epsilon^2}. \tag{3.24}$$

with Fourier transform

$$\hat{\delta}_\epsilon(k) = e^{-\epsilon |k|}. \tag{3.25}$$

Take the real part. This gives the approximate principal value of $1/x$ function

$$p_\epsilon(x) = \frac{x}{x^2 + \epsilon^2} \tag{3.26}$$

with Fourier transform

$$\hat{p}_\epsilon(k) = -\pi i [H(k) e^{-\epsilon k} - H(-k) e^{\epsilon k}]. \tag{3.27}$$

3.6 Problems

1. Let $f(x) = 1/(2a)$ for $-a \le x \le a$ and be zero elsewhere. Find the $L^1(R)$, $L^2(R)$, and $L^\infty(R)$ norms of f, and compare them.
2. Find the Fourier transform of f.
3. Find the $L^\infty(R')$, $L^2(R')$, and $L^1(R')$ norms of the Fourier transform, and compare them.
4. Compare the $L^\infty(R')$ and $L^1(R)$ norms for this problem. Compare the $L^\infty(R)$ and $L^1(R')$ norms for this problem.
5. Use the pointwise convergence at $x = 0$ to evaluate an improper integral.
6. Calculate the convolution of f with itself.
7. Find the Fourier transform of the convolution of f with itself. Verify in this case that the Fourier transform of the convolution is the product of the Fourier transforms.

3.7 Poisson summation formula

Theorem: Let f be in $L^1(R)$ with $\hat{f}$ in $L^1(R')$ and such that $\sum_k |\hat{f}(k)| < \infty$. Then

$$2\pi \sum_n f(2\pi n) = \sum_k \hat{f}(k). \tag{3.28}$$

Proof: Let

$$S(t) = \sum_n f(2\pi n + t). \tag{3.29}$$

Since $S(t)$ is 2π periodic, we can expand

$$S(t) = \sum_k a_k e^{ikt}. \tag{3.30}$$

It is easy to compute that

$$a_k = \frac{1}{2\pi} \int_0^{2\pi} S(t) e^{-ikt}\, dt = \frac{1}{2\pi} \hat{f}(k). \tag{3.31}$$

So the Fourier series of $S(t)$ is absolutely summable. In particular

$$S(0) = \sum_k a_k. \tag{3.32}$$

3.8 Problems

1. In this problem the Fourier transform is

$$\hat{f}(k) = \int_{-\infty}^{\infty} e^{-ixk} f(x)\, dx$$

and the inverse Fourier transform is

$$f(x) = \int_{-\infty}^{\infty} e^{ixk} f(k)\, \frac{dk}{2\pi}.$$

These provide an isomorphism between the Hilbert spaces $L^2(\mathbf{R}, dx)$ and $L^2(\mathbf{R}, \frac{dk}{2\pi})$. The norm of f in the first space is equal to the norm of $\hat{f}$ in the second space. We will be interested in the situation where the Fourier transform is band-limited, that is, only waves with $|k| \le a$ have non-zero amplitude.

Make the assumption that $|k| > a$ implies $\hat{f}(k) = 0$. That is, the Fourier transform of f vanishes outside of the interval $[-a, a]$.

Let

$$g(x) = \frac{\sin(ax)}{ax}.$$

The problem is to prove that

$$f(x) = \sum_{m=-\infty}^{\infty} f(\frac{m\pi}{a})g(x - \frac{m\pi}{a}).$$

This says that if you know f at multiples of π/a, then you know f at all points.

Hint: Let $g_m(x) = g(x - m\pi/a)$. The task is to prove that $f(x) = \sum_m c_m g_m(x)$ with $c_m = f(m\pi/a)$. It helps to use the Fourier transform of these functions. First prove that the Fourier transform of $g(x)$ is given by $\hat{g}(k) = \pi/a$ for $|k| \leq a$ and $\hat{g}(k) = 0$ for $|k| > a$. (Actually, it may be easier to deal with the inverse Fourier transform.) Then prove that $\hat{g}_m(k) = \exp(-im\pi k/a)\hat{g}(k)$. Finally, note that the functions $\hat{g}_m(k)$ are orthogonal.

2. In the theory of neural networks one wants to synthesize an arbitrary function from linear combinations of translates of a fixed function. Let f be a function in $L^2(R)$. Suppose that the Fourier transform $\hat{f}(k) \neq 0$ for all k. Define the translate f_a by $f_a(x) = f(x - a)$. The task is to show that the set of all linear combinations of the functions f_a, where a ranges over all real numbers, is dense in $L^2(R)$.

   Hint: It is sufficient to show that if g is in $L^2(R)$ with $(g, f_a) = 0$ for all a, then $g = 0$. (Why is this sufficient?) This can be done using Fourier analysis.

3.9 PDE Problems

1. Consider the initial value problem for the reaction-diffusion equation

$$\frac{\partial u}{\partial t} = \frac{\partial^2 u}{\partial x^2} + u - u^2.$$

   We are interested in solutions u with $0 \leq u \leq 1$. Find the constant solutions of this equation. Find the linear equations that are the linearizations about each of these constant solutions.

2. Find the dispersion relations for each of these linear equations. Find the range of wave numbers (if any) that are responsible for any instability of these linear equations.

3. Let $z = x - ct$ and $s = t$. Find $\partial/\partial x$ and $\partial/\partial t$ in terms of $\partial/\partial z$ and $\partial/\partial s$. Write the partial differential equation in these new variables. A traveling wave solution is a solution u for which $\partial u/\partial s = 0$. Write the ordinary differential equation for a traveling wave solution (in terms of du/dz).

4. Write this ordinary differential equation as a first order system. Take $c > 0$. Find the fixed points and classify them.

5. Look for a traveling wave solution that goes from 1 at $z = -\infty$ to 0 at $z = +\infty$. For which values of c are there solutions that remain in the interval from 0 to 1?

Chapter 4

Complex integration

4.1 Complex number quiz

1. Simplify $\frac{1}{3+4i}$.

2. Simplify $|\frac{1}{3+4i}|$.

3. Find the cube roots of 1.

4. Here are some identities for complex conjugate. Which ones need correction? $\overline{z+w} = \bar{z}+\bar{w}$, $\overline{z-w} = \bar{z}-\bar{w}$, $\overline{zw} = \bar{z}\bar{w}$, $\overline{z/w} = \bar{z}/\bar{w}$. Make suitable corrections, perhaps changing an equality to an inequality.

5. Here are some identities for absolute value. Which ones need correction? $|z+w| = |z|+|w|$, $|z-w| = |z|-|w|$, $|zw| = |z||w|$, $|z/w| = |z|/|w|$. Make suitable corrections, perhaps changing an equality to an inequality.

6. Define $\log(z)$ so that $-\pi < \Im \log(z) \leq \pi$. Discuss the identities $e^{\log(z)} = z$ and $\log(e^w) = w$.

7. Define $z^w = e^{w \log z}$. Find i^i.

8. What is the power series of $\log(1+z)$ about $z = 0$? What is the radius of convergence of this power series?

9. What is the power series of $\cos(z)$ about $z = 0$? What is its radius of convergence?

10. Fix w. How many solutions are there of $\cos(z) = w$ with $-\pi < \Re z \leq \pi$.

4.2 Complex functions

4.2.1 Closed and exact forms

In the following a region will refer to an open subset of the plane. A differential form $p\,dx + q\,dy$ is said to be closed in a region R if throughout the region

$$\frac{\partial q}{\partial x} = \frac{\partial p}{\partial y}. \tag{4.1}$$

It is said to be exact in a region R if there is a function h defined on the region with

$$dh = p\,dx + q\,dy. \tag{4.2}$$

Theorem. An exact form is closed.

The converse is not true. Consider, for instance, the plane minus the origin. The form $(-y\,dx + x\,dy)/(x^2 + y^2)$ is not exact in this region. It is, however, exact in the plane minus the negative axis. In this region

$$\frac{-y\,dx + x\,dy}{x^2 + y^2} = d\theta, \tag{4.3}$$

where $-\pi/2 < \theta < \pi/2$.

Green's theorem. If S is a bounded region with oriented boundary ∂S, then

$$\int_{\partial S} p\,dx + q\,dy = \int\int_S (\frac{\partial q}{\partial x} - \frac{\partial p}{\partial y})\,dx\,dy. \tag{4.4}$$

Consider a region R and an oriented curve C in R. Then $C \sim 0$ (C is homologous to 0) in R means that there is a bounded region S such that S and its oriented boundary ∂S are contained in R such that $\partial S = C$.

Corollary. If $p\,dx + q\,dy$ is closed in some region R, and if $C \sim 0$ in R, then

$$\int_C p\,dx + q\,dy = 0. \tag{4.5}$$

If C is an oriented curve, then $-C$ is the oriented curve with the opposite orientation. The sum $C_1 + C_2$ of two oriented curves is obtained by following one curve and then the other. The difference $C_1 - C_2$ is defined by following one curve and then the other in the reverse direction.

Consider a region R and two oriented curves C_1 and C_2 in R. Then $C_1 \sim C_2$ (C_1 is homologous to C_2) in R means that $C_1 - C_2 \sim 0$ in R.

Corollary. If $p\,dx + q\,dy$ is closed in some region R, and if $C_1 \sim C_2$ in R, then

$$\int_{C_1} p\,dx + q\,dy = \int_{C_2} p\,dx + q\,dy. \tag{4.6}$$

4.2.2 Cauchy-Riemann equations

Write $z = x + iy$. Define partial differential operators

$$\frac{\partial}{\partial z} = \frac{\partial}{\partial x} + \frac{1}{i}\frac{\partial}{\partial y} \tag{4.7}$$

and

$$\frac{\partial}{\partial \bar{z}} = \frac{\partial}{\partial x} - \frac{1}{i}\frac{\partial}{\partial y} \tag{4.8}$$

The justification for this definition is the following. Every polynomial in x, y may be written as a polynomial in $z, \bar{z}$, and conversely. Then for each term in such a polynomial

$$\frac{\partial}{\partial z} z^m \bar{z}^n = m z^{m-1} \bar{z}^n \tag{4.9}$$

and

$$\frac{\partial}{\partial \bar{z}} z^m \bar{z}^n = z^m \, n \bar{z}^{n-1}. \tag{4.10}$$

Let $w = u + iv$ be a function $f(z)$ of $z = x + iy$. Suppose that this satisfies the system of partial differential equations

$$\frac{\partial w}{\partial \bar{z}} = 0. \tag{4.11}$$

In this case we say that $f(z)$ is an analytic function of z in this region. Explicitly

$$\frac{\partial (u + iv)}{\partial x} - \frac{\partial (u + iv)}{\partial iy} = 0. \tag{4.12}$$

This gives the Cauchy-Riemann equations

$$\frac{\partial u}{\partial x} = \frac{\partial v}{\partial y} \tag{4.13}$$

and

$$\frac{\partial v}{\partial x} = -\frac{\partial u}{\partial y}. \tag{4.14}$$

4.2.3 The Cauchy integral theorem

Consider an analytic function $w = f(z)$ and the differential form

$$w \, dz = f(z) \, dz = (u + iv)\,(dx + i dy) = (u \, dx - v \, dy) + i(v \, dx + u \, dy). \tag{4.15}$$

According to the Cauchy-Riemann equations, this is a closed form.

Theorem (Cauchy integral theorem) If $f(z)$ is analytic in a region R, and if $C \sim 0$ in R, then

$$\int_C f(z) \, dz = 0. \tag{4.16}$$

Example: Consider the differential form $z^m\,dz$ for integer $m \neq 1$. When $m \geq 0$ this is defined in the entire complex plane; when $m < 0$ it is defined in the punctured plane (the plane with 0 removed). It is exact, since

$$z^m\,dz = \frac{1}{m+1} dz^{m+1}. \tag{4.17}$$

On the other hand, the differential form dz/z is closed but not exact in the punctured plane.

4.2.4 Polar representation

The exponential function is defined by

$$\exp(z) = e^z = \sum_{n=0}^{\infty} \frac{z^n}{n!}. \tag{4.18}$$

It is easy to check that

$$e^{x+iy} = e^x e^{iy} = e^x(\cos(y) + i\sin(y)). \tag{4.19}$$

Sometimes it is useful to represent a complex number in the polar representation

$$z = x + iy = r(\cos(\theta) + i\sin(\theta)). \tag{4.20}$$

This can also be written

$$z = re^{i\theta}. \tag{4.21}$$

From this we derive

$$dz = dx + i\,dy = dr\,e^{i\theta} + rie^{i\theta}\,d\theta. \tag{4.22}$$

This may also be written

$$\frac{dz}{z} = \frac{dr}{r} + i\,d\theta. \tag{4.23}$$

Notice that this does not say that dz/z is exact in the punctured plane. The reason is that the angle θ is not defined in this region. However dz/z is exact in a cut plane, that is, a plane that excludes some line running from the origin to infinity.

Let $C(0)$ be a circle of radius r centered at 0. We conclude that

$$\int_{C(0)} f(z)\,dz = \int_0^{2\pi} f(z) z\,i\,d\theta. \tag{4.24}$$

In particular,

$$\int_{C(0)} \frac{1}{z}\,dz = \int_0^{2\pi} i\,d\theta = 2\pi i. \tag{4.25}$$

By a change of variable, we conclude that for a circle $C(z)$ of radius r centered at z we have

$$\int_{C(z)} \frac{1}{\xi - z}\,d\xi = 2\pi i. \tag{4.26}$$

4.2.5 Branch cuts

Remember that

$$\frac{dz}{z} = \frac{dr}{r} + i\, d\theta \tag{4.27}$$

is exact in a cut plane. Therefore

$$\frac{dz}{z} = d\log(z) \tag{4.28}$$

in a cut plane,

$$\log(z) = \log(r) + i\theta \tag{4.29}$$

Two convenient choices are $0 < \theta < 2\pi$ (cut along the positive axis and $-\pi < \theta < \pi$ (cut along the negative axis).

In the same way one can define such functions as

$$\sqrt{z} = \exp(\frac{1}{2}\log(z)). \tag{4.30}$$

Again one must make a convention about the cut.

4.3 Complex integration and residue calculus

4.3.1 The Cauchy integral formula

Theorem. (Cauchy integral formula) Let $f(\xi)$ be analytic in a region R. Let $C \sim 0$ in R, so that $C = \partial S$, where S is a bounded region contained in R. Let z be a point in S. Then

$$f(z) = \frac{1}{2\pi i}\int_C \frac{f(\xi)}{\xi - z}\, d\xi. \tag{4.31}$$

Proof: Let $C_\delta(z)$ be a small circle about z. Let R' be the region R with the point z removed. Then $C \sim C_\delta(z)$ in R'. It follows that

$$\frac{1}{2\pi i}\int_C \frac{f(\xi)}{\xi - z}\, d\xi = \frac{1}{2\pi i}\int_{C_\delta(z)} \frac{f(\xi)}{\xi - z}\, d\xi. \tag{4.32}$$

It follows that

$$\frac{1}{2\pi i}\int_C \frac{f(\xi)}{\xi - z}\, d\xi - f(z) = \frac{1}{2\pi i}\int_{C_\delta(z)} \frac{f(\xi) - f(z)}{\xi - z}\, d\xi. \tag{4.33}$$

Consider an arbitrary $\epsilon > 0$. The function $f(\xi)$ is continuous at $\xi = z$. Therefore there is a δ so small that for ξ on $C_\delta(z)$ the absolute value $|f(\xi) - f(z)| \leq \epsilon$. Then the integral on the right hand side has integral with absolute value bounded by

$$\frac{1}{2\pi}\int_0^{2\pi} \frac{\epsilon}{\delta}\, \delta d\theta = \epsilon. \tag{4.34}$$

Therefore the left hand side has absolute value bounded by ϵ. Since ϵ is arbitrary, the left hand side is zero.

4.3.2 The residue calculus

Say that $f(z)$ has an isolated singularity at z_0. Let $C_\delta(z_0)$ be a circle about z_0 that contains no other singularity. Then the residue of $f(z)$ at z_0 is the integral

$$\mathrm{res}(z_0) = \frac{1}{2\pi i}\int_{C_\delta(z_0)} f(z)\,dz. \tag{4.35}$$

Theorem. (Residue Theorem) Say that $C \sim 0$ in R, so that $C = \partial S$ with the bounded region S contained in R. Suppose that $f(z)$ is analytic in R except for isolated singularities $z_1, \ldots, z_k$ in S. Then

$$\int_C f(z)\,dz = 2\pi i \sum_{j=1}^{k} \mathrm{res}(z_j). \tag{4.36}$$

Proof: Let R' be R with the singularities omitted. Consider small circles $C_1, \ldots, C_k$ around these singularities such that $C \sim C_1 + \cdots + C_k$ in R'. Apply the Cauchy integral theorem to $C - C_1 - \ldots - C_k$.

If $f(z) = g(z)/(z - z_0)$ with $g(z)$ analytic near z_0 and $g(z_0) \neq 0$, then $f(z)$ is said to have a pole of order 1 at z_0.

Theorem. If $f(z) = g(z)/(z - z_0)$ has a pole of order 1, then its residue at that pole is

$$\mathrm{res}(z_0) = g(z_0) = \lim_{z \to z_0} (z - z_0) f(z). \tag{4.37}$$

Proof. By the Cauchy integral formula for each sufficiently small circle C about z_0 the function $g(z)$ satisfies

$$g(z_0) = \frac{1}{2\pi i}\int_C \frac{g(z)}{z - z_0}\,d\xi = \frac{1}{2\pi i}\int_C f(z)\,dz. \tag{4.38}$$

This is the residue.

4.3.3 Estimates

Recall that for complex numbers we have $|zw| = |z||w|$ and $|z/w| = |z|/|w|$. Furthermore, we have

$$||z| - |w|| \leq |z \pm w| \leq |z| + |w|. \tag{4.39}$$

When $|z| > |w|$ this allows us to estimate

$$\frac{1}{|z \pm w|} \leq \frac{1}{|z| - |w|}. \tag{4.40}$$

Finally, we have

$$|e^z| = e^{\Re z}. \tag{4.41}$$

4.3.4 A residue calculation

Consider the task of computing the integral

$$\int_{-\infty}^{\infty} e^{-ikx} \frac{1}{x^2+1}\, dx \tag{4.42}$$

where k is real. This is the Fourier transform of a function that is in L^2 and also in L^1. The idea is to use the analytic function

$$f(z) = e^{-ikz} \frac{1}{z^2+1}. \tag{4.43}$$

The first thing is to analyze the singularities of this function. There are poles at $z = \pm i$. Furthermore, there is an essential singularity at $z = \infty$.

First look at the case when $k \leq 0$. The essential singularity of the exponential function has the remarkable feature that for $\Im z \geq 0$ the absolute value of e^{-ikz} is bounded by one. This suggests looking at a closed oriented curve C_a in the upper half plane. Take C_a to run along the x axis from $-a$ to a and then along the semicircle $z = ae^{i\theta}$ from $\theta = 0$ to $\theta = \pi$. If $a > 1$ there is a singularity at $z = i$ inside the curve. So the residue is the value of $g(z) = e^{-ikz}/(z+i)$ at $z = i$, that is, $g(i) = e^k/(2i)$. By the residue theorem

$$\int_{C_a} e^{-ikz} \frac{1}{z^2+1}\, dz = \pi e^k \tag{4.44}$$

for each $a > 1$.

Now let $a \to \infty$. The contribution from the semicircle is bounded by

$$\int_0^{\pi} \frac{1}{a^2-1}\, a\, d\theta = \pi \frac{a}{a^2-1}. \tag{4.45}$$

We conclude that for $k \leq 0$

$$\int_{-\infty}^{\infty} e^{-ikx} \frac{1}{x^2+1}\, dx = \pi e^k. \tag{4.46}$$

Next look at the case when $k \geq 0$. In this case we could look at an oriented curve in the lower half plane. The integral runs from a to $-a$ and then around a semicircle in the lower half plane. The residue at $z = -i$ is $e^{-k}/(-2i)$. By the residue theorem, the integral is $-\pi e^{-k}$. We conclude that for all real k

$$\int_{-\infty}^{\infty} e^{-ikx} \frac{1}{x^2+1}\, dx = \pi e^{-|k|}. \tag{4.47}$$

4.4 Problems

1. Evaluate

$$\int_0^{\infty} \frac{1}{\sqrt{x}(4+x^2)}\, dx$$

by contour integration. Show all steps, including estimation of integrals that vanish in the limit of large contours.

2. In the following problems $f(z)$ is analytic in some region. We say that $f(z)$ has a root of multiplicity m at z_0 if $f(z) = (z - z_0)^m h(z)$, where $h(z)$ is analytic with $h(z_0) \neq 0$. Find the residue of $f'(z)/f(z)$ at such a z_0.

3. Say that $f(z)$ has several roots inside the contour C. Evaluate

$$\frac{1}{2\pi i} \int_C \frac{f'(z)}{f(z)}\, dz.$$

4. Say that

$$f(z) = a_0 + a_1 z + a_2 z^2 + \cdots + a_n z^n$$

is a polynomial. Furthermore, suppose that C is a contour surrounding the origin on which

$$|a_k z^k| > |f(z) - a_k z^k|.$$

Show that on this contour

$$f(z) = a_k z^k g(z)$$

where

$$|g(z) - 1| < 1$$

on the contour. Use the result of the previous problem to show that the number of roots (counting multiplicity) inside C is k.

5. Find the number of roots (counting multiplicity) of $z^6 + 3z^5 + 1$ inside the unit circle.

4.5 More residue calculus

4.5.1 Jordan's lemma

Jordan's lemma says that for $b > 0$ we have

$$\frac{1}{\pi} \int_0^\pi e^{-b \sin(\theta)}\, d\theta \leq \frac{1}{b}. \tag{4.48}$$

To prove it, it is sufficient to estimate twice the integral over the interval from 0 to $\pi/2$. On this interval use the inequality $(2/\pi)\theta \leq \sin(\theta)$. This gives

$$\frac{2}{\pi} \int_0^{\frac{\pi}{2}} e^{-2b\theta/\pi}\, d\theta = \frac{1}{b}(1 - e^{-b}) \leq \frac{1}{b}. \tag{4.49}$$

4.5.2 A more delicate residue calculation

Consider the task of computing the integral

$$\int_{-\infty}^{\infty} e^{-ikx} \frac{1}{x-i}\, dx \tag{4.50}$$

where k is real. This is the Fourier transform of a function that is in L^2 but not in L^1. The idea is to use the analytic function

$$f(z) = e^{-ikz} \frac{1}{z-i}. \tag{4.51}$$

The first thing is to analyze the singularities of this function. There is a pole at $z = i$. Furthermore, there is an essential singularity at $z = \infty$.

First look at the case when $k < 0$. Take C_a to run along the x axis from $-a$ to a and then along the semicircle $z = ae^{i\theta}$ in the upper half plane from $\theta = 0$ to $\theta = \pi$. If $a > 1$ there is a singularity at $z = i$ inside the curve. So the residue is the value of $g(z) = e^{-ikz}$ at $z = i$, that is, $g(i) = e^k$. By the residue theorem

$$\int_{C_a} e^{-ikz} \frac{1}{z-i}\, dz = 2\pi i e^k \tag{4.52}$$

for each $a > 1$.

Now let $a \to \infty$. The contribution from the semicircle is bounded using Jordan's lemma:

$$\int_0^{\pi} e^{ka\sin(\theta)} \frac{1}{a-1}\, a\, d\theta \le \pi \frac{1}{-ka} \frac{a}{a-1} \tag{4.53}$$

We conclude that for $k < 0$

$$\int_{-\infty}^{\infty} e^{-ikx} \frac{1}{x-i}\, dx = 2\pi i e^k. \tag{4.54}$$

Next look at the case when $k < 0$. In this case we could look at an oriented curve in the lower half plane. The integral runs from a to $-a$ and then around a semicircle in the lower half plane. The residue is zero. We conclude using Jordan's lemma that for $k < 0$

$$\int_{-\infty}^{\infty} e^{-ikx} \frac{1}{x-i}\, dx = 0. \tag{4.55}$$

4.5.3 Cauchy formula for derivatives

Theorem. (Cauchy formula for derivatives) Let $f(\xi)$ be analytic in a region R including a point z. Let C be an oriented curve in R such that for each sufficiently small circle $C(z)$ about z, $C \sim C(z)$ in R. Then the mth derivative satisfies

$$\frac{1}{m!} f^{(m)}(z) = \frac{1}{2\pi i} \int_C \frac{f(\xi)}{(\xi - z)^{m+1}}\, d\xi. \tag{4.56}$$

Proof: Differentiate the Cauchy integral formula with respect to z a total of m times.

4.5.4 Poles of higher order

If $f(z) = g(z)/(z - z_0)^m$ with $g(z)$ analytic near z_0 and $g(z_0) \neq 0$ and $m \geq 1$, then $f(z)$ is said to have a pole of order m at z_0.

Theorem. If $f(z) = g(z)/(z - z_0)^m$ has a pole of order m, then its residue at that pole is

$$\text{res}(z_0) = \frac{1}{(m-1)!} g^{(m-1)}(z_0). \tag{4.57}$$

Proof. By the Cauchy formula for derivatives for each sufficiently small circle C about z the $m-1$th derivative satisfies

$$\frac{1}{(m-1)!} g^{(m-1)}(z_0) = \frac{1}{2\pi i} \int_C \frac{g(z)}{(z - z_0)^m}\, dz = \frac{1}{2\pi i} \int_C f(z)\, dz. \tag{4.58}$$

The expression given in the theorem is evaluated in practice by using the fact that $g(z) = (z - z_0)^m f(z)$ for z near z_0, performing the differentiation, and then setting $z = z_0$. This is routine, but it can be tedious.

4.5.5 A residue calculation with a double pole

Confider the task of computing the integral

$$\int_{-\infty}^{\infty} e^{-ikx} \frac{1}{(x^2+1)^2}\, dx \tag{4.59}$$

where k is real. This is the Fourier transform of a function that is in L^2 and also in L^1. The idea is to use the analytic function

$$f(z) = e^{-ikz} \frac{1}{(z^2+1)^2}. \tag{4.60}$$

The first thing is to analyze the singularities of this function. There are poles at $z = \pm i$. Furthermore, there is an essential singularity at $z = \infty$.

First look at the case when $k \leq 0$. Consider a closed oriented curve C_a in the upper half plane. Take C_a to run along the x axis from $-a$ to a and then along the semicircle $z = ae^{i\theta}$ from $\theta = 0$ to $\theta = \pi$. If $a > 1$ there is a singularity at $z = i$ inside the curve. The pole there is of order 2. So the residue is calculated by letting $g(z) = e^{-ikz}/(z + i)^2$, taking the derivative, and evaluating at $z = i$, that is, $g'(i) = (1 - k)e^k/(4i)$. By the residue theorem

$$\int_{C_a} e^{-ikz} \frac{1}{z^2+1}\, dz = \frac{1}{2}\pi(1-k)e^k \tag{4.61}$$

for each $a > 1$.

