# 1. Extensions of symmetric operators

References: Joachim Weidmann, Linear Operators in Hilbert Spaces, Springer-Verlag,

In what follows $\mathcal{H}$ is a **complex** Hilbert space.

Recall that an operator $A : D(A) \to H$ is symmetric if $D(A)$ is dense in $\mathcal{H}$ and for all $f, g \in D(A)$

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

Since $A \subset A^*$ it follows that a symmetric operator is closable and we shall henceforth assume that $A$ is a closed symmetric operator. Note that this assumption entails that the spaces $\mathrm{Ran}(A + iI)$ and $\mathrm{Ran}(A - iI)$ are closed subspaces of $\mathcal{H}$.

Further recall that the Cayley transform of $A$,

$$V : \mathrm{Ran}(A + iI) \to \mathrm{Ran}(A - iI)$$

is defined as follows. For $g \in \mathrm{Ran}(A + iI)$ there exists a unique $f \in D(A)$ with

$$g = (A + iI)f \ .$$

Define

$$Vg = (A - iI)f \ .$$

The operator $V$ satisfies $\|Vg\| = \|g\|$ and $V$ is onto. We call such operators **isometries**. Note that 'onto' is part of the definition. The point of the next theorem is that the study of symmetric operators can be reduced to the study of isometries.

**Theorem 1.1. (One to one correspondence between symmetric operators and isometries)** *Let $A$ be a closed symmetric operator and $V$ its Cayley transform. Then $\mathrm{Ran}(I - V)$ is dense in $\mathcal{H}$. Conversely let $F$ and $G$ be two closed subspaces of a Hilbert space and assume that $V : F \to G$ is an isometry such that $\mathrm{Ran}(I - V)$ is dense in $\mathcal{H}$. Then $V$ is the Cayley transform of a closed symmetric operator.*

*Proof.* Any $f \in D(A)$ there exists a unique $g = (A + iI)f$ such that $Vg = (A - iI)g$. Hence

$$f = \frac{1}{2i}(g - Vg) \text{ and } Af = \frac{1}{2}(g + Vg) \ ,$$

and

$$D(A) = \mathrm{Ran}(\frac{1}{2i}(I - V)) \ .$$

Because $D(A)$ is dense in $\mathcal{H}$, the first statement follows. To see the converse define $D(A) = \mathrm{Ran}(I - V)$, i.e., for $g \in D(A)$ there exists $f \in F$ such that

$$g = \frac{1}{2i}(f - Vf) \ .$$

By assumption this set is dense in $\mathcal{H}$. In fact the vector $f$ is unique. This is equivalent to the statement that $(I - V)$ is injective. If there exists $h \in F$ with $Vh = h$ then we have for all $f \in F$

$$(h, (I - V)f) = (h, f) - (h, Vf) = (h, f) - (Vh, Vf) = (h, f) - (h, f) = 0$$

since $V$ preserves the inner product. Since $\mathrm{Ran}(I-V)$ is dense it follows that $h=0$. Thus for any $g \in D(A)$ there exists a unique $f \in F$ such that $g = \frac{1}{2i}(f - Vf)$. Next we define

$$Ag = \frac{1}{2}(f + Vf)$$

and note that for any $g_1, g_2 \in D(A)$

$$(g_1, Ag_2) = \frac{1}{4i}((f_1 - Vf_1), (f_2 + Vf_2)) = \frac{1}{4i}\left[(f_1, f_2) + (f_1, Vf_2) - (Vf_1, f_2) - (Vf_1, Vf_2)\right] =$$
$$\frac{1}{4i}\left[(f_1, Vf_2) - (Vf_1, f_2)\right] .$$

Likewise,

$$(Ag_1, g_2) = -\frac{1}{4i}((f_1 + Vf_1), (f_2 - Vf_2)) = -\frac{1}{4i}\left[-(f_1, Vf_2) + (Vf_1, f_2)\right]$$

and hence $A$ is symmetric. To see that $A$ is closed let $g_n \in D(A)$ be a sequence converging to $g$ and $Ag_n$ converging to $h$. Then the sequence

$$f_n = (A + iI)g_n$$

converges to $f := h + ig$ which, since $F$ is closed, is also in $F$. Likewise, $Vf_n = (A - iI)g_n$ converges to $h - ig$ and since $G$ is closed we have that $h - ig \in G$. Since $V$ is bounded $Vf_n$ converges also to $h - ig$. Hence we have that

$$g = \frac{1}{2i}(f - Vf) \text{ and } h = \frac{1}{2}(f + Vf) ,$$

which means that $g \in D(A)$ and $h = Ag$. □

Our next theorem pushes this correspondence further by showing that extensions of symmetric operators correspond to extensions of isometries.

