Sturm–Liouville problem

Differential equations and eigenvalue problems: given a second-order differential operator $\hat{\mathscr{L}}$, a function $\psi(x): \mathbb{R} \to \mathbb{C}$ and $\lambda \in \mathbb{C}$, the differential equation

$$\hat{\mathscr{L}}\psi(x) = \lambda\psi(x)$$

subject to *boundary* conditions, defines an *eigenvalue problem* (a problem such that a scalar λ has the same effect on ψ than an operator $\hat{\mathscr{L}}$). Compared to linear algebra of matrices, the differential operator $\hat{\mathscr{L}}$ is equivalent to a matrix ad the functions $\psi(x)$ are equivalent to eigenvectors (here called *eigenfunctions*). The functions $\psi(x)$ subject to the boundary conditions form a Hilbert space. The operator $\hat{\mathscr{L}}$ has a general form

$$\hat{\mathscr{L}} = p_0(x)\frac{d^2}{dx^2} + p_1(x)\frac{d}{dx} + p_2(x).$$

where we limit ourselves to the case $p_j(x): \mathbb{R} \to \mathbb{R}$, $j \in \{0,1,2\}$.

> *Example*: the spatial part of a standing wave must satisfy the differential equation $\frac{d^2\psi}{dx^2} + k^2\psi = 0$ subject to the boundary conditions $\psi(0) = \psi(l) = 0$. Defining $\hat{\mathscr{L}} = \frac{d^2}{dx^2}$, one has $\hat{\mathscr{L}}\psi = -k^2\psi$. The eigenvalues are then $\lambda = -k^2$. The solution to this equation are the eigenfunctions $\psi_n(x) = A\sin(n\pi x/l)$, with $k^2 = n^2\pi^2/l^2$, $n \in \mathbb{N}$. We can show that those functions are orthogonal, i.e., $\langle\psi_n, \psi_m\rangle = 0 \iff n \neq m$ within the interval $[0,l]$.

Hermitian adjoint operator: consider the inner product of two functions, $\langle\hat{\mathscr{D}}f, g\rangle$, where $\hat{\mathscr{D}}$ is a differential operator acting on g. An adjoint operator $\hat{\mathscr{D}}^\dagger$ is defined such that $\langle\hat{\mathscr{D}}f, g\rangle = \langle f, \hat{\mathscr{D}}^\dagger g\rangle$ + extra terms due to the boundaries. If those extra terms are zero, then the operator is called *Hermitian adjoint*. (Remember that the inner product has the complex conjugate defined, as well as an interval and a weight!)

Self-adjoint operator: an operator for which $\hat{\mathscr{D}}^\dagger = \hat{\mathscr{D}}$. A Hermitian self-adjoint operator is simply called Hermitian. It can be shown that $\hat{\mathscr{L}}$ is self-adjoint if $p_0'(x) = p_1(x)$. This means that one can write $\hat{\mathscr{L}} = \frac{d}{dx}\left[p_0(x)\frac{d}{dx}\right] + p_2(x)$.

Orthogonality of the eigenfunctions (case without weight function): consider a Hermitian operator $\hat{\mathscr{L}}$ that satisfies $\hat{\mathscr{L}}u = \lambda_u u$, $\hat{\mathscr{L}}v = \lambda_v v$, where $u, v: \mathbb{R} \to \mathbb{C}$; $u(x), v(x)$ and no weight. Then,

$$\int_a^b \bar{v}\hat{\mathscr{L}}u\,dx = \int_a^b [\bar{v}(p_0u')' + \bar{v}p_2u]dx$$

= (int. by parts) = $[\bar{v}p_0u']_a^b + \int_a^b [-\bar{v}'p_0u' + \bar{v}p_2u]dx$ = (another int. by parts) =

$\int_a^b \bar{v}\hat{\mathscr{L}}u = [\bar{v}p_0u' - \bar{v}'p_0u]_a^b + \int_a^b [(p_0\bar{v}')'u + \bar{v}p_2u]dx = [\bar{v}p_0u' - \bar{v}'p_0u]_a^b + \int_a^b \overline{(\hat{\mathscr{L}}v)}u\,dx$. The boundary terms must vanish if $\hat{\mathscr{L}}$ is Hermitian, by definition. We see that if u, v are eigenfunctions, we can write $(\lambda_u - \lambda_v)\int_a^b \bar{v}u\,dx = [p_0(\bar{v}u' - \bar{v}'u)]_a^b$. For $u \neq v$ and in general $\lambda_u \neq \lambda_v$, and if the boundary terms vanish, then $\langle v, u\rangle = 0$ (i.e, the eigenfunctions must be orthogonal).

