1. Unbounded operators

In many applications, the linear operators one encounters are not bounded. The most elementary example is multiplication by x on the Hilbert space $L^2(\mathbb{R}, dx)$. Clearly

$$\int_{\mathbb{R}} |xf(x)|^2 dx$$

cannot be finite for all functions $f \in L^2(\mathbb{R}, dx)$, just take the function

$$\frac{1}{\sqrt{1+x^2}} \ .$$

In fact, the situation is somewhat worse because of the theorem of Hellinger and Toeplitz.

Theorem 1.1. *Let A be a linear operator defined everywhere on a Hilbert space $\mathcal{H}$, i.e., $A : \mathcal{H} \to \mathcal{H}$, and assume that for all $f, g \in \mathcal{H}$*

$$\langle Af, g \rangle = \langle f, Ag \rangle \ ,$$

then A is a boounded operator.

The proof of this theorem is a direct application of the uniform boundedness principle and we shall not repeat it here. Hence, we cannot talk about unbounded everywhere defined operators in general and have to restrict the domain of definition. We have a linear operator

$$A : D(A) \to \mathcal{H}$$

where $D(A)$ is a linear manifold, the **domain** of the operator A. An operator B is an **extension** of A if $D(A) \subset D(B)$ and $Af = Bf$ for all $f \in D(A)$. We write $A \subset B$.

Note that the domain is part of the definition of the operator. Consider, e.g., the linear operator $T_1 : C^1_c(\mathbb{R}) \to L^2(\mathbb{R})$ given by $T_1 f(x) = f'(x)$. The operator $T_2 : C^\infty_c(\mathbb{R}) \to \mathcal{H}$ is also given by $T_2 f(x) = f'(x)$. We treat these two operators as different operators. Clearly, $T_2 \subset T_1$. In general linear operators can be wild unless we impose some continuity.

Definition 1.2. Closed operators. *A linear operator $A : D(A) \to \mathcal{H}$ is* **closed** *if for any sequence of vectors $f_n \in D(A)$ such that, as $n \to \infty$, $f_n \to f$ and $Af_n \to g$, it follows that $f \in D(A)$ and $Af = g$.*

Bounded linear operators are obviously closed, in fact the convergence $f_n \to f$ entails the convergence of $Af_n \to Af$.

Another way of saying that an operator is closed is the following

Lemma 1.3. *A linear operator $A : D(A) \to \mathcal{H}$ is closed if and only if the domain $D(A)$ endowed with the norm $\|f\|_A := \sqrt{\|f\|^2 + \|Af\|^2}$ is a Banach space, i.e., a linear, normed, complete space.*

Proof. The argument is quite elementary. Assume that A is closed. Let f_n be a sequence in $D(A)$ such that f_n is a Cauchy sequence in the norm $\|f\|_A$. Hence $f_n \to f$ and $Af_n \to g$. Since A is closed, $f \in D(A)$ and $g = Af$ and hence $\|f_n - f\|_A \to 0$. Conversely, if $D(A)$ is a Banach space in the norm $\|\cdot\|_A$, and $f_n \in D(A)$ converges to f and Af_n converges to g, it follows that f_n is a Cauchy sequence in $D(A)$ with the norm $\|\cdot\|_A$ and hence converges to some f in this norm. Hence $f \in D(A)$ and $g = Af$. $\square$

You may guess that neither the operator T_1 nor T_2 defined above is closed. This is a standard situation that occurs in practice. Rarely can we compute explicitly what a closed operator does to all its element in its domain. Thus, we have the definition

Definition 1.4. Closable operators *A linear operator $A : D(A) \to \mathcal{H}$ is* **closable** *if it has a closed extension.*

Here is a simple statement about closable operators.

Lemma 1.5. *A linear operator $A : D(A) \to \mathcal{H}$ is closable if and only if for any sequence $f_n \in D(A)$ such that, as $n \to \infty$, $f_n \to 0$ and $Af_n \to g$, it follows that $g = 0$.*

Proof. Assume that A is closable and denote by B a closed extension. If $f_n \in D(A)$ then $f_n \in D(B)$. Since $Bf_n = Af_n \to g$ and since $f_n \to 0$, we have, since B is closed that $g = B0 = 0$. Conversely, consider the linear manifold

$$D = \{f \in \mathcal{H} : \text{ there exists } f_n \in D(A)\ , f_n \to f\ , Af_n \to g\}\ .$$

