We recall the basic steps of the method of separation of variables.

1. Search for basic solutions that are the products of one-variable functions using the equation and an appropriate subset of the initial/boundary conditions. Ideally, only countably many (that is, can be numbered by natural or integer numbers) such solutions exist.
2. Use the remaining initial/boundary conditions to determine an infinite sum involving the basic solutions.
3. Verify that this infinite sum indeed corresponds to a function and this function indeed satisfies the equation together with the initial/boundary conditions.

The first two steps are emphasized in our lectures, and the third step involves much mathematical theory and interested readers should take higher level PDE courses or consult more advanced books.

1. General boundary value problem.

We have seen that the method of separation of variables, with the help of the theory of Fourier series, can be applied to a wide variety of PDEs. However a closer inspection reveals that all of our previous examples have the following boundary conditions:

$$u(0,t)=u(l,t)=0. \tag{1}$$

How about problems with other boundary conditions? Let's check some examples.

Example 1. Consider the heat equation

$$\begin{aligned} u_t &= \kappa\, u_{xx} && 0<x<l, t>0 && (2)\\ u(x,0) &= f(x) && 0\leqslant x\leqslant l, && (3)\\ u_x(0,t) &= 0 && t\geqslant 0, && (4)\\ u_x(l,t) &= 0 && t\geqslant 0. && (5)\end{aligned}$$

This system models the change of temperature along a rod of length l whose both ends are insulated.
Solution. We apply the method of separation of variables. As we have seen, the method consists of the following steps:

1. First we try to find non-zero "basic" solutions whose variables are separated:

   $$u=X(x)\,T(t). \tag{6}$$

   Substituting this into the equation we obtain

   $$T'(t)\,X(x)=\kappa\,T(t)\,X''(x) \iff \frac{T'(t)}{T(t)}=\kappa\,\frac{X''(x)}{X(x)}. \tag{7}$$

   Thus we need to solve the ODE

   $$X''(x)-\lambda\,X(x)=0 \tag{8}$$

   with boundary conditions

   $$X'(0)=X'(t)=0. \tag{9}$$

   The solutions are

   $$\cos\Big(\frac{n\,\pi}{l}\,x\Big), \qquad n=0,1,2,\ldots \tag{10}$$

   Note that the sum starts from 0.

2. Represent the solution by an infinite sum.
   As $\lambda_n=-\left(\frac{n\,\pi}{l}\right)^2$, we see that

   $$T_n(t)=e^{-\left(\frac{n\,\pi}{l}t\right)} \tag{11}$$

   and therefore formally

   $$u(x,t)=\sum_{n=0}^{\infty} a_n\,e^{-\left(\frac{n\,\pi}{l}t\right)}\cos\Big(\frac{n\,\pi}{l}\,x\Big). \tag{12}$$

The coefficients a_n is determined by requiring

$$f(x) = \sum_{n=0}^{\infty} a_n \cos\left(\frac{n\,\pi}{l}\,x\right). \tag{13}$$

Noticing that this is simply a cosine series, we see that the coefficients can be computed through

$$a_n = \frac{2}{l} \int_0^l f(x) \cos\left(\frac{n\,\pi}{l}\,x\right) \qquad n > 0 \tag{14}$$

and

$$a_0 = \frac{1}{l} \int_0^l f(x)\,\mathrm{d}x. \tag{15}$$

We will see now that for other, more complicated, boundary conditions, the theory of Fourier series is not enough anymore.

Example 2. We still consider the heat equation modeling a rod. This time the temperature at 0 is kept 0 while the other end ($x = l$) is in contact with a medium of tempature 0.

$$\begin{aligned} u_t &= \kappa\, u_{xx} && 0 < x < l, t > 0 && (16)\\ u(x,0) &= f(x) && 0 \leqslant x \leqslant l, && (17)\\ u(0,t) &= 0 && t \geqslant 0, && (18)\\ u_x(l,t) &= -h\, u(l,t). && t \geqslant 0. && (19) \end{aligned}$$

Here $h > 0$.
Solution. Applying the method of separation of variables, we reach

$$X'' - \lambda\, X = 0, \qquad X(0) = 0, \quad h\, X(l) + X'(l) = 0. \tag{20}$$

We discuss the cases:

i. $\lambda > 0$. The general solution is

$$A\, e^{\sqrt{\lambda} x} + B\, e^{-\sqrt{\lambda} x}. \tag{21}$$

Now

$$X(0) = 0 \implies A + B = 0 \tag{22}$$

$$h\, X(l) + X'(l) = 0 \implies \left(h + \sqrt{\lambda}\right) e^{\sqrt{\lambda} l} A + \left(h - \sqrt{\lambda}\right) e^{-\sqrt{\lambda} l} B = 0. \tag{23}$$

The two equations can be written

$$\begin{pmatrix} 1 & 1 \\ \left(h + \sqrt{\lambda}\right) e^{\sqrt{\lambda} l} & \left(h - \sqrt{\lambda}\right) e^{-\sqrt{\lambda} l} \end{pmatrix} \begin{pmatrix} A \\ B \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \end{pmatrix}. \tag{24}$$

For the solution to be non-zero, we have to have

$$0 = \det \begin{pmatrix} 1 & 1 \\ \left(h + \sqrt{\lambda}\right) e^{\sqrt{\lambda} l} & \left(h - \sqrt{\lambda}\right) e^{-\sqrt{\lambda} l} \end{pmatrix} = \left(h - \sqrt{\lambda}\right) e^{-\sqrt{\lambda} l} - \left(h + \sqrt{\lambda}\right) e^{\sqrt{\lambda} l}. \tag{25}$$

As $h > 0$ and $\sqrt{\lambda} > 0$, this is not possible.

ii. $\lambda = 0$. The general solution is

$$A + B\, x \tag{26}$$

The boundary conditions lead to

$$A = 0, \qquad h\, A + (h\, l + 1)\, B = 0 \implies A = B = 0. \tag{27}$$

iii. $\lambda < 0$. The general solution is

$$A\cos\left(\sqrt{-\lambda}\,x\right) + B\sin\left(\sqrt{-\lambda}\,x\right). \tag{28}$$

Now

$$X(0) = 0 \iff A = 0, \tag{29}$$

$$h\,X(l) + X'(l) = 0 \iff h\sin\left(\sqrt{-\lambda}\,l\right) + \sqrt{-\lambda}\,\cos\left(\sqrt{-\lambda}\,l\right) = 0. \tag{30}$$

Therefore the solution is of the form $X = \sin(p\,x)$ with p satisfying

$$\tan(p\,l) = -p/h. \tag{31}$$

It is easy to see that the solutions form an infinite series

$$0 < p_1 < p_2 < \cdots < \cdots \tag{32}$$

Therefore our solution to the PDE can be written as

$$\sum_1^\infty b_n\,e^{-\kappa p_n^2 t}\sin(p_n\,x) \tag{33}$$

where b_n is determined by

$$f(x) = \sum_1^\infty b_n \sin(p_n\,x). \tag{34}$$

Now how should we determine b_n? And furthermore how can we know whether the infinite sum gives the solution – or equivalently whether similar properties as those hold for the Fourier series hold for our series with $\sin(p_n\,x)$? Keep in mind that it is not possible to obtain a formula for the p_ns.

Mimicking what we have done before, we compute, for $n \neq m$,

$$\begin{aligned}\int_0^l \sin(p_n\,x)\sin(p_m\,x)\,\mathrm{d}x &= \frac{1}{2}\int_0^l [\cos(p_n - p_m)\,x - \cos(p_n + p_m)\,x]\,\mathrm{d}x \\ &= \frac{1}{2}\left[\frac{\sin(p_n - p_m)\,l}{p_n - p_m} - \frac{\sin(p_n + p_m)\,l}{p_n + p_m}\right] \\ &= \frac{1}{2}\left[\frac{\sin(p_n\,l)\cos(p_m\,l) - \sin(p_m\,l)\cos(p_n\,l)}{p_n - p_m}\right. \\ &\quad \left. - \frac{\sin(p_n\,l)\cos(p_m\,l) + \sin(p_m\,l)\cos(p_n\,l)}{p_n + p_m}\right].\end{aligned} \tag{35}$$

Now using the fact that

$$h\sin(p_n\,l) + p_n\cos(p_n\,l) = 0 \Longrightarrow \sin(p_n\,l) = -\frac{p_n}{h}\cos(p_n\,l) \tag{36}$$

we have

$$\int_0^l \sin(p_n\,x)\sin(p_m\,x)\,\mathrm{d}x = 0. \tag{37}$$

Therefore we can determine b_n by

$$b_n = \frac{\int_0^l f(x)\sin(p_n\,x)\,\mathrm{d}x}{\int_0^l \sin^2(p_n\,x)\,\mathrm{d}x}. \tag{38}$$

But a convergence theory similar to that of the Fourier series is clearly beyond us here.

