Spectral theory on L^2: kernel operators and Hamiltonian

Arthur L. Limoge
Imperial College London

L^2 as a Hilbert Space

At the start of the 20th century, progress in analysis, especially spectral theory, led to define Hilbert spaces, and hence generalize notions previously established by figures including Fourier or Parseval. In particular, operator theory developed a lot under the influence of mathematicians such as Frigyes Riesz, who defined L^p spaces for the first time.

Fig. 1: Frigyes Riesz

Formally, for $p \in \mathbb{N}^*$, and $(X, \mathcal{F}, \mu)$ a measure space:

$$L^p(X) := \{f : \int_X |f|^p \mathrm{d}\mu < +\infty\}$$

In the following, we will simply consider X to be a subset of $\mathbb{R}$, μ to be the Lebesgue measure, and we will focus on the case $p = 2$.

For $X \subseteq \mathbb{R}$, $L^2(X)$ is a Hilbert Space. Its inner product is indeed well-defined due to the linearity of integration $\left(\text{where } \langle f|g\rangle^{1} = \int_X g(x)f(x)\mathrm{d}x\right)$; and the space has been proven to be complete by the Riesz-Fischer theorem [**1**]. We will here zoom in on integral operators of the form:

$$\mathcal{T}: \begin{array}{ccc} L^2(X) & \to & L^2(X) \\ f & \mapsto & \left(x \mapsto \int_X K(x,y)f(y)\mathrm{d}y\right) \end{array}$$

where $K : \mathbb{R}^2 \to \mathbb{R}$ is called the kernel of the transform.

Study of the spectrum

The spectrum of an operator is a generalization [**3**] of the set of eigenvalues to infinite dimension:

For two vectors $|\chi\rangle, |\varphi\rangle$ in a Hilbert space $\mathcal{H}$, and $z \in \mathbb{K}$, consider the equation

$$(zI - T)\,|\chi\rangle = |\varphi\rangle \tag{1}$$

If the image of $(zI - T)$ (I being the identity) is $\mathcal{H}$, then z is said to be a **regular value** of T, and the resolvent $(zI - T)^{-1}$ is well-defined. The spectrum is then defined to be the set of non-regular values of T. In our case, $\mathcal{H} = L^2(X)$, X being a subset of $\mathbb{R}$.

In some simple cases, this eigenvalue problem can be brought down to a linear algebra one. For example, with the operator satisfying $Tf(x) = \int K(x,y)f(y)\mathrm{d}y$:

Assume $K(x,y) = \sum_{k=1}^{n} \varphi_k(x)\psi_k(y)$ is the kernel of an operator T, where $\{\varphi_k\}$ and $\{\psi_k\}$ are sets of functions, and the $|\varphi_k\rangle$ are linearly independent (call V their span). Solving the eigenvalue problem is equivalent to diagonalizing the associated matrix in the side diagram; where u denotes the natural isomorphism $V \to \mathbb{R}^n$. We can check it by taking $|f\rangle \in V$, and then following the diagram to get $Au(|f\rangle) = u(T|f\rangle)$.

$$\begin{tikzcd} V \arrow[r, "T"] \arrow[d, "u"'] & V \arrow[d, "u"] \\ \mathbb{R}^n \arrow[r, "A"'] & \mathbb{R}^n \end{tikzcd}$$

Norm of operators

The norm of an operator T is defined as $||T||_2 := \sup_{f\neq 0} \frac{\langle Tf|f\rangle}{||f||^2}$. Its knowledge is quite useful because it provides an upper bound for the eigenvalues of the transform, [**4**]. However, some do not have eigenvalues. For instance, consider the operator $\mathcal{K}$ with kernel $K : (x,y) \mapsto \frac{1}{x+y}$, on $L^2(\mathbb{R}_+)$.

It has no (non-zero) eigenvalues, but it still has a non-empty spectrum: the function defined by $x \mapsto x^{-1/2}$ does not belong to $L^2(\mathbb{R}_+)$, but one can note that:

$$\int_0^{+\infty} \frac{1}{x+y} y^{-1/2}\mathrm{d}y = \pi x^{-1/2} \text{ (proved by setting } t = \frac{\sqrt{y}}{\sqrt{x}}) \tag{2}$$