On D we define $\overline{A}f = g$. We have to show that g is independent of the sequence f_n. Let $u_n \in D(A)$ be another sequence with $u_n \to f$ and $Au_n \to h$. We have to show that $h = g$. Since $f_n - u_n \to 0$ and since $A(f_n - u_n) \to g - h$ it follows that $f = g$. Hence, $\overline{A}$ is defined on D and it is easy to see that it is a linear operator. It remains to show $\overline{A}$ is closed. Let f_n be a sequence in D such that $f_n \to f$ and $\overline{A}f_n \to g$. We have to show that $f \in D$ and $\overline{A}f = g$. Since for each n $f_n \in D$ there exists $u_n \in D(A)$ such that

$$\|f_n - u_n\| + \|\overline{A}f_n - Au_n\| < \frac{1}{n}\ .$$

Hence, $u_n \to f$ and $Au_n \to g$, i.e., $f \in D$ and $g = \overline{A}f$. Hence $\overline{A}$ is closed. □

We call $\overline{A}$ the **closure** of the (closable) operator A. It is the **smallest** closed extension of A in the sense that if $A \subset B$ and B is closed, then $\overline{A} \subset B$. We leave this as an easy exercise to the reader.

The notion of adjoint operators can easily be generalized to our new situation.

Definition 1.6. Adjoint operator *Let $A; D(A) \to \mathcal{H}$ be a linear operator (not necessarily closed) with $D(A) \subset \mathcal{H}$ dense. Define $D(A^*)$ to be the set of all elements $f \in \mathcal{H}$ such that the linear functional*

$$g \to \langle Ag, f\rangle$$

extends to a bounded linear functional on all of $\mathcal{H}$. Since $D(A) \subset \mathcal{H}$ is dense, there exists, by the Riesz representation theorem a unique element $h \in \mathcal{H}$ such that

$$(f, Ag) = (h, g)\ .$$

We define $A^*f = h$. It is easily seen that A^* is a linear operator.

Note, that $D(A^*)$ is not empty since the zero vector is certainly in there. Here is another reason why the notion of closed operator makes sense.

Theorem 1.7. *Let A be a densely defined operator. Then the operator A^* is closed.*

Proof. Let $f_n \in D(A^*)$ such that $f_n \to f$ and $A^*f_n \to g$. Then for all $v \in D(A)$

$$(f, Av) = \lim_{n\to\infty}(f_n, Av) = \lim_{n\to\infty}(A^*f_n, v) = (g, v)\ .$$

Hence, $f \in D(A^*)$ and $g = A^*f$. □

Note, that we did not assume that A itself was closed, or even closable. The adjoint of any densely defined operator is automatically closed.

Here are a few simple facts.

Lemma 1.8. *a) If $A \subset B$ then $B^* \subset A^*$.*
b) If A is closable, then $(\overline{A})^* = A^*$.

Proof. $f \in D(B^*)$ means that there exists $h \in \mathcal{H}$ such that

$$(f, Bv) = (h, v)$$

for all $v \in D(B)$. Since $A \subset B$ we also have that

$$(f, Av) = (f, Bv) = (h, v)$$

for all $v \in D(A)$. Hence $B^* \subset A^*$. To prove b) note that since $A \subset \overline{A}$, $(\overline{A})^* \subset A^*$. Now let $f \in D(A^*)$. There exists a unique $h \in \mathcal{H}$ such that

$$(f, Av) = (h, v)$$

all $v \in D(A)$. If $w \in D(\overline{A})$ there exists $v_n \in D(A)$ such that $v_n \to w$ and $Av_n \to \overline{A}w$. Hence

$$(f, \overline{A}w) = \lim_{n\to\infty}(f, Av_n) = \lim_{n\to\infty}(h, v_n) = (h, w)$$

and hence $f \in D((\overline{A})^*)$. Since $h = A^*f$ we also have that $(\overline{A})^*f = h$. $\square$

We have learned that by passing to adjoint operators one obtains closed operators. There is a natural closed extension for a closable operator A and that would be $(A^*)^*$. This operator, however, exists only if A^* is densely defined. The following theorem is a bit trickier than we have seen so far.

Theorem 1.9. *An linear operator $A : D(A) \to \mathcal{H}$ is closable if and only if A^* is densely defined, in which case $\overline{A} = (A^*)^*$.*

Proof. First we assume that A^* is densely defined. $f \in D((A^*)^*)$ means that there exists a unique $h = (A^*)^*f \in \mathcal{H}$ so that

$$(f, A^*u) = (h, u) = ((A^*)^*f, u)$$

for all $u \in D(A^*)$. If $f \in D(A)$, then for all $u \in D(A^*)$

$$(u, Af) = ((A^*u, f)$$

from which it follows that $f \in D((A^*)^*)$ and $(A^*)^*f = Af$. Hence $A \subset (A^*)^*$ and since $(A^*)^*$ is closed, the operator A is closable.