Example 3. Consider the heat equation in a 2D disc $x^2 + y^2 \leqslant 1$:

$$\begin{aligned} u_t &= \kappa\,(u_{xx} + u_{yy}) && (39) \\ u(x,y,0) &= f(x,y) && (40) \\ u(x,y,t) &= 0 \qquad x^2 + y^2 = 1. && (41)\end{aligned}$$

Solution. Due to the special geometry of the domain, it is natural to consider the problem using polar coordinates (r, θ) satisfying

$$x = r\cos\theta, \quad y = r\sin\theta. \tag{42}$$

Now we change the variables from x, y to r, θ. Differentiating the above relation we have

$$\begin{aligned}(\cos\theta)\, r_x - r\,(\sin\theta)\,\theta_x &= 1 & (43)\\ (\cos\theta)\, r_y - r\,(\sin\theta)\,\theta_y &= 0 & (44)\\ (\sin\theta)\, r_x + r\,(\cos\theta)\,\theta_x &= 0 & (45)\\ (\sin\theta)\, r_y + r\,(\cos\theta)\,\theta_y &= 1 & (46)\end{aligned}$$

consequently

$$r_x = \frac{x}{r}, \quad r_y = \frac{y}{r}, \quad r_{xx} = \frac{1}{r} - \frac{x^2}{r^3}, \quad r_{yy} = \frac{1}{r} - \frac{y^2}{r^3}; \tag{47}$$

$$\theta_x = -\frac{\sin\theta}{r} = -\frac{y}{r^2}, \quad \theta_y = \frac{\cos\theta}{r} = \frac{x}{r^2}, \quad \theta_{xx} = \frac{2\,x\,y}{r^4}, \quad \theta_{yy} = -\frac{2\,x\,y}{r^4}$$

Therefore

$$\begin{aligned} u_{xx} &= u_{rr}\frac{x^2}{r^2} - u_{r\theta}\frac{2\,x\,y}{r^3} + u_{\theta\theta}\frac{y^2}{r^4} + u_r\left(\frac{1}{r} - \frac{x^2}{r^3}\right) + u_\theta\frac{2\,x\,y}{r^4}, & (48)\\ u_{yy} &= u_{rr}\frac{y^2}{r^2} + u_{r\theta}\frac{2\,x\,y}{r^3} + u_{\theta\theta}\frac{x^2}{y^4} + u_r\left(\frac{1}{r} - \frac{y^2}{r^3}\right) + u_\theta\left(-\frac{2\,x\,y}{r^4}\right). & (49)\end{aligned}$$

The equation and the initial-boundary conditions in polar coordinate form are

$$\begin{aligned} u_t &= \kappa\left(u_{rr} + \frac{1}{r}u_r + \frac{1}{r^2}u_{\theta\theta}\right) & (50)\\ u(r,\theta,0) &= f(r,\theta) & (51)\\ u(1,\theta,t) &= 0. & (52)\end{aligned}$$

We apply separation of variables to solve this equation.

First we try to find non-trivial "basic" solutions of the form

$$u(r,\theta,t) = R(r)\,\Theta(\theta)\,T(t). \tag{53}$$

Substituting this into the equation we reach

$$R(r)\,\Theta(\theta)\,T'(t) = \kappa\left(R''(r)\,\Theta(\theta) + \frac{1}{r}R'(r)\,\Theta(\theta) + \frac{1}{r^2}R(r)\,\Theta''(\theta)\right)T(t). \tag{54}$$

Dividing both sides by $R(r)\,\Theta(\theta)\,T(t)$ we reach

$$\frac{T'(t)}{T(t)} = \kappa\left(\frac{R''(r)}{R(r)} + \frac{1}{r}\frac{R'(r)}{R(r)} + \frac{1}{r^2}\frac{\Theta''(\theta)}{\Theta(\theta)}\right). \tag{55}$$

As the LHS only involves t and the RHS only r, θ there is a constant λ such that

$$\frac{T'(t)}{T(t)} = -\kappa\,\lambda \tag{56}$$

and

$$\frac{R''(r)}{R(r)} + \frac{1}{r}\frac{R'(r)}{R(r)} + \frac{1}{r^2}\frac{\Theta''(\theta)}{\Theta(\theta)} = -\lambda. \tag{57}$$

Multiply both sides by r^2 we have

$$\frac{r^2\,R''(r)}{R(r)} + \frac{r\,R'(r)}{R(r)} + \lambda\,r^2 = \frac{\Theta''(\theta)}{\Theta(\theta)}. \tag{58}$$

The LHS only involves r and the RHS only θ. Thus there is a constant μ such that

$$\frac{\Theta''(\theta)}{\Theta(\theta)} = \mu, \qquad \frac{r^2\,R''(r)}{R(r)} + \frac{r\,R'(r)}{R(r)} + \lambda\,r^2 = -\mu. \tag{59}$$

As $\Theta(\theta)$ is obviously 2π periodic, we have

$$\mu = -n^2, \qquad n = 1, 2, 3, \ldots \tag{60}$$

and

$$\Theta(\theta) = A\cos(n\theta) + B\sin(n\theta). \tag{61}$$

On the other hand, the equation for R now becomes

$$r^2 R'' + r R' + \left(\lambda r^2 - n^2\right) R = 0, \tag{62}$$

with the boundary condition

$$R(1) = 0. \tag{63}$$

Now it is clear that the success of our method depends on the following:

1. For each n, we have $\lambda_{n,k}$, such that the above equation has a solution $R_{n,k}$;
2. The initial data $f(r,\theta)$ have the following expansion

   $$f(r,\theta) = \sum_{n,k} a_{n,k} R_{n,k}(r)\cos(n\theta) + b_{n,k} R_{n,k}\sin(n\theta). \tag{64}$$

   As we can always expand $f(r,\theta)$ into Fourier series

   $$f(r,\theta) = \sum_n A_n(r)\cos(n\theta) + B_n(r)\sin(n\theta), \tag{65}$$

   The requirement becomes expanding

   $$A_n(r) = \sum_k a_{n,k} R_{n,k}(r), \quad B_n(r) = \sum_k b_{n,k} R_{n,k}(r). \tag{66}$$

3. The resulting infinite double summation

   $$\sum_{n,k} \left[a_{n,k} R_{n,k}(r)\cos(n\theta) + b_{n,k} R_{n,k}\sin(n\theta)\right] e^{-\lambda_{n,k} t} \tag{67}$$

   indeed gives the solution.

Clearly we see that a Fourier-type theory of the functions $R_{n,k}$ is crucial to the success of our method. We will see soon that these $R_{n,k}$'s are the so-called Bessel functions, which often arise in PDEs on discs and cylinders.

From the above example we see that as soon as the system becomes more and more complicated, the theory of Fourier series helps less and less. For simpler ones, we can still develop ad hoc theories following the idea of Fourier series, but for more complicated ones, it seems very hard to do things "on the fly". In particular, a complete understanding of solutions to equations like

$$r^2 R'' + r R' + \left(\lambda r^2 - n^2\right) R = 0 \tag{68}$$

is needed. Such understanding is obtained from the following Sturm-Liouville theory.

2. Sturm-Liouville theory.

The standard Sturm-Liouville (SL) problem is of the form

$$\begin{aligned}(p(x)\,y')' + q(x)\,y + \lambda\, r(x)\,y &= 0, \qquad a < x < b & (69)\\ \alpha_0\, y(a) + \alpha_1\, y'(a) &= 0, & (70)\\ \beta_0\, y(b) + \beta_1\, y'(b) &= 0. & (71)\end{aligned}$$

where all the functions and numbers are real. For simplicity we assume the coefficients are as smooth as we need.

The problem is called

- *regular* when p, q, r are bounded on $[a, b]$ (that is the interval $a \leqslant x \leqslant b$), $p, r > 0$ for all $a \leqslant x \leqslant b$, and α_0, α_1 real, not both 0, and β_0, β_1 real, not both 0.
- *singular* when any one or more of the following happens
  - → The interval (a, b) is infinite, that is either $a = -\infty$ or $b = +\infty$ or both occurs.
  - → $p(x) = 0$ for some $x \in [a, b]$ or $r(x) = 0$ for some $x \in [a, b]$.
  - → One or several coefficient function becomes ∞ at a or b, or both.

Example 4. We check the systems we have dealt with

-
$$y'' + \lambda\, y = 0, \qquad y(0) = y(l) = 0 \tag{72}$$
We have
$$a = 0,\ b = l;\ p(x) = 1,\ q(x) = 0,\ r(x) = 1;\ \alpha_0 = 1,\ \alpha_1 = 0,\ \beta_0 = 1,\ \beta_1 = 0. \tag{73}$$
The system is a regular SL problem.

-
$$y'' + \lambda\, y = 0, \qquad y'(0) = y'(l) = 0 \tag{74}$$
We have
$$a = 0,\ b = l;\ p(x) = 1,\ q(x) = 0,\ r(x) = 1;\ \alpha_0 = 0,\ \alpha_1 = 1,\ \beta_0 = 0,\ \beta_1 = 1. \tag{75}$$
This is also a regular SL problem.