**Theorem 1.2.** **(Extensions of symmetric operators correspond to extensions of isometries)** *The operator $A'$ is a closed symmetric extension of a closed symmetric operator $A$ if and only if for the corresponding Cayley transforms $V \subset V'$.*

*Proof.* Let $A'$ be a symmetric closed extension. Then $\mathrm{Ran}(A + iI) \subset \mathrm{Ran}(A' + iI)$ and $\mathrm{Ran}(A - iI) \subset \mathrm{Ran}(A' - iI)$. For $g \in \mathrm{Ran}(A + iI)$ there exists a unique $f \in D(A)$ such that $g = (A + iI)f$ and $Vg = (A - iI)f$. Since $A \subset A'$, $g = (A' + iI)f$ and $V'g = (A' - iI)f = Vg$. Hence $V \subset V'$. Conversely if $V \subset V'$ then for $g \in D(A)$ we have $g = \frac{1}{2i}(f - Vf)$ for a unique $f \in \mathrm{Ran}(A + iI)$. Since $V \subset V'$ we have that $\mathrm{Ran}(A + iI) \subset \mathrm{Ran}(A' + iI)$ and $\mathrm{Ran}(A - iI) \subset \mathrm{Ran}(A' - iI)$. Finally, $Ag = \frac{1}{2}(f + Vf) = \frac{1}{2}(f + V'f) = A'g$. Hence $A \subset A'$. □

The next step in our program consists of understanding extensions of isometries.

**Theorem 1.3.** **(Structure of isometric extensions)** *Let $F, G$ be two closed subspaces of $\mathcal{H}$ and $V : F \to G$ an isometry, i.e., $\|Vf\| = \|f\|$ for all $f \in F$ and $V$ is onto $G$. Let $F_+ \subset F^\perp$ and $F_- \subset G^\perp$ be closed subspaces. Then*

$$V' : F \oplus F_+ \to G \oplus F_-$$

*is an isometric extension of $V$ if and only if $\dim F_+ = \dim F_-$ and there exists an isometry $\widetilde{V} : F_+ \to F_-$ so that for any $f \in F \oplus F_+$, i.e., $f = f_0 + f_+, f_0 \in F, f_+ \in F_+$,*

$$V'f = Vf_0 + \widetilde{V}f_- . \qquad (1)$$

*Proof.* Clearly $V'$ of the form given above is an isometry. It is onto $G \oplus F_-$ since $V$ is onto $G$ and $\widetilde{V}$ is onto $F_-$. It preserves length since

$$(V'f, V'f) = (Vf_0 + \widetilde{V}f_+, Vf_0 + \widetilde{V}f_+) = (Vf_0, Vf_0) + (Vf_0, \widetilde{V}f_+) + (\widetilde{V}f_+, Vf_0) + (\widetilde{V}f_+, \widetilde{V}f_+) \ .$$

Since $Vf_0 \in G$ and $\widetilde{V}f_+ \in F_-$ they are perpendicular to each other and hence

$$\begin{aligned}(V'f, V'f) &= (Vf_0, Vf_0) + (\widetilde{V}f_+, \widetilde{V}f_+) \\ &= (f_0, f_0) + (f_+, f_+) = (f, f) \ .\end{aligned}$$