Now let $a \to \infty$. The contribution from the semicircle vanishes in that limit. We conclude that for $k \leq 0$

$$\int_{-\infty}^{\infty} e^{-ikx} \frac{1}{(x^2+1)^2}\, dx = \frac{1}{2}\pi(1-k)e^k. \tag{4.62}$$

Next look at the case when $k \geq 0$. In this case we could look at an oriented curve in the lower half plane. The integral runs from a to $-a$ and then around a semicircle in the lower half plane. The residue at $z = -i$ is $-(1+k)e^{-k}/(4i)$. By the residue theorem, the integral is $-\pi(1+k)e^{-k}/2$. We conclude that for all real k

$$\int_{-\infty}^{\infty} e^{-ikx} \frac{1}{(x^2+1)^2}\, dx = \frac{1}{2}\pi(1+|k|)e^{-|k|} \tag{4.63}$$

4.6 The Taylor expansion

4.6.1 Radius of convergence

Theorem. Let $f(z)$ be analytic in a region R including a point z_0. Let $C(z_0)$ be a circle centered at z_0 such that $C(z_0)$ and its interior are in R. Then for z in the interior of $C(z_0)$

$$f(z) = \sum_{m=0}^{\infty} \frac{1}{m!} f^{(m)}(z_0)(z - z_0)^m. \tag{4.64}$$

Proof. For each fixed ξ the function of z given by

$$\frac{1}{\xi - z} = \frac{1}{\xi - z_0 + z_0 - z} = \frac{1}{(\xi - z_0)} \frac{1}{1 - \frac{z - z_0}{\xi - z_0}} = \frac{1}{(\xi - z_0)} \sum_{m=0}^{\infty} \left(\frac{z - z_0}{\xi - z_0} \right)^m. \tag{4.65}$$

has a geometric series expansion. Multiply by $(1/2\pi i) f(\xi)\, d\xi$ and integrate around $C(z_0)$. On the left hand side apply the Cauchy integral formula to get $f(z)$.

In each term in the expansion on the right hand side apply the Cauchy formula for derivatives in the form

$$\frac{1}{2\pi i} \int_{C(z_0)} \frac{f(\xi)}{(\xi - z_0)^{m+1}}\, d\xi = \frac{1}{m!} f^{(m)}(z_0). \tag{4.66}$$

This theorem is remarkable because it shows that the condition of analyticity implies that the Taylor series always converges. Furthermore, take the radius of the circle $C(z_0)$ as large as possible. The only constraint is that there must be a function that is analytic inside the circle and that extends $f(z)$. Thus one must avoid the singularity of this extension of $f(z)$ that is closest to z_0. This explains why the radius of convergence of the series is the distance from z_0 to this nearest singularity.

The reason that we talk of an analytic extension is that artificialities in the definition of the function, such as branch cuts, should not matter. On the other hand, singularities such as poles, essential singularities, and branch points are intrinsic. The radius of convergence is the distance to the nearest such intrinsic singularity.

If one knows an analytic function near some point, then one knows it all the way out to the radius of convergence of the Taylor series about that point.

But then for each point in this larger region there is another Taylor series. The function is then defined out to the radius of convergence associated with that point. The process may be carried out over a larger and larger region, until blocked by some instrinsic singularity. It is known as analytic continuation.

If the analytic continuation process begins at some point and winds around a branch point, then it may lead to a new definition of the analytic function at the original point. This appears to lead to the necessity of introducing an artifical branch cut in the definition of the function. However this may be avoided by introducing the concept of Riemann surface.

4.6.2 Riemann surfaces

When an analytic function has a branch cut, it is an indicator of the fact that the function should not be thought of not as a function on a region of the complex plane, but instead as a function on a Riemann surface. A Riemann surface corresponds to several copies of a region in the complex plane. These copies are called sheets. Where one makes the transition from one sheet to another depends on the choice of branch cut. But the Riemann surface itself is independent of the notion of sheet.

As an example, take the function $w = \sqrt{z}$. The most natural definition of this function is as a function on the curve $w^2 = z$. This is a kind of two-dimensional parabola in a four dimensional space of two complex variables. The value of the square root function on the point with coordinates z, w on the parabola $w^2 = z$ is w. Notice that if z is given, then there are usually two corresponding values of w. Thus if we want to think of $\sqrt{z}$ as a function of a complex variable, then it is ambiguous. But if we think of it as a function on the Riemann surface, then it is perfectly well defined. The Riemann surface has two sheets. If we wish, we may think of sheet I as the complex plane cut along the negative axis. Sheet II is another copy of the complex plane cut along the negative axis. As z crosses the cut, it changes from one sheet to the other. The value of w also varies continuously, and it keeps track of what sheet the z is on.

As another example, take the function $w = \sqrt{z(z-1)}$. The most natural definition of this function is as a function on the curve $w^2 = z(z-1)$. This is a kind of two-dimensional circle in a four dimensional space of two complex variables. The value of the function on the point with coordinates z, w on the circle $w^2 = z(z-1)$ is w. Notice that if z is given, then there are usually two corresponding values of w. Thus if we want to think of $\sqrt{z(z-1)}$ as a function of a complex variable, then it is ambiguous. But if we think of it as a function on the Riemann surface, then it is perfectly well defined. The Riemann surface has two sheets. If we wish, we may think of sheet I as the complex plane cut between 0 and 1. Sheet II is another copy of the complex plane, also cut between 0 and 1. As z crosses the cut, it changes from one sheet to the other. The value of w also varies continuously, and it keeps track of what sheet the z is on.

As a final example, take the function $w = \log z$. The most natural definition of this function is as a function on the curve $\exp(w) = z$. This is a two-dimensional curve in a four dimensional space of two complex variables. The

value of the logarithm function on the point with coordinates z, w on the curve $\exp(w) = z$ is w. Notice that if z is given, then there are infinitely many corresponding values of w. Thus if we want to think of $\log z$ as a function of a complex variable, then it is ambiguous. But if we think of it as a function on the Riemann surface, then it is perfectly well defined. The Riemann surface has infinitely many sheets. If we wish, we may think of each sheet as the complex plane cut along the negative axis. As z crosses the cut, it changes from one sheet to the other. The value of w also varies continuously, and it keeps track of what sheet the z is on. The infinitely many sheets form a kind of spiral that winds around the origin infinitely many times.

Chapter 5

Distributions

5.1 Properties of distributions

Consider the space $C_c^\infty(R)$ of complex test functions. These are complex functions defined on the real line, infinitely differentiable and with compact support. A distribution is a linear functional from this space to the complex numbers. It must satisfy a certain continuity condition, but we shall ignore that. The value of the distribution F on the test function ϕ is written $\langle F, \phi \rangle$.

If f is a locally integrable function, then we may define a distribution

$$\langle F, \phi \rangle = \int_{-\infty}^{\infty} f(x)\phi(x)\,dx. \tag{5.1}$$

Thus many functions define distributions. This is why distributions are also called generalized functions.

A sequence of distributions F_n is said to converge to a distribution F if for each test function ϕ the numbers $\langle F_n, \phi \rangle$ converge to the number $\langle F, \phi \rangle$.

Example. The distribution δ_a is defined by

$$\langle \delta_a, \phi \rangle = \phi(a). \tag{5.2}$$

This is not given by a locally integrable function. However a distribution may be written as a limit of functions. For instance, let $\epsilon > 0$ and consider the function

$$\delta_\epsilon(x-a) = \frac{1}{\pi}\frac{\epsilon}{(x-a)^2+\epsilon^2}. \tag{5.3}$$

The limit of the distributions defined by these locally integrable functions as $\epsilon \downarrow 0$ is δ_a. For this reason the distribution is often written in the incorrect but suggestive notation

$$\langle \delta_a, \phi \rangle = \int_{-\infty}^{\infty} \delta(x-a)\phi(x)\,dx. \tag{5.4}$$

Operations on distributions are defined by looking at the example of a distribution defined by a function and applying the integration by parts formula

in that case. Thus, for instance, the derivative is defined by

$$\langle F', \phi \rangle = -\langle F, \phi' \rangle. \tag{5.5}$$

Example: Consider the locally integrable Heaviside function given by $H(x) = 1$ for $x > 0$, $H(x) = 0$ for $x < 0$. Then $H' = \delta$. Here δ is given by

$$\langle \delta, \phi \rangle = \phi(0). \tag{5.6}$$

Example: Consider the locally integrable log function $f(x) = \log |x|$. Then $f'(x) = \text{PV } 1/x$. Here the principal value PV $1/x$ is given by

$$\langle \text{PV } \frac{1}{x}, \phi \rangle = \lim_{\epsilon \downarrow 0} \int_{-\infty}^{\infty} \frac{x}{x^2 + \epsilon^2} \phi(x)\, dx.. \tag{5.7}$$

This can be seen by writing $\log |x| = \lim_\epsilon \log \sqrt{x^2 + \epsilon^2}$.

A distribution can be approximated by more than one sequence of functions. For instance, for each $a > 0$ let $\log_a(|x|) = \log(|x|)$ for $|x| \geq a$ and $\log_a(|x|) = \log(a)$ for $|x| < a$. Then $\log_a(|x|)$ also approaches $\log(|x|)$ as $a \to 0$. So its derivative is another approximating sequence for PV $1/x$. This says that

$$\langle \text{PV } \frac{1}{x}, \phi \rangle = \lim_{a \downarrow 0} \int_{|x|>a} \frac{1}{x} \phi(x)\, dx. \tag{5.8}$$

We can use this sequence to compute the derivative of PV $1/x$. We get

$$\int_{-\infty}^{\infty} \left(\frac{d}{dx} \text{PV } \frac{1}{x} \right) \phi(x)\, dx = -\lim_{a \to 0} \int_{|x|>a} \frac{1}{x} \phi'(x)\, dx = \lim_{a \to 0} \left[\int_{|x|>a} -\frac{1}{x^2} \phi(x)\, dx + \frac{\phi(a) + \phi(-a)}{a} \right]. \tag{5.9}$$

But $[\phi(a) + \phi(-a) - 2\phi(0)]/a$ converges to zero, so this is

$$\int_{-\infty}^{\infty} \left(\frac{d}{dx} \text{PV } \frac{1}{x} \right) \phi(x)\, dx = \lim_{a \to 0} \int_{|x|>a} -\frac{1}{x^2} [\phi(x) - \phi(0)]\, dx. \tag{5.10}$$

Another operator is multiplication of a distribution by a smooth function g in C^∞. This is defined in the obvious way by

$$\langle g \cdot F, \phi \rangle = \langle F, g\phi \rangle. \tag{5.11}$$

Distributions are not functions. They may not have values at points, and in general nonlinear operations are not defined. For instance, the square of a distribution is not always a well defined distribution.

Also, some algebraic operations involving distributions are quite tricky. Consider, for instance, the associative law. Apply this to the three distributions $\delta(x)$, x, and PV $1/x$. Clearly the product $\delta(x) \cdot x = 0$. On the other hand, the product $x \cdot \text{PV } 1/x = 1$ is one. So if the associate law were to hold, we would get

$$0 = 0 \cdot \text{PV } \frac{1}{x} = (\delta(x) \cdot x) \cdot \text{PV } \frac{1}{x} = \delta(x) \cdot (x \cdot \text{PV } \frac{1}{x}) = \delta(x) \cdot 1 = \delta(x). \tag{5.12}$$

5.2 Mapping distributions

A test function ϕ is naturally viewed as a covariant object, so the distribution F is contravariant. A proper function is a function such that the inverse image of each compact set is compact. It is natural to define the forward push of a distribution F by a smooth proper function g by $\langle g[F], \phi\rangle = \langle F, \phi\circ g\rangle$. Example: If F is the distribution $\delta(x-3)$ and if $u = g(x) = x^2 - 4$, then the forward push is $\delta(u-5)$. This is because $\int \delta(u-5)\phi(u)\,du = \int \delta(x-3)\phi(x^2-4)\,dx$.

On the other hand, it is actually more common to think of a distribution as being a covariant object, since a distribution is supposed to be a generalized function. The backward pull of the distribution by a smooth function g is defined in at least some circumstances by

$$\langle F \circ g, \phi\rangle = \langle F, g[\phi]\rangle. \tag{5.13}$$

Here

$$g[\phi](u) = \sum_{g(x)=u} \frac{\phi(x)}{|g'(x)|}. \tag{5.14}$$

Example. Let $u = g(x) = x^2 - 4$, with $a > 0$. Then the backward pull of $\delta(u)$ under g is $\delta(x^2-4) = (1/4)(\delta(x-2) + \delta(x+2))$. This is because

$$g[\phi](u) = \frac{\phi(\sqrt{u^2+4}) + \phi(-\sqrt{u^2+4})}{2\sqrt{u^2+4}}. \tag{5.15}$$

So if $F = \delta$, then

$$F \circ g = \frac{1}{4}(\delta_2 + \delta_{-2}) \tag{5.16}$$

Example: The backward pull is not always defined. To consider a distribution as a covariant object is a somewhat awkward act in general. Let $u = h(x) = x^2$. The backward pull of $\delta(u)$ by h is $\delta(x^2)$, which is not defined.

Example: The general formula for the pull back of the delta function is

$$\delta(g(x)) = \sum_{g(a)=0} \frac{1}{|g'(a)|}\delta(x-a). \tag{5.17}$$

The most important distributions are δ, PV $1/x$, $1/(x-i0)$, and $1/(x+i0)$. These are the limits of the functions $\delta_\epsilon(x), x/(x^2+\epsilon^2), 1/(x-i\epsilon), 1/(x+i\epsilon)$ as $\epsilon \downarrow 0$. The relations between these functions are given by

$$\delta_\epsilon(x) = \frac{1}{\pi}\frac{\epsilon}{x^2+\epsilon^2} = \frac{1}{2\pi i}\left(\frac{1}{x-i\epsilon} - \frac{1}{x+i\epsilon}\right). \tag{5.18}$$

and

$$\frac{x}{x^2+\epsilon^2} = \frac{1}{2}\left(\frac{1}{x-i\epsilon} + \frac{1}{x+i\epsilon}\right). \tag{5.19}$$

5.3 Radon measures

A Radon measure is a positive distribution. That is, it is a linear functional μ on $C_c^\infty(R)$ such that for each test function ϕ the condition $\phi \geq 0$ implies that the value $\langle \mu, \phi \rangle \geq 0$. Every Radon measure extends uniquely by continuity to a linear function on $C_c(R)$, the space of continuous functions with compact support. Each positive locally integrable function h defines a Radon measure by integrating $\phi(x)$ times $h(x)\,dx$. Also, the point mass distributions δ_a are Radon measures.

It is common to write the value of a Radon measure in the form

$$\langle \mu, \phi \rangle = \int \phi(x)\, d\mu(x). \tag{5.20}$$

What is remarkable is that the theory of Lebesgue integration works for Radon measures. That is, given a real function $f \geq 0$ that is only required to be Borel measurable, there is a natural definition of the integral such that

$$0 \leq \int f(x)\, d\mu(x) \leq +\infty. \tag{5.21}$$

Furthermore, if f is a complex Borel measurable function such that $|f|$ has finite integral, then the integral of f is defined and satisfies.

$$\left| \int f(x)\, d\mu(x) \right| \leq \int |f(x)|\, d\mu(x) < +\infty. \tag{5.22}$$

5.4 Approximate delta functions

It might seem that one could replace the notion of distribution by the notion of a sequence of approximating functions. This is true in some sense, but the fact is that many different sequences may approximate the same distribution. Here is a result of that nature.

Theorem. Let $\delta_1(u) \geq 0$ be a positive function with integral 1. For each $\epsilon > 0$ define $\delta_\epsilon(x) = \delta(x/\epsilon)/\epsilon$. Then the functions δ_ϵ converge to the δ distribution as ϵ tends to zero.

The convergence takes place in the sense of distributions (smooth test functions with compact support) or even in the sense of Radon measures (continuous test functions with compact support). Notice that there are no continuity or symmetry assumptions on the initial function.

The proof of this theorem is simple. Each δ_ϵ has integral one. Consider a bounded continuous function ϕ. Then

$$\int_{-\infty}^{\infty} \delta_\epsilon(x)\phi(x)\, dx = \int_{-\infty}^{\infty} \delta_1(u)\phi(\epsilon u)\, du. \tag{5.23}$$

The dominated convergence theorem shows that this approaches the integral

$$\int_{-\infty}^{\infty} \delta_1(u)\phi(0)\, du = \phi(0). \tag{5.24}$$

Here is an even stronger result.

Theorem. For each $\epsilon > 0$ let $\delta_\epsilon \geq 0$ be a positive function with integral 1. Suppose that for each $a > 0$ that

$$\int_{|x|>a} \delta_\epsilon(x)\,dx \to 0 \tag{5.25}$$

as $\epsilon \to 0$. Then the functions δ_ϵ converge to the δ distribution as ϵ tends to zero.

Here is a proof of this more general theorem. Let $H_\epsilon(a) = \int_0^a \delta_\epsilon(x)\,dx$. Then for each $a < 0$ we have $H_\epsilon(a) \to 0$, and for each $a > 0$ we have $1 - H_\epsilon(a) \to 0$. In other words, for each $a \neq 0$ we have $H_\epsilon(a) \to H(a)$ as $\epsilon \to 0$. Since the functions H_ϵ are uniformly bounded, it follows from the dominated convergence theorem that $H_\epsilon \to H$ in the sense of distributions. It follows by differentiation that $\delta_\epsilon \to \delta$ in the sense of distributions.

5.5 Problems

If F and G are distributions, and if at least one of them has compact support, then their convolution $F * G$ is defined by

$$\langle F * G, \phi \rangle = \langle F_x G_y, \phi(x + y) \rangle.$$

This product is commutative. It is also associative if at least two of the three factors have compact support.

1. If F and G are given by locally integrable functions f and g, and at least one has compact support, then $F * G$ is given by a locally integrable function

$$(f * g)(z) = \int_{-\infty}^{\infty} f(x)g(z - x)\,dx = \int_{-\infty}^{\infty} f(z - y)g(y)\,dy.$$

2. If G is given by a test function g, then $F * g$ is given by a smooth function

$$(F * g)(z) = \langle F_x, g(z - x) \rangle.$$

3. Calculate the convolution $1 * \delta'$.

4. Calculate the convolution $\delta' * H$, where H is the Heaviside function.

5. Calculate the convolution $(1 * \delta') * H$ and also calculate the convolution $1 * (\delta' * H)$. What does this say about the associative law for convolution?

6. Let L be a constant coefficient linear differential operator. Let u be a distribution that is a fundamental solution, that is, let $Lu = \delta$. Let G be a distribution with compact support. Show that the convolution $F = u * G$ satisfies the equation $LF = G$. Hint: Write $\langle LF, \phi \rangle = \langle F, L^\dagger \phi \rangle$, where $L^\dagger$ is adjoint to L.

7. Take $L = -d^2/dx^2$. Is there a fundamental solution that has support in a bounded interval? Is there a fundamental solution that has support in a semi-infinite interval?

5.6 Tempered distributions

Let d/dx be the operator of differentiation, and let x be the operator of multiplication by the coordinate x. The space $\mathcal{S}$ of rapidly decreasing smooth test functions consists of the functions ϕ in L^2 such that every finite product of the operators d/dx and x applied to ϕ is also in L^2. The advantage of this definition is that the space $\mathcal{S}$ is clearly invariant under Fourier transformation.

A tempered distribution is a linear functional on $\mathcal{S}$ satisfying the appropriate continuity property. Every tempered distribution restricts to define a distribution. So tempered distributions are more special.

The advantage of tempered distributions is that one can define Fourier transforms $\hat{F}$ of tempered distributions F. The definition is

$$\langle \hat{F}, \phi \rangle = \langle F, \hat{\phi} \rangle. \tag{5.26}$$

Here $\hat{\phi}$ is the Fourier transform of ϕ.

Here are some Fourier transforms for functions. The first two are easy. They are

$$\int_{-\infty}^{\infty} e^{-ikx} \frac{1}{x - i\epsilon}\, dx = 2\pi i e^{\epsilon k} H(-k) \tag{5.27}$$

and

$$\int_{-\infty}^{\infty} e^{-ikx} \frac{1}{x + i\epsilon}\, dx = -2\pi i e^{-\epsilon k} H(k). \tag{5.28}$$

Subtract these and divide by $2\pi i$. This gives

$$\int_{-\infty}^{\infty} e^{-ikx} \delta_\epsilon(x)\, dx = e^{-\epsilon|k|}. \tag{5.29}$$

Instead, add these and divide by 2. This gives

$$\int_{-\infty}^{\infty} e^{-ikx} \frac{x}{x^2 + \epsilon^2}\, dx = -\pi i e^{-\epsilon|k|} \mathrm{sign}(k). \tag{5.30}$$

The corresponding Fourier transforms for distributions are

$$F[1/(x - i0)] = 2\pi i H(-k) \tag{5.31}$$

and

$$F[1/(x + i0)] = -2\pi i H(k). \tag{5.32}$$

Also,

$$F[\delta(x)] = 1 \tag{5.33}$$

and

$$F[\text{PV } \frac{1}{x}] = -\pi i \text{sign}(k). \tag{5.34}$$

Example: Here is a more complicated calculation. The derivative of PV $1/x$ is the distribution

$$\frac{d}{dx}\text{PV } \frac{1}{x} = -\frac{1}{x^2} + c\delta(x), \tag{5.35}$$

where c is the infinite constant

$$c = \int_{-\infty}^{\infty} \frac{1}{x^2}\, dx. \tag{5.36}$$

This makes rigorous sense if interprets it as

$$\int_{-\infty}^{\infty} \left(\frac{d}{dx}\text{PV } \frac{1}{x}\right) \phi(x)\, dx = \lim_{a\to 0} \int_{|x|>a} -\frac{1}{x^2}[\phi(x) - \phi(0)]\, dx. \tag{5.37}$$

One can get an intuitive picture of this result by graphing the approximating functions. The key formula is

$$\frac{d}{dx}\frac{x}{x^2+\epsilon^2} = -\frac{x^2}{(x^2+\epsilon^2)^2} + c_\epsilon \frac{2\epsilon^3}{\pi(x^2+\epsilon^2)^2}, \tag{5.38}$$

where $c_\epsilon = \pi/(2\epsilon)$. This is an approximation to $-1/x^2$ plus a big constant times an approximation to the delta function.

The Fourier transform of the derivative is obtained by multiplying the Fourier transform of PV $1/x$ by ik. Thus the Fourier transform of $-1/x^2 + c\delta(x)$ is ik times $-\pi i \text{sign}(k)$ which is $\pi|k|$.

This example is interesting, because it looks at first glance that the derivative of PV $1/x$ should be $-1/x^2$, which is negative definite. But the correct answer for the derivative is $-1/x^2 + c\delta(x)$, which is actually positive definite. And in fact its Fourier transform is positive.

For each of these formula there is a corresponding inverse Fourier transform. For, instance, the inverse Fourier transform of 1 is

$$\delta(x) = \int_{\infty}^{\infty} e^{ikx} \frac{dk}{2\pi} = \int_0^{\infty} \cos(kx) \frac{dk}{2\pi}. \tag{5.39}$$

Of course such an equation is interpreted by integrating both sides with a test function.

Another formula of the same type is gotten by taking the inverse Fourier transform of $-\pi i \text{sign}(k)$. This is

$$\text{PV } \frac{1}{x} = -\pi i \int_{-\infty}^{\infty} e^{ikx} \text{sign}(k) \frac{dk}{2\pi} = \int_0^{\infty} \sin(kx)\, dk. \tag{5.40}$$

5.7 Poisson equation

We begin the study of fundamental solutions of partial differential equations. These are solutions of the equation $Lu = \delta$, where L is the differential operator, and δ is a point source.

Let us start with the equation in one space dimension:

$$\left(-\frac{d^2}{dx^2} + m^2\right) u = \delta(x). \tag{5.41}$$

This is an equilibrium equation that balances a source with losses due to diffusion and to dissipation (when $m > 0$). Fourier transform. This gives

$$\left(k^2 + m^2\right) \hat{u}(k) = 1. \tag{5.42}$$

The solution is

$$\hat{u}(k) = \frac{1}{k^2 + m^2}. \tag{5.43}$$

There is no problem of division by zero. The inverse Fourier transform is

$$u(x) = \frac{1}{2m} e^{-m|x|}. \tag{5.44}$$

This is the only solution that is a tempered distribution. (The solutions of the homogeneous equation all grow exponentially.)

What happens when $m = 0$? This is more subtle. The equation is

$$-\frac{d^2}{dx^2} u = \delta(x). \tag{5.45}$$

Fourier transform. This gives

$$k^2 \hat{u}(k) = 1. \tag{5.46}$$

Now there is a real question about division by zero. Furthermore, the homogeneous equation has solutions that are tempered distributions, namely linear combinations of $\delta(k)$ and $\delta'(k)$. The final result is that the inhomogeneous equation does have a tempered distribution solution, but it needs careful definition. The solution is

$$\hat{u}(k) = \frac{1}{k^2} + \infty \delta(k). \tag{5.47}$$

This may be thought of as the derivative of $-\text{PV } 1/k$. The inverse Fourier transform of PV $1/k$ is $(1/2)i\text{sign}(x)$. So the inverse Fourier transform of $-d/dk\text{PV } 1/k$ is $-(-ix)(1/2)i\text{sign}(x) = -(1/2)|x|$. Thus

$$u(x) = -\frac{1}{2}|x| \tag{5.48}$$

is a solution of the inhomogeneous equation. The solutions of the homogeneous equation are linear combinations of 1 and x. None of these solutions are a

good description of diffusive equilibrium. In fact, in one dimension there is no diffusive equilibrium.

The next case that is simple to compute and of practical importance is the equation in dimension 3. This is

$$\left(-\nabla^2 + m^2\right) u = \delta(x). \tag{5.49}$$

This is an equilibrium equation that balances a source with losses due to diffusion and to dissipation (when $m > 0$). Fourier transform. This gives

$$\left(k^2 + m^2\right) \hat{u}(k) = 1. \tag{5.50}$$

The solution is

$$\hat{u}(k) = \frac{1}{k^2 + m^2}. \tag{5.51}$$

The inverse Fourier transform in the three dimension case may be computed by going to polar coordinates. It is

$$u(x) = \frac{1}{4\pi|x|} e^{-m|x|}. \tag{5.52}$$

What happens when $m = 0$? The situation is very different in three dimensions. The equation is

$$\nabla^2 u = \delta(x). \tag{5.53}$$

Fourier transform. This gives

$$k^2 \hat{u}(k) = 1. \tag{5.54}$$

The inhomogeneous equation has a solution

$$\hat{u}(k) = \frac{1}{k^2}. \tag{5.55}$$

But now this is a locally integrable function. It defines a tempered distribution without any regularization. Thus

$$u(x) = \frac{1}{4\pi|x|} \tag{5.56}$$

is a solution of the inhomogeneous equation. In three dimensions there is diffusive equilibrium. There is so much room that the effect of the source can be completely compensated by diffusion alone.