-
$$y'' + \lambda\, y = 0, \qquad y(0) = 0,\ y'(l) = -h\, y(l). \tag{76}$$
We have
$$a = 0,\ b = l;\ p(x) = 1,\ q(x) = 0,\ r(x) = 1;\ \alpha_0 = 1,\ \alpha_1 = 0,\ \beta_0 = h,\ \beta_1 = 1. \tag{77}$$

-
$$x^2\, y'' + x\, y' + \left(\lambda\, x^2 - n^2\right) y = 0, \qquad y(0) \text{ bounded},\ y(1) = 0. \tag{78}$$
At first sight this problem is not an SL problem. However we can transform it through the following operations:

We search for a multiplier $h(x)$ such that
$$h(x) \left[x^2\, y'' + x\, y' + \left(\lambda\, x^2 - n^2\right) y\right] = (p\, y')' + q\, y + \lambda\, r\, y. \tag{79}$$
Comparing the two sides, we have
$$h(x)\, x^2 = p(x), \qquad h(x)\, x = p(x)' \tag{80}$$
which leads to
$$p(x)' = \frac{1}{x}\, p(x) \implies p(x) = x \implies h(x) = \frac{1}{x}. \tag{81}$$
Thus we see that the equation is equivalent to
$$(x\, y')' - \frac{n^2}{x}\, y + \lambda\, x\, y = 0 \tag{82}$$
which corresponds to
$$a = 0,\ b = 1;\ p(x) = x,\ q(x) = -\frac{n^2}{x},\ r(x) = x;\ \beta_0 = 1,\ \beta_1 = 0. \tag{83}$$
This is a singular SL problem.

Any λ that the problem has non-trivial solutions is called an eigenvalue, the corresponding solutions are called eigenfunctions.

2.1. Properties of regular Sturm-Liouville problems.

We see from the following theorem that the solutions to a SL problem enjoy similar properties as the functions $\sin\left(\frac{n\pi}{l}x\right)$ and $\cos\left(\frac{n\pi}{l}x\right)$ in the Fourier series.

Theorem 5. *A regular SL problem has the following properties.*

1. *It has nonzero solutions for a countably infinite set of values of λ. These eigenvalues are all real. The set of eigenvalues does not have any limit points. These eigenvalues are bounded from below if $\alpha_0\,\alpha_1 \leqslant 0$ and $\beta_0\,\beta_1 \geqslant 0$. These eigenvalues are bounded from below by 0 if furthermore $q \leqslant 0$.*
2. *For each fixed eigenvalue λ, the solution space is one-dimensional. That is, there is y_λ such that all other solutions for the same λ is a multiple of y_λ.*
3. *If we enumerate the eigenvalues as $\lambda_1, \lambda_2, \ldots$, then for each λ_n we can pick one eigenfunction φ_n. These eigenfunctions satisfy*

   a) $\displaystyle\int_a^b \varphi_n(x)\,\varphi_m(x)\,r(x)\,\mathrm{d}x = 0$ *for any $n \neq m$.*

   b) *For any f having two continuous derivatives on $[a,b]$ and satisfying the boundary conditions, the infinite sum*

   $$\sum_{n=1}^{\infty} c_n\,\varphi_n \tag{84}$$

   where

   $$c_n = \frac{\int_a^b f(x)\,\varphi_n(x)\,r(x)\,\mathrm{d}x}{\int_a^b \varphi_n(x)^2\,r(x)\,\mathrm{d}x} \tag{85}$$

   converges absolutely uniformly to $f(x)$. By "absolutely uniformly" we mean

   $$\sum_1^{\infty} |c_n|\,|\varphi_n| < \infty \tag{86}$$

   and the convergence to f is uniform.

   c) *The only continuous function f on $[a,b]$ with $\int_a^b f(x)\,\varphi_n(x)\,r(x)\,\mathrm{d}x = 0$ for all n is $f \equiv 0$.*

   d) *If φ_n's are chosen such that*

   $$\int_a^b \varphi_n(x)^2\,r(x)\,\mathrm{d}x = 1 \tag{87}$$

   We have the following Parseval-type relation

   $$\int_a^b f(x)^2\,r(x)\,\mathrm{d}x = \sum_{n=1}^{\infty} |c_n|^2. \tag{88}$$

Proof. The proofs for many of the above claims are either too technical or beyond our course. We omit them.

1. Properties of the eigenvalues.
   - It has nonzero solutions for a countably infinite set of values of λ.

     Omitted. Interested readers should check §1.3 of Anthony W. Knapp **Advanced Real Analysis**.
   - These eigenvalues are all real.

Let λ be an eigenvalue and let φ be a corresponding eigenfunction. We compute

$$\begin{aligned} 0 &= \int_a^b \left[(p\,y')' + q\,y + \lambda\,r\,y \right] \bar{y}\,\mathrm{d}x \\ &= \int_a^b (p\,y')'\,\bar{y} + \int_a^b q\,|y|^2 + \lambda \int_a^b r\,|y|^2 \\ &= (p\,y')\,\bar{y}\,|_a^b - \int_a^b p\,y'\,\bar{y}\,' + \int_a^b q\,|y|^2 + \lambda \int_a^b r\,|y|. \end{aligned} \tag{89}$$

On the other hand, taking the complex conjugate of

$$(p\,y')' + q\,y + \lambda\,r\,y = 0 \tag{90}$$

we obtain

$$(p\,\bar{y}\,')' + q\,\bar{y} + \bar{\lambda}\,r\,\bar{y} = 0. \tag{91}$$

In other words, $\bar{\lambda}$ is also an eigenvalue with eigenfunction $\bar{y}$. Multiplying this equation by y and integrate, we have

$$\begin{aligned} 0 &= \int_a^b \left[(p\,\bar{y}\,')' + q\,\bar{y} + \bar{\lambda}\,r\,\bar{y} \right] y \\ &= \int_a^b (p\,\bar{y}\,')'\,y + \int_a^b q\,|y|^2 + \bar{\lambda} \int_a^b r\,|y|^2 \\ &= (p\,\bar{y}\,')\,y\,|_a^b - \int_a^b p\,y'\,\bar{y}\,' + \int_a^b q\,|y|^2 + \bar{\lambda} \int_a^b r\,|y|^2. \end{aligned} \tag{92}$$

Combining the above, we reach

$$(\lambda - \bar{\lambda}) \int_a^b r\,|y|^2 = p(b)\,[y'(b)\,\bar{y}\,(b) - \bar{y}\,'(b)\,y(b)] - p(a)\,[y'(a)\,\bar{y}\,(a) - \bar{y}\,'(a)\,y(a)]. \tag{93}$$

Using the boundary conditions

$$\alpha_0\,y(a) + \alpha_1\,y'(a) = 0, \tag{94}$$

$$\beta_0\,y(b) + \beta_1\,y'(b) = 0. \tag{95}$$

we see that

$$y'(b)\,\bar{y}\,(b) - \bar{y}\,'(b)\,y(b) = 0, \qquad y'(a)\,\bar{y}\,(a) - \bar{y}\,'(a)\,y(a) = 0. \tag{96}$$

Therefore

$$(\lambda - \bar{\lambda}) \int_a^b r\,|y|^2\,\mathrm{d}x = 0 \tag{97}$$

which leads to $\lambda = \bar{\lambda}$, or λ is real.

- The set of eigenvalues does not have any limit points.

  Omitted.

- These eigenvalues are bounded from below if $\alpha_0\,\alpha_1 \leqslant 0$ and $\beta_0\,\beta_1 \geqslant 0$. These eigenvalues are bounded from below by 0 if furthermore $q \leqslant 0$.

  We have

$$\begin{aligned} 0 &= \int_a^b \left[(p\,y')' + q\,y + \lambda\,r\,y \right] \bar{y}\,\mathrm{d}x \\ &= \int_a^b (p\,y')'\,\bar{y} + \int_a^b q\,|y|^2 + \lambda \int_a^b r\,|y|^2 \\ &= (p\,y')\,\bar{y}\,|_a^b - \int_a^b p\,y'\,\bar{y}\,' + \int_a^b q\,|y|^2 + \lambda \int_a^b r\,|y|^2. \\ &= p(b)\,y'(b)\,\bar{y}\,(b) - p(a)\,y'(a)\,\bar{y}\,(a) - \int_a^b \left[p\,|y'|^2 - q\,|y|^2 \right] + \lambda \int_a^b r\,|y|^2. \end{aligned} \tag{98}$$

Thus

$$\lambda = \frac{\left\{ - p(b)\, y'(b)\, \bar{y}\,(b) + p(a)\, y'(a)\, \bar{y}\,(a) + \int_a^b \left[p\, |y'|^2 - q\, |y|^2 \right] \right\}}{\int_a^b r\, |y|^2}. \tag{99}$$

Using the boundary conditions we have

$$- p(b)\, y'(b)\, \bar{y}\,(b) = p(b)\, \frac{\beta_0}{\beta_1}\, |y(b)|^2, \tag{100}$$

$$p(a) y'(a)\, \bar{y}\,(a) = - p(a)\, \frac{\alpha_0}{\alpha_1}\, |y(a)|^2. \tag{101}$$

When $\alpha_0\, \alpha_1 \leqslant 0$ and $\beta_0\, \beta_1 \geqslant 0$, both terms are non-negative which means

$$\lambda \geqslant \frac{- \int_a^b q\, |y|^2}{\int_a^b r\, |y|^2}. \tag{102}$$

If furthermore $q \leqslant 0$, we see that $\lambda \geqslant 0$ too.