Suppose that $V' : F \oplus F_+ \to G \oplus F_-$ is an isometry that extends $V$. For any vector $f_+ \in F_+$ define

$$\widetilde{V}f_+ := V'f_+ \in G \oplus F_- \ .$$

Pick any $g \in G$ and note that since $V$ is onto $G$, there exists $f \in F$ with $g = Vf$. Hence

$$(g, \widetilde{V}f_+) = (Vf, V'f_+) = (V'f, V'f_+) = (f, f_+) = 0 \ .$$

Since $g \in G$ is arbitrary, $\widetilde{V}f_+ \perp G$ and hence $\widetilde{V}$ maps $F_+$ into $F_-$. That $\widetilde{V}$ preserves the norm follows from the fact that $V'$ does. We have to show that $\widetilde{V}$ is onto. For any $f_- \in F_-$ there exists $f \in F \oplus F_+$ so that $V'f = f_-$ because $V'$ is onto. For any $f_0 \in F$ we have that

$$0 = (Vf_0, V'f) = (V'f_0, V'f) = (f_0, f)$$

Hence $f \in F_+$ and $\widetilde{V}f = f_-$. The formula (1) is obvious. □

With these results we can now completely characterize all closed symmetric extensions of a closed symmetric operator.

**Theorem 1.4. (Closed symmetric extensions)** *Let $A : D(A) \to \mathcal{H}$ be a closed symmetric operator. A closed symmetric operator $A' : D(A') \to \mathcal{H}$ is an extension of $A$ if and only if the following holds:*
*There exists closed subspaces $F_+ \subset \mathrm{Ker}(A^* - iI) = \mathrm{Ran}(A + iI)^\perp, F_- \subset \mathrm{Ker}(A^* + iI) = \mathrm{Ran}(A - iI)^\perp$ and an isometry $\widetilde{V} : F_+ \to F_-$ so that the Cayley transform of $A', V'$, is of the form*

$$\begin{aligned}V' : \mathrm{Ran}(A + iI) \oplus F_+ &\to \mathrm{Ran}(A - iI) \oplus F_- \\ V'f &= Vf_0 + \widetilde{V}f_+ \end{aligned} \tag{2}$$

*with $f = f_0 + f_+$.*
*In particular this entails that $\mathrm{dim} F_+ = \mathrm{dim} F_-$.*

*Proof.* If $A'$ is a closed symmetric extension of $A$ then we know that for their respective Cayley transforms $V \subset V'$ by Theorem 1.2. Since $\mathrm{Ran}(A \pm iI) \subset \mathrm{Ran}(A' \pm iI)$ we can define $F_\pm$ to be the orthogonal complement of $\mathrm{Ran}(A \pm iI)$ in $\mathrm{Ran}(A' \pm iI)$. The conclusion follows from Theorem 1.3. Conversely, if $V'$ is given by (2) then $\mathrm{Ran}(I - V')$ is dens in $\mathcal{H}$ because $\mathrm{Ran}(I - V)$ is and hence by Theorem 1.1 $V'$ is the Cayley transform of a closed symmetric operator and since $V \subset V'$ we have that $A'$ extends $A$. Since $\widetilde{V}$ is bijective we must have that $\mathrm{dim} F_+ = \mathrm{dim} F_-$. □

**Corollary 1.5.** *A closed symmetric operator has self-adjoint extensions if and only if the* **deficiency indices**

$$n_\pm := \dim\ \mathrm{Ker}(A^* \mp iI)$$

*are equal.*

*Proof.* Recall that a closed symmetric operator is self-adjoint if and only if its Cayley transform is unitary. Then Theorem 1.4 implies that $n_- = n_+$. □

So far this has been rather abstract. More useful are the following two theorems of von Neumann. The first one is simple but instructive since it allows, in principle, to compute a special extension of $A$, namely $A^*$.

**Theorem 1.6.** *Let $A : D(A) \to \mathcal{H}$ be a closed symmetric operator. Then*

$$D(A^*) = D(A) + \mathrm{Ker}(A^* - iI) + \mathrm{Ker}(A^* + iI)$$

*where the sum is direct. Moreover, writing an arbitrary $f \in D(A^*)$ as $f = f_0 + f_+ + f_-$ where $f_0 \in D(A)$, $f_+ \in \mathrm{Ker}(A^* - iI)$ and $f_- \in \mathrm{Ker}(A^* + iI)$ we have*

$$A^* f = Af_0 + if_+ - if_- \ .$$

*Proof.* Since $A \subset A^*$ we have that $D(A) \subset D(A^*)$. The inclusions $\mathrm{Ker}(A - iI) \subset D(A^*)$ and $\mathrm{Ker}(A^* + iI) \subset D(A^*)$ are obvious. Hence