5.8 Diffusion equation

The diffusion equation or heat equation is

$$\left(\frac{\partial}{\partial t} - \frac{1}{2}\sigma^2 \frac{\partial^2}{\partial x^2}\right) u = \delta(x)\delta(t). \tag{5.57}$$

It says that the time rate of change is entirely due to diffusion. Fourier transform. We get

$$(i\omega + \frac{1}{2}\sigma^2 k^2)\hat{u}(k,\omega) = 1. \tag{5.58}$$

This has solution

$$\hat{u}(k,\omega) = \frac{1}{i\omega + \frac{1}{2}\sigma^2 k^2} = \frac{1}{i}\frac{1}{\omega - i\frac{1}{2}\sigma^2 k^2}. \tag{5.59}$$

Here the only division by zero is when both ω and k are zero. But this is not so serious, because it is clear how to regularize. We can use the fact that the inverse Fourier transform of $1/(\omega - i\epsilon)$ with $\epsilon > 0$ is $iH(t)e^{-\epsilon t}$. So we have

$$\hat{u}(k,t) = H(t)e^{-\frac{\sigma^2 t k^2}{2}}. \tag{5.60}$$

This is a Gaussian, so the fundamental solution is

$$u(x,t) = H(t)\frac{1}{\sqrt{2\pi\sigma^2 t}}e^{-\frac{x^2}{2\sigma^2 t}}. \tag{5.61}$$

5.9 Wave equation

We will look for the solution of the wave equation with a point source at time zero that lies in the forward light cone. The wave equation in $1+1$ dimensions is

$$\left(\frac{\partial^2}{\partial t^2} - c^2\frac{\partial^2}{\partial x^2}\right)u = \delta(x)\delta(t). \tag{5.62}$$

Fourier transform. We get

$$(-\omega^2 + c^2 k^2)\hat{u}(k,\omega) = 1. \tag{5.63}$$

This has solution

$$\hat{u}(k,\omega) = -\frac{1}{(\omega - i0)^2 - c^2 k^2}. \tag{5.64}$$

The division by zero is serious, but it is possible to regularize. The choice of regularization is not the only possible one, but we shall see that it is the convention that gives propagation into the future. We can write this also as

$$\hat{u}(k,\omega) = -\frac{1}{2c|k|}\left(\frac{1}{\omega - i0 - c|k|} - \frac{1}{\omega - i0 + c|k|}\right). \tag{5.65}$$

We can use the fact that the inverse Fourier transform of $1/(\omega - i0)$ is $iH(t)$. So we have

$$\hat{u}(k,t) = -\frac{1}{2c|k|}iH(t)\left[e^{ic|k|t} - e^{-ic|k|t}\right] = \frac{1}{c|k|}\sin(c|k|t)H(t). \tag{5.66}$$

It is easy to check that this is the Fourier transform of

$$u(x,t) = \frac{1}{2c}\left[H(x+ct) - H(x-ct)\right] H(t). \tag{5.67}$$

The wave equation in $3+1$ dimensions is

$$\left(\frac{\partial^2}{\partial t^2} - c^2\nabla^2\right) u = \delta(x)\delta(t). \tag{5.68}$$

Fourier transform. We get

$$(-\omega^2 + c^2k^2)\hat{u}(k,\omega) = 1. \tag{5.69}$$

This has solution

$$\hat{u}(k,\omega) = -\frac{1}{(\omega - i0)^2 - c^2k^2}. \tag{5.70}$$

Again we can write this as

$$\hat{u}(k,\omega) = -\frac{1}{2c|k|}\left(\frac{1}{\omega - i0 - c|k|} - \frac{1}{\omega - i0 + c|k|}\right). \tag{5.71}$$

Thus we have again

$$\hat{u}(k,t) = -\frac{1}{2c|k|} iH(t)\left[e^{ic|k|t} - e^{-ic|k|t}\right] = \frac{1}{c|k|}\sin(c|k|t)H(t). \tag{5.72}$$

However the difference is that the k variable is three dimensional. It is easy to check that this is the Fourier transform of

$$u(x,t) = \frac{1}{4\pi c|x|}\delta(|x| - ct)H(t). \tag{5.73}$$

This is a beautiful formula. It represents an expanding sphere of influence, going into the future. Inside the sphere it is dark. The solution has an even more beautiful expression that exhibits the symmetry:

$$u(x,t) = \frac{1}{2\pi c}\delta(x^2 - c^2t^2)H(t). \tag{5.74}$$

5.10 Homogeneous solutions of the wave equation

The polynomial $\omega^2 - k^2$ vanishes on an entire cone, so it is not surprising that the wave equation has a number of interesting homogeneous solutions. The most important ones are

$$\hat{u}(k,t) = \frac{1}{c|k|}\sin(c|k|t) \tag{5.75}$$

and its derivative

$$\hat{v}(k,t) = \cos(c|k|t). \tag{5.76}$$

These are the solutions that are used in constructing solutions of the initial value problem.

It is interesting to see what these solutions look like in the frequency representation. The result is

$$\hat{u}(k,\omega) = -\pi i \frac{1}{c|k|}[\delta(\omega - c|k|) - \delta(\omega + c|k|)] = -2\pi i \delta(\omega^2 - c^2k^2)\text{sign}(\omega) \tag{5.77}$$

and

$$\hat{v}(k,\omega) = i\omega\hat{u}(k,\omega) = \pi[\delta(\omega - c|k|) + \delta(\omega + c|k|)] = 2\pi|\omega|\delta(\omega^2 - c^2k^2). \tag{5.78}$$

5.11 Problems

1. Show that $\frac{1}{x^{\frac{1}{3}}}$ is a locally integrable function and thus defines a distribution. Show that its distribution derivative is

$$\frac{d}{dx}\frac{1}{x^{\frac{1}{3}}} = -\frac{1}{3}\frac{1}{x^{\frac{4}{3}}} + c\delta(x), \tag{5.79}$$

where

$$c = \frac{1}{3}\int_{-\infty}^{\infty} \frac{1}{x^{\frac{4}{3}}}\, dx \tag{5.80}$$

Hint: To make this rigorous, consider $x/(x^2+\epsilon^2)^{\frac{2}{3}}$.

2. Show that $\frac{1}{|x|^{\frac{1}{3}}}$ is a locally integrable function and thus defines a distribution. Show that its distribution derivative is

$$\frac{d}{dx}\frac{1}{x^{\frac{1}{3}}} = -\frac{1}{3}\frac{1}{x^{\frac{4}{3}}}\text{sign}(x). \tag{5.81}$$

The right hand side is not locally integrable. Explain the definition of the right hand side as a distribution. Hint: To make this rigorous, consider $1/(x^2+\epsilon^2)^{\frac{1}{6}}$.

3. Discuss the contrast between the results in the last two problems. It may help to draw some graphs of the functions that approximate these distributions.

4. Let $m > 0$. Use Fourier transforms to find a tempered distribution u that is the fundamental solution of the equation

$$-\frac{d^2}{dx^2}u + m^2 u = \delta(x). \tag{5.82}$$

Is this a unique tempered distribution solution? Explain.

5. Let $m > 0$. Consider Euclidian space of dimension $n = 3$. Use Fourier transforms to find a tempered distribution u that is the fundamental solution of the equation

$$-\nabla^2 u + m^2 u = \delta(x). \tag{5.83}$$

5.12 Answers to first two problems

1. The function $\frac{1}{x^{\frac{1}{3}}}$ is locally integrable, while its pointwise derivative $-\frac{1}{3}\frac{1}{x^{\frac{4}{3}}}$ is not. But we do have

$$\frac{d}{dx}\frac{x}{(x^2+\epsilon^2)^{\frac{2}{3}}} = -\frac{1}{3}\frac{x^2}{(x^2+\epsilon^2)^{\frac{5}{3}}} + \frac{\epsilon^2}{(x^2+\epsilon^2)^{\frac{5}{3}}}. \tag{5.84}$$

Let

$$c_\epsilon = \int_{-\infty}^{\infty} \frac{1}{3}\frac{x^2}{(x^2+\epsilon^2)^{\frac{5}{3}}}\,dx \tag{5.85}$$

which is easily seen to be proportional to $1/\epsilon^{\frac{1}{3}}$. From the fundamental theory of calculus

$$\int_{-\infty}^{\infty} \frac{\epsilon^2}{(x^2+\epsilon^2)^{\frac{5}{3}}}\,dx = c_\epsilon. \tag{5.86}$$

Write

$$\delta_\epsilon(x) = \frac{1}{c_\epsilon}\frac{\epsilon^2}{(x^2+\epsilon^2)^{\frac{5}{3}}}. \tag{5.87}$$

Then $\delta_\epsilon(x) \to \delta(x)$ in the sense of distributions. Furthermore,

$$\int_{-\infty}^{\infty} \frac{d}{dx}\frac{1}{x^{\frac{1}{3}}}\phi(x)\,dx = \lim_{\epsilon\to 0}\int_{-\infty}^{\infty}[-\frac{1}{3}\frac{x^2}{(x^2+\epsilon^2)^{\frac{5}{3}}} + c_\epsilon\delta_\epsilon(x)]\phi(x)\,dx. \tag{5.88}$$

Since for ϕ smooth enough

$$\int c_\epsilon\delta_\epsilon(x)[\phi(x)-\phi(0)]\,dx \to 0, \tag{5.89}$$

this may be written in the simple form

$$\int_{-\infty}^{\infty} \frac{d}{dx}\frac{1}{x^{\frac{1}{3}}}\phi(x)\,dx = \int_{-\infty}^{\infty} -\frac{1}{3}\frac{1}{x^{\frac{4}{3}}}[\phi(x)-\phi(0)]\,dx. \tag{5.90}$$

Notice that the integrand is integrable for each test function ϕ.

2. The function $\frac{1}{|x|^{\frac{1}{3}}}$ is locally integrable, while its pointwise derivative $-\frac{1}{3}\frac{1}{x^{\frac{4}{3}}}\text{sign}(x)$ is not. We have

$$\frac{d}{dx}\frac{1}{(x^2+\epsilon^2)^{\frac{1}{6}}} = -\frac{1}{3}\frac{x}{(x^2+\epsilon^2)^{\frac{7}{6}}}. \tag{5.91}$$

Since this derivative is an odd function, we have

$$\int_{-\infty}^{\infty} \frac{d}{dx}\frac{1}{|x|^{\frac{1}{3}}}\phi(x)\,dx = \lim_{\epsilon\to 0}\int_{-\infty}^{\infty} -\frac{1}{3}\frac{x}{(x^2+\epsilon^2)^{\frac{7}{6}}}[\phi(x)-\phi(0)]\,dx. \quad (5.92)$$

We can write this as

$$\int_{-\infty}^{\infty} \frac{d}{dx}\frac{1}{|x|^{\frac{1}{3}}}\phi(x)\,dx = \int_{-\infty}^{\infty} -\frac{1}{3}\frac{1}{x^{\frac{4}{3}}}\text{sign}(x)[\phi(x)-\phi(0)]\,dx. \quad (5.93)$$

Again the integrand is integrable.

Chapter 6

Bounded Operators

6.1 Introduction

This chapter deals with bounded linear operators. These are bounded linear transformations of a Hilbert space into itself. In fact, the chapter treats four classes of operators: finite rank, Hilbert-Schmidt, compact, and bounded. Every finite rank operator is Hilbert-Schmidt. Every Hilbert-Schmidt operator is compact. Every compact operator is bounded.

We shall see in the next chapter that it is also valuable to look at an even broader class of operators, those that are closed and densely defined. Every bounded operator (everywhere defined) is closed and densely defined. However the present chapter treats only bounded operators.

6.2 Bounded linear operators

Let H be a Hilbert space (a vector space with an inner product that is a complete metric space). A linear transformation $K : H \to H$ is said to be bounded if it maps bounded sets into bounded sets. This is equivalent to there being a constant M with

$$\|Ku\| \leq M\|u\|. \tag{6.1}$$

Let M_2 be the least such M. This is called uniform norm of K and is written $\|K\|_\infty$ or simply $\|K\|$ when the context makes this clear. [The subscript in M_2 is supposed to remind us that we are dealing with Hilbert spaces like L^2. The subscript in $\|K\|_\infty$, on the other hand, tells that we are looking at a least upper bound.]

If K and L are bounded operators, their sum $K + L$ and product KL are bounded. Furthermore, we have $\|K + L\|_\infty \leq \|K\|_\infty + \|L\|_\infty$ and $\|KL\|_\infty \leq \|K\|_\infty\|L\|_\infty$.

A bounded operator K always has an adjoint K^* that is a bounded operator.

It is the unique operator with the property that

$$(u, K^*v) = (Ku, v) \tag{6.2}$$

for all u, v in H. Furthermore $K^{**} = K$, and $\|K^*\|_\infty = \|K\|_\infty$. For products we have $(KL)^* = L^*K^*$, in the opposite order.

It is also possible to define the adjoint of an operator from one Hilbert space to another. Here is a special case. Let g be a vector in the Hilbert space H. Then g defines a linear transformation from $\mathbf{C}$ to H by sending z to the vector zg. The adjoint is a linear transformation from H to $\mathbf{C}$, denoted by g^*. It is the transformation that sends v to (g, v), so $g^*v = (g, v)$. The adjointness relation is $\bar{z}\, g^*v = (zg, v)$ which is just $\bar{z}(g, v) = (zg, v)$.

Let f be another vector. Define the operator K from H to H by $Ku = f(g, u)$, that is, $K = fg^*$. Then the adjoint of K is $K^* = gf^*$.

Example: Hilbert-Schmidt integral operators. Let

$$(Kf)(x) = \int k(x, y) f(y)\, dy. \tag{6.3}$$

with k in L^2, that is,

$$\|k\|_2^2 = \int \int |k(x, y)|^2\, dx\, dy < \infty. \tag{6.4}$$

Then K is bounded with norm $\|K\|_\infty \leq \|k\|_2$.

Proof: Fix x. Apply the Schwarz inequality to the integral over y in the definition of the operator. This gives that $|(Kf)(x)|^2 \leq \int |k(x, y)|^2\, dy \int |f(y)|^2\, dy$. Now integrate over x.

Example: Interpolation integral operators. Let K be an integral operator such that

$$M_1 = \sup_y \int |k(x, y)|\, dx < \infty \tag{6.5}$$

and

$$M_\infty = \sup_x \int |k(x, y)|\, dy < \infty. \tag{6.6}$$

(Here we choose to think of $k(x, y)$ as a function of x and y, not as a Schwartz distribution like $\delta(x - y)$.) Let $1/p + 1/q = 1$. Then for each p with $1 \leq p \leq \infty$ the norm M_p of K as an operator on L^p is bounded by $M_p \leq M_1^{\frac{1}{p}} M_\infty^{\frac{1}{q}}$. In particular as an operator on L^2 the norm $M_2 = \|K\|_\infty$ of K is bounded by

$$M_2 \leq \sqrt{M_1 M_\infty}. \tag{6.7}$$

The reason for the name interpolation operator (which is not standard) is that the bound interpolates for all p from the extreme cases $p = 1$ (where the bound is M_1) and $p = \infty$ (where the bound is M_∞).

Proof: Write

$$|(Kf)(x)| \leq \int |k(x, y)||f(y)|\, dy = \int |k(x, y)|^{\frac{1}{q}} \cdot |k(x, y)|^{\frac{1}{p}} |f(y)|\, dy. \tag{6.8}$$

Apply the Hölder inequality to the integral. This gives

$$|(Kf)(x)| \le \left(\int |k(x,y)|\, dy \right)^{\frac{1}{q}} \left(\int |k(x,y)||f(y)|^p\, dy \right)^{\frac{1}{p}} \le M_\infty^{\frac{1}{q}} \left(\int |k(x,y)||f(y)|^p\, dy \right)^{\frac{1}{p}}. \tag{6.9}$$

It follows that

$$\int |(Kf)(x)|^p\, dx \le M_\infty^{\frac{p}{q}} \int \int |k(x,y)||f(y)|^p\, dy\, dx \le M_\infty^{\frac{p}{q}} M_1 \int |f(y)|^p\, dy. \tag{6.10}$$

Take the pth root to get the bound

$$\left(\int |(Kf)(x)|^p\, dx \right)^{\frac{1}{p}} \le M_\infty^{\frac{1}{q}} M_1^{\frac{1}{p}} \left(\int |f(y)|^p\, dy \right)^{\frac{1}{p}}. \tag{6.11}$$

For a bounded operator K the set of points μ such that $(\mu I - K)^{-1}$ is a bounded operator is called the resolvent set of K. The complement of the resolvent set is called the spectrum of K. When one is only interested in values of $\mu \neq 0$ it is common to define $\lambda = 1/\mu$ and write

$$\mu(\mu I - K)^{-1} = (I - \lambda K)^{-1} \tag{6.12}$$

While one must be alert to which convention is being employed, this should be recognized as a trivial relabeling.

Theorem. If complex number μ satisfies $\|K\|_\infty < |\mu|$, then μ is in the resolvent set of K.

Proof: This is the Neumann series expansion

$$(\mu I - K)^{-1} = \frac{1}{\mu} \sum_{j=0}^{\infty} \frac{1}{\mu^j} K^j. \tag{6.13}$$

The jth term has norm $\|K^j\|_\infty / |\mu|^j \le (\|K\|_\infty / |\mu|)^j$. This is the jth term of a convergent geometric series.

Theorem. If for some $n \ge 1$ the complex number μ satisfies $\|K^n\|_\infty < |\mu|^n$, then μ is in the resolvent set of K.

This is the Neumann series again. But now we only require the estimate for the nth power of the operator. Write $j = an + b$, where $0 \le b < n$. Then $\|K^j\|_\infty / |\mu|^j$ is bounded by $(\|K\|_\infty / |\mu|)^b ((\|K^n\|_\infty / |\mu|^n)^a$. So this is the sum of n convergent geometric series, one for each value of b between 0 and $n-1$.

The spectral radius of an operator is the largest value of $|\mu|$, where μ is in the spectrum. The estimate of this theorem gives an upper bound on the spectral radius.

This is a remarkable result, since it has no analog for scalars. However for a matrix the norm of a power can be considerably smaller than the corresponding power of the norm, so this result can be quite useful. The most spectacular application is to Volterra integral operators.

Example: Volterra integral operators. Let $H = L^2(0,1)$ and

$$(Kf)(x) = \int_0^x k(x,y) f(y)\, dy. \tag{6.14}$$

Suppose that $|k(x,y)| \le C$ for $0 \le y \le x \le 1$ and $k(x,y) = 0$ for $0 \le x < y \le 1$. Then

$$\|K^n\|_\infty \le \frac{C^n}{(n-1)!}. \tag{6.15}$$

As a consequence every complex number $\mu \neq 0$ is in the resolvent set of K.

Proof: Each power K^n with $n \ge 1$ is also a Volterra integral operator. We claim that it has kernel $k^n(x,y)$ with

$$|k^n(x,y)| \le \frac{C^n}{(n-1)!}(x-y)^{n-1}. \tag{6.16}$$

for $0 \le y \le x \le 1$ and zero otherwise. This follows by induction.

Since $|k^n(x,y)| \le C^n/(n-1)!$, the Hilbert-Schmidt norm of K is also bounded by $C^n/(n-1)!$. However this goes to zero faster than every power. So the Neumann series converges.

The norm of a bounded operator can always be found by calculating the norm of a self-adjoint bounded operator. In fact, $\|K\|_\infty^2 = \|K^*K\|_\infty$. Furthermore, the norm of a self-adjoint operator is its spectral radius. This shows that to calculate the norm of a bounded operator K exactly, one needs only to calculate the spectral radius of K^*K and take the square root. Unfortunately, this can be a difficult problem. This is why it is good to have other ways of estimating the norm.

6.3 Compact operators

Let H be a Hilbert space. A subset S is totally bounded if for every $\epsilon > 0$ there is a cover of S by a finite number N of ϵ balls. A totally bounded set is bounded.

Thus for instance, if H is finite dimensional with dimension n and S is a cube of side L, then $N \approx (L/\epsilon)^n$. This number N is finite, though it increases with ϵ. One expects a cube or a ball to be totally bounded only in finite dimensional situations.

However the situation is different for a rectangular shaped region in infinite dimensions. Say that the sides are $L_1, L_2, L_3, \ldots, L_k, \ldots$ and that these decrease to zero. Consider $\epsilon > 0$. Pick k so large that $L_{k+1}, L_{k+1}, \ldots$ are all less than ϵ. Then $N \approx (L_1/\epsilon)(L_2/\epsilon)\cdots(L_k/\epsilon)$. This can increase very rapidly with ϵ. But such a region that is fat only in finitely many dimensions and increasingly thin in all the others is totally bounded.

A linear transformation $K : H \to H$ is said to be compact if it maps bounded sets into totally bounded sets. (One can take the bounded set to be the unit ball.) A compact operator is bounded.

If K and L are compact operators, then so is their sum $K + L$. If K is compact and L is bounded, then KL and LK are compact.

If the self-adjoint operator K^*K is compact, then K is compact.

Proof: Let $\epsilon > 0$. Then there are $u_1, \ldots, u_k$ in the unit ball such that for each u in the unit ball there is a j with $\|K^*K(u - u_j)\| < \epsilon/2$. But this says that

$$\|K(u-u_j)\| = (K(u-u_j), K(u-u_j)) = ((u-u_j), K^*K(u-u_j)) \leq \|u-u_j\| \, \|K^*K(u-u_j)\| < \epsilon. \tag{6.17}$$

The adjoint K^* of a compact operator K is a compact operator.

Proof: Say that K is compact. Then since K^* is bounded, it follows that KK^* is compact. It follows from the last result that K^* is compact.

Approximation theorem. If K_n is a sequence of compact operators, and K is a bounded operator, and if $\|K_n - K\|_\infty \to 0$ and $n \to \infty$, then K is also compact.

The proof is a classical $\epsilon/3$ argument. Let $\epsilon > 0$. Choose n so large that $\|K-K_n\|_\infty < \frac{\epsilon}{3}$. Since K_n is compact, there are finitely many vectors $u_1, \ldots, u_k$ in the unit ball such that every vector $K_n u$ with u in the unit ball is within $\epsilon/3$ of some $K_n u_j$. Consider an arbitrary u in the unit ball and pick the corresponding u_j. Since

$$Ku - Ku_j = (K - K_n)u + (K_n u - K_n u_j) + (K_n - K)u_j, \tag{6.18}$$

it follows that

$$\|Ku-Ku_j\| \leq \|(K-K_n)u\| + \|K_n u - K_n u_j\| + \|(K_n - K)u_j\| \leq \frac{\epsilon}{3} + \frac{\epsilon}{3} + \frac{\epsilon}{3} = \epsilon. \tag{6.19}$$

This shows that the image of the unit ball under K is totally bounded.

Spectral properties of compact operators. Let K be a compact operator. The only non-zero points in the spectrum of K are eigenvalues of finite multiplicity. The only possible accumulation point of the spectrum is 0.

Notice that there is no general claim that the eigenvectors of K form a basis for the Hilbert space. The example of a Volterra integral operator provides a counterexample: The only point in the spectrum is zero.

Let K be a compact operator. We want to consider equations of the form

$$\mu u = f + Ku, \tag{6.20}$$

where μ is a parameter. If $\mu = 0$, then this is an equation of the first kind. If $\mu \neq 0$, then this is an equation of the second kind. Very often an equation of the second kind is written $u = f_1 + \lambda K u$, where $\lambda = 1/\mu$, and where $f_1 = \lambda f$.

The condition for a unique solution of an equation of the first kind is the existence of the inverse K^{-1}, and the solution is $u = -K^{-1}f$. Thus the issue for an equation of the first kind is whether $\mu = 0$ is not an eigenvalue of K. If $\mu = 0$ is not an eigenvalue, the operator K^{-1} will be typically be an unbounded operator that is only defined on a linear subspace of the Hilbert space.

The condition for a unique solution of an equation of the second kind is the existence of the inverse $(\mu I - K)^{-1}$ for a particular value of $\mu \neq 0$, and the solution is $u = (\mu I - K)^{-1} f$. The issue for an equation of the second kind is whether $\mu \neq 0$ is not an eigenvalue of K. In this case, if $\mu \neq 0$ is not an eigenvalue, then $(\mu I - K)^{-1}$ will be a bounded operator. Thus equations of the second kind are much nicer. This is because compact operators have much better spectral properties away from zero.

Spectral theorem for compact self-adjoint operators. Let K be a compact self-adjoint operator. Then there is an orthonormal basis u_j of eigenvectors of K. The eigenvalues μ_j of K are real. Each non-zero eigenvalue is of finite multiplicity. The only possible accumulation point of the eigenvalues is zero. The operator K has the representation

$$Kf = \sum_j \mu_j u_j (u_j, f). \tag{6.21}$$

In abbreviated form this is

$$K = \sum_j \mu_j u_j u_j^*. \tag{6.22}$$

There is yet another way of writing the spectral theorem for compact operators. Define the unitary operator U from H to ℓ^2 by $(Uf)_j = (u_j, f)$. Its inverse is the unitary operator form ℓ^2 to H given by $(U^* c) = \sum c_j u_j$. Let M be the diagonal operator from ℓ^2 to ℓ^2 defined by multiplication by μ_j. Then

$$K = U^* M U. \tag{6.23}$$

The norm of a compact operator can always be found by calculating the norm of a self-adjoint compact operator. In fact, $\|K\|_\infty^2 = \|K^* K\|_\infty$. Furthermore, the norm of a compact self-adjoint operator is its spectral radius, which in this case is the largest value of $|\mu|$, where μ is an eigenvalue. Unfortunately, this can be a difficult computation.

Singular value decomposition for compact operators. Let K be a compact operator. Then there is an orthonormal family u_j and an orthonormal family w_j and a sequence of numbers $\chi_j \geq 0$ (singular values of K) approaching zero such that the operator K has the representation

$$Kf = \sum_j \chi_j w_j (u_j, f). \tag{6.24}$$

In abbreviated form this is

$$K = \sum_j \chi_j w_j u_j^*. \tag{6.25}$$

Sketch of proof: The operator $K^* K$ is self-adjoint with positive eigenvalues χ_j^2. We can write

$$K^* K f = \sum_j \chi_j^2 u_j (u_j, f). \tag{6.26}$$

Then

$$\sqrt{K^*K}f = \sum_j \chi_j u_j (u_j, f). \tag{6.27}$$

Since $\|Kf\| = \|\sqrt{K^*K}f\|$ for each f, we can write $K = V\sqrt{K^*K}$, where $\|Vg\| = \|g\|$ for all $g = \sqrt{K^*K}f$ in the range of $\sqrt{K^*K}$. This is the well-known polar decomposition. Then

$$Kf = \sum_j \chi_j w_j (u_j, f), \tag{6.28}$$

where $w_j = Vu_j$.

There is another way of writing the singular value decomposition of K. Let $\sqrt{K^*K} = U^*DU$ be the spectral representation of $\sqrt{K^*K}$, where D is diagonal with entries $\chi_j \geq 0$. Then $K = VU^*DU = WDU$.