2. For each fixed eigenvalue λ, the solution space is one-dimensional. That is, there is y_λ such that all other solutions for the same λ is a multiple of y_λ.

   Fix λ. Let $y(x)$ and $z(x)$ be two eigenfunctions. That is

$$\begin{aligned} (p(x)\, y')' + q(x)\, y + \lambda\, r(x)\, y &= 0, \qquad a < x < b & (103)\\ \alpha_0\, y(a) + \alpha_1\, y'(a) &= 0, & (104)\\ \beta_0\, y(b) + \beta_1\, y'(b) &= 0. & (105) \end{aligned}$$

and

$$\begin{aligned} (p(x)\, z')' + q(x)\, z + \lambda\, r(x)\, z &= 0, \qquad a < x < b & (106)\\ \alpha_0\, z(a) + \alpha_1\, z'(a) &= 0, & (107)\\ \beta_0\, z(b) + \beta_1\, z'(b) &= 0. & (108) \end{aligned}$$

Multiplying the y equation by z and z equation by y, and subtract, we have

$$0 = (p\, y')'\, z - (p\, z')'\, y = (p\, (y'\, z - z'\, y))'. \tag{109}$$

We conclude that

$$p(x)\, (y'\, z - z'\, y)(x) = p(a)\, (y'\, z - z'\, y)(a). \tag{110}$$

As y, z both satisfy the boundary conditions, we have

$$p(a)\, (y'(a)\, z(a) - z'(a)\, y(a)) = 0 \tag{111}$$

which leads to

$$p\, (y'\, z - z'\, y) = 0 \implies y'\, z - z'\, y = 0 \tag{112}$$

for all $a \leqslant x \leqslant b$ as $p(x) > 0$.

   Finally,

$$y'\, z - z'\, y = 0 \implies \frac{y'}{y} = \frac{z'}{z} \implies \ln y - \ln z = \text{constant} \implies y/z = \text{constant}. \tag{113}$$

3. We enumerate the eigenvalues by λ_1, λ_2, ... and denote the corresponding eigenfunctions by φ_1, $\varphi_2, \ldots$.

   a) $\displaystyle\int_a^b \varphi_n(x)\, \varphi_m(x)\, r(x)\, \mathrm{d}x = 0$ for any $n \neq m$.

      It suffices to show that if λ, μ are two distinct eigenvalues, and y, z the corresponding eigenfunctions, then $\int_a^b y\, z\, r\, \mathrm{d}x = 0$.

Using the equations we have

$$\int_a^b \left[(p\,y')' + q\,y + \lambda\,r\,y \right] z - \left[(p\,z')' + q\,z + \mu\,r\,z \right] y\,\mathrm{d}x = 0. \tag{114}$$

After using the boundary conditions, we can show that

$$\text{LHS} = (\lambda - \mu) \int y\,z\,r\,\mathrm{d}x. \tag{115}$$

Therefore

$$(\lambda - \mu) \int_a^b y(x)\,z(x)\,r(x)\,\mathrm{d}x = 0. \tag{116}$$

As $\lambda \neq \mu$, we have

$$\int_a^b y(x)\,z(x)\,r(x)\,\mathrm{d}x = 0. \tag{117}$$

b) Omitted.

c) Omitted.

d) Omitted.

□

2.2. Properties of singular Sturm-Liouville problems.

Recall that the problem is "singular" when any one (or more) of the following is true:

→ The interval (a, b) is infinite, that is either $a = -\infty$ or $b = +\infty$ or both occurs.

→ $p(x) = 0$ for some $x \in [a, b]$ or $r(x) = 0$ for some $x \in [a, b]$.

→ One or several coefficient function becomes ∞ at a or b, or both.

For singular SL problems, appropriate boundary conditions should be specified. In particular, if p vanishes at a or b, we should require y and y' to be bounded at a or b respectively.

Similar to the regular SL problems, the eigenfunctions for singular SL problems are also orthogonal with respect to weight $r(x)$.

Example 6. Consider the Legendre's equation

$$\left[\left(1 - x^2\right)\, y' \right]' + \lambda\,y = 0, \qquad -1 < x < 1. \tag{118}$$

As $p(x) = 1 - x^2$ vanishes at both ends, the boundary conditions should be taken as

$$y, y' \text{ remain bounded as } x \to \pm 1. \tag{119}$$

The eigenvalues are $\lambda_n = n\,(n+1)$. Here $r(x) = 1$, so the corresponding eigenfunctions satisfy

$$\int_{-1}^1 P_m(x)\,P_n(x)\,\mathrm{d}x = 0, \qquad n \neq m. \tag{120}$$

Example 7. Consider the Bessel's equation

$$(x\,y')' + \left(\lambda\,x - \frac{\nu^2}{x} \right) y = 0, \qquad 0 < x < a \tag{121}$$

$p(x) = x$ vanishes at $x = 0$. Therefore we can assign the usual boundary condition

$$\beta_0\,y + \beta_1\,y' = 0 \tag{122}$$

at $x = a$ but need to require

$$y, y' \text{ remain bounded as } x \to 0+. \tag{123}$$

The eigenvalues are n^2. As $r(x) = x$, the corresponding eigenfunctions satisfy

$$\int_0^a y_n(x)\, y_m(x)\, x\, \mathrm{d}x = 0, \qquad n \neq m. \tag{124}$$

Example 8. Consider the Hermite's equation

$$u'' - 2\,x\,u' + \lambda\,u = 0, \qquad -\infty < x < \infty \tag{125}$$

To write this problem into a SL problem, we multiply the equation by e^{-x^2} to obtain

$$\left(e^{-x^2} u'\right)' + \lambda\, e^{-x^2} u = 0, \qquad -\infty < x < \infty. \tag{126}$$

Now that we have $p(x) = e^{-x^2}$ which tends to 0 as $x \to \pm\infty$, the boundary conditions should be

$$u, u' \text{ remain bounded as } x \to \pm\infty. \tag{127}$$

The eigenvalues are $\lambda_n = 2\,n$ for nonnegative integers n. Since $r(x) = e^{-x^2}$, the orthogonality property reads

$$\int_{-\infty}^{\infty} H_n(x)\, H_m(x)\, e^{-x^2}\, \mathrm{d}x = 0, \qquad n \neq m. \tag{128}$$

3. Special functions.

To apply this theory to solve PDEs, we need to obtain more information of the eigenfunctions. This leads to the theory of special functions.

3.1. Bessel function.

Recall our example problem: Consider the heat equation in a 2D disc $x^2 + y^2 \leqslant 1$:

$$\begin{aligned} u_t &= \kappa\,(u_{xx} + u_{yy}) && (129)\\ u(x,y,0) &= f(x,y) && (130)\\ u(x,y,t) &= 0 \qquad x^2 + y^2 = 1. && (131) \end{aligned}$$

which leads to "basic" solutions of the form

$$R(r)\,\Theta(\theta)\,T(t) \tag{132}$$

where R solves

$$r^2 R'' + r\,R' + \left(\lambda\,r^2 - n^2\right) R = 0, \tag{133}$$

with the boundary condition

$$R(0) \text{ bounded, } R(1) = 0. \tag{134}$$

We have seen that the above equation can be written into the Sturm-Liouville system

$$(r\,R')' - \frac{n^2}{r} R + \lambda\,r\,R = 0 \tag{135}$$

which means that after detemining the eigenvalues λ_m and the corresponding eigenfunctions $R_{n,m}$, we can expand any function of r into

$$f(r) = \sum_m A_m\, R_{n,m}(r) \tag{136}$$

with

$$A_m = \frac{\int_0^1 f(r)\, R_{n,m}(r)\, r\, \mathrm{d}r}{\int_0^1 R_{n,m}(r)^2\, r\, \mathrm{d}r}. \tag{137}$$

One problem to this approach is that neither λ_m nor $R_{n,m}$ has a formula. However, we can qualitatively solve the equation as follows.

First we determine the general solutions. Notice that, if $R(r)$ solves the following equation

$$r^2 R'' + r R' + (r^2 - n^2) R = 0, \tag{138}$$

then we have (replacing each r by $\sqrt{\lambda}\, r$)

$$\left(\sqrt{\lambda}\, r\right)^2 R''\left(\sqrt{\lambda}\, r\right) + \left(\sqrt{\lambda}\, r\right) R'\left(\sqrt{\lambda}\, r\right) + \left(\left(\sqrt{\lambda}\, r\right)^2 - n^2\right) R\left(\sqrt{\lambda} r\right) = 0 \tag{139}$$

which means $R_\lambda(r) \equiv R\left(\sqrt{\lambda}\, r\right)$ solves

$$r^2 R_\lambda'' + r R_\lambda' + (\lambda r^2 - n^2) R_\lambda = 0. \tag{140}$$

Therefore we first consider the singular SL equation

$$x^2 y'' + x y' + (x^2 - \nu^2) y = 0 \tag{141}$$

where ν is a non-negative real number. We have seen that this is closely related to solving equations involving the 2D Laplacian $\partial_{xx} + \partial_{yy}$ in a disc.