$$D(A) + \mathrm{Ker}(A^* - iI) + \mathrm{Ker}(A^* + iI) \subset D(A^*).$$

To see the converse, consider any $f \in D(A^*)$. Since the subspaces $\mathrm{Ran}(A + iI)$ and $\mathrm{Ran}(A + iI)^\perp = \mathrm{Ker}(A^* - iI)$ are closed we can split the split the vector $(A^* + iI)f$ uniquely into $u + f_+$ where $u = (A + iI)f_0$ for some unique $f_0 \in D(A)$ and $A^* f_+ = if_+$ or $(A^* + iI)vf_+ = 2if_+$. Thus,

$$(A^* + iI)f = (A + iI)f_0 + (A^* + iI)\frac{1}{2i}f_+ = (A^* + iI)f_0 + (A^* + iI)\frac{1}{2i}f_+$$

since $D(A) \subset D(A^*)$. Hence

$$(A^* + iI)\left[f - f_0 - \frac{1}{2i}f_+\right] = 0 \ .$$

This means that $f - f_0 - \frac{1}{2i}f_+ \in \mathrm{Ker}(A^* + iI)$ and hence

$$D(A^*) = D(A) + \mathrm{Ker}(A^* - iI) + \mathrm{Ker}(A^* + iI) \ .$$

To see that the sum is direct, assume that $f_0 + f_+ + f_- = 0$ where $f_0 \in D(A)$, $f_+ \in \mathrm{Ker}(A^* - iI)$ and $f_- \in \mathrm{Ker}(A^* + iI)$. Now

$$(A + iI)f_0 = (A^* + iI)f_0 = -(A^* + iI)f_+ = -2if_+$$

This says that $f_+ \in \mathrm{Ker}(A^* - iI) \cap \mathrm{Ran}(A + iI)$ which are orthogonal complements. Hence $f_+ = 0$. In a similar fashion we see that $f_- = 0$ and hence $f_0 = 0$ and the sum is direct. Finally, for $f \in D(A^*)$, i.e., $f = f_0 + f_+ + f_-$ we compute

$$A^* f = Af_0 + A^* f_+ + A^* f_- = Af_0 + if_+ - if_- \ .$$

□

There is an analog of this theorem for arbitrary closed symmetric extensions. This time, we will make use of the Cayley transform.

**Theorem 1.7.** *Let $A$ be a closed symmetric operator. The operator $A'$ is a closed symmetric extension of $A$ if and only if there are subspaces $F_\pm \subset \mathrm{Ker}(A^* \mp iI)$ and an isometry $\widetilde{V} : F_+ \to F_-$ such that*

$$D(A') = D(A) + (I - \widetilde{V})(F_+) \tag{3}$$

*where the sum is direct and*

$$A'(f_0 + g - \widetilde{V}g) = Af_0 + ig + i\widetilde{V}g \ . \tag{4}$$

*The operator $A'$ is self adjoint if and only if $F_\pm = \mathrm{Ker}(A^* \mp iI)$ .*

*Proof.* Using Theorem 1 it remains to show the displayed formulas. The domain of $A'$ is given by $\mathrm{Ran}(I - V') = (I - V)(\mathrm{Ran}(A + iI) + \mathrm{Ran}(I - \widetilde{V})(F_+)$. Since $(I - V)(\mathrm{Ran}(A + iI) = D(A)$ the formula (3) is established. Since $F_\pm \subset \mathrm{Ker}(A^* \mp iI)$ it follows from the proof of the previous theorem that the sum is direct. Let $f \in D(A')$. There exists a unique $h \in \mathrm{Ran}(A' + iI) = \mathrm{Ran}(A + iI) \oplus F_+$ such that

$$f = (h - V'h)$$

and $A'$ is then given by

$$A'f = i(h + V'h) \ .$$

Since $h$ can be written as $h_0 + f_+$, $h_0 \in \mathrm{Ran}(A + iI)$, $f_+ \in F_+$ and $V'(h_0 + f_+) = Vh_0 + \widetilde{V}f_+$ we have

$$f = (h_0 - Vh_0) + (f_+ - \widetilde{V}f_+) = f_0 + (f_+ - \widetilde{V}f_+)$$

where $f_0 = h_0 - Vh_0$, and hence

$$A'f = A'(f_0 + f_+ - \widetilde{V}f_+) = A'f_0 + A'(f_+ - \widetilde{V}f_+) = Af_0 + i(f_+ + \widetilde{V}f_+) \ .$$