Orthogonality of the eigenfunctions (with weight function): if the operator $\hat{\mathscr{L}}_{\text{nsa}}$ is not self-adjoint (nsa), then there can be a function $w(x)$ (the weight function) such that, when $w(x)\hat{\mathscr{L}}_{\text{nsa}}\psi(x) = w(x)\lambda\psi(x)$, it makes the operator self-adjoint (sa) (i.e., $\hat{\mathscr{L}}_{\text{sa}} = w\hat{\mathscr{L}}_{\text{nsa}}$). One can show that such a function is $w(x)=p_0^{-1}(x)\exp\left[\int\frac{p_1(x)}{p_0(x)}dx\right]$. The equation becomes $(p(x)\psi_n'(x))'=-(s(x)+\lambda_n w(x))\psi_n(x)$ and after the same procedure as the case without the weight function, we find $p(x)[\psi_m(x)\psi_n'(x)-\psi_m'(x)\psi_n(x)]_a^b=(\lambda_m-\lambda_n)\int_a^b dx\, w(x)\,\psi_{\lambda_n}(x)\,\psi_{\lambda_m}(x)$, meaning that the inner product requires the weight function for the functions to be considered orthogonal.

Sturm-Liouville equation: The second-order linear ordinary differential equation $\hat{\mathscr{L}}[y(x)]=-\lambda w(x)y(x)$ with the Hermitian operator $\hat{\mathscr{L}}:=\frac{d}{dx}\left[p(x)\frac{d}{dx}\right]-s(x)$, subject to suitable boundary conditions, is called a *Sturm-Liouville problem*. (Note: from now on, $\lambda\to-\lambda$)

Comment: the boundary conditions must be such that $[p(\bar{v}u'-\bar{v}'u)]_a^b$ for two eigenfunctions. There are several possibilities. For real eigenfunctions, here are some examples:

- *Dirichlet boundary conditions*: $u(a)=u(b)=v(a)=v(b)=0$
- *Neumann boundary conditions:* $u'(a)=u'(b)=v'(a)=v'(b)=0$
- *Periodic boundary conditions:* $p(a)=p(b);\ \ v(a)=v(b);\ \ v'(a)=v'(b)$
- Other combinations of the eigenfunctions or their derivatives such that the term in the parenthesis is zero at the boundaries
- Making $p(x)$ to be zero at the boundaries.

Series expansion of a function: one can develop a given function $f(x)$ into a series (i.e., set the function as the limit value to which the series must converge) of a set of (orthogonal) eigenfunctions $\{g_k(x)\}$ ($k\in\mathbb{Z}$) that form the basis of a vector space:

$$f(x)=\sum_k c_k g_k(x).$$

The limit of the series can be, e.g., from $k=-\infty$ to ∞, or from $k=0$ to ∞. If the eigenfunctions are not orthonormal, one can find the normalization constant N_k as $N_k^2=\langle g_k,g_k\rangle$. The coefficients $c_k\in\mathbb{C}$ can be found using the inner product (multiplying from the right by $g_\ell(x)$ with a different index $\ell\in\mathbb{Z}$):

$$\langle f(x),g_\ell(x)\rangle=\sum_k c_k\langle g_k(x),g_\ell(x)\rangle=\sum_k c_k N_k^2\delta_{\ell k}\quad (\delta_{\ell k}\text{ is the Kronecker delta}).$$

$$\implies c_\ell=\langle f(x),g_\ell(x)\rangle/N_\ell^2.$$

Classical orthogonal polynomials: there are some orthogonal polynomials $C_n(x)$ that satisfy the Sturm-Liouville equation and are called *classical orthogonal polynomials*. Remember: there are functions that satisfy the Sturm-Liouville equation and that are not polynomials.