As we have mentioned, it is not possible to obtain a formula for the solutions. We have to rely on the so-called Frobenius method: We search for solutions of the form

$$y(x) = \sum_{n=0}^{\infty} a_n x^{s+n} \tag{142}$$

with s to be determined.

Substituting this formula into the equation, we obtain

$$\begin{aligned}
0 &= x^2 y'' + x y' + (x^2 - \nu^2) y \\
&= x^2 \left(\sum_{n=0}^{\infty} a_n (s+n)(s+n-1) x^{s+n-2} \right) \\
&\quad + x \left(\sum_{n=0}^{\infty} a_n (s+n) x^{s+n-1} \right) + (x^2 - \nu^2) \left(\sum_{n=0}^{\infty} a_n x^{s+n} \right) \\
&= \sum_{n=0}^{\infty} a_n (s+n)(s+n-1) x^{s+n} + \sum_{n=0}^{\infty} a_n (s+n) x^{s+n} \\
&\quad + \sum_{n=2}^{\infty} a_{n-2} x^{s+n} - \sum_{n=0}^{\infty} \nu^2 a_n x^{s+n} \\
&= \sum_{n=0}^{\infty} a_n \left[(s+n)^2 - \nu^2 \right] x^{s+n} + \sum_{n=2}^{\infty} a_{n-2} x^{s+n} \\
&= (s^2 - \nu^2) a_0 x^s + \left[(s+1)^2 - \nu^2 \right] a_1 x^{s+1} + \sum_{n=2}^{\infty} \left\{ a_n \left[(s+n)^2 - \nu^2 \right] + a_{n-2} \right\} x^{s+n}.
\end{aligned} \tag{143}$$

Therefore the solution should satisfy

$$(s^2 - \nu^2) a_0 = 0 \tag{144}$$

$$\left[(s+1)^2 - \nu^2 \right] a_1 = 0 \tag{145}$$

$$a_n \left[(s+n)^2 - \nu^2 \right] + a_{n-2} = 0 \qquad n = 2, 3, \ldots \tag{146}$$

As we are discussing the general case here, we assume $a_0 \neq 0$. As a consequence,

$$s^2 = \nu^2 \iff s = \pm \nu. \tag{147}$$

We see that close to $x = 0$, the solution behaves as either x^ν or $x^{-\nu}$. The former satisfies $y(0) = 0$ while the latter is unbounded. Thus we discuss the two cases separately.

– $s = \nu$.

In this case, $(s+n)^2 \neq \nu^2$ for all $n>0$. Consequently we have

$$\begin{aligned}
a_1 &= 0 &(148)\\
a_2 &= -\frac{a_0}{2\,(2\,\nu+2)} &(149)\\
a_3 &= -\frac{a_1}{3\,(2\,\nu+3)} = 0 &(150)\\
a_4 &= -\frac{a_2}{4\,(2\,\nu+4)} &(151)\\
&\vdots\\
a_{2n} &= -\frac{a_{2n-2}}{2\,n\,(2\,\nu+2\,n)} = -\frac{a_{2n-2}}{4\,n\,(\nu+n)}, &(152)\\
a_{2n+1} &= 0 &(153)\\
&\vdots
\end{aligned}$$

From the above we have the formula

$$a_{2n} = \frac{(-1)^n\,a_0}{4^n\,n!\,(\nu+n)\cdots(\nu+1)}. \tag{154}$$

The formula for $y(x)$ is then

$$y(x) = a_0 \sum_{n=0}^{\infty} \frac{(-1)^n}{4^n\,n!\,(\nu+n)\cdots(\nu+1)}\,x^{2n+\nu}. \tag{155}$$

This is called the *Bessel function of the first kind of order* ν, denoted by $J_\nu(x)$.

– $s=-\nu$.

In this case

$$(s+n)^2-\nu^2 = (-\nu+n)^2-\nu^2 = n^2-2\,n\,\nu = 0 \tag{156}$$

when $n=2\,\nu$. Thus we discuss two cases.

→ $2\,\nu$ is not an integer. In this case none of $(s+n)^2-\nu^2$ is 0 unless $n=0$. Thus we have the interative relation

$$a_{2n} = \frac{-a_{2n-2}}{2\,n\,(2\,n-2\,\nu)} = \frac{-a_{2n-2}}{4\,n\,(n-\nu)} = \cdots = \frac{(-1)^n\,a_0}{4^n\,n!\,(n-\nu)\cdots(1-\nu)}, \qquad a_{2n-1}=0. \tag{157}$$

Thus

$$J_{-\nu}(x) \equiv y(x) = a_0 \sum_{n=0}^{\infty} \frac{(-1)^n\,a_0}{4^n\,n!\,(n-\nu)\cdots(1-\nu)}\,x^{2n-\nu}. \tag{158}$$

→ $2\,\nu$ is an integer.

→ ν is an integer. For convenience we denote ν by m_0. Then from

$$a_n\left[(s+n)^2-\nu^2\right] + a_{n-2} = 0 \tag{159}$$

we have

$$a_{2m_0-2}=0 \Longrightarrow a_{2m_0-4}=0 \Longrightarrow a_0=0. \tag{160}$$

On the other hand, the same iteration process gives $a_{2n-1}=0$ for all $n>0$. As a consequence, the first term in the series is actually $x^{2m_0-\nu}=x^\nu$. In other words, when ν is an integer, the solution for $s=-\nu$ is regular. In fact one can show that the solution $J_{-n}(x)$ is simply $(-1)^n\,J_n(x)$.

→ ν is not an integer but $2\,\nu$ is. Thus necessarily $2\,\nu$ is odd, denote it by $2\,n_0-1$. In this case, using the iteration relation

$$a_n\left[(s+n)^2-\nu^2\right] + a_{n-2} = 0 \tag{161}$$

we can show that $a_{2n-1} = 0$ for all $n < n_0$. Now if we define

$$J_{-\nu}(x) \equiv y(x) = a_0 \sum_{n=0}^{\infty} \frac{(-1)^n a_0}{4^n n! (n-\nu) \cdots (1-\nu)} x^{2n-\nu}, \tag{162}$$

it can be shown that the solution $y(x)$ is in fact a linear combination of $J_{-\nu}$ and J_ν.

Summarizing, we have

$$J_{-\nu}(x) \equiv y(x) = a_0 \sum_{n=0}^{\infty} \frac{(-1)^n a_0}{4^n n! (n-\nu) \cdots (1-\nu)} x^{2n-\nu} \tag{163}$$

when ν is not an integer, and

$$J_{-\nu}(x) = (-1)^n J_\nu(x) \tag{164}$$

when ν is an integer.

Recall that our purpose is to find out the general behavior of the solutions to the Bessel equation

$$x^2 y'' + x y' + (x^2 - \nu^2) y = 0. \tag{165}$$

When ν is not an integer, we have two linear independent solutions $J_{\pm\nu}$ therefore the general solution can be written as

$$y(x) = A J_\nu(x) + B J_{-\nu}(x). \tag{166}$$

However when ν is an integer, $J_{\pm\nu}$ are linearly dependent of each other and we have to find another solution which is linearly independent of J_ν.

To remedy this, we define

$$Y_\nu(x) = \frac{(\cos \nu \pi) J_\nu(x) - J_{-\nu}(x)}{\sin \nu \pi}, \tag{167}$$

which should be explained as the limit $\nu \longrightarrow n$ when ν is an negative integer. That is

$$Y_{-n} = \lim_{\nu \longrightarrow n} Y_{-\nu}. \tag{168}$$

It turns out that J_ν and Y_ν are always linearly independent. That is

$$y(x) = A J_\nu(x) + B Y_\nu(x). \tag{169}$$

The coefficients A, B are determined by the boundary conditions, taking advantage of the fact that $J_\nu(0) = 0$, $Y_\nu(0) = \infty$.

Recall our example which leads to the discussion of Sturm-Liouville problems: Consider the heat equation in a 2D disc $x^2 + y^2 \leqslant 1$:

$$u_t = \kappa (u_{xx} + u_{yy}) \tag{170}$$

$$u(x, y, 0) = f(x, y) \tag{171}$$

$$u(x, y, t) = 0 \qquad x^2 + y^2 = 1. \tag{172}$$

Separating the variables in polar coordinates

$$u(x, y, t) = R(r) \Theta(\theta) T(t) \tag{173}$$

we reach the following problem for R:

$$r^2 R'' + r R' + (\lambda r^2 - n^2) R = 0, \tag{174}$$

with the boundary condition

$$R(0) \text{ bounded}, R(1) = 0. \tag{175}$$

We know that the general solution is of the form

$$R(r) = A J_n\left(\sqrt{\lambda} r\right) + B Y_n\left(\sqrt{\lambda} \rho\right). \tag{176}$$

To determine the coefficients we need the boundary conditions. Besides $R(1)=0$, we need to specify another condition at $r=0$. The reasonable one is $R(0)$ being bounded.