It follows from the approximation theorem and from the singular value decomposition that an operator is compact if and only if it is a norm limit of a sequence of finite rank operators.

Notice that this theorem gives a fairly clear picture of what a compact operator acting on L^2 looks like. It is an integral operator with kernel

$$k(x,y) = \sum_j \chi_j w_j(x)\overline{u_j(y)}, \tag{6.29}$$

where the $\chi_j \to 0$. Of course this representation may be difficult to find in practice. What happens in the case of a Hilbert-Schmidt integral operator is special: the χ_j go to zero sufficiently rapidly that $\sum_j |\chi_j|^2 < \infty$.

6.4 Hilbert-Schmidt operators

Let H be a Hilbert space. For a positive bounded self-adjoint operator B the trace is defined by $\mathrm{tr}B = \sum_j (e_j, Be_j)$, where the e_j form an orthonormal basis. A bounded linear operator $K : H \to H$ is said to be Hilbert-Schmidt if $\mathrm{tr}(K^*K) < \infty$. The Hilbert-Schmidt norm is $\|K\|_2 = \sqrt{\mathrm{tr}(K^*K)}$.

Theorem. If K is a Hilbert-Schmidt integral operator with $(Kf)(x) = \int k(x,y)f(y)\,dy$ then

$$\|K\|_2^2 = \int\int |k(x,y)|^2\,dx\,dy. \tag{6.30}$$

Proof: Let $\{e_1, e_2, ...\}$ be an orthonormal basis for H. We can always expand a vector in this basis via

$$u = \sum_j e_j (e_j, u). \tag{6.31}$$

(Remember the convention adopted here that inner products are linear in the second variable, conjugate linear in the first variable.) Write

$$Kf = \sum_i e_i \sum_j (e_i, Ke_j)(e_j, f). \tag{6.32}$$

The matrix elements (e_i, Ke_j) satisfy

$$\sum_i \sum_j |(e_i, Ke_j)|^2 = \sum_j \sum_i (Ke_j, e_i)(e_i, Ke_j) = \sum_j ||Ke_j||^2 = \sum_j (e_j, K^*Ke_j) = \mathrm{tr}(K^*K). \tag{6.33}$$

So the kernel of the integral operator K is

$$k(x, y) = \sum_i \sum_j (e_i, Ke_j) e_i(x) \overline{e_j(y)}. \tag{6.34}$$

This sum is convergent in $L^2(dxdy)$.

A Hilbert-Schmidt operator is a bounded operator. It is always true that $\|K\|_\infty \leq \|K\|_2$.

Theorem. A Hilbert-Schmidt operator is compact.

Proof: Let K be a Hilbert-Schmidt operator. Then K is given by a square-summable matrix. So K may be approximated by a sequence of finite-rank operators K_n such that $\|K_n - K\|_2 \to 0$. In particular, $\|K_n - K\|_\infty \to 0$. Since each K_n is compact, it follows from the approximation theorem that K is compact.

If K and L are Hilbert-Schmidt operators, their sum $K + L$ is a Hilbert-Schmidt operator and $\|K + L\|_2 \leq \|K\|_2 + \|L\|_2$. If K is a Hilbert-Schmidt operator and L is a bounded operator, then the products KL and LK are Hilbert-Schmidt. Furthermore, $\|KL\|_2 \leq \|K\|_2 \|L\|_\infty$ and $\|LK\|_2 \leq \|L\|_\infty \|K\|_2$.

The adjoint of a Hilbert-Schmidt operator is a Hilbert-Schmidt operator. Furthermore, $\|K^*\|_2 = \|K\|_2$.

Notice that the Hilbert-Schmidt norm of a bounded operator is defined in terms of a self-adjoint operator. In fact, $\|K\|_2$ is the square root of the trace of the self-adjoint operator K^*K, and the trace is the sum of the eigenvalues. However we do not need to calculate the eigenvalues, since, as we have seen, there are much easier ways to calculate the trace.

6.5 Problems

1. Let $H = L^2$ be the Hilbert space of square integrable functions on the line. Create an example of a Hilbert-Schmidt operator that is not an interpolation operator.

2. Let $H = L^2$ be the Hilbert space of square integrable functions on the line. Create an example of an interpolation operator that is not a Hilbert-Schmidt operator. Make the example so that the operator is not compact.

3. Find an example of a compact bounded operator on $H = L^2$ that is neither a Hilbert-Schmidt or an interpolation operator.

4. Find an example of a bounded operator on $H = L^2$ that is neither a Hilbert-Schmidt nor an interpolation operator, and that is also not a compact operator.

5. Let H be a Hilbert space. Give an example of a Hilbert-Schmidt operator for which the spectral radius is equal to the uniform norm.

6. Let H be a Hilbert space. Give an example of a Hilbert-Schmidt operator for which the spectral radius is very different from the uniform norm.

7. Let H be a Hilbert space. Is it possible for a Hilbert-Schmidt operator to have its Hilbert-Schmidt norm equal to its uniform norm? Describe all possible such situations.

6.6 Finite rank operators

Let H be a Hilbert space. A bounded linear transformation $K : H \to H$ is said to be finite rank if its range is finite dimensional. The dimension of the range of K is called the rank of K. A finite rank operator may be represented in the form

$$Kf = \sum_j z_j (u_j, f), \tag{6.35}$$

where the sum is finite. In a more abbreviated notation we could write

$$K = \sum_j z_j u_j^*. \tag{6.36}$$

Thus in L^2 this is an integral operator with kernel

$$k(x, y) = \sum_j z_j(x)\overline{u_j(y)}. \tag{6.37}$$

If K and L are finite rank operators, then so is their sum $K + L$. If K is finite rank and L is bounded, then KL and LK are finite rank.

The adjoint K^* of a finite rank operator K is finite rank. The two operators have the same rank.

Every finite rank operator is Hilbert-Schmidt and hence compact. If K is a compact operator, then there exists a sequence of finite rank operators K_n such that $\|K_n - K\|_\infty \to 0$ as $n \to \infty$.

If K is a finite rank operator and $\mu \neq 0$, then the calculation of $(\mu I - K)^{-1}$ or of $(I - \lambda K)^{-1}$ may be reduced to a finite-dimensional matrix problem in the finite dimensional space $R(K)$. This is because K leaves $R(K)$ invariant. Therefore if $\mu = 1/\lambda$ is not an eigenvalue of K acting in $R(K)$, then there is an inverse $(I - \lambda K)^{-1}$ acting in $R(K)$. However this gives a corresponding inverse in the original Hilbert space, by the formula

$$(I - \lambda K)^{-1} = I + (I - \lambda K)^{-1}\lambda K. \tag{6.38}$$

Explictly, to solve

$$u = \lambda K u + f, \tag{6.39}$$

write

$$u = (I - \lambda K)^{-1} f = f + (I - \lambda K)^{-1} \lambda K f. \tag{6.40}$$

To solve this, let w be the second term on the right hand side, so that $u = f + w$. Then $(I - \lambda K)w = \lambda K f$. Write $w = \sum_j a_j z_j$. Then

$$\sum_j a_j z_j - \lambda \sum_j z_j (u_j, \sum_r a_r z_r) = \lambda \sum_j z_j (u_j, f). \tag{6.41}$$

Thus

$$a_j - \lambda \sum_r (u_j, z_r) a_r = (u_j, f). \tag{6.42}$$

This is a matrix equation that may be solved whenever $1/\lambda$ is not an eigenvalue of the matrix with entries (u_j, z_r).

6.7 Problems

It may help to recall that the problem of inverting $I - \lambda K$ is the same as the problem of showing that $\mu = 1/\lambda$ is not in the spectrum of K.

1. Consider functions in $L^2(-\infty, \infty)$. Consider the integral equation

$$f(x) - \lambda \int_{-\infty}^{\infty} \cos(\sqrt{x^2 + y^4}) e^{-|x|-|y|} f(y)\, dy = g(x).$$

   It is claimed that there exists $r > 0$ such that for every complex number λ with $|\lambda| < r$ the equation has a unique solution. Prove or disprove. Interpret this as a statement about the spectrum of a certain linear operator.

2. Consider functions in $L^2(-\infty, \infty)$. Consider the integral equation

$$f(x) - \lambda \int_{-\infty}^{\infty} \cos(\sqrt{x^2 + y^4}) e^{-|x|-|y|} f(y)\, dy = g(x).$$

   It is claimed that there exists $R < \infty$ such that for every complex number λ with $|\lambda| > R$ the equation does not have a unique solution. Prove or disprove. Interpret this as a statement about the spectrum of a certain linear operator.

3. Consider functions in $L^2(-\infty, \infty)$. Consider the integral equation

$$f(x) - \lambda \int_{-\infty}^{\infty} e^{-|x|-|y|} f(y)\, dy = g(x).$$

   Find all complex numbers λ for which this equation has a unique solution. Find the solution. Interpret this as a statement about the spectrum of a certain linear operator.

4. Consider functions in $L^2(0,1)$. Consider the integral equation

$$f(x) - \lambda \int_0^x f(y)\, dy = g(x).$$

Find all complex numbers λ for which this equation has a unique solution. Find the solution. Interpret this as a statement about the spectrum of a certain linear operator. Hint: Differentiate. Solve a first order equation with a boundary condition.

5. Consider functions in $L^2(0,1)$. Consider the integral equation

$$f(x) - \lambda \left[\int_0^x y(1-x) f(y)\, dy + \int_x^1 x(1-y) f(y)\, dy \right] = g(x).$$

Find all complex numbers λ for which this equation has a unique solution. Interpret this as a statement about the spectrum of a certain linear operator. Hint: The integral operator K has eigenfunctions $\sin(n\pi x)$. Verify this directly. This should also determine the eigenvalues.

Chapter 7

Densely Defined Closed Operators

7.1 Introduction

This chapter deals primarily with densely defined closed operators. Each everywhere defined bounded operator is in particular a densely defined closed operator.

If L is a densely defined closed operator, then so is its adjoint L^*. Furthermore, $L^{**} = L$. If both L and L^* have trivial null spaces, then both L^{-1} and L^{*-1} are densely defined closed operators.

A complex number λ is in the resolvent set of a densely defined closed operator L if $(L - \lambda I)^{-1}$ is an everywhere defined bounded operator. A complex number λ is in the spectrum of L if it is not in the resolvent set. A complex number λ is in the spectrum of L if and only if $\bar{\lambda}$ is in the spectrum of the adjoint L^*.

It is common to divide the spectrum into three disjoint subsets: point spectrum, continuous spectrum, and residual spectrum. (This terminology is misleading, in that it treats limits of point spectrum as continuous spectrum.) In this treatment we divide the spectrum into four disjoint subsets: standard point spectrum, pseudo-continuous spectrum, anomalous point spectrum, and residual spectrum. The adjoint operation maps the first two kind of spectra into themselves, but it reverses the latter two.

7.2 Subspaces

Let H be a Hilbert space. Let M be a vector subspace of H. The closure $\bar{M}$ is also a vector subspace of H. The subspace M is said to be closed if $M = \bar{M}$. The orthogonal complement $M^\perp$ is a closed subspace of H. Furthermore, $(\bar{M})^\perp = M^\perp$. Finally $M^{\perp\perp} = \bar{M}$. The nicest subspaces are closed subspaces.

For a closed subspace M we always have $M^{\perp\perp} = M$.

A subspace M is dense in H if $\bar{M} = H$. This is equivalent to the condition $M^{\perp} = \{0\}$.

7.3 Graphs

Let H be a Hilbert space. The direct sum $H \oplus H$ with itself consists of all ordered pairs $[u, v]$, where u, v are each vectors in H. The inner product of $[u, v]$ with $[u', v']$ is

$$([u, v], [u', v']) = (u, u') + (v, v'). \tag{7.1}$$

A graph is a linear subspace of $H \oplus H$. If we have two graphs L_1 and L_2 and if $L_1 \subset L_2$, then we say that L_1 is a *restriction* of L_2 or L_2 is an *extension* of L_1.

If L is a graph, then its domain $D(L)$ is the set of all u in H such that there exists a v with $[u, v]$ in L. Its range $R(L)$ is the set of all v in H such that there exists u with $[u, v]$ in L.

If L is a graph, then its null space $N(L)$ is the set of all u in H such that $[u, 0]$ is in L.

If L is a graph, then the inverse graph L^{-1} consists of all $[v, u]$ such that $[u, v]$ is in L.

We say that a graph L is an operator if $[0, v]$ in L implies $v = 0$. It is easy to see that this is equivalent to saying that $N(L^{-1}) = \{0\}$ is the zero subspace. When L is an operator and $[u, v]$ is in L, then we write $Lu = v$. We shall explore the properties of operators in the next section.

Write $\bar{L}$ for the closure of L. We say L is closed if $L = \bar{L}$.

If L is a graph, then the adjoint graph L^* consists of the pairs $[w, z]$ such that for all $[u, v]$ in L we have $(z, u) = (w, v)$.

If L is a graph, then the adjoint graph L^* is always closed. Furthermore, the adjoint of its closure $\bar{L}$ is the same as the adjoint of L.

Remark: One way to think of the adjoint graph is to define the negative inverse $-L^{-1}$ of a graph L to consist of all the ordered pairs $[v, -u]$ with $[u, v]$ in L. Then the adjoint L^* is the orthogonal complement in $H \oplus H$ of $-L^{-1}$. That is, the pair $[z, w]$ in the graph L^* is orthogonal to each $[v, -u]$ with $[u, v]$ in the graph of L. This says that $([z, w], [v, -u]) = (z, u) - (w, v) = 0$ for all such $[u, v]$. [This says to take the graph with negative reciprocal slope, and then take the perpendicular graph to that.]

Another way to think of this is to define the anti-symmetric form $\omega([z, w], [u, v]) = (z, u) - (w, v)$. Then the adjoint A^* consists of the orthogonal complement of A with respect to ω.

Theorem. If L is a graph, then $L^{**} = \bar{L}$.

Perhaps the nicest general class of graphs consists of the closed graphs L. For such a graph the adjoint L^* is a graph, and $L^{**} = L$.

It is not hard to check that $L^{*-1} = L^{-1*}$.

Theorem. $N(L^*) = R(L)^{\perp}$.

Corollary. $\overline{R(L)} = N(L^*)^\perp$.

This corollary is very important in the theory of linear equations. Let L be a linear operator. Suppose that $R(L)$ is a closed subspace of H. Then in this special case the corollary says that $R(L) = N(L^*)^\perp$. Thus a linear equation $Lu = g$ has a solution u if and only if g is orthogonal to all solutions v of $L^*v = 0$. This is called the Fredholm alternative.

7.4 Operators

If L is a graph, then L is an operator if $[0, v]$ in L implies $v = 0$. It is easy to see that L is an operator precisely when $N(L^{-1}) = \{0\}$ is the zero subspace. When L is an operator and $[u, v]$ is in L, then we write $Lu = v$.

Corollary. L is densely defined if and only if L^* is an operator.

Proof: Apply the last theorem of the previous section to L^{-1}. This gives $N(L^{*-1}) = D(L)^\perp$.

Corollary. $\bar{L}$ is an operator if and only if L^* is densely defined.

Proof: Apply the previous corollary to L^* and use $L^{**} = \bar{L}$.

An operator L is said to be closable if $\bar{L}$ is also an operator. For a densely defined closable operator the adjoint L^* is a densely defined closed operator, and $L^{**} = \bar{L}$. Furthermore, the definition of the adjoint is that w is in the domain of L^* and $L^*w = z$ if and only if for all u in the domain of L we have $(z, u) = (w, Lu)$, that is,

$$(L^*w, u) = (w, Lu). \tag{7.2}$$

Perhaps the nicest general class of operators consists of the densely defined closed operators L. For such an operator the adjoint L^* is a densely defined closed operator, and $L^{**} = L$.

7.5 The spectrum

Theorem. (Closed graph theorem) Let H be a Hilbert space. Let L be a closed operator with domain $D(L) = H$. Then L is a bounded operator. (The converse is obvious.)

0. Let L be a closed operator. We say that λ is in the resolvent set of L if $N(L-\lambda I) = \{0\}$ and $R(L-\lambda I) = H$. In that case $(L-\lambda I)^{-1}$ is a closed operator with domain $D((L - \lambda I)^{-1}) = H$. By the closed graph theorem, $(L - \lambda I)^{-1}$ is a bounded operator.

We shall usually refer to $(L - \lambda I)^{-1}$ as the resolvent of L. However in some contexts it is convenient to use instead $(\lambda I - L)^{-1}$, which is of course just the negative. There is no great distinction between these two possible definitions of resolvent. However it is important to be alert to which one is being used.

1. Let L be a closed operator. We say that λ is in the standard point spectrum of L if $N(L - \lambda I) \neq \{0\}$ and $R(L - \lambda I)^\perp \neq \{0\}$.

2. Let L be a closed operator. We say that λ is in the anomalous point spectrum of L if $N(L-\lambda I) \neq \{0\}$ and $R(L-\lambda I)^{\perp} = \{0\}$ (that is, $R(L-\lambda I)$ is dense in H).

3. Let L be a closed operator. We say that λ is in the pseudo-continuous spectrum of L if $N(L-\lambda I) = \{0\}$ and $R(L-\lambda I)^{\perp} = \{0\}$ (so $R(L-\lambda I)$ is dense in H) but $R(L-\lambda I) \neq H$. In that case $(L-\lambda I)^{-1}$ is a closed operator with dense domain $D((L-\lambda I)^{-1})$ not equal to H.

4. Let L be a closed operator. We say that λ is in the residual spectrum of L if $N(L-\lambda I) = \{0\}$ and $R(L-\lambda I)^{\perp} \neq \{0\}$. In that case $(L-\lambda I)^{-1}$ is a closed operator with a domain that is not dense.

Theorem. Let L be a densely defined closed operator and let L^* be its adjoint operator. Then:

0. The number λ is in the resolvent set of L if and only if $\bar{\lambda}$ is in the resolvent set of L^*.

1. The number λ is in the standard point spectrum of L if and only if $\bar{\lambda}$ is in the standard point spectrum of L^*.

2. The number λ is in the anomalous point spectrum of L if and only if $\bar{\lambda}$ is in the residual spectrum of L^*.

3. λ is in the pseudo-continuous spectrum of L if and only if $\bar{\lambda}$ is in the pseudo-continuous spectrum of L^*.

4. λ is in the residual spectrum of L if and only if $\bar{\lambda}$ is in the anomalous point spectrum of L^*.

For finite dimensional vector spaces only cases 0 and 1 can occur.

Summary: Let L be a closed, densely defined operator. The complex number λ is in the point spectrum of L is equivalent to λ being an eigenvalue of L. Similarly, λ in the pseudo-continuous spectrum of L is equivalent to $(L-\lambda I)^{-1}$ being a densely defined, closed, but unbounded operator. Finally, λ in the residual spectrum of L is equivalent to $(L-\lambda I)^{-1}$ being a closed operator that is not densely defined.

7.6 Spectra of inverse operators

Consider a closed, densely defined operator with an inverse L^{-1} that is also a closed, densely defined operator. Let $\lambda \neq 0$. Then λ is in the resolvent set of L if and only if $1/\lambda$ is in the resolvent set of L^{-1}. In fact, we have the identity

$$\left(I-\lambda^{-1}L\right)^{-1} + \left(I-\lambda L^{-1}\right)^{-1} = I. \tag{7.3}$$

One very important situation is when $K = L^{-1}$ is a compact operator. Then we know that all non-zero elements μ of the spectrum of $K = L^{-1}$ are eigenvalues of finite multiplicity, with zero as their only possible accumulation point. It follows that all elements $\lambda = 1/\mu$ of the spectrum of L are eigenvalues of finite multiplicity, with infinity as their only possible accumulation point.

7.7 Problems

If K is a bounded everywhere defined operator, then in particular K is a closed densely defined operator.

If K is a closed densely defined operator, and if both K and K^* have trivial nullspaces, then $L = K^{-1}$ is also a closed densely defined operator.

1. Let $K = L^{-1}$ be as above. Let $\lambda \neq 0$ and let $\mu = 1/\lambda$. Find a formula relating the resolvent $(L - \lambda)^{-1}$ to the resolvent $(K - \mu)^{-1}$.

2. Consider functions in $L^2(0, 1)$. Consider the integral operator K given by

$$(Kf)(x) = \int_0^x f(y)\, dy.$$

   Show that $L = K^{-1}$ exists and is closed and densely defined. Describe the domain of L. Be explicit about boundary conditions. Describe how L acts on the elements of this domain. Show that $L^* = K^{*-1}$ is closed and densely defined. Describe the domain of L^*. Describe how L^* acts on the elements of this domain. Hint: Differentiate.

3. In the preceding problem, find the spectrum of L. Also, find the resolvent $(L - \lambda)^{-1}$ of L. Hint: Solve a first order linear ordinary differential equation.

4. Consider functions in $L^2(0, 1)$. Consider the integral operator K given by

$$(Kf)(x) = \left[\int_0^x y(1 - x)f(y)\, dy + \int_x^1 x(1 - y)f(y)\, dy \right].$$

   Show that $L = K^{-1}$ exists and is closed and densely defined. Describe the domain of L. Be explicit about boundary conditions. Describe how L acts on the elements of this domain. Hint: Differentiate twice.

5. In the preceding problem, find the spectrum of L. Find the resolvent $(L - \lambda)^{-1}$ of L. Hint: Use $\sin(\sqrt{\lambda}x)$ and $\sin(\sqrt{\lambda}(1 - x))$ as a basis for the solutions of a homogeneous second order linear ordinary differential equation. Solve the inhomogeneous equation by variation of parameters.

6. Let K be a compact operator. Suppose that K and K^* have trivial nullspaces, so that $L = K^{-1}$ is a closed densely defined operator. Prove that the spectrum of $L = K^{-1}$ consists of isolated eigenvalues of finite multiplicity. To what extent does this result apply to the examples in the previous problems?

7. Let K be a compact self-adjoint operator. Suppose that K has trivial null-space, so that $L = K^{-1}$ is a self-adjoint operator. Prove that there exists an orthogonal basis consisting of eigenvectors of L. To what extent does this result apply to the examples in the previous problems?

7.8 Self-adjoint operators

It is difficult to do algebraic operations with closed, densely defined operators, because their domains may differ. It is always true that $(zL)^* = \bar{z}L^*$. If K is bounded everywhere defined, then $(L+K)^* = L^*+K^*$ and $(K+L)^* = K^*+L^*$. Furthermore, if K is bounded everywhere defined, then $(KL)^* = L^*K^*$.

An operator A is self-adjoint if $A = A^*$. A self-adjoint operator is automatically closed and densely defined. (Every adjoint A^* is automatically closed. If A^* is an operator, then A is densely defined.)

If a self-adjoint operator has trivial null space, then its inverse is also a self-adjoint operator.

If L is a closed, densely defined operator, then L^*L is defined on the domain consisting of all u in $D(L)$ such that Lu is in $D(L^*)$. It is not obvious that this is closed and densely defined, much less that it is self-adjoint. However this is all a consequence of the following theorem.

Theorem. If L is a closed and densely defined operator, then L^*L is a self-adjoint operator.

Proof: If L is a closed and densely defined operator, then L^* is also a closed and densely defined operator. Furthermore, LL^* is an operator with $LL^* \subset (LL^*)^*$.

The Hilbert space $H \oplus H$ may be written as the direct sum of the two closed graphs $-L^{-1}$ and L^* Therefore an arbitrary $[0, h]$ for h in H may be written as the sum $[0, h] = [-Lf, f] + [g, L^*g]$. This says that $0 = -Lf + g$ and $h = f + L^*g$. As a consequence $h = f + L^*Lf$. Furthermore, by properties of projections we have $\|Lf\|^2 + \|f\|^2 \leq \|h\|^2$. We have shown that for each h we can solve $(I + L^*L)f = h$ and that $\|f\|^2 \leq \|h\|^2$. Thus $(I + L^*L)^{-1}$ is everywhere defined and is a bounded operator with norm bounded by one.

Since $L^*L \subset (L^*L)^*$, we have $(I + L^*L)^{-1} \subset (I + L^*L)^{-1*}$. It follows that $(I + L^*L)^{-1} = (I + L^*L)^{-1*}$ is a self-adjoint operator. The conclusion follows.

7.9 First order differential operators with a bounded interval: point spectrum

In this section we shall see examples of operators with no spectrum at all. However we shall also see a very pretty and useful example of an operator with standard point spectrum. This operator is the one behind the theory of Fourier series.

Example 1A: This example is one where the correct number of boundary conditions are imposed. In the case of a first order differential operator this number is one. Let H be the Hilbert space $L^2(0, 1)$. Let L_0 be the operator d/dx acting on functions of the form $f(x) = \int_0^x g(y)\,dy$ where g is in H. The value of L_0 on such a function is $g(x)$. Notice that functions in the domain of L_0 automatically satisfy the boundary condition $f(0) = 0$. This is an example of a closed operator. The reason is that $(L_0^{-1}g)(x) = \int_0^x g(y)\,dy$. This is a bounded operator defined on the entire Hilbert space. So L_0^{-1} and L_0 are both closed.

The adjoint of the inverse is given by $(L_0^{-1*})h(x) = \int_x^1 h(y)\,dy$. It follows that L_0^* is the operator $-L_1$, where L_1 is given by d/dx acting on functions of the form $f(x) = -\int_x^1 g(y)\,dy$ where g is in H. The value of L_1 on such a function is $g(x)$. Notice that functions in the domain of L_1 automatically satisfy the boundary condition $f(1) = 0$.

The operators L_0 and L_1 each have one boundary condition. They are negative adjoints of each other. They each have a spectral theory, but it is extremely pathological. For instance, the resolvent of L_0 is given by

$$((L_0 - \lambda I)^{-1}g)(x) = \int_0^x e^{\lambda(x-y)}g(y)\,dy.$$

So there are no points at all in the spectrum of L_0. It is in some sense located all at infinity.

To see this, consider the operator L_0^{-1}. This operator has spectrum consisting of the point zero. All the spectral information is hidden at this one point. This is, by the way, an example of pseudo-continuous spectrum.

This is one important though somewhat technical point. The domain of L_0 consists precisely of the functions in the range of $K_0 = L_0^{-1}$. In the example where K_0 is the integration operator, this is all functions of the form

$$u(x) = \int_0^x f(y)dy, \tag{7.4}$$

where f is in $L^2(0,1)$. These functions u need not be C^1. They belong to a larger class of functions that are indefinite integrals of L^2 functions. Such functions are continuous, but they may have slope discontinuities. The functions u of course satisfy the boundary condition $u(0) = 0$. The action of L_0 on a function u is given by $L_0u = u'$, where the derivative exists except possible on a set of measure zero. However L^2 functions such as f are defined only up to sets of measure zero, so this is not a problem.