Therefore, the spectrum contains π, which we can prove is an upper bound for the norm. Indeed, take $|f\rangle \in L^2(\mathbb{R}_+)$ and consider:

$$\begin{aligned} \langle Kf|f\rangle &= \iint_0^{+\infty} \frac{f(y)f(x)}{x+y}\mathrm{d}y\,\mathrm{d}x = \iint_0^{+\infty} \frac{f(xt)f(x)}{1+t}\mathrm{d}t\,\mathrm{d}x \text{ (set } y = tx), \\ &= \int_0^{+\infty} \frac{\langle f(x)|f(xt)\rangle}{1+t}\mathrm{d}t \leq \int_0^{+\infty} \frac{1}{1+t} \times \frac{||f||}{\sqrt{t}}||f||\,\mathrm{d}t \text{ (Cauchy-Schwarz)} \\ &= ||f||^2 \int_0^{+\infty} \frac{t^{-1/2}}{1+t}\mathrm{d}t = \pi||f||^2 \implies ||K||_2 \leq \pi. \end{aligned}$$

As-a-matter-of-fact, this norm **is** π: note that though the function $x \mapsto x^{-1/2}$ is not in L^2; for $a > 1$, the function defined by $f_a(x) = \begin{cases} x^{-1/2} \text{ if } 0 < x < a \\ 0 \text{ else} \end{cases}$ **is**[2]. And by taking bigger values of a, we can expect $\frac{\langle Kf_a|f_a\rangle}{||f_a||^2}$ to get arbitrarily close to π:

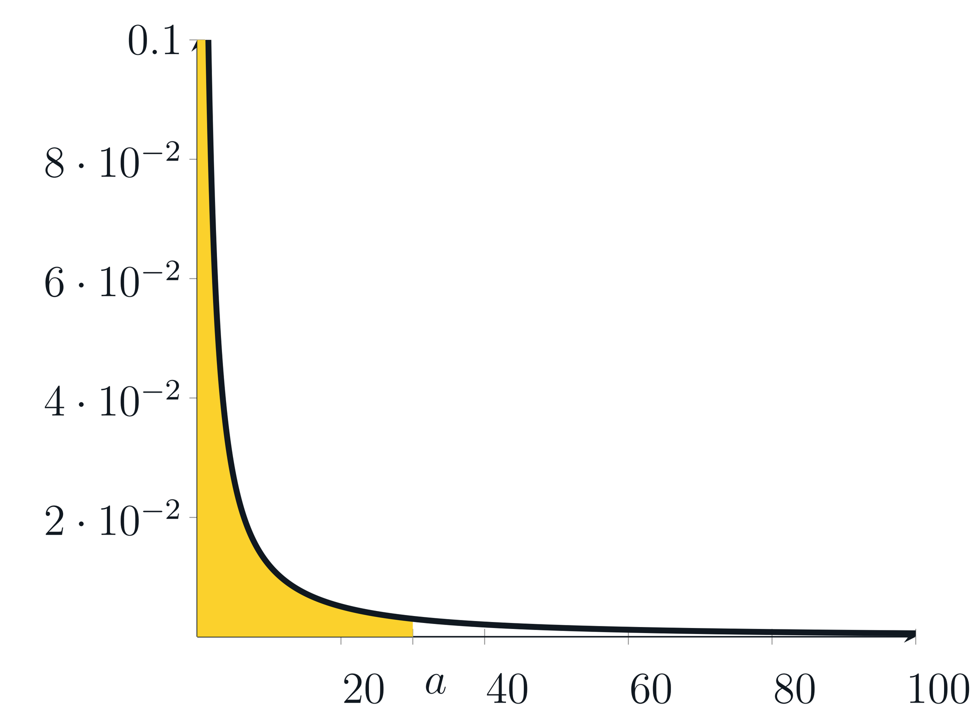

Fig. 2: Plot of the curve $y = x^{-1/2} \times Kf_a(x)$. The yellow area represents $\langle Kf_a|f_a\rangle$.

And it does! $\frac{\langle Kf_a|f_a\rangle}{||f_a||^2} = \frac{1}{\ln(a)}\int_0^{+\infty} \frac{2}{x}\arctan\left(\frac{\sqrt{a}}{\sqrt{x}}\right)\mathrm{d}x \geq \frac{1}{\ln(a)}\int_{a^{\varepsilon/\pi}}^{a} \frac{2}{x}\arctan\left(\frac{\sqrt{a}}{\sqrt{a^{\varepsilon/\pi}}}\right)\mathrm{d}x$

$$= 2\frac{\ln(a^{1-\varepsilon/\pi})}{\ln(a)}\arctan\left(\frac{\sqrt{a}}{\sqrt{a^{\varepsilon/\pi}}}\right) \longrightarrow \pi(1 - \frac{\varepsilon}{\pi}) = \pi - \varepsilon, \text{ as } a \longrightarrow +\infty$$