As $Y_n(0)=\infty$, the boundary conditions become

$$R(0) \text{ bounded} \Longrightarrow B=0, \tag{177}$$

$$R(1)=0 \Longrightarrow J_n\left(\sqrt{\lambda}\right)=0 \Longrightarrow \lambda=\lambda_n, \; n=1,2,3,\ldots \tag{178}$$

Thus the solutions are

$$R_n(r)=J_n\left(\sqrt{\lambda_n}\, r\right), \qquad n=1,2,3,\ldots \tag{179}$$

Example 9. (§10.13 15) Solve the heat conduction problem in a circular plate

$$u_t=k\left(u_{rr}+\frac{1}{r}u_r+\frac{1}{r^2}u_{\theta\theta}\right), \quad r<1, \quad 0<\theta<2\pi, \quad t>0, \tag{180}$$

$$u(r,\theta,0)=f(r,\theta), \qquad u(1,\theta,t)=0. \tag{181}$$

Solution. We solve the problem using separation of variables.

First we search for "basic" solutions which are non-zero and of the form

$$u=R(r)\,\Theta(\theta)\,T(t). \tag{182}$$

Substituting this into the equation we obtain

$$R(r)\,\Theta(\theta)\,T'(t)=k\left(R''(r)\,\Theta(\theta)\,T(t)+\frac{1}{r}R'(r)\,\Theta(\theta)\,T(t)+\frac{1}{r^2}R(r)\,\Theta''(\theta)\,T(t)\right). \tag{183}$$

Divide by $R(r)\,\Theta(\theta)\,T(t)$ we obtain

$$\frac{T'(t)}{T(t)}=k\left[\frac{R''(r)}{R(r)}+\frac{1}{r}\frac{R'(r)}{R(r)}+\frac{1}{r^2}\frac{\Theta''(\theta)}{\Theta(\theta)}\right]. \tag{184}$$

As the LHS is a function of t only and the RHS a function of r,θ only, there is a constant $-\lambda$ such that

$$\frac{T'(t)}{T(t)}=-k\lambda, \qquad \frac{R''(r)}{R(r)}+\frac{1}{r}\frac{R'(r)}{R(r)}+\frac{1}{r^2}\frac{\Theta''(\theta)}{\Theta(\theta)}=-\lambda. \tag{185}$$

Now multiply the R,Θ equation by r^2, we reach

$$\frac{r^2R''(r)}{R(r)}+\frac{rR'(r)}{R(r)}+\frac{\Theta''(\theta)}{\Theta(\theta)}=-\lambda r^2 \Longleftrightarrow \frac{r^2R''(r)}{R(r)}+\frac{rR'(r)}{R(r)}+\lambda r^2=-\frac{\Theta''(\theta)}{\Theta(\theta)}. \tag{186}$$

Now the LHS is a function of r only while the RHS a function of θ only. Therefore there is another constant μ such that

$$\frac{r^2R''(r)}{R(r)}+\frac{rR'(r)}{R(r)}+\lambda r^2=\mu, \qquad \frac{\Theta''(\theta)}{\Theta(\theta)}=-\mu. \tag{187}$$

Summarizing, we have the following equations to solve (and along the way determine λ,μ):

$$\frac{T'(t)}{T(t)}=-k\lambda, \text{ with } T(0) \text{ to be specified;} \tag{188}$$

$$\frac{\Theta''(\theta)}{\Theta(\theta)}=-\mu, \qquad \Theta \text{ periodic with period } 2\pi; \tag{189}$$

$$\frac{r^2R''(r)}{R(r)}+\frac{rR'(r)}{R(r)}+\lambda r^2=\mu, \qquad R(1)=0. \tag{190}$$

It is clear that we should first solve the Θ equation. We have

$$\Theta''(\theta)+\mu\,\Theta(\theta)=0, \qquad \Theta \text{ periodic with period } 2\pi. \tag{191}$$

The boundary condition can also be written as

$$\Theta(0)=\Theta(2\,\pi), \qquad \Theta'(0)=\Theta'(2\,\pi) \tag{192}$$

as this, together with the equation, guarantees $\Theta^{(k)}(0)=\Theta^{(k)}(2\,\pi)$ for all k which in turn guarantees periodicity.

We discuss the three cases.

i. $\mu<0$. The general solution is

$$\Theta=A\,e^{\sqrt{-\mu}\,\theta}+B\,e^{-\sqrt{-\mu}\,\theta} \tag{193}$$

which cannot be periodic unless $A=B=0$.

ii. $\mu=0$. The general solution is

$$\Theta=A+B\,\theta \tag{194}$$

which again cannot be periodic unless $A=B=0$.

iii. $\mu>0$. The general solution is

$$\Theta=A\cos\sqrt{\mu}\,\theta+B\sin\sqrt{\mu}\,\theta \tag{195}$$

which is $2\,\pi$-periodic if and only if

$$\mu=n^2 \tag{196}$$

for some integer n. As the cosine function is even and the sine function is odd, it suffices to consider the case $n\geqslant 0$.

Thus the possible (μ,Θ) pairs are

$$\mu_n=n^2, \qquad \Theta_n=\cos n\,\theta \text{ and } \sin n\,\theta. \tag{197}$$

Now that we have μ, we turn to the equation for R. Replacing μ by n^2 we have

$$\frac{r^2\,R''(r)}{R(r)}+\frac{r\,R'(r)}{R(r)}+\lambda\,r^2=n^2, \qquad R(1)=0 \tag{198}$$

which becomes

$$r^2\,R''(r)+r\,R'(r)+\left(\lambda\,r^2-n^2\right)R(r)=0, \qquad R(1)=0. \tag{199}$$

The theory of Bessel functions tells us that

$$R(r)=A\,J_n\!\left(\sqrt{\lambda}\,r\right)+B\,Y_n\!\left(\sqrt{\lambda}\,r\right) \tag{200}$$

where J_n and Y_n are Bessel functions of the first and the second kinds or order n.

Integrating the boundary condition $R(0)$ bounded, we conclude $B=0$. On the other hand, requiring $R(1)=0$ leads to $\lambda=\lambda_m$ where $\sqrt{\lambda_m}$ is the m-th root of J_n. Therefore the possible (λ,R) pairs are

$$\lambda_m, \qquad R_m=J_n\!\left(\sqrt{\lambda_m}\,r\right). \tag{201}$$

Finally we solve the equation for T. For each λ_m, solving

$$\frac{T'(t)}{T(t)}=-\,k\,\lambda_m. \tag{202}$$

would give us a function T_m and finally the solution can be written as a sum

$$u(r,\theta,t)=\sum_{m=1}^{\infty}\sum_{n=0}^{\infty}\left[T_{m,n,1}(t)\cos(n\,\theta)+T_{m,n,2}(t)\sin(n\,\theta)\right]J_n\!\left(\sqrt{\lambda_m}\,r\right). \tag{203}$$

Setting $t=0$ we have

$$f(r,\theta)=\sum_{m=1}^{\infty}\sum_{n=0}^{\infty}\left[T_{m,n,1}(0)\cos(n\,\theta)+T_{m,n,2}(0)\sin(n\,\theta)\right]J_n\!\left(\sqrt{\lambda_m}\,r\right). \tag{204}$$

To obtain these initial values, notice that $J_n\big(\sqrt{\lambda_m}\,r\big)$ depens on both indices while $\sin(n\,\theta)$ and $\cos(n\,\theta)$ only depends on n, we first expand

$$f(r,\theta)=\sum_{n=0}^{\infty}\,[f_{n,1}(r)\cos(n\,\theta)+f_{n,2}(r)\sin(n\,\theta)] \tag{205}$$

with

$$f_{n,1}(r)=\begin{cases}\dfrac{1}{2\,\pi}\displaystyle\int_0^{2\pi}f(r,\theta)\,\mathrm{d}\theta & n=0\\ \dfrac{1}{\pi}\displaystyle\int_0^{2\pi}f(r,\theta)\cos(n\,\theta)\,\mathrm{d}\theta & n>0\end{cases},\quad f_{n,2}(r)=\frac{1}{\pi}\int_0^{2\pi}f(r,\theta)\sin(n\,\theta)\,\mathrm{d}\theta. \tag{206}$$

Now writing

$$\begin{aligned} f(r,\theta) &= \sum_{m=1}^{\infty}\sum_{n=0}^{\infty}\,[T_{m,n,1}(0)\cos(n\,\theta)+T_{m,n,2}(0)\sin(n\,\theta)]\,J_n\big(\sqrt{\lambda_m}\,r\big) &(207)\\ &= \sum_{n=0}^{\infty}\left\{\left[\sum_{m=1}^{\infty}T_{m,n,1}(0)\,J_n\big(\sqrt{\lambda_m}\,r\big)\right]\cos(n\,\theta)+\left[\sum_{m=1}^{\infty}T_{m,n,2}(0)\,J_n\big(\sqrt{\lambda_m}\,r\big)\right]\sin(n\,\theta).\right. &(208)\end{aligned}$$

Therefore

$$f_{n,1}(r)=\sum_{m=1}^{\infty}\,T_{m,n,1}(0)\,J_n\big(\sqrt{\lambda_m}\,r\big) \tag{209}$$

and

$$f_{n,2}(r)=\sum_{m=1}^{\infty}\,T_{m,n,2}(0)\,J_n\big(\sqrt{\lambda_m}\,r\big). \tag{210}$$