Now for a really picky question: If u is also regarded as an L^2 function, then it is also defined only up to sets of measure zero. So what does $u(0)$ mean? After all, the set consisting of 0 alone is of measure zero. The answer is that the general indefinite integral is a function of the form

$$u(x) = \int_0^x f(y)dy + C. \tag{7.5}$$

Among all L^2 functions given by such an integral expression, there is a subclass of those for which $C = 0$. These are the ones satisfying the boundary condition $u(0) = 0$. There is another subclass for which $C = -\int_0^1 f(y)dy$. These are the ones satisfying $u(1) = 0$.

A densely defined operator L is said to be self-adjoint if $L = L^*$. Similarly, L is said to be skew-adjoint if $L = -L^*$.

Example 1B: Here is another example with the correct number of boundary conditions. Let H be the Hilbert space $L^2(0,1)$. Let $L_=$ be the operator d/dx

acting on functions of the form $f(x) = \int_0^x g(y)\,dy + C$ where g is in H and $\int_0^1 g(y)\,dy = 0$. The value of $L_=$ on such a function is $g(x)$. Notice that functions in the domain of $L_=$ automatically satisfy the boundary condition $f(0) = f(1)$. The operator $L_=$ is skew-adjoint.

The operator $L_=$ has periodic boundary conditions. Since it is skew-adjoint, it has an extraordinarily nice spectral theory. The resolvent is

$$((L_= - \lambda I)^{-1} g)(x) = \frac{1}{1 - e^{\lambda}} \int_0^x e^{\lambda(x-y)} g(y)\,dy - \frac{1}{1 - e^{-\lambda}} \int_x^1 e^{-\lambda(y-x)} g(y)\,dy.$$

The spectrum consists of the numbers $2\pi i n$. These are all point spectrum. The corresponding eigenvectors form a basis that gives the Fourier series expansion of an arbitrary periodic function with period one.

A densely defined operator L is said to be *Hermitian* if $L \subset L^*$. This is simply the algebraic property that

$$(Lu, w) = (u, Lw)$$

for all u, w in $D(L)$. Similarly, L is said to be skew-Hermitian if $L \subset -L^*$.

Example 2: The following example illustrates what goes wrong when one imposes the wrong number of boundary conditions. Let H be the Hilbert space $L^2(0,1)$. Let L_{01} be the operator d/dx acting on functions of the form $f(x) = \int_0^x g(y)\,dy$ where g is in H and $\int_0^1 g(y)\,dy = 0$. The value of L_{01} on such a function is $g(x)$. Notice that functions in the domain of L_{01} automatically satisfy the boundary conditions $f(0) = 0$ and $f(1) = 0$. The adjoint of L_{01} is the operator $-L$, where L is given by d/dx acting on functions of the form $\int_0^x g(y)\,dy + C$, where g is in H. The value of L on such a function is $g(x)$. Notice that functions in the domain of L need not satisfy any boundary conditions. From this we see that L_{01} is skew-Hermitian.

The operator L is d/dx. It has too few boundary conditions. The operator L_{01} has a boundary condition at 0 and at 1. This is too many boundary conditions. Each of these operators is the negative of the adjoint of the other. The spectrum of L consists of the entire complex plane, and it is all point spectrum. The spectrum of L_{01} also consists of the entire complex plane, and it is all residual spectrum.

Remark: The operators L_0 and L_1 have $L_{01} \subset L_0 \subset L$ and with $L_{01} \subset L_1 \subset L$. Furthermore, the operator $L_=$ has $L_{01} \subset L_= \subset L$. Thus there are various correct choices of boundary conditions, but they may have different spectral properties.

7.10 Spectral projection and reduced resolvent

Consider a closed densely defined operator L. In this section we shall assume that the eigenvectors of L span the entire Hilbert space. Consider also an isolated eigenvalue λ_n. The spectral projection corresponding to λ_n is a (not

necessarily orthogonal) projection onto the corresponding eigenspace. It is given in terms of the resolvent by

$$P_n = \lim_{\lambda \to \lambda_n} (\lambda_n - \lambda)(L - \lambda I)^{-1}. \tag{7.6}$$

This is the negative of the residue of the resolvent at λ_1. The reason this works is that $L = \sum_m \lambda_m P_m$ and consequently

$$(L - \lambda I)^{-1} = \sum_m \frac{1}{\lambda_m - \lambda} P_m, \tag{7.7}$$

at least in the case under consideration, when the eigenvectors span the entire Hilbert space.

The reduced resolvent corresponding to λ_n is defined as the operator that inverts $(L - \lambda_n I)$ in the range of $(I - P_n)$ and is zero in the range of P_n. It is a solution of the equations

$$S_n P_n = P_n S_n = 0 \tag{7.8}$$

and

$$(L - \lambda_n I) S_n = 1 - P_n \tag{7.9}$$

It may be expressed in terms of the resolvent by

$$S_n = \lim_{\lambda \to \lambda_n} (L - \lambda I)^{-1}(1 - P_n). \tag{7.10}$$

When the eigenvectors span this is

$$S_n = \sum_{m \neq n} \frac{1}{\lambda_m - \lambda_n} P_m. \tag{7.11}$$

Example: Take the skew-adjoint operator $L_= = d/dx$ acting in $L^2(0,1)$ with periodic boundary conditions. The spectral projection corresponding to eigenvalue $2\pi i n$ is the self-adjoint operator

$$(P_n g)(x) = \int_0^1 \exp(2\pi i n(x - y)) g(y)\, dy. \tag{7.12}$$

The reduced resolvent corresponding to eigenvalue 0 is the skew-adjoint operator

$$(S_0 g)(x) = \int_0^x (\frac{1}{2} - x + y) g(y)\, dy + \int_x^1 (-\frac{1}{2} - x + y) g(y)\, dy. \tag{7.13}$$

7.11 Generating second-order self-adjoint operators

This section exploits the theorem that says that if L is an arbitrary closed densely defined operator, then L^*L is a self-adjoint operator. Remember that $L^{**} = L$, so LL^* is also a self-adjoint operator.

It would be easy to conclude that first order differential operators such as L_{01} and its adjoint L are of no interest for spectral theory. This is not the case. From the general theorem LL_{01} and $L_{01}L$ are self-adjoint second-order differential operators. These, as we shall see, have a nice spectral theory. The operator LL_{01} is the operator $-d^2/dx^2$ with Dirichlet boundary conditions $u(0) = 0$ and $u(1) = 0$. The operator $L_{01}L$ is the operator $-d^2/dx^2$ with Neumann boundary conditions $u'(0) = 0$ and $u'(1) = 0$. It is amusing to work out other self-adjoint second order differential operators that may be generated from the first order differential operators of the preceding sections.

7.12 First order differential operators with a semi-infinite interval: residual spectrum

In this example we shall see examples of operators with anomalous point spectrum and residual spectrum. These operators underly the theory of the Laplace transform.

Example: Let H be the Hilbert space $L^2(0, \infty)$. Let L_0 be the operator d/dx acting on functions f in H of the form $f(x) = \int_0^x g(y)\, dy$ where g is in H. The value of L_0 on such a function is $g(x)$. Notice that functions in the domain of L_0 automatically satisfy the boundary condition $f(0) = 0$.

If $\Re\lambda < 0$, then we can find always find a solution of the equation $(L_0 - \lambda I)f = g$. This solution is

$$f(x) = \int_0^x e^{\lambda(x-y)} g(y)\, dy. \tag{7.14}$$

This equation defines the bounded operator $(L_0 - \lambda I)^{-1}$ that sends g into f, at least when $\Re\lambda < 0$. Notice that if $\Re\lambda > 0$, then the formula gives a result in L^2 only if g is orthogonal to $e^{-\bar{\lambda}x}$. Thus $\Re\lambda > 0$ corresponds to residual spectrum.

Again let H be the Hilbert space $L^2(0, \infty)$. Let L be the operator d/dx with no boundary condition. If $\Re\lambda > 0$, then we can find always find a solution of the equation $(L - \lambda I)f = g$. This solution is

$$f(x) = -\int_x^\infty e^{\lambda(x-y)} g(y)\, dy. \tag{7.15}$$

This equation defines the bounded operator $(L - \lambda I)^{-1}$ that sends g into f, at least when $\Re\lambda > 0$. On the other hand, if $\Re\lambda < 0$, then we have point spectrum.

The relation between these two operators is $L_0^* = -L$. This corresponds to the fact that $(L_0 - \lambda I)^{-1*} = (-L - \bar{\lambda})^{-1}$, which is easy to check directly.

7.13 First order differential operators with an infinite interval: continuous spectrum

In this section we shall see an example of an operator with continuous spectrum. This is the example that underlies the theory of the Fourier transform.

Example: Let H be the Hilbert space $L^2(-\infty, \infty)$. Let L be the operator d/dx acting on functions f in H with derivatives f' in H.

If $\Re\lambda < 0$, then we can find always find a solution of the equation $(L-\lambda I)f = g$. This solution is

$$f(x) = \int_{-\infty}^{x} e^{\lambda(x-y)} g(y)\, dy. \tag{7.16}$$

This equation defines the bounded operator $(L - \lambda I)^{-1}$ that sends g into f, at least when $\Re\lambda < 0$. If $\Re\lambda > 0$, then we can find always find a solution of the equation $(L - \lambda I)f = g$. This solution is

$$f(x) = -\int_{x}^{\infty} e^{\lambda(x-y)} g(y)\, dy. \tag{7.17}$$

This equation defines the bounded operator $(L - \lambda I)^{-1}$ that sends g into f, at least when $\Re\lambda > 0$.

The operator L is skew-adjoint, that is, $L^* = -L$. This corresponds to the fact that $(L - \lambda I)^{-1*} = (-L - \bar{\lambda})^{-1}$, which is easy to check directly.

7.14 Problems

1. Let $H = L^2(0, 1)$. Let $L = -id/dx$ with periodic boundary conditions. Find an explicit formula for $(\lambda - L)^{-1}g$. Hint: Solve the first order ordinary differential equation $(\lambda - L)f = g$ with the boundary condition $f(0) = f(1)$.

2. Find the eigenvalues and eigenvectors of L. For each eigenvalue λ_n, find the residue P_n of $(\lambda - L)^{-1}$ at λ_n.

3. Find the explicit form of the formula $g = \sum_n P_n g$.

4. Let $H = L^2(-\infty, \infty)$. Let $L = -id/dx$. Let k be real and $\epsilon > 0$. Find an explicit formula for $(L - k - i\epsilon)^{-1}g$. Also, find an explicit formula for $(L - k + i\epsilon)^{-1}g$. Find the explicit form of the expression

$$\delta_\epsilon(L - k)g = \frac{1}{2\pi i}[(L - k - i\epsilon)^{-1} - (L - k + i\epsilon)^{-1}]g.$$

5. Find the explicit form of the formula

$$g = \int_{-\infty}^{\infty} \delta_\epsilon(L - k)g\, dk.$$

6. Let $\epsilon \to 0$. Find the explicit form of the formula

$$g = \int_{-\infty}^{\infty} \delta(L - k)g\, dk.$$

7.15 A pathological example

Consider $H = L^2(R)$ and fix g in H. Define K as the integral operator with kernel $k(x, y) = g(x)\delta(y)$. Consider the domain $D(K)$ to be the set of all continuous functions in H. Then

$$(Ku)(x) = g(x)f(0). \tag{7.18}$$

This K is densely defined but not closed. It has a closure $\bar{K}$, but this is not an operator. To see this, let $u_n \to u$ and $Ku_n = u_n(0)g \to v$. Then the pair $[u, v]$ is in the graph $\bar{K}$. But we can take $u_n \to 0$ in the Hilbert space sense, yet with each $u_n(0) = C$. So this gives the pair $[0, Cg]$ in the graph $\bar{K}$. This is certainly not an operator!

Consider the adjoint K^*. This is the integral operator with kernel $\delta(x)\overline{g(y)}$. That is,

$$(K^*w)(x) = \delta(x) \int_{-\infty}^{\infty} \overline{g(y)}w(y)\, dy. \tag{7.19}$$

Since

$$\int_{-\infty}^{\infty} \delta(x)^2\, dx = +\infty, \tag{7.20}$$

the $\delta(x)$ is not in L^2. Hence the domain of K^* consists of all w with $(g, w) = 0$, and $K^* = 0$ on this domain. This is an operator that is closed but not densely defined. According to the general theory, its adjoint is $K^{**} = \bar{K}$, which is not an operator.

Chapter 8

Normal operators

8.1 Spectrum of a normal operator

Theorem (von Neumann) Let L be a densely defined closed operator. Then L^*L and LL^* are each self-adjoint operators.

A densely defined closed operator is said to be normal if $L^*L = LL^*$.

There are three particularly important classes of normal operators.

1. A self-adjoint operator is an operator L with $L^* = L$.

2. A skew-adjoint operator is an operator L with $L^* = -L$.

3. A unitary operator is an operator L with $L^* = L^{-1}$. A unitary operator is bounded.

For a self-adjoint operator the spectrum is on the real axis. For a skew-adjoint operator the spectrum is on the imaginary axis. For a unitary operator the spectrum is on the unit circle.

For normal operators there is a different classification of spectrum. Let L be a normal operator acting in a Hilbert space H. The point spectrum consists of the eigenvalues of L. The corresponding eigenvectors span a closed subspace M_p of the Hilbert space. The spectrum of L in this space consists of either what we have previously called standard point spectrum or of what we have previously called pseudo-continuous spectrum. This kind of pseudo-continuous spectrum is not really continuous at all, since it consists of limits of point spectrum.

Let M_c be the orthogonal complement in H of M_p. Then the spectrum of L restricted to M_c is called the continuous spectrum of L. In our previous classification the spectrum of L in this space would be pseudo-continuous spectrum.

With this classification for normal operators the point spectrum and continuous spectrum can overlap. But they really have nothing to do with each other, since they take place in orthogonal subspaces.

Spectral theorem for compact normal operators. Let K be a compact normal operator. (This includes the cases of self-adjoint operators and skew-adjoint operators.) Then K has an orthogonal basis of eigenvectors. The non-zero

eigenvalues have finite multiplicity. The only possible accumulation point of eigenvalues is zero.

Spectral theorem for normal operators with compact resolvent. Let L be a normal operator with compact resolvent. (This includes the cases of self-adjoint operators and skew-adjoint operators.) Then L has an orthogonal basis of eigenvectors. The eigenvalues have finite multiplicity. The only possible accumulation point of eigenvalues is infinity.

8.2 Problems

1. Perhaps the most beautiful self-adjoint operator is the spherical Laplacian

$$\Delta_S = \frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\sin\theta\frac{\partial}{\partial\theta} + \frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\phi^2}.$$

   Show by explicit computation that this is a Hermitian operator acting on L^2 of the sphere with surface measure $\sin\theta\, d\theta\, d\phi$. Pay explicit attention to what happens at the north pole and south pole when one integrates by parts.

2. Let r be the radius satisfying $r^2 = x^2 + y^2 + z^2$. Let

$$L = r\frac{\partial}{\partial r}$$

   be the Euler operator. Show that the Laplace operator

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

   is related to L and Δ_S by

$$\Delta = \frac{1}{r^2}[L(L+1) + \Delta_S].$$

3. Let p be a polynomial in x, y, z that is harmonic and homogeneous of degree ℓ. Thus $\Delta p = 0$ and $Lp = \ell p$. Such a p is called a solid spherical harmonic. Show that each solid spherical harmonic is an eigenfunction of Δ_S and find the corresponding eigenvalue as a function of ℓ.

4. The restriction of a solid spherical harmonic to the sphere $r^2 = 1$ is called a surface spherical harmonic. The surface spherical harmonics are the eigenfunctions of Δ_S. Show that surface spherical harmonics for different values of ℓ are orthogonal in the Hilbert space of L^2 functions on the sphere.

5. The dimension of the eigenspace indexed by ℓ is $2\ell + 1$. For $\ell = 0$ the eigenspace is spanned by 1. For $\ell = 1$ it is spanned by z, $x + iy$, and $x - iy$. For $\ell = 2$ it is spanned by $3z^2 - r^2$, $z(x + iy)$, $z(x - iy)$, $(x + iy)^2$,

and $(x-iy)^2$. For $\ell = 3$ it is spanned by $5z^3 - 3zr^2$, $(5z^2 - r^2)(x+iy)$. $(5z^2 - r^2)(x-iy)$, $z(x+iy)^2$, $z(x-iy)^2$, $(x+iy)^3$, $(x-iy)^3$. Express the corresponding surface spherical harmonics in spherical coordinates.

6. In the case $\ell = 1$ we can write the general spherical harmonic as $ax+by+cz$. In the case $\ell = 2$ we can write it as $ax^2 + by^2 + cz^2 + dxy + eyz + fzx$ with an additional condition on the coefficients. What is this condition? In the case $\ell = 3$ we can write it as $a_1x^3 + b_1y^2x + c_1z^2x + a_2y^3 + b_2z^2y + c_2x^2y + a_3z^3 + b_3x^2z + c_3y^2z + dxyz$ with additional conditions. What are they?

8.3 Variation of parameters and Green's functions

First look at first order linear ordinary differential operators. Let $Lu = p(x)u' + r(x)u$. Let u_1 be a non-zero solution of the homogeneous equation $Lu = 0$. The general solution of the homogeneous equation $Lu = 0$ is $u(x) = c_1u_1(x)$, where c_1 is a parameter. The method of variation of parameters gives a solution of the inhomogeneous equation $Lu = f$ in the form $u(x) = c_1(x)u_1(x)$.

The condition on the parameter is given by plugging u into $Lu = f$. This gives $p(x)c_1'(x)u_1(x) = f(x)$. The solution is $c_1'(x) = f(x)/(p(x)u_1(x))$. The only difficult part is to integrate this to get the general solution

$$u(x) = \int_a^x \frac{u_1(x)}{p(y)u_1(y)} f(y)\,dy + Cu_1(x). \tag{8.1}$$

Now look at second order linear ordinary differential operators. Let $Lu = p(x)u'' + r(x)u' + q(x)u$. Let u_1 and u_2 be independent solutions of the homogeneous equation $Lu = 0$. The general solution of the homogeneous equation $Lu = 0$ is $u(x) = c_1u_1(x) + c_2u_2(x)$, where c_1 and c_2 are parameters. The method of variation of parameters gives a solution of the inhomogeneous equation $Lu = f$ in the form $u(x) = c_1(x)u_1(x) + c_2(x)u_2(x)$. Not only that, it has the property that the derivative has the same form, that is, $u'(x) = c_1(x)u_1'(x) + c_2(x)u_2'(x)$.

If this is to be so, then $c_1'(x)u_1(x) + c_2'(x)u_2(x) = 0$. This is the first equation. The second equation is given by plugging u into $Lu = f$. This gives $p(x)(c_1'u_1'(x) + c_2'(x)u_2'(x)) = f(x)$. This system of two linear equations is easily solved. Let $w(x) = u_1(x)u_2'(x) - u_2(x)u_1'(x)$. The solution is $c_1'(x) = -u_2(x)f(x)/(p(x)w(x))$ and $c_2'(x) = u_1(x)f(x)/(p(x)w(x))$.

A solution of $Lu = f$ is thus

$$u(x) = \int_x^b \frac{u_1(x)u_2(y)}{p(y)w(y)} f(y)\,dy + \int_a^x \frac{u_2(x)u_1(y)}{p(y)w(y)} f(y)\,dy. \tag{8.2}$$

Furthermore,

$$u'(x) = \int_x^b \frac{u_1'(x)u_2(y)}{p(y)w(y)} f(y)\,dy + \int_a^x \frac{u_2'(x)u_1(y)}{p(y)w(y)} f(y)\,dy. \tag{8.3}$$

Notice that $u(a) = Au_1(a)$ and $u'(a) = Au_1'(a)$, while $u(b) = Bu_2(b)$ and $u'(b) = Bu_2'(b)$. So this form of the solution is useful for specifying boundary conditions at a and b.

The general solution is obtained by adding an arbitrary linear combination $C_1u_1(x)+C_2u_2(x)$. However often we want a particular solution with boundary conditions at a and b. Then we use the form above. This can also be written

$$u(x) = (Kf)(x) = \int_a^b k(x,y)f(y)\,dy, \tag{8.4}$$

where

$$k(x,y) = \begin{cases} \frac{u_1(x)u_2(y)}{p(y)w(y)} & \text{if } x < y \\ \frac{u_2(x)u_1(y)}{p(y)w(y)} & \text{if } x > y \end{cases} \tag{8.5}$$

Sometime one thinks of y as a fixed source and write the equation

$$L_x k(x,y) = \delta(x-y). \tag{8.6}$$

Of course this is just another way of saying that $LK = I$.

8.4 Second order differential operators with a bounded interval: point spectrum

Example. Consider the self-adjoint differential operator $L_D = -d^2/dx^2$ on $L^2(0,1)$ with Dirichlet boundary conditions $f(0) = 0$ and $f(1) = 0$ at 0 and 1. Take the solutions $u_1(x) = \sin(\sqrt{\lambda}x)/\sqrt{\lambda}$ and $u_2(x) = \sin(\sqrt{\lambda}(1-x))/\sqrt{\lambda}$. These are defined in a way that does not depend on which square root of λ is taken. (Furthermore, they have obvious values in the limit $\lambda \to 0$.) Then $p(x) = -1$ and $w(x) = -\sin(\sqrt{\lambda})/\sqrt{\lambda}$. This also does not depend on the cut. The resolvent is thus $((L_D - \lambda)^{-1}g)(x) = f(x)$ where

$$f(x) = \frac{1}{\sqrt{\lambda}\sin(\sqrt{\lambda})}\left[\int_0^x \sin(\sqrt{\lambda}(1-x))\sin(\sqrt{\lambda}y)g(y)\,dy + \int_x^1 \sin(\sqrt{\lambda}x)\sin(\sqrt{\lambda}(1-y))g(y)\,dy\right]. \tag{8.7}$$

The spectrum consists of the points $\lambda = n^2\pi^2$ for $n = 1, 2, 3, \ldots$. This is standard point spectrum. It is amusing to work out the spectral projection at the eigenvalue $n^2\pi^2$. This is the negative of the residue and is explicitly

$$(P_n g)(x) = 2\int_0^1 \sin(n\pi x)\sin(n\pi y)g(y)\,dy. \tag{8.8}$$

Example. Consider the self-adjoint differential operator $L_N = -d^2/dx^2$ on $L^2(0,1)$ with Neumann boundary conditions $f'(0) = 0$ and $f'(1) = 0$ at 0 and 1. Take the solutions $u_1(x) = \cos(\sqrt{\lambda}x)$ and $u_2(x) = \cos(\sqrt{\lambda}(1-x))$. Then $p(x) = -1$ and $w(x) = \sqrt{\lambda}\sin(\sqrt{\lambda})$. This also does not depend on the cut. The

resolvent is thus

$$((L_N-\lambda)^{-1}g)(x) = -\frac{1}{\sqrt{\lambda}\sin(\sqrt{\lambda})}\left[\int_0^x \cos(\sqrt{\lambda}(1-x))\cos(\sqrt{\lambda}y)g(y)\,dy + \int_x^1 \cos(\sqrt{\lambda}x)\cos(\sqrt{\lambda}(1-y))g(y)\,dy\right]. \tag{8.9}$$

The spectrum consists of the points $\lambda = n^2\pi^2$ for $n = 0, 1, 2, 3, \ldots$. This is standard point spectrum. The spectral projection at the eigenvalue $n^2\pi^2$ for $n = 1, 2, 3, \ldots$ is

$$(P_n g)(x) = 2\int_0^1 \cos(n\pi x)\cos(n\pi y)g(y)\,dy. \tag{8.10}$$

For $n = 0$ it is

$$(P_0 g)(x) = \int_0^1 g(y)\,dy. \tag{8.11}$$

It is interesting to compute the reduced resolvent of L_N at the eigenvalue 0. Thus we must compute $(L_N - \lambda)^{-1}\bar{g}$, where $\bar{g} = (1-P)g$ has zero average, and then let λ approach zero. This is easy. Expand the cosine functions to second order. The constant terms may be neglected, since they are orthogonal to $\bar{g}$. This gives

$$(S_0\bar{g})(x) = \int_0^x (\frac{1}{2}(1-x)^2 + \frac{1}{2}y^2)\bar{g}(y)\,dy + \int_x^1 (\frac{1}{2}x^2 + \frac{1}{2}(1-y)^2)\bar{g}(y)\,dy. \tag{8.12}$$

From this it is easy to work out that

$$(S_0 g)(x) = \int_0^x (\frac{1}{2}(1-x)^2 + \frac{1}{2}y^2 - \frac{1}{6})g(y)\,dy + \int_x^1 (\frac{1}{2}x^2 + \frac{1}{2}(1-y)^2 - \frac{1}{6})g(y)\,dy. \tag{8.13}$$

8.5 Second order differential operators with a semibounded interval: continuous spectrum

Example. Consider the self-adjoint differential operator $L_D = -d^2/dx^2$ on $L^2(0,\infty)$ with Dirichlet boundary condition $f(0) = 0$ at 0. Take the solutions $u_1(x) = \sinh(\sqrt{-\lambda}x)/\sqrt{-\lambda}$ and $u_2(x) = e^{-\sqrt{-\lambda}x}$. Since $\sinh(iz) = i\sin(z)$, this is the same $u_1(x)$ as before. In $u_2(x)$ the square root is taken to be cut on the negative axis. Then $p(x) = -1$ and $w(x) = -1$. The resolvent is

$$((L_D-\lambda)^{-1}g)(x) = \frac{1}{\sqrt{-\lambda}}\left[\int_0^x e^{-\sqrt{-\lambda}x}\sinh(\sqrt{-\lambda}y)g(y)\,dy + \int_x^\infty \sinh(\sqrt{-\lambda}x)e^{-\sqrt{-\lambda}y}g(y)\,dy\right]. \tag{8.14}$$

The spectrum consists of the positive real axis and is continuous.

It is instructive to compute the resolvent of the self-adjoint differential operator $L_N = -d^2/dx^2$ on $L^2(0,\infty)$ with Neumann boundary condition $f'(0) = 0$ at 0. Again the spectrum consists of the positive real axis and is continuous.

8.6 Second order differential operators with an infinite interval: continuous spectrum

Example. Consider the self-adjoint differential operator $L = -d^2/dx^2$ on $L^2(-\infty, \infty)$. There is now no choice of boundary conditions. The resolvent is

$$((L-\lambda)^{-1}g)(x) = \frac{1}{2\sqrt{-\lambda}}\left[\int_{-\infty}^{x} e^{-\sqrt{-\lambda}x}e^{\sqrt{-\lambda}y}g(y)\,dy + \int_{x}^{\infty} e^{\sqrt{-\lambda}x}e^{-\sqrt{-\lambda}y}g(y)\,dy\right]. \tag{8.15}$$

This can also be written in the form

$$((L-\lambda)^{-1}g)(x) = \frac{1}{2\sqrt{-\lambda}}\int_{-\infty}^{\infty} e^{-\sqrt{-\lambda}|x-y|}g(y)\,dy. \tag{8.16}$$

The spectrum consists of the positive real axis and is continuous.