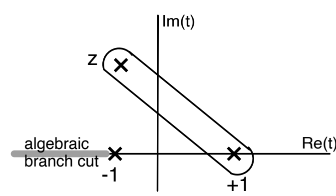
Generalized Rodrigues's formula: $C_n(x)=\frac{K_n}{w}\frac{d^n}{dx^n}[wp_0^n]$. Where: $p_0(x):\mathbb{R}\to\mathbb{R}$ is a polynomial of degree ≤ 2 with only real roots; $w(x):\mathbb{R}\to\mathbb{R}$ strictly positive function ("weight function"), integrable within $[a,b]$ and such that $w(a)s(a)=0=w(b)s(b)$; $C_1(x)$ is a first-degree polynomial in x. The generalized Rodrigues's formula generates classical orthogonal polynomials in the interval $[a,b]$. The constant K_n depends on the standard normalization of the polynomials (chosen so for historical reasons).

Comment: It can be proven that the Rodrigues's formula generates polynomials that satisfy the differential equation $(wp_0C_n')'=w\lambda_nC_n$, i.e., they satisfy a Sturm-Liouville problem.

Generating function: it is also possible to generate all orthogonal polynomials that satisfy a given Sturm-Liouville problem by repeated differentiations of a *generating function* $g(x,t)$ that can be expanded as $g(x,t) = \sum_{n=0}^{\infty} a_n t^n C_n(x)$ with some constants a_n. Note that the ***nth*** derivative w.r.t. ***t*** brings out the polynomials and changes of variables to the index in the series create terms like C_{n-1} or C_{n+1}. This means that derivatives of the generating function can create recurrence relations.

Schläfli representation: in order to extend the definition of orthogonal polynomials to the complex plane, we start by the complex Rodrigues's formula, $C_n(z) = \frac{K_n}{w(z)} \frac{d^n}{dz^n}[w(z)(p_0(z))^n]$, $n \in \mathbb{N}_0$, $z \in \mathbb{Z}$ ($\implies C_n(z) : \mathbb{Z} \to \mathbb{Z}$ because $C_n(z)$ is a polynomial). Using Cauchy's integral formula $\oint_{|z-z_0|=r} \frac{f(z)}{(z-z_0)^{n+1}} dz = 2\pi i f^{(n)}(z_0)/n!$ to integrate n times, we find $C_n(z) = \frac{K_n}{w(z)} \frac{n!}{2\pi i} \oint_C \frac{w(y)[p_0(y)]^n}{(y-z)^{n+1}} dy$, where C encloses the point z, $y \in \mathbb{C}$ and the numerator inside the integral is analytic on and within C.

Example: contrary to the Rodrigues's formula, the Schläfli representation doesn't need $n \in \mathbb{N}_0$ to make sense. Therefore, one can use the Schläfli representation for generalizing a polynomial to a function with non-integer values of n. As a concrete example, consider the Legendre polynomials. Substituting from the table, we find $P_\nu(z) = \frac{1}{2\pi i} \oint_C \frac{1}{2^\nu} \frac{(t^2-1)^\nu}{(t-z)^{\nu+1}} dt$. The contour is in the figure on the right. Generalizing for $\nu \in \mathbb{R}$ and using the change of variable $t = z + \sqrt{z^2-1}\, e^{i\phi}$, it is possible to show that $P_{-1/2}(x)$ can be written as an elliptical integral $\frac{2}{\pi} K(\sqrt{(1-x)/2})$, which is another kind of special function. Integral representations are useful for finding relations (sometimes unexpected) between special functions.