Recalling the orthogonality property

$$\int_0^1 J_n\big(\sqrt{\lambda_m}\,r\big)\,J_n\big(\sqrt{\lambda_k}\,r\big)\,r\,\mathrm{d}r=0, \tag{211}$$

we conclude

$$T_{m,n,1}(0)=\frac{\displaystyle\int_0^1 f_{n,1}(r)\,J_n\Big(\sqrt{\lambda_m}\,r\Big)\,r\,\mathrm{d}r}{\displaystyle\int_0^1 J_n\big(\sqrt{\lambda_m}\,r\big)^2\,r\,\mathrm{d}r},\qquad m=1,2,\ldots \tag{212}$$

and

$$T_{m,n,2}(0)=\frac{\displaystyle\int_0^1 f_{n,2}(r)\,J_n\Big(\sqrt{\lambda_m}\,r\Big)\,r\,\mathrm{d}r}{\displaystyle\int_0^1 J_n\big(\sqrt{\lambda_m}\,r\big)^2\,r\,\mathrm{d}r},\qquad m=1,2,\ldots \tag{213}$$

Now inserting the formulas for $f_{n,1}(r)$ and $f_{n,2}(r)$, we reach

$$T_{m,n,1}(0)=a_{m,n,1}=\begin{cases}\dfrac{\displaystyle\int_0^{2\pi}\int_0^1 f(r,\theta)\,J_0\Big(\sqrt{\lambda_m}\,r\Big)\,r\,\mathrm{d}r}{2\,\pi\displaystyle\int_0^1 J_0\big(\sqrt{\lambda_m}\,r\big)^2\,r\,\mathrm{d}r} & n=0\\ \dfrac{\displaystyle\int_0^{2\pi}\int_0^1 f(r,\theta)\,J_n\Big(\sqrt{\lambda_m}\,r\Big)\,r\cos(n\,\theta)\,\,\mathrm{d}r\,\mathrm{d}\theta}{\pi\displaystyle\int_0^1 J_n\big(\sqrt{\lambda_m}\,r\big)^2\,r\,\mathrm{d}r} & n\geqslant 1\end{cases}, \tag{214}$$

$$T_{m,n,2}(0)=a_{m,n,2}=\frac{\displaystyle\int_0^{2\pi}\int_0^1 f(r,\theta)\,J_n\Big(\sqrt{\lambda_m}\,r\Big)\,r\sin(n\,\theta)\,\,\mathrm{d}r\,\mathrm{d}\theta}{\pi\displaystyle\int_0^1 J_n\big(\sqrt{\lambda_m}\,r\big)^2\,r\,\mathrm{d}r}. \tag{215}$$

Solving

$$\frac{T'(t)}{T(t)} = -k\,\lambda_{m,n,1} \text{ and } -k\,\lambda_{m,n,2} \tag{216}$$

with initial values $a_{m,n,1}$ and $a_{m,n,2}$ we obtain

$$T_{m,n,1}(t) = a_{m,n,1}\, e^{-k\lambda_m t}, \qquad T_{m,n,2}(t) = a_{m,n,2}\, e^{-k\lambda_m t}. \tag{217}$$

Finally, putting everything together, we reach

$$u(r,\theta,t) = \sum_{m=1}^{\infty} \sum_{n=0}^{\infty} \left[a_{m,n,1} \cos(n\,\theta) + a_{m,n,2}\,\sin(n\,\theta)\right] J_n\!\left(\sqrt{\lambda_m}\, r\right) e^{-k\lambda_m t} \tag{218}$$

with

$$a_{m,n,1} = \begin{cases} \dfrac{\displaystyle\int_0^{2\pi}\int_0^1 f(r,\theta)\, J_0\!\left(\sqrt{\lambda_m}\, r\right) r\,\mathrm{d}r}{\displaystyle 2\,\pi \int_0^1 J_0\!\left(\sqrt{\lambda_m}\, r\right)^2 r\,\mathrm{d}r} & n=0 \\ \dfrac{\displaystyle\int_0^{2\pi}\int_0^1 f(r,\theta)\, J_n\!\left(\sqrt{\lambda_m}\, r\right) r\cos(n\,\theta)\;\mathrm{d}r\,\mathrm{d}\theta}{\displaystyle \pi \int_0^1 J_n\!\left(\sqrt{\lambda_m}\, r\right)^2 r\,\mathrm{d}r} & n \geqslant 1 \end{cases}, \tag{219}$$

$$a_{m,n,2} = \frac{\displaystyle\int_0^{2\pi}\int_0^1 f(r,\theta)\, J_n\!\left(\sqrt{\lambda_m}\, r\right) r\sin(n\,\theta)\;\mathrm{d}r\,\mathrm{d}\theta}{\displaystyle \pi \int_0^1 J_n\!\left(\sqrt{\lambda_m}\, r\right)^2 r\,\mathrm{d}r}. \tag{220}$$

The formula above is the same as the one in the book given on page 733. The equivalence follows from (8.6.30).

3.2. Legendre function.

Legendre functions arise from PDEs on domains with sperical symmetry.[1]

Example 10. We consider the Laplace equation in a sphere:

$$u_{xx} + u_{yy} + u_{zz} = 0 \qquad x^2 + y^2 + z^2 < a^2, \tag{223}$$

$$u = f \qquad x^2 + y^2 + z^2 = a^2. \tag{224}$$

Consider the case where $f = f(\theta)$ is independent of the longitudinal coordinate ϕ in the spherical coordinates

$$r = \sqrt{x^2 + y^2 + z^2}, \quad 0 < \theta < \pi, \quad 0 < \phi < 2\,\pi. \tag{225}$$

In this case u is also a function of r, θ only.

The problem now becomes

$$\left(r^2\, u_r\right)_r + \frac{1}{\sin\theta}\left[(\sin\theta)\, u_\theta\right]_\theta = 0, \tag{226}$$

$$u(a,\theta) = f(\theta). \tag{227}$$

1. **Spherical coordinates.** Consider a vector in $\mathbb{R}^3$ (x-y-z space). Let r be its length, and let θ be the angle between this vector and the z-axis. Then the projection of this vector onto the x-y plane is $r\sin\theta$. Now we introduce a second angle φ which is the angle in the polar coordinates of the x-y plane. Thus we have

$$x = r\cos\varphi\sin\theta, \qquad y = r\sin\varphi\sin\theta, \qquad z = r\cos\theta \tag{221}$$

with $r > 0, 0 \leqslant \varphi < 2\,\pi, 0 \leqslant \theta < \pi$.

One can also try to make θ measuring the (signed) angle between the vector and the x-y plane, in that case the change-of-variable relation changes to

$$x = r\cos\varphi\cos\theta, \qquad y = r\sin\varphi\cos\theta, \qquad z = r\sin\theta. \tag{222}$$

This means the spherical coordinate form of $u_{xx} + u_{yy} + u_{zz}$ also changes.

We look for a "basic" solution with separated variables

$$u(r,\theta) = R(r)\,\Theta(\theta). \tag{228}$$

Substituting into the equation, we have

$$\frac{1}{R}\left(r^2 R'\right)' = -\frac{1}{\Theta\sin\theta}\left[(\sin\theta)\,\Theta'\right]'. \tag{229}$$

Thus there is a constant λ such that

$$\left(r^2 R'\right)' - \lambda R = 0, \qquad 0 < r < a \tag{230}$$

$$\left[(\sin\theta)\,\Theta'\right]' + \lambda\,(\sin\theta)\,\Theta = 0, \qquad 0 < \theta < \pi. \tag{231}$$

The R equation can be solve through the following. Write the equation as

$$r\,(r\,R')' + r\,R' - \lambda\,R = 0, \tag{232}$$

and set

$$x = \ln r. \tag{233}$$

Then we have

$$\frac{\mathrm{d}R}{\mathrm{d}r} = \frac{\mathrm{d}R}{\mathrm{d}x}\frac{\mathrm{d}x}{\mathrm{d}r} = r^{-1}\frac{\mathrm{d}R}{\mathrm{d}x} \Longrightarrow r\,R' = \frac{\mathrm{d}R}{\mathrm{d}x} \tag{234}$$

therefore the equation becomes

$$\frac{\mathrm{d}^2R}{\mathrm{d}x^2} + \frac{\mathrm{d}R}{\mathrm{d}x} - \lambda\,R = 0 \tag{235}$$

whose general solution is

$$R(r) = A\,r^{\nu} + B\,r^{-(1+\nu)} \tag{236}$$

with

$$\nu = \frac{-1 + \sqrt{1+4\lambda}}{2} \qquad \text{solves} \qquad \nu^2 + \nu - \lambda = 0. \tag{237}$$

For the Θ equation, a change of variable and unknown

$$x = \cos\theta, \qquad y(x) = \Theta(\theta) \tag{238}$$

leads to

$$\frac{\mathrm{d}\Theta}{\mathrm{d}\theta} = \frac{\mathrm{d}y}{\mathrm{d}x}\frac{\mathrm{d}x}{\mathrm{d}\theta} = y'\,(-\sin\theta) \tag{239}$$

therefore

$$\frac{\mathrm{d}}{\mathrm{d}\theta}[(\sin\theta)\,\Theta'] = \frac{\mathrm{d}}{\mathrm{d}\theta}\left[(-\sin^2\theta)\,y'\right] = \frac{\mathrm{d}}{\mathrm{d}x}\left[\left(x^2-1\right)y'\right]\frac{\mathrm{d}x}{\mathrm{d}\theta} = \left[\left(x^2-1\right)y'\right]'(-\sin\theta). \tag{240}$$

Thus the equation becomes

$$\left[\left(1-x^2\right)y'\right]' + \lambda\,y = 0 \tag{241}$$

which can be expanded to

$$\left(1-x^2\right)y'' - 2\,x\,y' + \lambda\,y = 0, \qquad -1 < x < 1. \tag{242}$$

or equivalently

$$\left(1-x^2\right)y'' - 2\,x\,y' + \nu\,(\nu+1)\,y = 0, \qquad -1 < x < 1 \tag{243}$$

as

$$\nu\,[-(1+\nu)] = -\lambda. \tag{244}$$

The solutions are called Legendre functions.