8.7 The spectral theorem for normal operators

Throughout the discussion we make the convention that the inner product is conjugate linear in the first variable and linear in the second variable.

The great theorem of spectral theory is the following.

Let H be a Hilbert space. Let L be a normal operator. Then there exists a set K (which may be taken to be a disjoint union of copies of the line) and a measure μ on K and a unitary operator $U : H \to L^2(K, \mu)$ and a complex function λ on K such that

$$(ULf)(k) = \lambda(k)(Uf)(k). \tag{8.17}$$

Thus if we write Λ for the operator of multiplication by the function λ, we get the representation

$$L = U^*\Lambda U. \tag{8.18}$$

The theorem is a generalization of the theorem on diagonalization of normal matrices. If the measure μ is discrete, then the norm in the space $L^2(\mu)$ is given by $\|g\|^2 = \sum_k |g(k)|^2\mu(\{k\})$. The λ_k are the eigenvalues of L. The equation then says

$$(ULf)_k = \lambda_k(Uf)_k. \tag{8.19}$$

The unitary operator U is given by

$$(Uf)_k = (\psi_k, f), \tag{8.20}$$

where the ψ_k are eigenvectors of L normalized so that $\mu(\{k\}) = 1/(\psi_k, \psi_k)$. The inverse of U is given by

$$U^*g = \sum_k g_k\psi_k\,\mu(\{k\}). \tag{8.21}$$

The equation

$$Lf = U^*\Lambda U f \tag{8.22}$$

says explicitly that

$$Lf = \sum_k \lambda_k(\psi_k, f)\psi_k\, \mu(\{k\}). \tag{8.23}$$

If the measure μ is continuous, then the norm in the space $L^2(K, \mu)$ is given by $\|g\|^2 = \int |g(k)|^2\, d\mu(k)$. Then $\lambda(k)$is a function of the continuous parameter k. The equation then says

$$(ULf)(k) = \lambda(k)(Uf)(k). \tag{8.24}$$

In quite general contexts the unitary operator U is given by

$$(Uf)(k) = (\psi_k, f), \tag{8.25}$$

but now this equation only makes sense for a dense set of f in the Hilbert space, and the ψ_k resemble eigenvectors of L, but do not belong to the Hilbert space, but instead to some larger space, such as a space of slowly growing functions or of mildly singular distributions. The inverse of U is given formally by

$$U^*g = \int g(k)\psi_k\, d\mu(k), \tag{8.26}$$

but this equation must be interpreted in some weak sense. The equation

$$Lf = U^*\Lambda U f \tag{8.27}$$

says formally that

$$Lf = \int \lambda(k)(\psi_k, f)\psi_k\, d\mu(k). \tag{8.28}$$

Since the eigenvectors ψ_k are not in the Hilbert space, it is convenient in many contexts to forget about them and instead refer to the measure μ and the function λ and to the operators U and U^*. The theorem says simply that every normal operator L is isomorphic to multiplication by a function λ. The simplicity and power of the equation $L = U^*\Lambda U$ cannot be overestimated.

The spectral theorem for normal operators says that every normal operator is isomorphic (by a unitary operator mapping the Hilbert space to an L^2 space) to a multiplication operator (multiplication by some complex valued function λ). The spectrum is the essential range of the function. This is the set of points ω such that for each $\epsilon > 0$ the set of all points k such that $\lambda(k)$ is within ϵ of w has measure > 0. This is obvious; a function $\lambda(k)$ has $1/(\lambda(k) - w)$ bounded if and only if w is not in the essential range of $\lambda(k)$.

8.8 Examples: compact normal operators

The theorem on compact normal operators is a corollary of the general spectral theorem. Consider a compact normal operator L. Say that it is isomorphic to multiplication by λ. Fix $\epsilon > 0$ and look at the part of the space where $|L| \geq \epsilon$. This is just the part of the space that is isomorphic to the part of L^2 where $|\lambda| \geq \epsilon$. More explicitly, this is the subspace consisting of all functions g in L^2 such that $g(k) \neq 0$ only where $|\lambda(k)| \geq \epsilon$. On this part of the space the operator L maps the unit ball onto a set that contains the ball of radius ϵ. Since L is compact, it follows that this part of the space is finite dimensional. This shows that the spectrum in the subspace where $|L| \geq \epsilon$ is finite dimensional. Therefore there are only finitely many eigenvectors of finite multiplicity in this space. Since $\epsilon > 0$ is arbitrary, it follows that there are only countably many isolated eigenvectors of finite multiplicity in the part of the space where $|L| > 0$. In the part of the space where $L = 0$ we can have an eigenvalue 0 of arbitrary multiplicity (zero, finite, or infinite).

8.9 Examples: translation invariant operators and the Fourier transform

The nicest examples for the continuous case are given by translation invariant operators acting in $H = L^2(R, dx)$. In this case the Fourier transform maps H into $L^2(R, dk/(2\pi))$. The Fourier transform is given formally by

$$(Ff)(k) = (\psi_k, f) = \int_{-\infty}^{\infty} e^{-ikx} f(x)\, dx. \tag{8.29}$$

Here $\psi_k(x) = e^{ikx}$, and we are using the convention that the inner product is linear in the second variable. The inverse Fourier transform is

$$(F^{-1}g)(x) = \int_{-\infty}^{\infty} e^{ikx} g(k)\, \frac{dk}{2\pi}. \tag{8.30}$$

Here are some examples:

Example 1: Translation. Let U_a be defined by

$$(T_a f)(x) = f(x - a). \tag{8.31}$$

Then T_a is unitary. The spectral representation is given by the Fourier transform. In fact

$$(FT_a f)(k) = \exp(-ika)(Ff)(k). \tag{8.32}$$

Example 2: Convolution. Let C be defined by

$$(Cf)(x) = \int_{-\infty}^{\infty} c(x - y) f(y)\, dy = \int_{-\infty}^{\infty} c(a) f(x - a)\, da, \tag{8.33}$$

where c is an integrable function. Then C is bounded normal. Then by integrating the first example we get

$$(FCf)(k) = \hat{c}(k)(Ff)(k), \tag{8.34}$$

where $\hat{c}$ is the Fourier transform of c.

Example 3: Differentiation. Let D be defined by

$$(Df)(x) = \frac{df(x)}{dx}. \tag{8.35}$$

Then D is skew-adjoint. Furthermore, we get

$$(FDf)(k) = ik(Ff)(k). \tag{8.36}$$

Notice that the unitary operator in Example 1 may be written

$$U_a = \exp(-aD). \tag{8.37}$$

Example 4. Second differentiation. Let D^2 be defined by

$$(D^2f)(x) = \frac{d^2f(x)}{dx^2}. \tag{8.38}$$

Then D is self-adjoint. Furthermore, we get

$$(FDf)(k) = -k^2(Ff)(k). \tag{8.39}$$

We can take interesting functions of these operator. For instance $(-D^2 + m^2)^{-1}$ is convolution by $1/(2m)e^{-m|x|}$. And $\exp(tD^2)$ is convolution by $1/\sqrt{2\pi t}e^{\frac{-x^2}{2t}}$.

8.10 Examples: Schrödinger operators

If $V(x)$ is a real locally integrable function that is bounded below, then

$$H = -D^2 + V(x) \tag{8.40}$$

is a well-defined self-adjoint operator. Such an operator is called a Schrödinger operator.

If $V(x) \to \infty$ as $|x| \to \infty$, then the spectrum of H is point spectrum. Finding the eigenvalues is a challenge. One case where it is possible to obtain explicit formulas is when $V(x)$ is a quadratic function.

Also there is an interesting limiting case. If $V(x) = 0$ for $0 < x < 1$ and $V(x) = +\infty$ elsewhere, then we may think of this as the operator $H = -D^2$ with Dirichlet boundary conditions at the end points of the unit interval. We know how to find the spectrum in this case.

If on the other hand, $V(x)$ is integrable on the line, then the spectrum of H consists of positive continuous spectrum and possibly some strictly negative eigenvalues. A nice example of this is the square well, where there is a constant

$a > 0$ with $V(x) = -a$ for $0 < x < 1$ and $V(x) = 0$ otherwise. This is another case where computations are possible.

The calculation of the spectral properties of Schrödinger operators is the main task of quantum physics. However we shall see that Schrödinger operators play a role in other contexts as well. (One example will be in calculus of variations.)

8.11 Subnormal operators

The spectral theorem for normal operators is a landmark. However not every operator is normal. One important class of operators with fascinating spectral properties consists of the subnormal operators. A subnormal operator is an operator that is the restriction of a normal operator to an invariant subspace. First consider the case of bounded operators. An operator $S : H \to H$ is subnormal if there exists a larger Hilbert space H' with $H \subset H'$ as a closed subspace, a normal operator $N : H' \to H'$ that leaves H invariant, and such that N restricted to H is S.

Example: Let $H = L^2([0, \infty), dt)$. For each $a \geq 0$ define

$$(S_a f)(t) = f(t - a) \tag{8.41}$$

for $a \leq t$ and

$$(S_a f)(t) = 0 \tag{8.42}$$

for $0 \leq t < a$. Then S_a is subnormal.

To see this, consider the bigger space $H' = L^2(R, dt)$ and consider H as the subspace of functions that vanish except on the positive reals. Let U_a be translation by a on H'. If $a \geq 0$, then the subspace H is left invariant by U_a. Then S_a is U_a acting in this subspace.

It follows from the spectral theorem that a subnormal operator S is isomorphic by a unitary operator $U : H \to M$ to a multiplication operator that sends $g(k)$ to $\lambda(k)g(k)$. Here M is a closed subspace of an L^2 space. For each f in H we have Uf in M and $USf(k) = \lambda(k)(Uf)(k)$ in M.

Now it is more difficult to characterize the spectrum. A number w is in the resolvent set if $1/(\lambda(k) - w)g(k)$ is in M for every function $g(k)$ in M. However it is not sufficient that this is a bounded function. If, for instance, every function $g(k)$ in M has an extension to an analytic function $g(z)$ defined on some larger region, then one would want $1/(\lambda(z) - w)g(z)$ to also be an analytic function in this region. So we need to require also that w is not in the range of the extension $\lambda(z)$.

Example: Let F be the Fourier transform applied to the Hilbert space H of L^2 functions that vanish except on the positive axis. Then the image of this transform consists of the subspace M of L^2 functions $g(k)$ that are boundary values of analytic functions $g(z)$ in the lower half plane. The operator S_a for $a > 0$ is isomorphic to multiplication by $\lambda(k) = \exp(-iak)$ acting in this subspace. This function extends to a function $\lambda(z) = \exp(-iaz)$ defined in the lower half

plane. So the spectrum is the range of this function. But the image of $\Im z \le 0$ under $\exp(-iaz)$ is the unit circle $|w| \le 1$. So this is the spectrum.

The adjoint of a subnormal operator $S : H \to H$ is another operator $S^* : H \to H$. The adjoint S^* need not be subnormal.

Lemma. If $N : H' \to H'$ is normal, $H \subset H'$, and $S : H \to H$ is the restriction of N to H, then $S^* : H \to H$ is given by $S^* = PN^*$, where P is the orthogonal projection of H' onto H.

Proof: If u is in H, for each v in H we have

$$(S^*u, v) = (u, Sv) = (u, Nv) = (N^*u, v). \tag{8.43}$$

This says that $N^*u - S^*u$ is orthogonal to every v in H. Since S^*u is in H, this implies that S^*u is the orthogonal projection of N^*u onto H.

Theorem. If S is a subnormal operator, then $SS^* \le S^*S$ as quadratic forms, that is, $(u, SS^*u) \le (u, S^*Su)$ for all u in H.

Proof: First note that for u in H' we have

$$(N^*u, N^*u) = (u, NN^*u) = (u, N^*Nu) = (Nu, Nu). \tag{8.44}$$

Then for u in H we have

$$(S^*u, S^*u) = (PN^*u, PN^*u) \le (N^*u, N^*u) = (Nu, Nu) = (Su, Su). \tag{8.45}$$

Corollary. If S is a subnormal operator and $Su = 0$, then $S^*u = 0$. Thus the null space of S is contained in the null space of S^*.

Corollary. If S is a subnormal operator and $Su = \lambda u$, then $S^*u = \bar{\lambda}u$. Thus every eigenvector of S is an eigenvector of S^*.

It is not true that every eigenvalue of S^* is an eigenvalue of S. It is more typical that S^* has eigenvalues while S does not. In fact we shall see examples in which S^* has anomalous point spectrum, while S has residual spectrum.

Theorem. If the Hilbert space is finite dimensional, then every subnormal operator is normal.

Proof: Let S be a subnormal operator acting in H. Since the space H is finite dimensional, S has an eigenvector u in H with $Su = \lambda u$. Since S is subnormal, it follows that $S^*u = \bar{\lambda}u$. Let v be a vector in H that is orthogonal to u. Then $(Sv, u) = (v, S^*u) = \bar{\lambda}(v, u) = 0$. Thus the orthogonal complement of u in H is also an invariant space, so the operator S restricted to this smaller space is also subnormal. Continue in this way until one finds an orthogonal basis of eigenvectors for S.

There are examples in which one might want to consider unbounded subnormal operators. One possible definition might be the following. Consider an unbounded normal operator N. Thus there is a dense domain $D(N) \subset H'$ such that $N : D(N) \to H'$ is normal. Let H be a Hilbert space that is a closed subspace of H'. Suppose that $D(N) \cap H$ is dense in H and that N sends vectors in this dense subspace into H. Then if $D(S) = D(N) \cap H$ and S is the restriction of N to $D(S)$, the operator S is subnormal. Then $D(S)$ is dense in H, and $S : D(S) \to H$ is a closed, densely defined operator.

Example: Let $H = L^2([0,\infty), dt)$. Define

$$(Sf)(t) = f'(t) \tag{8.46}$$

on the domain consisting of all f in H such that f' is also in H and $f(0) = 0$. Then S is subnormal.

To see this, consider the bigger space $H' = L^2(R, dt)$ and consider H as the subspace of functions that vanish except on the positive reals. Let N be differentiation on H'. Notice that if f is in $D(N)$ and is also in H, then $f(0) = 0$ automatically.

If N is a normal operator acting in H', so $N : D(N) \to H'$, then its adjoint N^* is also a normal operator, and in fact $D(N^*) = D(N)$. So if $S : D(S) \to H$ is subnormal, then $D(S) = D(N) \cap H = D(N^*) \cap H$. Furthermore, if u is in $D(N^*) \cap H$, then u is in $D(S^*)$ and $S^*u = PN^*u$. This can be seen from the computation $(u, Sv) = (u, Nv) = (N^*u, v)$ for all v in $D(S)$.

We conclude that for a subnormal operator $D(S) \subset D(S^*)$ and $(S^*, S^*u) \leq (Su, Su)$ for all u in $D(S)$. This is also an easy computation: $(S^*u, S^*u) = (PN^*u, PN^*u) \leq (N^*u, N^*u) = (Nu, Nu) = (Su, Su)$.

Example: For the operator S in the last example we have

$$(S^*f)(t) = -f'(t) \tag{8.47}$$

on the domain consisting of all f in H such that f' is also in H. There is no boundary condition at zero. This is a case where $D(S) \subset D(S^*)$ and the two domains are not equal.

8.12 Examples: forward translation invariant operators and the Laplace transform

The example in the last section is the operator theory context for the theory of the Laplace transform.

The Laplace transform of a function f in $L^2([0,\infty), dt)$ is

$$(Lf)(z) = \int_0^\infty e^{-zt} f(t)\, dt. \tag{8.48}$$

If we think of $z = i\omega$ on the imaginary axis, then when regarded as a function of ω this is the Fourier transform . However it extends as an analytic function to ω in the lower half plane, that is, to z in the right half plane.

Let $a \geq 0$ and let S_a be the operator of right translation filling in with zero as defined in the previous section. Then

$$(LS_a f)(z) = \int_a^\infty e^{-zt} f(t-a)\, dt = e^{-az}(Lf)(z). \tag{8.49}$$

So S_a is isomorphic to multiplication by e^{-az} acting on the Hilbert space of functions analytic in the right half plane. Its spectrum consists of the closed unit disk.

Let c be an integrable function defined on the positive axis, and let the causal convolution C be defined by

$$(Cf)(t) = \int_0^t c(t-u)f(u)\,du = \int_0^t c(a)f(t-a)\,da. \tag{8.50}$$

Then C is subnormal, and

$$(LCf)(z) = \hat{c}(z)(Lf)(z), \tag{8.51}$$

where $\hat{c}$ is the Laplace transform of c.

Let $D_0 = d/dt$ be differentiation with zero boundary conditions at the origin. Then

$$(LD_0f)(z) = z(Lf)(z). \tag{8.52}$$

Notice that the boundary condition is essential for integration by parts. The spectrum of D_0 consists of the closed right half plane. We can write $\exp(-aD_0) = S_a$ for $a \geq 0$. This operator satisfies the differential equation $dS_af/da = -D_0S_af$ for $a \geq 0$, provided that f is in the domain of D_0 (and in particular satisfies the boundary condition).

The adjoint of a subnormal operator need not be subnormal. Thus, for instance, the adjoint of S_a is

$$(S_a^*f)(t) = f(t+a). \tag{8.53}$$

Its spectrum is also the closed unit disc, but the interior of the disk consists of point spectrum. Notice that the Laplace transform does not send this into a multiplication operator. In fact,

$$(LS_a^*f)(z) = \int_0^\infty e^{-zt}f(t+a)\,dt = e^{az}\left[(Lf)(z) - \int_0^a e^{-zt}f(t)\,dt\right]. \tag{8.54}$$

Similarly, the adjoint of D_0 is $-D$, where $D = d/dt$ with no boundary condition. Again the Laplace transform does not make this into a multiplication operator. In fact, we have

$$(LDf)(z) = z(Lf)(z) - f(0). \tag{8.55}$$

The spectrum of D consists of the closed left half plane. The interior consists of point spectrum. We can write $\exp(aD) = \exp(-aD_0^*) = S_a^*$ for $a \geq 0$. Even though D does not have a spectral representation as a multiplication operator, this operator satisfies the differential equation $dS_a^*f/da = DS_a^*f$ for $a \geq 0$, provided f is in the domain of D.

Example: Solve the differential equation $(D+k)f = g$, with $k > 0$, with boundary condition $f(0) = c$. The operator $D + k$ is not invertible, since $-k$ is an eigenvalue of D. However we can write $f = u - ce^{-kt}$ and solve

$$(D_0 + k)u = g. \tag{8.56}$$

The solution is $u = (D_0 + k)^{-1} g$. In terms of Laplace transforms this is $\hat{u}(z) = 1/(z+k)\hat{g}(z)$. It follows that u is given by the causal convolution

$$u(t) = \int_0^t e^{-k(t-u)} g(u)\, du. \tag{8.57}$$

Thus

$$f(t) = f(0)e^{-kt} + \int_0^t e^{-k(t-u)} g(u)\, du. \tag{8.58}$$

8.13 Quantum mechanics

Here is a dictionary of the basic concepts. Fix a Hilbert space. A *quantum observable* is a self-adjoint operator L. A *quantum state* is a unit vector u. The *expectation* of the observable L in the state u in $D(L)$ is

$$\mu = (u, Lu). \tag{8.59}$$

The *variance* of the observable L in the state u in $D(L)$ is

$$\sigma^2 = \|(L - \mu I)u\|^2. \tag{8.60}$$

Here are some observables. The Hilbert space is $L^2(R, dx)$. The *momentum observable* is $p = -i\hbar d/dx$. Here $\hbar > 0$ is Planck's constant. The *position observable* is q which is multiplication by the coordinate x. The *Heisenberg uncertainty principle* says that for every state the product $\sigma_p \sigma_q \geq \hbar/2$.

If L is an observable and f is a real function, then $f(L)$ is an observable. Take the case where the function is 1_A, the indicator function of a set A of position coordinate values. Then $1_A(q)$ has expectation

$$(u, 1_A(q)u) = \int_A |u(x)|^2\, dx. \tag{8.61}$$

This is the probability that the position is in A. Similarly, take the case where the function is 1_B, the indicator function of a set B of momentum coordinate values. Since in the Fourier transform representation p is represented by multiplication by $\hbar k$, it follows that $1_B(p)$ has expectation

$$(u, 1_B(p)u) = \int_{\{k \mid \hbar k \in B\}} |\hat{u}(k)|^2 \, \frac{dk}{2\pi}. \tag{8.62}$$

This is the probability that the momentum is in B.

Energy observables are particularly important. The *kinetic energy observable* is $H_0 = p^2/(2m) = -\hbar^2/(2m)d^2/dx^2$. Here $m > 0$ is the mass. The spectrum of H_0 is the positive real axis. The *potential energy observable* is $V = v(q)$ which is multiplication by $v(x)$. Here v is a given real function that represents potential energy as a function of the space coordinate. The spectrum of V is the range of the function v. The *total energy observable* or *quantum Hamiltonian* is

$$H = H_0 + V = \frac{p^2}{2m} + v(q) = -\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + v(x). \tag{8.63}$$

If we assume that the function v is bounded, then H is a self-adjoint operator. (In many cases when v is only bounded below it remains a self-adjoint operator.) The problem of investigating its spectrum is of the utmost importance for quantum mechanics. Since H_0 and V do not commute, this is not an easy problem.

Suppose that the total energy observable H is a self-adjoint operator. Then the *time evolution operator* is the unitary operator $\exp(-itH/\hbar)$. A central problem of quantum mechanics is to compute this operator. This is not easy, because while $\exp(-itH_0/\hbar)$ and $\exp(-itV/\hbar)$ are easy to compute, the operators H_0 and V do not commute. So there is no direct algebraic way to express $\exp(-itH/\hbar)$ in terms of the simpler operators. Nevertheless, we shall encounter a beautiful formula for this time evolution operator in the next chapter.

8.14 Problems

1. A particularly fascinating self-adjoint operator is the quantum harmonic oscillator. (This operator also occurs in disguised form in other contexts.) It is
$$N = \frac{1}{2}\left(-\frac{d^2}{dx^2} + x^2 - 1\right)$$
acting in $L^2(-\infty, \infty)$. Show that it factors as
$$N = A^*A,$$
where
$$A = \frac{1}{\sqrt{2}}\left(x + \frac{d}{dx}\right)$$
and
$$A^* = \frac{1}{\sqrt{2}}\left(x - \frac{d}{dx}\right).$$

2. Show that $AA^* = A^*A + I$.

3. Solve the equation $Au_0 = 0$. Show that $Nu_0 = 0$.

4. Show that if $Nu_n = nu_n$ and $u_{n+1} = A^*u_n$, then $Nu_{n+1} = (n+1)u_{n+1}$. Thus the eigenvalues of N are the natural numbers. These are the standard type of point spectrum.

5. Show that each eigenfunction u_n is a polynomial in x times $u_0(x)$. Find the polynomials for the cases of $n = 0, 1, 2, 3$ explicitly (up to constant factors). Verify that each u_n belongs to the Hilbert space.

6. It may be shown that A^* is a subnormal operator and so A is the adjoint of a subnormal operator. Find all eigenvalues (point spectrum) of A. Find each corresponding eigenvector. Verify that it belongs to the Hilbert space.

7. Find all eigenvalues (point spectrum) of A^*. Find the spectrum of A^*. What kind of spectrum is it?

8. If A^* is indeed a subnormal operator, then we should have $A^*A \leq AA^*$ as quadratic forms. Is this the case?

Chapter 9

Calculus of Variations

9.1 The Euler-Lagrange equation

The problem is to find the critical points of

$$F(y) = \int_{x_1}^{x_2} f(y, y_x, x)\, dx. \tag{9.1}$$

The differential of F is

$$dF(y)h = \int_{x_1}^{x_2} (f_y h + f_{y_x} h_x)\, dx = \int_{x_1}^{x_2} (f_y - \frac{d}{dx} f_{y_x}) h\, dx + f_{y_x} h \mid_{x_1}^{x_2} . \tag{9.2}$$

Thus for the differential to be zero we must have the Euler-Lagrange equation

$$f_y - \frac{d}{dx} f_{y_x} = 0. \tag{9.3}$$

This is an equation for the critical function y. It is second order, and it has the explicit form

$$f_y - f_{y y_x} \frac{dy}{dx} - f_{y_x y_x} \frac{d^2 y}{dx^2} - f_{x y_x} = 0. \tag{9.4}$$

This equation is linear in d^2y/dx^2. However the coefficients are in general nonlinear expressions in y, dy/dx, and x.

If the y are required to have fixed values $y = y_1$ at $x = x_1$ and $y = y_2$ at $x = x_2$ at the end points, then the h are required to be zero at the end points. The corresponding boundary term is automatically zero.

If the y and h are free to vary at an end point, then at a critical point one must have $f_{y_x} = 0$ at at the end points.

Sometimes one wants to think of

$$\frac{\delta F}{\delta y(x)} = \frac{\partial f}{\partial y} - \frac{d}{dx} \frac{\partial f}{\partial y_x} \tag{9.5}$$

as the gradient of F, where the inner product is given by the integral. This expression is then known as the variational derivative. The Euler-Lagrange equation then says that the variational derivative is zero.

Example. Consider the problem of minimizing the length

$$F(y) = \int_{x_1}^{x_2} \sqrt{1 + y_x^2}\, dx \tag{9.6}$$

between the points (x_1, y_1) and (x_2, y_2). The boundary condition are $y(x_1) = y_1$ and $y(x_2) = y_2$. The solution of the Euler-Lagrange equation is $y_x = C$, a curve of constant slope. So the solution is $y - y_1 = m(x - x_1)$, where $m = (y_2 - y_1)/(x_2 - x_1)$.

Example. Consider the problem of minimizing the length

$$F(y) = \int_{x_1}^{x_2} \sqrt{1 + y_x^2}\, dx \tag{9.7}$$

between the lines $x = x_1$ and $x = x_2$. The boundary conditions for the Euler-Lagrange equation are $y_x(x_1) = 0$ and $y_x(x_2) = 0$. The solution of the Euler-Lagrange equation is $y_x = C$, a curve of constant slope. But to satisfy the boundary conditions $C = 0$. So the solution is $y = A$, where A is a arbitrary constant.

9.2 A conservation law

Say that one has a solution of the Euler-Lagrange equation. Then

$$\frac{d}{dx} f = f_y y_x + f_{y_x} y_{xx} + f_x = \frac{d}{dx}(y_x f_{y_x}) + f_x. \tag{9.8}$$

Thus

$$\frac{d}{dx} H + f_x = 0, \tag{9.9}$$

where

$$H = y_x f_{y_x} - f. \tag{9.10}$$

If $f_x = 0$, then this says that H is constant. This is the conservation law. It is a nonlinear equation for y and dy/dx. It takes the explicit form

$$y_x f_{y_x} - f = C. \tag{9.11}$$

Thus it is first order, but in general fully nonlinear in y_x. How in practice does one solve a problem in calculus of variations? There is a way when the function $f(y, y_x)$ does not depend on x. Use the conservation law $H(y, dy/dx) = C$ to solve for $dy/dx = \alpha(y)$. Perhaps this equation can be solved directly. Or write $dx = dy/\alpha(y)$. Integrate both sides to get x in terms of y. Or make a substitution expressing y in terms of a new variable u, and get x and y each in terms of u.