Schläfli integral for non-polynomials and its relation to generating functions: the Bessel functions of the first kind are not polynomials, but they have a generating function $g(x,t) = e^{(x/2)(t-1/t)} = \sum_n J_n(x) t^n$ (see table). If we apply the residue theorem to an integral containing the generating function, we get $\oint_C \frac{e^{(x/2)(t-1/t)}}{t^{n+1}} dt = \oint_C \sum_m J_m(x) t^{m-n-1} = 2\pi i J_n(x)$ with C encircling $t = 0$. With the change of variable $t = e^{i\theta} \implies e^{(x/2)(t-1/t)} = e^{ix\sin\theta}$, and C being the unit circle, we find $2\pi i J_n(x) = \int_0^{2\pi} e^{i(x\sin\theta - n\theta)} i\, d\theta$ in general for $x \in \mathbb{C}$ or $J_n(x) = \frac{1}{\pi}\int_0^{\pi} \cos(x\sin\theta - n\theta) d\theta$ for $x \in \mathbb{R}$. In this case, the generating function was used to get (a) Schläfli representation, but we can also derive generating functions (for example, for polynomials) using the/a Schläfli representation.

References

- Dennery, P., Krzywicki, A. (1967) *Mathematics for Physicists.* Dover publications.
- Lang, C.B., Pucker, N. (2016) *Mathematische Methoden in der Physik* (3.ª ed., en alemán). Springer.
- Hassani, S. (1999) *Mathematical Physics.* Springer.
- Korn, G.A.; Korn, T.M. (1968) *Mathematical handbook for scientists and engineers.* Dover publications.
- Boas, M. (1983) *Mathematical Methods in the Physical Sciences.* Wiley.
- Weber & Arfken (2003) *Essential Mathematical Methods for Physicists.* Academic Press.

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Some (definitely not all!) **orthogonal polynomials and eigenfunctions of the Sturm-Liouville problem**

Polynomial/ Function	**Interval**	$w(x)$	$p(x)$ **(nb 1)**	$s(x)$	λ	**Standard normalization** N^2	**Generating function (nb 2)**	K_n **for Rodrigues's formula**
Harmonic $\{e^{inx}\}$	$[-\pi,\pi]$	1	1	0	n^2	π	-	not a polynomial
Legendre $P_l(x)$	$[-1,1]$	1	$1-x^2$	0	$l(l+1)$	$\frac{2}{2l+1}$	$(1-2xt+t^2)^{-1/2}$	$\frac{1}{2^l l!}\cdot(-1)^l$ **(nb 3)**
Associated Legendre $P_l^m(x)$	$[-1,1]$	1	$1-x^2$	$\frac{m^2}{1-x^2}$	$l(l+1)$	$\frac{2}{2l+1}\cdot\frac{(l+m)!}{(l-m)!}$	Modifications needed. Main definition: $P_l^m(x)=(-1)^m\frac{d^m}{dx^m}P_l(x)$	
Bessel of the first kind $J_p(x)$	$[0,1]$	x	x	$-\frac{p^2}{x}$	1 **(nb 4)**	$\int_0^1[J_p(ax)]^2x\,dx$ $=\frac{1}{2}[J_p'(a)]^2$ (boundary condition $J_p(a)=0$) **(nb 5)**	$e^{(x/2)(t-1/t)}$	not a polynomial
Laguerre $L_n(x)$	$[0,\infty]$	e^{-x}	xe^{-x}	0	n	1	$\frac{e^{-xt/(1-t)}}{1-t}$, $a_n=1/n!$	$\frac{1}{n!}$
Associated Laguerre $L_n^k(x)$ **(nb 6)**	$[0,\infty]$	x^ke^{-x}	$x^{k+1}e^{-x}$	0	$-n$	$\frac{(n+k)!}{n!}$	$\frac{e^{-xt/(1-t)}}{(1-t)^{k+1}}$, $a_n=1/n!$	$\frac{1}{n!}$
Hermite $H_n(x)$ **(nb 7)**	$[-\infty,\infty]$	e^{-x^2}	e^{-x^2}	0	$2n$	$2^n\pi^{1/2}n!$	e^{-t^2+2tx}, $a_n=1/n!$	$(-1)^n$
Chebyshev polynomials $T_n(x)$	$[-1,1]$	$\frac{1}{\sqrt{1-x^2}}$	$(1-x^2)^{\frac{1}{2}}$	0	$-n^2$	$\pi/2$, if $n\neq 0$; π, if $n=0$	$\frac{1-tx}{1-2tx+t^2}$	$\frac{(-2)^n n!}{(2n)!}$

Checked against: Weber & Arfken (2003) *Essential Mathematical Methods for Physicists*, Academic Press. Chapters 9-13.
The Chebyshev polynomials are taken from Korn & Korn (1968) *Mathematical handbook...* , table 21.7-1.
However: please be careful and always check.