The proof of the converse is more difficult. Assume that A is closable. We have to show that $D(A^*)$ is dense. We want to show that the assumption that $D(A^*)$ is not dense leads to a contradiction. Since $(\overline{A})^* = A^*$ we may assume that $A = \overline{A}$, i.e., that A is closed. Since $D(A^*)$ is not dense, there exists a non-zero vector $f \in \mathcal{H}$ such that $f \perp D(A^*)$. Consider the minimization problem

$$D^2 = \inf_{g\in D(A)} \left[\|f - Ag\|^2 + \|g\|^2\right] \ . \tag{1}$$

The idea for this expression is to approximate the pair $f, 0 \in \mathcal{H} \times \mathcal{H}$ by elements of the form $Ag, g \in \mathcal{H} \times D(A)$. To see the relevance of (1) assume that the infimum is attained at h, i.e.,

$$D^2 = \|f - Ah\|^2 + \|h\|^2 \ .$$

Pick any $v \in D(A)$ and consider

$$\|f - A(h+tv)\|^2 + \|(h+tv)\|^2 \ge D^2 \ .$$

Taking the derivative in t at $t = 0$ yields, as usual,

$$-(f - Ah, Av) + (h, v) = 0$$

for all $v \in D(A)$ or

$$(f - Ah, Av) = (h, v)$$

for all $v \in D(A)$. This means that $f - Ah \in D(A^*)$ and $A^*(f - Ah) = h$. Now, since $f \perp f - Ah$ we have that

$$\|f\|^2 = (f, Ah) \ ,$$

and in particular

$$\|f\| \le \|Ah\| \ .$$

Further, since $h \in D(A)$

$$\|h\|^2 = (h, A^*(f - Ah) = (Ah, f) - \|Ah\|^2 = \|f\|^2 - \|Ah\|^2 \le 0 \ .$$

Hence $h = 0$ and hence $Ah = 0$, a contradiction, since $f \neq 0$.

We shall prove that the infimum is attained. Let $g_n \in D(A)$ be a minimizing sequence. As in the proof of the projection theorem we find that

$$\|\frac{(f - Ag_n) + (f - Ag_m)}{2}\|^2 + \|\frac{g_n + g_m}{2}\|^2 + \|\frac{(f - Ag_n) - (f - Ag_m)}{2}\|^2 + \|\frac{g_n - g_m}{2}\|^2$$

$$= \frac{1}{2}\left[\|(f - Ag_n)\|^2 + \|f - Ag_m)\|^2 + \|g_n\|^2 + |g_m\|^2\right] \ .$$

From this we see that g_n as well as Ag_n is a Cauhy sequence. Hence $g_n \to h$ for some $h \in \mathcal{H}$ and $Ag_n \to v \in \mathcal{H}$. Since A is closed $h \in D(A)$ and $Ah = v$. Thus, we have that

$$D^2 = \|f - Ah\|^2 + \|h\|^2 \ .$$

It remains to show that $\overline{A} = (A^*)^*$. We have seen before that, $\overline{A} \subset (A^*)^*$. To show the converse we may assume that A is closed and pick any $f \in D((A^*)^*)$. As before the problem

$$D^2 = \inf_{g \in D(A)} \left[\|f - g\|^2 + \|(A^*)^* f - Ag\|^2\right]$$

has a minimizer $h \in D(A)$ (since A is closed). Again, we consider for $v \in D(A)$ arbitrary

$$\|f - (h+tv)\|^2 + \|(A^*)^* f - A(h+tv)\|^2 \ge D^2$$

and find

$$(f - h, v) + ((A^*)^* f - Ah, Av) = 0 \ .$$

This means that $(A^*)^* f - Ah \in D(A^*)$ and

$$A^*((A^*)^* f - Ah) = -(f - h)$$

Taking the inner product with $f - h$ yields

$$-\|f - h\|^2 = (A^*((A^*)^*(f - h), f - h) = (((A^*)^*(f - h), (A^*)^*(f - h)) \ge 0 \ .$$

Hence $f = g \in D(A)$ and $(A^*)^* f = Ag$. $\square$

Our goal is to study a certain class of operators, the self-adjoint operators. We start with a defintion.

Definition 1.10. Symmetric operators *A linear operator $A : D(A) \to \mathcal{H}$ is symmetric if $D(A)$ is dense in $\mathcal{H}$ and for all $f, g \in D(A)$*

$$(Af, g) = (f, Ag) \ .$$

A simple consequence is that any symmetric operator A is extended by its adjoint, i.e.,

$$A \subset A^* \ ,$$

in other words **a symmetric operator is always closable**. If B is any symmetric extension of A,i.e., $A \subset B$ we have that $B^* \subset A^*$, i.e., we have

$$A \subset B \subset B^* \subset A^* \ .$$

A symmetric operator A with $A = A^*$ is called **self-adjoint**. Note that a self adjoint operator is automatically closed. Moreover, it does not have symmetric extensions. A symmetric operator A that has not symmetric extensions but $A \neq A^*$ is called maximally symmetric.