Example 1: This example comes from minimizing the area of a surface of revolution. The unknown is a function y of x between $-a$ and a. The value of y at $\pm a$ is r. The element of area is proportional to $2\pi y\,ds = 2\pi y\sqrt{1+y_x^2}\,dx$. Let $f(y, y_x) = 2\pi y\sqrt{1+y_x^2}$. Then $H = -2\pi y/\sqrt{1+y_x^2} = -C$. The differential equation to be solved is $(dy/dx)^2 = (k^2y^2 - 1)$, where $k = 2\pi/C$. This has solution $y = (1/k)\cosh(k(x - x_0))$. By symmetry $x_0 = 0$. So we need to solve $rk = \cosh(ak)$. This equation has to be solved for k. Fix r and vary a. When a is small enough, then $\cosh(ak)$ cuts the line rk in two points. Thus there are two solutions of the Euler-Lagrange equations, corresponding to $y = (1/k)\cosh(kx)$ with the two values of k. The derivative is $dy/dx = \sinh(kx)$. The smaller value of k gives the smaller derivative, so this is the minimum area surface satisfying the boundary conditions.

Example 2: This example comes up finding the maximum area for given arc length. For simplicity consider y as a function of x between $-a$ and a, with value 0 at the two end points. For simplicity let the arc length κ satisfy $2a < \kappa < \pi a$. The area is the integral from $-a$ to a of $y\,dx$, while the length is the integral from $-a$ to a of $ds = \sqrt{1+y_x^2}\,dx$. This is a Lagrange multiplier problem. The function is $f(y, y_x) = y - \lambda\sqrt{1+y_x^2}$. The conserved quantity is $H = -\lambda 1/\sqrt{1+y_x^2} - y = -c_1$. The differential equation is $dx/dy = (y - c_1)/\sqrt{(\lambda^2 - (y-c_1)^2}$. Thus $x - c_2 = \sqrt{\lambda^2 - (y-c_1)^2}$, which is the equation of a circle $(x-c_2)^2 + (y-c_1)^2 = \lambda^2$. The Lagrange multiplier turns out to be the radius of the circle. By symmetry $c_2 = 0$. Furthermore $c_1 = -\sqrt{\lambda^2 - a^2}$. If we let $\sin(\theta) = a/\lambda$, then the equation $\sin(\theta) < \theta < (\pi/2)\sin(\theta)$ translates into $2a < \kappa = 2\lambda\theta < \pi a$.

9.3 Second variation

Say that y is a solution of the Euler-Lagrange equation that has fixed values at the end points. Then the second differential of F is obtained by expanding $F(y+h) = F(y) + dF(y)h + \frac{1}{2}d^2F(y)(h,h) + \cdots$. The result is

$$d^2F(y)(h,h) = \int_{x_1}^{x_2} (f_{yy}h^2 + 2f_{yy_x}hh_x + f_{y_xy_x}h_x^2)\,dx. \tag{9.12}$$

The functions h have value 0 at the end points, so we may freely integrate by parts. The result may thus also be written

$$d^2F(y)(h,h) = \int_{x_1}^{x_2} ((f_{yy} - \frac{d}{dx}f_{yy_x})h^2 + f_{y_xy_x}h_x^2)\,dx. \tag{9.13}$$

Yet another form is

$$d^2F(y)(h,h) = \int_{x_1}^{x_2} [-\frac{d}{dx}(f_{y_xy_x}h_x) + (f_{yy} - \frac{d}{dx}f_{yy_x})h]h\,dx = (Lh, h). \tag{9.14}$$

We recognize

$$Lh = -\frac{d}{dx}(f_{y_xy_x}h_x) + (f_{yy} - \frac{d}{dx}f_{yy_x})h \tag{9.15}$$

as a Sturm-Liouville operator. In fact, if $f(y, y_x, x) = \frac{1}{2}y_x^2 + g(y, x)$, then

$$Lh = -h_{xx} + g_{yy}h \tag{9.16}$$

is a Schrödinger operator. The coefficient g_{yy} has the solution of the Euler-Lagrange inserted, so it is regarded as a function of x. The operator has Dirichlet boundary conditions at the end points of the interval from x_1 to x_2.

9.4 Interlude: The Legendre transform

The Legendre transform of a function L of v is defined as follows. Let $p = dL/dv$. Find the inverse function defining v as a function of p. Then the Legendre transform is a function H of p satisfying $dH/dp = v$. The constant of integration is chosen so that $H(0) + L(0) = 0$.

Example: Let $L = e^v - v - 1$. Then the derivative is $p = e^v - 1$. The inverse function is $v = \log(1 + p)$. The integral is $H = (1 + p)\log(1 + p) - p$.

There is a remarkable formula relating the Legendre transform of a function to the original function. Let L be a function of v. Define

$$p = \frac{dL}{dv}. \tag{9.17}$$

Then

$$H = pv - L. \tag{9.18}$$

is the Legendre transform of L. In the following we want to think of L as a function of the v, while H is a function of the dual variable p. The variable p is covariant and is dual to the variable v, which is contravariant. Thus in this formula v is defined in terms of p by solving the equation $p = dL/dv$ for v.

The fundamental theorem about the Legendre transform is

$$v = \frac{dH}{dp}. \tag{9.19}$$

Proof: Let $H = pv - L$ as above By the product rule and the chain rule and the definition of p we get

$$\frac{dH}{dp} = v + p\frac{dv}{dp} - \frac{dL}{dv}\frac{dv}{dp} = v + p\frac{dv}{dp} - p\frac{dv}{dp} = v. \tag{9.20}$$

Thus the situation is symmetric, and one can go back from H to L in the same way as one got from L to H. Conclusion: Two functions are Legendre transforms of each other when their derivatives are inverse functions to each other.

One would like a condition that guarantees that the equations that define the Legendre transform actually have solutions. In order for $p = dL/dv$ to have a unique solution v, it would be useful to have dL/dv to be strictly increasing. This is the same as saying that $dp/dv = d^2L/dv^2 > 0$. The inverse function then has derivative given by the inverse $dv/dp = d^2H/dp^2 > 0$.

Example: Let $L = e^v - v - 1$. Then we have seen that $H = (p+1)\log(p+1) - p$. This also follows from the general formula $H = pv - L$. In fact, since $p = e^v - 1$ has inverse $v = \log(1+p)$, we have $H = pv - L = p\log(1+p) - [(1+p) - \log(1+p) - 1] = (1+p)\log(1+p) - p$. In this example the second derivatives are e^v and $1/(p+1)$. These are both positive, and they are reciprocals of each other.

Example: Let $L = v^a/a$ with $1 < a < \infty$ defined for $v \geq 0$. Then $H = p^b/b$ with $1 < b < \infty$ defined for $p \geq 0$. In this case $p = v^{a-1}$ and $v = p^{b-1}$. The relation between a and b is $(a-1)(b-1) = 1$. This may also be written as $1/a + 1/b = 1$. Thus a and b are conjugate exponents. The second derivatives are $(a-1)v^{a-2}$ and $(b-1)p^{b-2}$. Again they are reciprocals.

The Legendre transform plays a fundamental role in thermodynamics and in mechanics. Here are examples from mechanics involving kinetic energy.

Example: Start with $L = (1/2)mv^2$. Then $p = mv$. So $v = p/m$ and $H = pv - L = p^2/(2m)$. This H is the Legendre transform of L.

Example: If we start instead with $H = p^2/(2m)$, then $v = p/m$. So $p = mv$ and $L = pv - H = (1/2)mv^2$. The Legendre transform of L brings us back to the original H.

Example: A famous relativistic expression for energy is $H = \sqrt{m^2c^4 + p^2c^2}$. It is an amusing exercise to compute that $L = -mc^2\sqrt{1 - v^2/c^2}$. The key is the relation $p = mv/\sqrt{1 - v^2/c^2}$ between the derivatives.

The Legendre transform has a generalization to several dimensions. Let L be a function of $v_1, \ldots, v_n$. Define

$$p_j = \frac{\partial L}{\partial v_j}, \tag{9.21}$$

so $dL = \sum_j p_j \, dv_j$. (This is the differential of L, so it is a one-form.) Then

$$H = \sum_k p_k v_k - L. \tag{9.22}$$

is the Legendre transform of L. In the following we want to think of L as a function of the v_j, while H is a function of the dual variables p_k. The variables p_k are covariant and dual to the variable v_j, which are contravariant. Thus in this formula the v_j are defined in terms of p_k by solving the equation $p_k = \partial L/\partial v_k$ for the v_j.

The fundamental theorem about the Legendre transform in this context is

$$v_k = \frac{\partial H}{\partial p_k}. \tag{9.23}$$

Proof: Let $H = \sum_k p_k v_k - L$ as above By the product rule and the chain rule and the definition of p we get

$$\frac{\partial H}{\partial p_j} = v_j + \sum_k p_k \frac{\partial v_k}{\partial p_j} - \sum_k \frac{\partial L}{\partial v_k}\frac{\partial v_k}{\partial p_j} = v_j + \sum_k p_k \frac{\partial v_k}{\partial p_j} - \sum_k p_k \frac{\partial v_k}{\partial p_j} = v_j. \tag{9.24}$$

Thus the situation is symmetric, and one can go back from H to L in the same way as one got from L to H. Conclusion: Two functions are Legendre

transforms of each other when their derivatives are inverse functions to each other.

One would like a condition that guarantees that the equations that define the Legendre transform actually have solutions. In order for the equation to have a solution locally, the matrix

$$\frac{\partial p_k}{\partial v_j} = \frac{\partial^2 L}{\partial v_k \partial v_j} \tag{9.25}$$

should be invertible. A particularly nice condition is that this matrix is strictly positive definite. The inverse matrix is then

$$\frac{\partial v_j}{\partial p_k} = \frac{\partial^2 H}{\partial p_j \partial p_k}. \tag{9.26}$$

It is then also strictly positive definite.

9.5 Lagrangian mechanics

One is given a Lagrangian function L that is a function of position q and velocity $\dot{q}$ and possibly time t. The problem is to find the critical points of

$$S(q) = \int_{t_1}^{t_2} L(q, q_t, t)\, dt. \tag{9.27}$$

The function q represents position as a function of time. It has fixed values q_1 and q_2 at the end points t_1 and t_2. The differential of S is

$$dS(q)h = \int_{t_1}^{t_2} (L_q h + L_{\dot{q}} h_t)\, dt = \int_{t_1}^{t_2} (L_q - \frac{d}{dt} L_{\dot{q}}) h\, dt. \tag{9.28}$$

Here h is a function with values 0 at the end points. Thus for the differential to be zero we must have the Euler-Lagrange equation

$$\frac{\partial L}{\partial q} - \frac{d}{dt}\frac{\partial L}{\partial \dot{q}} = 0. \tag{9.29}$$

Say that one has a solution of the Euler-Lagrange equation. Then

$$\frac{d}{dt} L = L_q q_t + L_{\dot{q}} q_{tt} + L_t = \frac{d}{dt}(q_t L_{\dot{q}}) + L_t. \tag{9.30}$$

Thus along a solution

$$\frac{d}{dt} H + \frac{\partial L}{\partial t} = 0, \tag{9.31}$$

where

$$H = q_t L_{\dot{q}} - L. \tag{9.32}$$

If $L_t = 0$, then this says that H is constant. This is the energy conservation law.

Define

$$p = \frac{\partial L}{\partial \dot{q}}. \tag{9.33}$$

This is the momentum variable. Then the Euler-Lagrange equation says that along a solution

$$\frac{dp}{dt} = \frac{\partial L}{\partial q}. \tag{9.34}$$

9.6 Hamiltonian mechanics

Let

$$H = p\dot{q} - L. \tag{9.35}$$

be the Legendre transform of L, where $\dot{q}$ is defined in terms of p implicitly by $p = \partial L/\partial \dot{q}$.

In the following we want to think of L as a function of q and $\dot{q}$ and possibly t, while H is a function of q and p and possibly t. The momentum variable p is covariant and is dual to the velocity variable $\dot{q}$, which is contravariant. However p is expressed in terms of q and $\dot{q}$ by solving the Legendre transform equation $p = \partial L/\partial \dot{q}$. According to the properties of the Legendre transform we have

$$\dot{q} = \frac{\partial H}{\partial p}. \tag{9.36}$$

In fact, the proof is simple if we remember that q is fixed:

$$\frac{\partial H}{\partial p} = \dot{q} + p\frac{\partial \dot{q}}{\partial p} - \frac{\partial L}{\partial \dot{q}}\frac{\partial \dot{q}}{\partial p} = \dot{q}. \tag{9.37}$$

It also follows that

$$\frac{\partial H}{\partial q} = -\frac{\partial L}{\partial q}. \tag{9.38}$$

This also has an easy proof if we remember that p is fixed and so $\dot{q}$ depends on q:

$$\frac{\partial H}{\partial q} = p\frac{\partial \dot{q}}{\partial q} - \frac{\partial L}{\partial q} - \frac{\partial L}{\partial \dot{q}}\frac{\partial \dot{q}}{\partial q} = -\frac{\partial L}{\partial q}. \tag{9.39}$$

The Euler-Lagrange equation says that along a solution we have

$$\frac{dp}{dt} = -\frac{\partial H}{\partial q}. \tag{9.40}$$

Since $p = \partial L/\partial \dot{q}$ determines the function p in terms of q, dq/dt, and t, it follows that along a solution

$$\frac{dq}{dt} = \frac{\partial H}{\partial p} \tag{9.41}$$

determines the function dq/dt in terms of q, p, and t. The last two equations are Hamilton's equations. They are a first order system, linear in dq/dt and dp/dt, but nonlinear in q, p, t.

It is easy to check from Hamilton's equations that along a solution

$$\frac{dH}{dt} = \frac{\partial H}{\partial t}. \tag{9.42}$$

When H does not depend explicitly on t, then this has an integral in which H is constant. This integral is conservation of energy. It gives a situation in which p is related to q. This allows an equation in which dq/dt is related to q. This relation may be highly nonlinear.

9.7 Kinetic and potential energy

The most classical situation is when

$$L = \frac{1}{2}m\dot{q}^2 - V(q). \tag{9.43}$$

The Euler-Lagrange equation is just.

$$-V'(q) - \frac{dq_t}{dt} = 0. \tag{9.44}$$

This is Newton's law of motion.

In this problem the momentum is $p = m\dot{q}$. The Hamiltonian is

$$H = \frac{1}{2m}p^2 + V(q). \tag{9.45}$$

Let us look at this from the point of view of maximum and minimum. The second differential is determined by the Schrödinger operator

$$L = -m\frac{d^2}{dt^2} - V''(q(t)). \tag{9.46}$$

Here $q(t)$ is a function of t satisfying the Euler-Lagrange equation and the boundary conditions. So for instance if this operator with Dirichlet boundary conditions at t_1 and t_2 has strictly positive eigenvalues, then the solution will be a minimum. This will happen, for instance, if $V''(q) \leq 0$. In many other cases, the solution will not be a minimum of the action, but only a stationary point.

Example: Take an example with $V''(q) < 0$. Then the problem is to find $q(t)$ that minimizes the integral from t_1 to t_1 of $(1/2)m\dot{q}^2 - V(q)$. Here $q(t_1) = q_1$ and $q(t_2) = q_2$ are fixed. Clearly there is tradeoff. One would like the solution to linger as long as possible in the region where $V(q)$ is large. On the other hand, to satisfy the boundary conditions the solution should not move too fast. The solution will start at the point y_1 at time t_1. Then it go reasonably, but not excessively, rapidly to the region where $V(q)$ is large. There it will linger. Then it will fall back to the point y_2, arriving there at time t_2. This minimization problem seems to have nothing to do with Newton's laws. But it gives the same answer.

9.8 Problems

Let L be a function of q and $\dot{q}$ given by

$$L = \frac{1}{2}m\dot{q}^2 - V(q).$$

Let

$$S(q) = \int_{t_1}^{t_2} L dt,$$

with functions q of t satisfying $q = q_1$ at $t = t_1$ and $q = q_2$ at $t = t_2$.

1. Show that
$$dS(q)h = (-m\frac{d}{dt}\dot{q} - V'(q), h),$$
where h satisfies Dirichlet boundary conditions at t_1 and t_2.

2. Consider a $q(t)$ for which $dS(q) = 0$. Show that
$$d^2S(q)(h,h) = \int_{t_1}^{t_2} [m\left(\frac{dh}{dt}\right)^2 - V''(q)h^2]\, dt.$$
where the functions h satisfy Dirichlet boundary conditions at t_1 and t_2.

3. Consider a $q(t)$ for which $dS(q) = 0$. Show that
$$d^2S(q)(h,h) = (h, [-m\frac{d^2}{dt^2} - V''(q)]h),$$
where the operator satisfies Dirichlet boundary conditions at t_1 and t_2.

4. Show that if $V(q)$ is concave down, then the solution $q(t)$ of the variational problem is actually a minimum.

5. Let $H = m\dot{q}^2 - L = (1/2)m\dot{q}^2 + V(q)$. Show that $H = E$ along a solution, where E is a constant.

6. From now on take the example $V(q) = -(1/2)kq^2$. Here $k > 0$. Note the sign. We are interested in solutions with $E > 0$. Let $\omega = \sqrt{k/m}$. Show that $q = C\sinh(\omega t)$ is a solution, and find the constant C in terms of E.

7. Take $t_1 = -T$ and $t_2 = T$. Take $q_1 = -a$ and $q_2 = a$. Fix a. Write the boundary condition $a = C\sinh(\omega T)$ as a relation between T and E. Show that $T \to 0$ implies $E \to \infty$, while $T \to \infty$ implies $E \to 0$.

8. Interpret the result of the last problem intuitively in terms of particle motion satisfying conservation of energy.

9. Interpret the result of the same problem intuitively in terms of a minimization problem.

9.9 The path integral

Let us return to the problem of evaluating the quantum mechanical time evolution $\exp(-iitH/\hbar)$. Here the total energy operator $H = H_0 + V$ is the sum of two non-commuting operators, corresponding to potential energy and kinetic energy.

The problem is easy when we just have kinetic energy. Then we must evaluate $\exp(-itH_0/\hbar)$, where $H_0 = p^2/(2m) = -\hbar^2/(2m)d^2/dx^2$. In the Fourier transform representation this is multiplication by $\hbar^2/(2m)k^2$. So in the Fourier transform representation the unitary time evolution is multiplication by $\exp(-it(\hbar/m)k^2/2)$. This is like the heat equation with complex diffusion coefficient $i\sigma^2 = i(\hbar/m)$. So the solution is convolution by the inverse Fourier transform, which is $1/\sqrt{2\pi i\sigma^2 t}\exp(-x^2/(2i\sigma^2 t)) = 1/\sqrt{2\pi i(\hbar/m)t}\exp(ix^2/(2(\hbar/m)t)$. In other words,

$$(\exp(-\frac{itH_0}{\hbar})u)(x) = \int_{-\infty}^{\infty} \exp(\frac{im(x-x')^2}{t\hbar})u(x')\,\frac{dx'}{\sqrt{2\pi i(\hbar/m)t}}. \tag{9.47}$$

The calculation of the exponential is also easy when we just have potential energy. In fact,

$$(\exp(-\frac{itV}{\hbar})u)(x) = \exp(-\frac{itv(x)}{\hbar})u(x). \tag{9.48}$$

The Trotter product formula is a remarkable formula that expresses the result for the sum $H = H_0 + V$ in terms of the separate results for H_0 and for V. It may be proved under various circumstances, for example when V is a bounded operator. The formula says that

$$\exp(-\frac{itH}{\hbar})u = \lim_{n\to\infty}\left(\exp(-\frac{i(t/n)H_0}{\hbar})\exp(-\frac{i(t/n)V}{\hbar})\right)^n u. \tag{9.49}$$

We can write out the Trotter product formula in detail using the results obtained before for H_0 and for V separately. Write $\Delta t = t/n$. Then the quantity of interest is $(\exp(-\frac{itH}{\hbar})u)(x) = u(x,t)$ given by the Trotter formula. This works out to be

$$u(x,t) = \lim_{n\to\infty}\int_{-\infty}^{\infty}\cdots\int_{-\infty}^{\infty}\exp\left(\frac{i\sum_{j=0}^{n-1}\left[\left(\frac{x_{j+1}-x_j}{\Delta t}\right)^2 - V(x_j)\right]\Delta t}{\hbar}\right)u(x_0)\frac{dx_{n-1}\cdots dx_0}{(\sqrt{2\pi i(\hbar/m)\Delta t})^n}, \tag{9.50}$$

where $x_n = x$.

So far this has been rigorous. However now we follow Feynman and take the formal limit as $n\to\infty$ and $\Delta t\to 0$ with $n\Delta = t$ fixed. This gives

$$(\exp(-\frac{itH}{\hbar})u)(x) = \int \exp\left(\frac{i\int_0^t\left[\left(\frac{dx(t')}{dt}\right)^2 - V(x(t'))\right]dt'}{\hbar}\right)u(x_0)\,\mathcal{D}x, \tag{9.51}$$

where the integral is over all paths x from some x_0 at time 0 to fixed final x at time t. This can also be written

$$(\exp(-\frac{itH}{\hbar})u)(x) = \int \exp\left(\frac{i\int_0^t L(x(t'), \frac{dx(t')}{dt})\,dt'}{\hbar}\right) u(x_0)\,\mathcal{D}x, \tag{9.52}$$

where

$$L(x(t'), \frac{dx(t')}{dt}) = \left(\frac{dx(t')}{dt}\right)^2 - V(x(t')) \tag{9.53}$$

is the Lagrangian. Thus the integrand in the path integral is the exponential of i times the action divided by $\hbar$.

This expression goes some way toward an explanation of the principle of stationary action. Consider a part of the integral near a path that is not a critical point of the action. Then nearby paths will have considerably different values of the action, and after division by $\hbar$ the phase will be very different. So there will be a lot of cancelation. On the other hand, the part of the integral near a path that is a critical point will contribute more or less the same value of the action. So there will be no cancelation.

9.10 Appendix: Lagrange multipliers

In this section y will represent the coordinates $y_1, \ldots, y_n$. We are interested in finding the critical points of a scalar function $F(y) = F(y_1, \ldots, y_n)$.

Consider first the problem of finding a critical point of $F(y)$ with no constraints. The usual method is to compute the differential and set it equal to zero, so that the equation to be solved is $dF(y) = 0$.

Consider the problem of finding a critical point of $F(y)$ subject to a constraint $G(y) = \kappa$.

The method of Lagrange multipliers is to say that the differential of $F(y)$ without the constraint must satisfy

$$dF(y) = \lambda dG(y) \tag{9.54}$$

for some λ. That is, the function can vary only by relaxing the constraint. The change in the function must be proportional to the change in the constraint. This fundamental equation is an equation for differential forms, and it takes the same form in every coordinate system.

Example: Maximize $y_1 y_2$ subject to $y_1^2 + y_2^2 = \kappa$. The equation is $y_2\,dy_1 + y_1\,dy_2 = \lambda(2y_1\,dy_1 + 2y_2\,dy_2)$. This gives $y_2 = 2\lambda y_1$ and $y_1 = 2\lambda y_2$. Eliminating λ we get $y_1^2 = y_2^2$. Combine this with $y_1^2 + y_2^2 = \kappa$. We get $y_1 = \pm\sqrt{\kappa/2}$ and $y_2 = \pm\sqrt{\kappa/2}$. The value of $y_1 y_2$ at these points are $\pm\kappa/2$. If you care, you can also compute that $\lambda = \pm 1/2$.

Say that $\bar{y}$ is a critical point, so in particular it satisfies the constraint $G(\bar{y}) = \kappa$. Then $dG(\bar{y}) = d\kappa$. It follows that $dF(\bar{y}) = \lambda dG(\bar{y}) = \lambda d\kappa$. The conclusion is that the Lagrange multiplier λ is the rate of change of the value of the function at the critical point as a function of the constraint parameter, that is, $\lambda = \frac{dF(\bar{y})}{d\kappa}$.

Example: In the last example the derivative of the maximum value $\pm\kappa/2$ with respect to κ is $\lambda = \pm 1/2$.

In calculations, one wants to maximize $F(y)$ subject to the constraint $G(y) = \kappa$. The idea is to take λ arbitrary. Set $\bar{F}(y) = F(y) - \lambda G(y)$ and require $d\bar{F}(y) = 0$. This gives the above equation for y and λ. However one also has the constraint equation for y and λ. These two are then solved simultaneously.

The method of Lagrange multipliers extends to the case when there are several constraints.

Consider the problem of finding a critical point of $F(y)$ subject to constraint $G_1(y) = \kappa_1, \ldots, G_m(y) = \kappa_m$..

The method of Lagrange multipliers is to say that the differential of $F(y)$ without the constraint must satisfy

$$dF(y) = \sum_{j=1}^{m} \lambda_j dG_j(y) \tag{9.55}$$

for some λ. That is, the function can vary only by relaxing the constraint. The change in the function must be proportional to the change in the constraints. This fundamental equation is an equation for differential forms, and it takes the same form in every coordinate system.

Say that $\bar{y}$ is a critical point, so in particular it satisfies the constraints $G_j(\bar{y}) = \kappa_j$. Then $dG_j(\bar{y}) = d\kappa_j$. It follows that $dF(\bar{y}) = \sum_j \lambda_j dG_j(\bar{y}) = \sum_j \lambda_j d\kappa_j$. The conclusion is that the Lagrange multiplier λ_j is the rate of change of the value of the function at the critical point as a function of the constraint parameter κ_j, with the other constraint parameters fixed. Thus $\lambda_j = \frac{\partial F(\bar{y})}{\partial \kappa_j}$.

Chapter 10

Perturbation theory

10.1 The implicit function theorem: scalar case

Let $f(u, \epsilon)$ be a function of u and ϵ. Let $f_u(u, \epsilon)$ be the partial derivative of F as a function of u. The assumption for the implicit function theorem is that $f(u_0, 0) = 0$ and the partial derivative $f_u(u_0, 0) \neq 0$. There are some other technical assumptions. The conclusion is that the equation

$$f(u, \epsilon) = 0 \tag{10.1}$$

defines u as a function of ϵ for ϵ sufficiently near 0, in such a way that $\epsilon = 0$ is mapped into u_0.

The intuition behind the theorem is that one can expand

$$f(u, \epsilon) \approx f_u(u_0, 0)(u - u_0) + f_\epsilon(u_0, 0)\epsilon. \tag{10.2}$$

Then we can solve

$$u \approx u_0 - f_u(u_0, 0)^{-1} f_\epsilon(u_0, u)\epsilon. \tag{10.3}$$

For ϵ small this is a very good approximation. In fact, this says that at the point $\epsilon = 0$ we have

$$\frac{du}{d\epsilon} = -f_u(u_0, 0)^{-1} f_\epsilon(u_0, 0). \tag{10.4}$$

This result is called first order perturbation theory.