□

**Example:**

We apply now this theory to a concrete problem (taken from Reed -Simon, Modern methods of mathematical physics, volume I). Consider the Hilbert space $L^2(0,1)$ of complex valued square integrable functions. Consider the dense domain

$$D = \{f \in L^2(0,1) : f \in AC[0,1], f(0) = f(1) = 0\} \ .$$

Here AC[0,1] is the space of absolute continuous functions whose derivative is square integrable. On $D$ consider the operator

$$Af = \frac{1}{i}f' \ .$$

$A$ is closed (this is a bit tedious but not difficult to show), symmetric but not self adjoint. We shall determine all its self adjoint extensions. It is not very difficult to see that the adjoint of $A$, $A^*$ is given by

$$A^*f = \frac{1}{i}f'$$

for $f$ in the domain AC[01] with no boundary conditions, but the neat thing is that we do not have to know that. First we pretend that we know what $A^*$ is and do a formal calculation. That $f_+ \in \mathrm{Ker}(A^* - iI)$ means that $\frac{1}{i}f_+' = if_+$, i.e., $f_+' = -f_+$. Hence

$$f_+(x) = \frac{\sqrt{2}}{\sqrt{e^2 - 1}}e^{-(x-1)} \ .$$

Note that the pre-factor renders the function normalized in $L^2(0,1)$. Likewise to find $f_- \in \mathrm{Ker}(A^* + iI)$ amounts to solving the equation $f' = f$ and we get

$$f_-(x) = \frac{\sqrt{2}}{\sqrt{e^2 - 1}}e^{x} \ .$$

Now we give a rigorous argument for for this result. Assume that $f \in \mathrm{Ker}(A^* - iI)$. Consider $\phi_\varepsilon(x) = \varepsilon^{-1}\phi(x/\varepsilon)$ where $\phi(x) \geq 0 \in C_c^\infty(-1,1)$, $\int_{\mathbb{R}} \phi(x)dx = 1$ and write $f_\varepsilon(x) := \int_0^1 \phi_\varepsilon(x-y)f(y)dy$. For each fixed $x \in (0,1)$ we have, for $\varepsilon$ sufficiently small, that $\phi_\varepsilon \in D(A)$ and hence we can write that

$$f_\varepsilon(x) = \langle \phi_\varepsilon(x - \cdot), f\rangle$$

so that

$$\frac{1}{i} f_\varepsilon'(x) = \frac{1}{i}\langle \phi_\varepsilon'(x-\cdot), f\rangle = -\langle A\phi_\varepsilon(x-\cdot), f\rangle = \langle \phi_\varepsilon(x-\cdot), A^* f\rangle \ .$$

(Note that the minus sign is there since we $f$ appears and not $\overline{f}$.) Since $f \in \mathrm{Ker}(A^* - iI)$, we find that

$$\frac{1}{i} f_\varepsilon'(x) = \langle \phi_\varepsilon(x-\cdot), if\rangle = i f_\varepsilon(x) \ ,$$

so that $f_\varepsilon'(x) = f_\varepsilon(x)$ and hence $f_\varepsilon(x) = c_\varepsilon e^x$ where $c_\varepsilon$ is a constant. Since $f$ is continuous, we have that $\lim_{\varepsilon\to 0} f_\varepsilon(x) = f(x)$ and hence $f(x) = ce^x$ where $c$ is a constant. Thus, there are no other solutions and hence $f_+$ furnishes a basis for $\mathrm{Ker}(A^* - iI)$. A similar computation shows that $f_-$ is a basis for the space $\mathrm{Ker}(A^* + iI)$. Thus, the operator $A$ has deficiency indices $(1,1)$ and therefore has self-adjoint extensions.