Here is a first simple criterion for self-adjointess.

Theorem 1.11. *Let $A : D(A) \to \mathcal{H}$ be a symmetric operator with the property that $Ran(A) = \mathcal{H}$. Then A is selfadjoint.*

Proof. Since $D(A) \subset D(A^*)$ all we have to show is that $f \in D(A^*)$ implies $f \in D(A)$. Consider $g = A^* f$. Since $Ran(A) = \mathcal{H}$ there exists $h \in D(A)$ so that $g = Ah$. Now for all $v \in D(A)$

$$(f, Av) = (A^* f, v) = (g, v) = (Ah, v) = (h, Av) \ .$$

If $u \in \mathcal{H}$ is arbitrary, there exists $v \in D(A)$ such that $u = Av$. Hence we have for all $u \in \mathcal{H}$

$$(f, u) = (h, u)$$

and thus, $f = h \in D(A)$. $\square$

The following surprising theorem is due to von Neumann.

Theorem 1.12. *Let $A : D(A) \to \mathcal{H}$ be a densely defined closed operator. Then, $D = \{h \in D(A) : Ah \in D(A^*)\}$ is dense and A^*A is a self-adjoint operator with domain D.*

Proof. We use a similar technique as before. For $f \in \mathcal{H}$ consider the minimization problem

$$D^2 = \inf_{g \in D(A)} \left[\|f - g\|^2 + \|Ag\|^2 \right] \ .$$

Let $g_n \in D(A)$ be a minimizing sequence, i.e.,

$$\|f - g_n\|^2 + \|Ag_n\|^2 \to D^2 \ .$$

Let us go through the argument in detail. By the parallelogram identity we find

$$\|\frac{(f - g_n) + (f - g_m)}{2}\|^2 + \|\frac{(f - g_n) - (f - g_m)}{2}\|^2 + \|\frac{Ag_n + Ag_m}{2}\|^2 + \|\frac{Ag_n - Ag_m}{2}\|^2$$

$$= \frac{1}{2}\|f - g_n\|^2 + \frac{1}{2}\|Ag_n\|^2 + \frac{1}{2}\|f - g_m\|^2 + \frac{1}{2}\|Ag_m\|^2 \ .$$

Put in another way

$$\|f - \frac{g_n + g_m}{2}\|^2 + \|\frac{A(g_n + g_m)}{2}\|^2 + \|\frac{g_n - g_m}{2}\|^2 + +\|\frac{Ag_n - Ag_m}{2}\|^2$$

converges as $n, m \to \infty$ to D^2. Since

$$D^2 \le \|f - \frac{g_n + g_m}{2}\|^2 + \|\frac{A(g_n + g_m)}{2}\|^2$$

we must have that g_n as well as Ag_n are Cauchy sequences and hence converge to h resp. v. Since A is closed, $h \in D(A)$ and $Ah = v$. Hence

$$D^2 = \|f - h\|^2 + \|Ah\|^2 \ .$$

The usual variational argument $h \to h + tv, v \in D(A)$ leads to

$$-(f - h, v) + (Ah, Av) = 0$$

all $v \in D(A)$. Since $D(A)$ is dense $Ah \in D(A^*)$ and

$$A^*Ah = f - h$$

or

$$A^*Ah + h = f \ .$$

This means that for any $f \in \mathcal{H}$ there exists $h \in D$ with $A^*Ah + h = f$. This means that the operator $A^*A + I$ is surjective. If $h_1, h_2 \in D$ and $A^*Ah_1 + h_1 = f = A^*Ah_2 + h_2$ it follows that

$$A^*A(h_2 - h_1) + (h_2 - h_1) = 0 \ .$$

Since $h_2 - h_1 \in D$ we have that

$$\|A(h_2 - h_1)\|^2 + \|h_2 - h_1\|^2 = 0$$

and hence $A^*A + I$ is injective on D. It remains to show that the operator A^*A is symmetric. The domain D is dense, for suppose that $f \perp D$ then

$$f = A^*Ah + h$$

for a unique $h \in D$. Hence

$$0 = (h, f) = (h, A^*Ah) + (h, h) = \|Ah\|^2 + \|h\|^2$$

which implies that h and hence $f = 0$. Finally, A^*A is symmetric on D since for $f, g \in D$

$$(f, A^*Ag) = (Af, Ag) = (A^*Af, g) \ .$$

Hence, $A^*A + I$ is symmetric on D and its range is the whole Hilbert space and hence it is self-adjoint.

$\square$