For practical calculations one wants to compute higher derivatives $u^{(n)}$ as a function of ϵ. These are used in the Taylor expansion

$$u = \sum_{n=0}^{\infty} \frac{u^{(n)}}{n!} \epsilon^n. \tag{10.5}$$

In first order we have

$$f_u u^{(1)} + f_\epsilon = 0 \tag{10.6}$$

which gives the first order result

$$u^{(1)} = -f_u^{-1} f_\epsilon. \tag{10.7}$$

Usually we are interested in evaluating this expression at $u = u_0$ and $\epsilon = 0$.

The second order result is obtained by differentiating the first order equation. This gives

$$f_u u^{(2)} + f_{uu}(u^{(1)})^2 + 2f_{u\epsilon}u^{(1)} + f_{\epsilon\epsilon} = 0. \tag{10.8}$$

Thus the result of second order perturbation theory is that

$$u^{(2)} = -f_u^{-1}[f_{uu}(u^{(1)})^2 + 2f_{u\epsilon}u^{(1)} + f_{\epsilon\epsilon}]. \tag{10.9}$$

Again we are interested in evaluating this expression at $u = u_0$ and $\epsilon = 0$.

The general pattern is this. The nth derivative is given by

$$f_u u^{(n)} + r_n = 0 \tag{10.10}$$

Differentiate again. This gives

$$f_u u^{(n+1)} + [f_{uu}u^{(1)} + f_{u\epsilon}]u^{(n)} + [r_{nu}u^{(1)} + r_{n\epsilon}] = 0. \tag{10.11}$$

Thus at every stage one only has to invert the first derivative f_u.

Example: Here is a simple example. Fix a. We want to solve $u = a + \epsilon g(u)$ to find u as a function of ϵ. The first derivative is $u_\epsilon = g(u) + \epsilon g'(u)u_\epsilon$. The second derivative is $u_{\epsilon\epsilon} = 2g'(u)u_\epsilon + \epsilon g'(u)u_{\epsilon\epsilon} + \epsilon g''(u)u_\epsilon^2$. The third derivative is $u_{\epsilon\epsilon\epsilon} = 3g''(u)u_\epsilon^2 + 3g'(u)u_{\epsilon\epsilon} + \epsilon$ times other junk. Evaluate these at $\epsilon = 0$, that is, at $u = a$. This gives $u_\epsilon = g(a)$, $u_{\epsilon\epsilon} = 2g(a)g'(a)$, and $u_{\epsilon\epsilon\epsilon} = 3g(a)^2 g''(a) + 6g(a)g'(a)^2$. It is difficult to see the pattern. However in the next section we will see that there is one, at least in this case.

Example: Another popular way of solving the problem is to substitute $u = a + u'\epsilon + \frac{1}{2}u''\epsilon^2 + \frac{1}{6}u'''\epsilon^3 + \cdots$ in the equation. This gives

$$a+u'\epsilon+\frac{1}{2}u''\epsilon^2+\frac{1}{6}u'''\epsilon^3+\cdots = a+\epsilon[g(a)+g'(a)(u'\epsilon+\frac{1}{2}u''\epsilon^2+\cdots)+\frac{1}{2}\epsilon^2 g''(a)(u'\epsilon+\cdots)^2+\cdots]. \tag{10.12}$$

Equating powers of ϵ gives the same equations, and these are solved recursively the same way.

10.2 Problems

There is at least one case when one can evaluate Taylor coefficients to all orders. Say that x is a fixed parameter and one wants to solve

$$u = x + tg(u) \tag{10.13}$$

for u as a function of t. When $t = 0$ the solution is $u = x$. The Lagrange expansion says that for arbitrary $n \geq 1$ we have

$$\frac{d^n u}{dt^n} \mid_{t=0} = \frac{d^{n-1}}{dx^{n-1}} g(x)^n. \tag{10.14}$$

So the expansion to all orders is

$$u = x + tg(x) + \frac{t^2}{2}\frac{d}{dx}g(x)^2 + \frac{t^3}{6}\frac{d^2}{dx^2}g(x)^3 + \cdots + \frac{t^n}{n!}\frac{d^{n-1}}{dx^{n-1}}g(x)^n + \cdots. \quad (10.15)$$

1. Let $w = g(u)$. Show that the equation becomes

$$w = g(x + wt). \quad (10.16)$$

2. Show that the function w is the solution of the partial differential equation

$$\frac{\partial w}{\partial t} = w\frac{\partial w}{\partial x} \quad (10.17)$$

with initial condition $w = g(x)$ at $t = 0$.

3. Prove the conservation laws

$$\frac{\partial w^n}{\partial t} = \frac{n}{n+1}\frac{\partial w^{n+1}}{\partial x}. \quad (10.18)$$

4. Prove that for $n \geq 1$ we have

$$\frac{\partial^{n-1} w}{\partial t^{n-1}} = \frac{1}{n}\frac{\partial^{n-1}}{\partial x^{n-1}}w^n. \quad (10.19)$$

5. Prove that at $t = 0$

$$w = g(x) + \frac{t}{2}\frac{d}{dx}g(x)^2 + \frac{t^2}{6}\frac{d^2}{dx^2}g(x)^3 + \cdots + \frac{t^{n-1}}{n!}\frac{d^{n-1}}{dx^{n-1}}g(x)^n + \cdots. \quad (10.20)$$

6. Use $u = x + tw$ to prove the Lagrange expansion.

Note: The partial differential equation has a physical interpretation. If $v = -w$, then the equation is

$$\frac{\partial v}{\partial t} + v\frac{\partial v}{\partial x} = 0 \quad (10.21)$$

with initial condition $v = h(x)$ at time zero. This is the equation for the velocity of a gas of particles moving freely in one dimension. The motion of a particle moving with the gas is given by

$$\frac{dx}{dt} = v. \quad (10.22)$$

The acceleration of a particle is

$$\frac{dv}{dt} = \frac{\partial v}{\partial t} + \frac{dx}{dt}\frac{\partial v}{\partial x} = 0 \quad (10.23)$$

That is why it is considered free particle motion. Since v is constant along particle paths $x = x_0 + vt$, we have that v at arbitrary x, t is given in terms of the initial $v = h(x_0)$ at time zero by $v = h(x_0) = h(x - vt)$. So the solution of the equation is

$$v = h(x - vt). \quad (10.24)$$

10.3 The implicit function theorem: systems

We can take $F(u, \epsilon) = 0$ to be a system of n equations for n variables u and an extra variable ϵ. Or more generally we can take $F(u, \epsilon)$ to be a function of u and ϵ, where u ranges over a region U in some Banach space E. Then $F(u, \epsilon)$ takes values in a Banach space E'. The parameter ϵ is still real.

We shall often abbreviate the function by F. Let F_u be the partial derivative of F as a function of u. In the case of a system this is the n by n matrix of partial derivatives of the components of F with respect to the components of u. More generally, it is a function on U with values that are linear transformations from E to E'.

The assumption for the implicit function theorem is that $F(u_0, 0) = 0$ and the partial derivative $F_u(u_0, 0)$ has a bounded inverse. There are some other technical assumptions. The conclusion is that the equation

$$F(u, \epsilon) = 0 \tag{10.25}$$

defines u as a function of ϵ for ϵ sufficiently near 0, in such a way that $\epsilon = 0$ is mapped into u_0.

For practical calculations one wants to compute higher derivatives $u^{(n)}$ as a function of ϵ. These are used in the Taylor expansion

$$u = \sum_{n=0}^{\infty} \frac{u^{(n)}}{n!} \epsilon^n. \tag{10.26}$$

In first order we have

$$F_u u^{(1)} + F_\epsilon = 0 \tag{10.27}$$

which gives the first order result

$$u^{(1)} = -F_u^{-1} F_\epsilon. \tag{10.28}$$

Note that F_ϵ has values in E'. On the other hand, F_u^{-1} has values that are linear transformation from E' to E. So the right hand side has values in E, as it must. Usually we are interested in evaluating this expression at $u = u_0$ and $\epsilon = 0$.

The second order result is obtained by differentiating the first order equation. This gives

$$F_u u^{(2)} + F_{uu}(u^{(1)}, u^{1)}) + 2F_{u\epsilon} u^{(1)} + F_{\epsilon\epsilon} = 0. \tag{10.29}$$

Thus the result of second order perturbation theory is that

$$u^{(2)} = -F_u^{-1}[F_{uu}(u^{(1)}, u^{1)}) + 2F_{u\epsilon} u^{(1)} + F_{\epsilon\epsilon}]. \tag{10.30}$$

Note that F_{uu} has values that are bilinear functions from $E \times E$ to E'. On the other hand, $F_{u\epsilon}$ has values that are linear functions from E to E'. Again the right hand side has values in E. Again we are interested in evaluating this expression at $u = u_0$ and $\epsilon = 0$.

The general pattern is this. The nth derivative is given by

$$F_u u^{(n)} + R_n = 0 \tag{10.31}$$

Differentiate again. This gives

$$F_u u^{(n+1)} + [F_{uu} u^{(1)} + F_{u\epsilon}] u^{(n)} + [R_{nu} u^{(1)} + R_{n\epsilon}] = 0. \tag{10.32}$$

Thus at every stage one only has to invert the first derivative F_u.

10.4 Nonlinear differential equations

Let us look at the simplest non-linear differential equation

$$Lu = \epsilon g(u). \tag{10.33}$$

Here L is the restriction of a linear operator to satisfy an inhomogeneous boundary condition. For example, we could have $L = \partial/\partial t + 1$ acting on functions with $u(0) = 1$. When $\epsilon = 0$ there is a solution $u = u_0$. In the example $u_0(t) = e^{-t}$.

The derivative of L is L_0, where L_0 is a linear operator with zero boundary conditions. For instance, we could have $L_0 = \partial/\partial t + 1$ acting on functions h with $h(0) = 0$. Thus the first order perturbation equation is $L_0 u_\epsilon = g(u) + \epsilon g'(u) u_\epsilon$. The second order equation is $L_0 u_{\epsilon\epsilon} = 2g'(u)u_\epsilon +$ terms with ϵ. One can continue in this way. Thus the hierarchy of equations begins $Lu_0 = 0$, $L_0 u_\epsilon = g(u_0)$, $L_0 u_{\epsilon\epsilon} = 2g'(u_0)u_\epsilon$.

It is possible to think of this in another way. Write $u = u_0 + w$. Then the equation $Lu = \epsilon g(u)$ becomes $L_0 w = \epsilon g(u)$, where L_0 is the operator defined with zero boundary conditions. Suppose that L_0 has an inverse. Then

$$u = u_0 + \epsilon L_0^{-1} g(u). \tag{10.34}$$

This is very close in form to the scalar equation examined in the first two sections.

This equation may be solved by the usual procedure. The first derivative is $u_\epsilon = L_0^{-1} g(u) + \epsilon L_0^{-1} g'(u) u_\epsilon$. The second derivative is $u_{\epsilon\epsilon} = 2L_0^{-1} g'(u) u_\epsilon + \epsilon L_0^{-1} g'(u) u_{\epsilon\epsilon} + \epsilon L_0^{-1}[g''(u) u_\epsilon^2]$. The third derivative is $u_{\epsilon\epsilon\epsilon} = 3L_0^{-1}[g''(u)u_\epsilon^2] + 3L_0^{-1}[g'(u)u_{\epsilon\epsilon}] + \epsilon$ times other junk. Evaluate these at $\epsilon = 0$, that is, at $u = u_0$. This gives

$$u_\epsilon = L_0^{-1} g(u_0), \tag{10.35}$$

and

$$u_{\epsilon\epsilon} = 2L_0^{-1}[g'(u_0) L_0^{-1} g(u_0)], \tag{10.36}$$

and

$$u_{\epsilon\epsilon\epsilon} = 3L_0^{-1}[g''(u_0)(L_0^{-1}(g(u_0))^2] + 6L_0^{-1}[g'(u_0) L_0^{-1}(g'(u_0) L_0^{-1} g(u_0))]. \tag{10.37}$$

Notice how the linear operators occur in various places, making it impossible to do the simplification that we found in the scalar case.

10.5 A singular perturbation example

In quantum mechanics one often wants to solve a problem of the form

$$-\frac{\hbar^2}{2m}u'' + v(x)u = \lambda u. \tag{10.38}$$

Here $v(x)$ is a given real function. In many contexts λ plays the role of an eigenvalue parameter. The constant $m > 0$ is fixed. The constant $\hbar > 0$ is the perturbation parameter.

The characteristic feature of this problem is that the zero order perturbation is not apparent. Thus setting $\hbar = 0$ it is not clear that there will be a solution at all.

The resolution of this problem is to write the equation in new variables. For simplicity think of the case when $\lambda > v(x)$. Thus

$$u = Ae^{i\frac{S}{\hbar}}. \tag{10.39}$$

The equation becomes

$$A\left[\frac{1}{2m}(S')^2 + v(x) - \lambda\right] = \frac{\hbar^2}{2m}A'' \tag{10.40}$$

together with

$$2A'S' + AS'' = 0. \tag{10.41}$$

Now we can recognize the $\hbar = 0$ limit as

$$\frac{1}{2m}(S')^2 + v(x) = \lambda. \tag{10.42}$$

The other equation may be written

$$(A^2S')' = 0. \tag{10.43}$$

These equations have a physical interpretation. The function S' is a velocity that depends on position. The first equation is the classical equation for conservation of energy. The function A^2 is a density. The second equation is the conservation law that says that the current A^2S' is constant in space. Of course these equations are only valid in the zero order approximation, which in this case is called the WKB approximation.

This approximation is relevant to a heuristic understanding of Schrödinger operators of the form

$$H = -\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + v(x). \tag{10.44}$$

The Hilbert space is the space of L^2 functions on the line. If $v(x)$ is bounded below, then one expects this to be a well-defined self-adjoint operator. In fact, for $\lambda < 0$ sufficiently negative, one expects $(H - \lambda I)^{-1}$ to be a well-defined bounded self-adjoint operator. The reason is that the solutions of the differential

equation either decay rapidly at infinity or grow rapidly at infinity. The Green's function is defined by the solutions that decay rapidly at infinity. There is a solution of $Hu = \lambda u$ that is in L^2 at $-\infty$ and by another solution of the same equation that is in L^2 at $+\infty$. The two solutions are matched by a jump condition to form the kernel of the integral operator.

When $v(x)$ is very badly unbounded below, then something quite different happens. Let us look at the example of $v(x) \sim \epsilon x^{2n}$ with $\epsilon < 0$. According to the WKB approximation, we have $S'(x) \sim \pm|x|^n$. It follows that $A^2 \sim |x|^{-n}$. Thus it is plausible that if $n > 1$ then every solution is in L^2. These solutions are highly oscillatory and decrease at infinity at a moderate rate.

If this is indeed the case, then the operator H is not self-adjoint. The problem is that when one wants to define a Green's function, there are two linearly independent solutions, and they are both in L^2 at $\pm\infty$. So there is no boundary condition at infinity that determines the Green's function in a natural way.

10.6 Eigenvalues and eigenvectors

We have an operator $H_0 + \epsilon V$. We are interested in an isolated eigenvalue λ of multiplicity 1. The corresponding eigenvector is p. It is only determined up to a constant multiple. The adjoint operator has eigenvalue $\bar{\lambda}$ with eigenvalue q. It is convenient to choose p and q so that the inner product $(q, p) = 1$. The associated projection onto the eigenspace is P satisfying $P^2 = P$. It is given by $Pu = (q, u)p$. Thus p is an eigenvector with

$$(H_0 + \epsilon V - \lambda)p = 0. \tag{10.45}$$

Furthermore, $(q, (H_0 + \epsilon V - \lambda)u) = 0$ for all u. We also have the reduced resolvent S with $SP = PS = 0$ and $S(H_0 + \epsilon V - \lambda I) = 1 - P$.

If we indicate the dependence on ϵ explicitly, then the equation we want to solve is

$$(H_0 + \epsilon V - \lambda(\epsilon))p(\epsilon) = 0. \tag{10.46}$$

We would like to find the perturbation expansion in terms of the λ and p and q and S associated with $\epsilon = 0$.

The following discussion is meant to establish two formulas, one for the eigenvalue and one for the eigenvector (not normalized). The first is the formula for the eigenvalue to second order

$$\lambda(\epsilon) = \lambda + (q, Vp)\epsilon - (q, VSVp)\epsilon^2 + \cdots. \tag{10.47}$$

The other is the formula for the (unnormalized) eigenvector to second order

$$p(\epsilon) = p - SVp\epsilon + [SVSVp - S^2Vp(q, Vp)]\epsilon^2 + \cdots. \tag{10.48}$$

These formulas are so important that they should be memorized, at least the one for the eigenvalues.

We now proceed to the derivations. Differentiate the eigenvector equation with respect to ϵ. This gives

$$(H_0 + \epsilon V - \lambda)\dot{p} - \dot{\lambda}p + Vp = 0. \tag{10.49}$$

Now take the inner product with q on the left. This gives

$$\dot{\lambda} = (q, Vp). \tag{10.50}$$

This gives the first order change of the eigenvalue. That is,

$$\lambda(\epsilon) = \lambda + (q, Vp)\epsilon \cdots. \tag{10.51}$$

Next apply $I - P$ on the left. This gives

$$(I - P)(H_0 + \epsilon V - \lambda)\dot{p} + (I - P)Vp = 0, \tag{10.52}$$

or

$$(I - P)\dot{p} = -SVp. \tag{10.53}$$

Thus

$$\dot{p} = -SVp + c_1 p. \tag{10.54}$$

Notice that the derivative of the eigenvector is not uniquely determined. It ordinarily harmless to take $c_1 = 0$. This gives the first order change of the eigenvector

$$p(\epsilon) = p + [-SVp + c_1 p]\epsilon. \tag{10.55}$$

Now differentiate again. This gives

$$(H_0 + \epsilon V - \lambda)\ddot{p} + \ddot{\lambda}p + 2V\dot{p} - 2\dot{\lambda}\dot{p} = 0. \tag{10.56}$$

Take the inner product with q on the left. This gives

$$\ddot{\lambda} + 2(q, V\dot{p}) - 2\dot{\lambda}(q, \dot{p}), \tag{10.57}$$

or

$$\frac{1}{2}\ddot{\lambda} = -(q, VSVp). \tag{10.58}$$

This gives the second order change of the eigenvalue. That is,

$$\lambda(\epsilon) = \lambda + (q, Vp)\epsilon - (q, VSVp)\epsilon^2 + \cdots. \tag{10.59}$$

Now apply $1 - P$ on the left. This gives

$$(1 - P)(H_0 + \epsilon V - \lambda)\ddot{p} + 2(1 - P)V\dot{p} - 2\dot{\lambda}(1 - P)\dot{p} = 0. \tag{10.60}$$

Thus

$$\frac{1}{2}(1 - P)\ddot{p} = SVSVp - \frac{1}{2}c_1 SVp - S^2 Vp(q, Vp). \tag{10.61}$$

Hence

$$\frac{1}{2}\ddot{p} = SVSVp - S^2Vp(q, Vp) - \frac{1}{2}c_1SVp + \frac{1}{2}c_2p. \tag{10.62}$$

This gives the second order change of the eigenvector

$$p(\epsilon) = p + [-SVp + c_1p]\epsilon + [SVSVp - S^2Vp(q, Vp) - \frac{1}{2}c_1SVp + \frac{1}{2}c_2p]\epsilon^2 + \cdots. \tag{10.63}$$

Now let us change notation. We will think of a basis p_n for the Hilbert space and a dual basis q_m, with $(q_m, p_n) = \delta_{mn}$. We write q_m^* for the functional that takes u to (q_m, u). Then the various operators have special forms. We take the p_n to be the eigenvectors of H_0. Thus $H_0p_n = \lambda_n p_n$. The operator $P_n = p_n q_n^*$ is the spectral projection associated with the nth eigenvalue λ_n of H_0. The operator $S_n = \sum_{j\neq n} p_j q_j^*/(\lambda_k - \lambda_n)$.

Then the second order expression for the eigenvalue can be written as

$$\lambda_n(\epsilon) = \lambda_n + (q_n, Vp_n)\epsilon - (q_n, VS_nVp_n)\epsilon^2 + \cdots. \tag{10.64}$$

Even more explicitly, this is

$$\lambda_n(\epsilon) = \lambda_n + (q_n, Vp_n)\epsilon - \sum_{j\neq n}(q_n, Vp_j)\frac{1}{\lambda_j - \lambda_n}(q_j, Vp_n)\epsilon^2 + \cdots. \tag{10.65}$$

The second order expression for the eigenvector $p_n(\epsilon)$ is (taking $c_1 = 0$)

$$p_n(\epsilon) = p_n - S_nVp_n\epsilon + [S_nVS_nVp_n - S_n^2Vp_n(q_n, Vp_n) + \frac{1}{2}c_2p_n]\epsilon^2 + \cdots. \tag{10.66}$$

If H_0 has discrete spectrum, then (leaving out the last term) this may be written

$$p_n(\epsilon) = p_n - \sum_{j\neq n}\frac{1}{\lambda_j - \lambda_n}(q_j, Vp_n)p_j\epsilon \tag{10.67}$$

$$+ \sum_{j\neq n}\frac{1}{\lambda_j - \lambda_n}[\sum_{k\neq n}(q_j, Vp_k)\frac{1}{\lambda_k - \lambda_n}(q_k, Vp_n) - \frac{1}{\lambda_j - \lambda_n}(q_j, Vp_n)(q_n, Vp_n)]p_j\epsilon^2 + \cdots.$$

10.7 The self-adjoint case

In the self-adjoint case $q = p$ and it is natural to normalize so that $(p(\epsilon), p(\epsilon)) = 1$ to second order. This gives $c_1 = 0$ and

$$c_2 = -(p, VS^2Vp). \tag{10.68}$$

So in this case

$$\lambda(\epsilon) = \lambda + (p, Vp)\epsilon - (p, VSVp)\epsilon^2 + \cdots. \tag{10.69}$$

and

$$p(\epsilon) = p - SVp\epsilon + [SVSVp - S^2Vp(p, Vp) - \frac{1}{2}(p, VS^2Vp)p]\epsilon^2 + \cdots. \tag{10.70}$$

If $\lambda = \lambda_n$ and $p = p_n$, we can write the coefficient c_2 even more explicitly as

$$c_2 = -\sum_{j \neq n} (p_n, V p_j) \frac{1}{(\lambda_j - \lambda_n)^2} (p_j, V p_n). \tag{10.71}$$

Example: Take

$$H_0 = \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix} \tag{10.72}$$

and

$$V = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}. \tag{10.73}$$

The eigenvalues are $\lambda(\epsilon) = \pm\sqrt{1+\epsilon^2}$. However it is interesting to compare this exact result with the result of second order perturbation theory.

Let us look at the perturbation of the eigenvalue -1 of H_0. For this eigenvalue the spectral projection is

$$P = \begin{bmatrix} 0 & 0 \\ 0 & 1 \end{bmatrix} \tag{10.74}$$

and the eigenvector p is the second column of P. The reduced resolvent is

$$S = \begin{bmatrix} \frac{1}{1-(-1)} & 0 \\ 0 & 0 \end{bmatrix} = \begin{bmatrix} \frac{1}{2} & 0 \\ 0 & 0 \end{bmatrix}. \tag{10.75}$$

So the coefficient in second order perturbation theory is

$$-(p, VSVp) = -\frac{1}{2}. \tag{10.76}$$

Thus

$$\lambda(\epsilon) = -1 - \frac{1}{2}\epsilon^2 + \cdots. \tag{10.77}$$

10.8 The anharmonic oscillator

In this section we let

$$H_0 = \frac{1}{2}\left[\frac{d^2}{dx^2} + x^2 - 1\right]. \tag{10.78}$$

The perturbation V is multiplication by

$$v(x) = \epsilon x^4. \tag{10.79}$$

Let

$$A = \frac{1}{\sqrt{2}}\left(x + \frac{d}{dx}\right) \tag{10.80}$$

and

$$A^* = \frac{1}{\sqrt{2}}\left(x - \frac{d}{dx}\right). \tag{10.81}$$

Then $AA^* = A^*A + I$ and $H_0 = A^*A$. Furthermore, the solution of $Au_0 = 0$ is

$$u_0(x) = \frac{1}{\sqrt[4]{\pi}} e^{-\frac{x^2}{2}}. \tag{10.82}$$

Define for each $n = 0, 1, 2, 3, \ldots$ the vector

$$u_n = \frac{1}{n!} A^{*n} u_0. \tag{10.83}$$

We have $A^* u_m = \sqrt{m+1}\, u_{m+1}$ and $A u_m = \sqrt{m}\, u_{m-1}$. Then the u_n form an orthonormal basis consisting of eigenvectors of H_0. Furthermore,

$$H_0 u_n = n u_n. \tag{10.84}$$

Say that we are interested in a particular n. The corresponding reduced resolvent S_n is given by

$$S_n u_m = \frac{1}{m-n} u_m \tag{10.85}$$

for $m \neq n$, and by $S_n u_n = 0$.

The operator multiplication by x may be expressed in terms of A and A^* by

$$x = \frac{1}{\sqrt{2}}(A + A^*). \tag{10.86}$$

This allows us to calculate the matrix elements of x. These are given by

$$(u_{m+1}, x u_m) = \frac{1}{\sqrt{2}}(u_{m+1}, A^* u_m) = \frac{1}{\sqrt{2}}\sqrt{m+1} \tag{10.87}$$

and

$$(u_{m-1}, x u_m) = \frac{1}{\sqrt{2}}(u_{m-1}, A u_m) = \frac{1}{\sqrt{2}}\sqrt{m}. \tag{10.88}$$

So each transition is to a neighboring natural number.

As a warmup, let us compute the matrix element $(u_n, x^2 u_n)$. This is the sum of two possible transition paths, one up-down and one down-up. The result is $(n+1)/2 + (n/2) = (2n+1)/2$.

To compute the first order perturbation coefficient $(u_n, x^4 u_n)$. we need to look at all transitions that go from n to n in 4 steps. After two steps one is either at u_{n-2}, at u_n, or at u_{n+2}. So

$$(u_n, x^4 u_n) = (u_n, x^2 u_{n-2})^2 + (u_n, x^2 u_n)^2 + (u_n, x^2 u_{n+2})^2. \tag{10.89}$$

This is

$$(u_n, x^4 u_n) = \frac{n(n-1)}{4} + (\frac{2n+1}{2})^2 + \frac{(n+1)(n+2)}{4} = \frac{6n^2 + 6n + 3}{4}. \tag{10.90}$$

Higher order perturbations may be computed with more labor. It turns out that the perturbation series in ϵ does not converge. Some intuition for this is provided by the observation that $H_0 + \epsilon V$ is not a self-adjoint operator for $\epsilon < 0$. So for $\epsilon < 0$ the eigenvalue problem is meaningless. On the other hand, if the Taylor series had a positive radius of convergence, then it would converge also for some values of $\epsilon < 0$.