This holds for any fixed $\varepsilon \in (0, \pi)$, and *a fortiori* for all $\varepsilon > 0$.

$$\therefore \forall\varepsilon > 0\ \exists a > 1, \frac{\langle Kf_a|f_a\rangle}{||f_a||^2} \geq \pi - \varepsilon \implies \boxed{\pi = \sup_{f\neq 0}\frac{\langle Kf|f\rangle}{||f||^2} = ||K||_2} \qquad \square$$

Hamiltonian in Quantum Mechanics

The study of L^2 operators turns out to be important in quantum mechanics, as many problems consist in solving the eigenvalue equation of the Hamiltonian operator $\hat{H} := -\frac{\hbar}{2m}\nabla^2 + \hat{V}$ (where $\hbar = \frac{h}{2\pi}$ is the reduced Planck constant, and $\hat{V}$ is the potential operator)[3].

For example, consider the one-dimensional *infinite* potential well problem presented in [**2**]. Assume a particle of mass m is confined to an infinite tube of diameter L. By convention say the potential within is 0. Let the potential outside be $+\infty$, so that the particle can never escape no matter its kinetic energy.

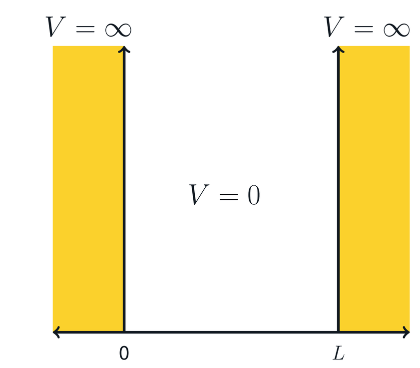

Fig. 3: 1-D potential well

Let $|\psi\rangle$ be the quantum state of the system, and ψ its associated wave function, *ie* it defines a probability amplitude. Hence, $\psi(x) = 0\ \forall x \notin (0, L)$ (value at the barriers is enforced by the continuity of ψ). We can now solve:

Time-independent Schrödinger's equation

$$\boxed{\hat{H}\,|\psi\rangle = E\,|\psi\rangle, \text{ with } E \text{ the energy of the system.}}$$

in one-dimension. Since $\hat{V} = 0$ within the tube, we get: $-\frac{\hbar}{2m}\frac{\mathrm{d}^2\psi(x)}{\mathrm{d}x^2} = E\psi(x)$, which yields $\psi(x) = A\sin(kx)$ by using the boundary conditions above. And $\psi(L) = 0$ enforces that k depends on $n \in \mathbb{N}$: $k_n = \pi n/L$.

Now, the particle has to be **somewhere** between 0 and L, and since ψ is a probability amplitude, this implies we need to normalize $\int_0^L \psi(x)^2\mathrm{d}x$ for it to equal 1. This condition enforces $A = \sqrt{2/L}$.

Now, the original ODE tells us that $k = \frac{\sqrt{2mE}}{\hbar}$

$\implies E = \frac{\hbar^2 k_n^2}{2m}$. Energy **is** quantified!

Fig. 4: Max Planck

Remarks

1. To use the quantum mechanics notation, often used with infinite-dimensional Hilbert spaces, denote by $|.\rangle$ vectors, and by $\langle .|.\rangle$ the inner product on the space.
2. This choice of function was inspired by that of the user robjohn in a post on the 14th of May 2013 on *Math StackExchange* [**5**]. I, however, tried to simplify the calculations as much as I could to make them easier, and aimed to add a geometrical meaning to that « trick ».
3. Note that $\hat{H}$ is an example of unbounded operator (as it is frequent in quantum physics). One can indeed easily find a bounded function whose laplacian is unbounded.

References

[1] J. Horvath, "On the Riesz-Fischer theorem," *University of Maryland*, Feb. 1942.
[2] F. L. Quéré, "Cours de mécanique quantique," *alpha.univ-mlv.fr/meca*, 2014.
[3] M. L. Bellac, *Physique Quantique, 2e édition.* CNRS Éditions, 2003, pp. 241–252.
[4] P. R. Helmos, *A Hilbert Space Problem Book.* D. Van Nostrand Company, Inc, 1974, pp. 130–136.
[5] *Post by robjohn*, `https://math.stackexchange.com/questions/384546/show-that-the-linear-operator-tfx-frac1-pi-int-0-infty-fracfy`, Accessed: 2019-06-02.