Now, we use Theorem 1.7. Any isometry $\widetilde{V} : \mathrm{Ker}(A^* - iI) \to \mathrm{Ker}(A^* + iI)$ is given by

$$\widetilde{V}_\beta f_+ = \beta f_-$$

where $\beta$ is a complex number of absolute value 1. Hence the domain of $A_\beta$, the self-adjoint extension corresponding to this isometry $\widetilde{V}_\beta$, is given by functions of the form

$$f_0 + c(f_+ - \beta f_-) = f_0 + c\frac{\sqrt{2}}{\sqrt{e^2-1}}(e^{-(x-1)} - \beta e^x)$$

where $f_0 \in D$ and $c$ is an arbitrary complex constant. Further,

$$A_\beta(f_0 + c(f_+ - \beta f_-)) = Af_0 + ic(f_+ + \beta f_-) = Af_0 + ic\frac{\sqrt{2}}{\sqrt{e^2-1}}(e^{-(x-1)} + \beta e^x) \ .$$

The domain $D(A_\beta)$. Has another characterization. Any function of the form $f := f_0 + c\frac{\sqrt{2}}{\sqrt{e^2-1}}(e^{-(x-1)} - \beta e^x)$ where $f_0 \in D(A)$ satisfies

$$f(0) = c\frac{\sqrt{2}}{\sqrt{e^2-1}}(e - \beta) \text{ and } f(1) = c\frac{\sqrt{2}}{\sqrt{e^2-1}}(1 - \beta e) \ .$$

In other words

$$f(1) = \frac{1-\beta e}{e-\beta} f(0) \ .$$

Note that the constant

$$\alpha := \frac{1-\beta e}{e-\beta}$$

is a complex constant of absolute value 1. Also note that

$$\beta = \frac{\alpha e - 1}{\alpha - e} \ .$$

Now let's turn things around, and consider the operator $B_\alpha f = \frac{1}{i} f'$ on the domain

$$D(B_\alpha) = \{f \in L^2(0,1) : f \in AC[0,1], f(1) = \alpha f(0)\} \ ,$$

where $\alpha \in \mathbb{C}$ has magnitude 1. One expects that $A_\beta = B_\alpha$. To see this we have to show that the domains are equal. We have seen that $D(A_\beta) \subset D(B_\alpha)$. Now pick any $f \in D(B_\alpha)$ and consider the function

$$f_0 := f + af_+ + bf_-$$

and try to adjust the constants $a$ and $b$ so that $f_0(0) = f_0(1) = 0$, i.e., $f_0 \in D(A)$. This amounts to solving the equations

$$af_+(0) + bf_-(0) + f(0) = 0 \text{ and } af_+(1) + bf_-(1) + f(1) = 0 \ .$$

We find

$$\begin{bmatrix} a \\ b \end{bmatrix} = -\frac{1}{f_+(0)f_-(1) - f_-(0)f_+(1)} \begin{bmatrix} f_-(1) & -f_-(0) \\ -f_+(1) & f_+(0) \end{bmatrix} \begin{bmatrix} f(0) \\ f(1) \end{bmatrix}$$
$$= -f(0)\frac{1}{2}\frac{\sqrt{2}}{\sqrt{e^2-1}} \begin{bmatrix} e-\alpha \\ e\alpha - 1 \end{bmatrix}$$

which leads to

$$af_+ + bf_- = -f(0)\frac{e-\alpha}{e^2-1}[e^{-(x-1)} - \frac{\alpha e - 1}{\alpha - e}e^x] = c\frac{\sqrt{2}}{\sqrt{e^2-1}}[e^{-(x-1)} - \beta e^x] \ .$$

This shows that $D(A_\beta) = D(B\alpha)$.

It is now very easy to compute the eigenvalues of $B_\beta$. It amounts to solving the equation

$$\frac{1}{i}f' = \lambda f$$

with the condition $f(1) = \beta f(0)$. The general solution is $ce^{i\lambda x}$ and the boundary condition requires

$$ce^{i\lambda} = c\beta$$

or

$$e^{i\lambda} = \beta$$

$(c \neq 0!)$ Write

$$\beta = e^{i\phi}$$

where $\phi \in [0, 2\pi)$ and then find that the eigenvalues are given by

$$\lambda_k = \phi + 2\pi k \ , \ k = 0, \pm 1, \pm 2, \dots \ .$$

The corresponding eigenfunctions are

$$e^{i(\phi + 2\pi k)x} \ .$$