(nb 1) Warning, when computing the Rodrigues's formula: $p_0(x)=p(x)/w(x)$.
(nb 2) Here, $a_n=1$ in the respective series expansion, unless otherwise specified. Warning: generating functions are not unique.
(nb 3) In most books, they take in Rodrigues's formula $p_0(x)\to -p_0(x)$ and therefore they show no factor $(-1)^l$ in K_l. However, they only do it in the Rodrigues's formula and not in the differential equation, so this is why we prefer to modify the K_l and introduce the minus sign there instead.
(nb 4) It is customary to make the change of variables $x=k\rho\implies\frac{d}{dx}=\frac{1}{k}\frac{d}{d\rho}$. After this change of variables, $\lambda=k^2$ and the interval is rescaled to $[0,\alpha]$ where the boundary condition is now $J_p(k\alpha)=0$. Then, the normalization changes to $\int_0^\alpha\rho[J_p(k\rho)]^2d\rho=\frac{\alpha^2}{2}\left[J_p'(c_{pm})\right]^2$ where c_{pm} are the zeros of the Bessel function.
(nb 5) See also nb 4. Because of recurrence formulae, one can express the normalization in other ways, for example, in terms of $J_\nu'(k_{\mu\nu})=-J_{\nu+1}(k_{\nu\mu})$. The orthogonalization is achieved by considering Dirichlet boundary conditions, i.e., $J_\nu(ka)=0$. The Bessel function is oscillatory, so one needs to choose a zero at the right distance a to satisfy the boundary condition.
(nb 6) Similarly to the case of the associated Legendre polynomials, the Associated Laguerre polynomials are defined in terms of a derivative of the Laguerre polynomials, namely, $L_n^k(x)=(-1)^k\frac{d^k}{dx^k}L_{k+n}(x)$.
(nb 7) There is an alternative way of defining the Hermite polynomials and its differential equation. Here we take the "Physicist Hermite polynomials".

Generalized Bessel ODE

The ODE $y'' + \frac{1-2a}{x} y' + \left[(bcx^{c-1})^2 + \frac{a^2 - p^2c^2}{x^2} \right] y = 0$
with $a, b, c, p \in \mathbb{C}$ has the solution $y(x) = x^a Z_p(bx^c)$, where Z_p is a combination of Bessel $[J_p(x)]$ and Neumann $[Y_p(x) = (\cos(\pi p) J_p(x) - J_{-p}(x))/\sin(\pi p)]$ functions (multiplied by constants).

Equation	**Solutions**	a	b	c	p
Bessel	$J_p(x), Y_p(x)$ $H_p^{(1,2)} = J_p(x) \pm i Y_p(x)$	0	1	1	p
Bessel (rescaled)	$J_p(k\rho), Y_p(k\rho), H_p(k\rho)$	0	k	1	p
Modified Bessel	$I_p(x) = i^{-p} J_p(ix)$ $K_p(x) = \frac{\pi}{2} i^{p+1} H_p^{(1)}(ix)$	0	i	1	p
Spherical Bessel	$j_n(x) = \sqrt{\frac{\pi}{2x}} J_{(2n+1)/2}(x)$ $y_n(x) = \sqrt{\frac{\pi}{2x}} Y_{(2n+1)/2}(x)$ $h_n^{(1,2)} = j_n(x) \pm i y_n(x)$	$-1/2$	1	1	$n + \frac{1}{2}, n \in \mathbb{Z}$
Ber, bei, ker, kei functions	$J_0(i^{3/2}x) = \mathrm{ber}\, x + i\, \mathrm{bei}\, x$ $K_0(i^{3/2}x) = \mathrm{ker}\, x + i\, \mathrm{kei}\, x$	0	$i^{3/2}$	1	0