Remark 11. When the problem is not independent of the variable φ, the resulting Θ equation would lead to the so-called "associated Legendre functions".

The Legendre equation reads

$$\left(1-x^2\right) y''-2\,x\,y'+\nu\,(\nu+1)\,y=0. \tag{245}$$

We search for solutions of the form

$$y(x)=\sum_{m=0}^{\infty} a_m\,x^m. \tag{246}$$

Substituting into the equation and collecting the same powers, we have

$$\sum_{m=0}^{\infty} [(m+1)\,(m+2)\,a_{m+2}+(\nu-m)\,(\nu+m+1)\,a_m]\,x^m=0. \tag{247}$$

As a consequence, we must have

$$a_{m+2}=-\frac{(\nu-m)\,(\nu+m+1)}{(m+1)\,(m+2)}\,a_m, \qquad m\geqslant 0. \tag{248}$$

Iterating, we have the formulas for the coefficients

$$a_{2k} = \frac{(-1)^k\,\nu\,(\nu-2)\cdots(\nu-2\,k+2)\,(\nu+1)\,(\nu+3)\cdots(\nu+2\,k-1)}{(2\,k)!}\,a_0, \tag{249}$$

$$a_{2k+1} = \frac{(-1)^k\,(\nu-1)\,(\nu-3)\cdots(\nu-2\,k+1)\,(\nu+2)\,(\nu+4)\cdots(\nu+2\,k)}{(2\,k+1)!}\,a_0. \tag{250}$$

It can be shown that when n is an integer, the solution is a sum of one polynomial of order n, and an infinite series solution. The polynomial solution is denoted $P_n(x)$, and called the *Legendre polynomial of degree* n or *the Legendre function of the first kind of order* n. The infinite series is denoted $Q_n(x)$ and called the *Legendre function of the second kind*.

Therefore the general solutions to the Legendre equation are

$$y(x)=A\,P_\nu(x)+B\,Q_\nu(x). \tag{251}$$

In practice one usually requires $y(x)$ to be bounded at $x=\pm 1$, this is true if and only if $\nu=n$ is an integer and $B=0$, that is

$$y(x)=P_n(x) \tag{252}$$

A simple formula for the Legendre polynomials is

$$P_n(x)=\frac{1}{2^n\,n!}\,\frac{\mathrm{d}^n}{\mathrm{d}x^n}\Big[\left(x^2-1\right)^n\Big]. \tag{253}$$

From this the first few Legendre polynomials can be easily computed as

$$P_0(x) = 1 \tag{254}$$

$$P_1(x) = x \tag{255}$$

$$P_2(x) = \frac{1}{2}\left(3\,x^2-1\right) \tag{256}$$

$$P_3(x) = \frac{1}{2}\left(5\,x^2-3\,x\right). \tag{257}$$

From the Sturn-Liouville theory, we know that $P_n(x)$ enjoys the orthogonality relation

$$\int_{-1}^{1} P_n(x)\,P_m(x)\,\mathrm{d}x=0 \qquad n\neq m. \tag{258}$$

Or equivalently

$$\int_0^{\pi} P_n(\cos\theta)\,P_m(\cos\theta)\sin\theta\,\mathrm{d}\theta=0 \qquad n\neq m. \tag{259}$$

Now we state one fact that is very useful when solving equations. Observe that any polynomial of degree k can be represented as a linear combination of the first k Legendre polynomials. Therefore the orthogonality condition leads to

$$\int_{-1}^{1} P_n(x)\,p(x)\,\mathrm{d}x=0 \tag{260}$$

for any polynomial $p(x)$ with degree $k < n$.

Finally it can be shown that

$$\int_{-1}^{1} P_n^2(x)\,\mathrm{d}x = \frac{2}{2\,n+1} \tag{261}$$

therefore the coefficients in

$$f(x) = \sum_{0}^{\infty} A_n\,P_n(x) \tag{262}$$

is determined by

$$A_n = \frac{\int_{-1}^{1} f(x)\,P_n(x)\,\mathrm{d}x}{\int_{-1}^{1} P_n(x)^2\,\mathrm{d}x} = \frac{2\,n+1}{2}\int_{-1}^{1} f(x)\,P_n(x)\,\mathrm{d}x. \tag{263}$$

Example 12. (§10.13 5) Find the solution of the Dirichlet problem for a sphere

$$\nabla^2 u = 0, \quad r < a, \quad 0 < \theta < \pi, \quad 0 < \varphi < 2\,\pi \tag{264}$$

$$u(a, \theta, \varphi) = \cos^2\theta. \tag{265}$$

Solution. As the boundary value is $\cos^2\theta$ which is independent of φ, and furthermore the Laplacian operator is invariant with respect to translations in φ, the solution is also independent of φ, that is $u = u(r, \theta)$.

In this case the equation becomes

$$\left(r^2\,u_r\right)_r + \frac{1}{\sin\theta}\left[(\sin\theta)\,u_\theta\right]_\theta = 0, \tag{266}$$

$$u(a, \theta) = \cos^2(\theta). \tag{267}$$

Setting $u = R(r)\,\Theta(\theta)$, we reach

$$\frac{1}{R}\left(r^2\,R'\right)' = -\frac{1}{\Theta\sin\theta}\left[(\sin\theta)\,\Theta'\right]'. \tag{268}$$

Thus there is a constant λ such that

$$\left(r^2\,R'\right)' - \lambda\,R = 0, \qquad 0 < r < a \tag{269}$$

$$\left[(\sin\theta)\,\Theta'\right]' + \lambda\,(\sin\theta)\,\Theta = 0, \qquad 0 < \theta < \pi. \tag{270}$$

Setting

$$x = \cos\theta, \qquad y(x) = \Theta(\theta) \tag{271}$$

we have

$$\left(1 - x^2\right) y'' - 2\,x\,y' + \lambda\,y = 0, \qquad -1 < x < 1. \tag{272}$$

Therefore

$$\lambda_n = n\,(n+1), \qquad y_n = P_n(x), \qquad n = 0, 1, 2, \ldots \tag{273}$$

Returning to θ, we have

$$\lambda_n = n\,(n+1), \qquad \Theta_n(\theta) = P_n(\cos\theta), \qquad n = 0, 1, 2, \ldots \tag{274}$$

Now back to the R equation we have

$$R(r) = A\,r^n + B\,r^{-(n+1)} \tag{275}$$

where B is forced to 0 as we require $R(0)$ to be bounded.

Finally the solution can be written as

$$\sum_{n=0}^{\infty} A_n\,r^n\,P_n(\cos\theta). \tag{276}$$

To determine A_n we use the boundary value. Setting $r = a$ we have

$$\cos^2\theta = \sum_{n=0}^{\infty} A_n\, a^n\, P_n(\cos\theta) \tag{277}$$

or equivalently

$$x^2 = \sum_{n=1}^{\infty} A_n\, a^n\, P_n(x). \tag{278}$$

The coefficients are computed by

$$A_n\, a^n = \frac{2\,n+1}{2} \int_{-1}^{1} x^2\, P_n(x)\, \mathrm{d}x. \tag{279}$$

As x^2 is a polynomial of degree 2, we immediately know that $A_n = 0$ for all $n \geqslant 3$. Now we compute

$$A_0 = \frac{1}{2} \int_{-1}^{1} x^2\, \mathrm{d}x = \frac{1}{3}; \tag{280}$$

$$A_1\, a = \frac{3}{2} \int_{-1}^{1} x^3\, \mathrm{d}x = 0; \tag{281}$$

$$A_2\, a^2 = \frac{5}{2} \int_{-1}^{1} \frac{1}{2} \left(3\,x^2 - 1\right) x^2\, \mathrm{d}x = \frac{15}{4} \int_{-1}^{1} x^4\, \mathrm{d}x - \frac{5}{4} \int_{-1}^{1} x^2\, \mathrm{d}x = \frac{3}{2} - \frac{5}{6} = \frac{2}{3}. \tag{282}$$

Finally we have

$$u(r, \theta) = \frac{1}{3}\, P_0(\cos\theta) + \frac{2}{3}\, \frac{r^2}{a^2}\, P_2(\cos\theta) \tag{283}$$

We can further simplify it to

$$u(r, \theta) = \frac{1}{3} + \frac{1}{3}\, \frac{r^2}{a^2} \left(3\cos^2\theta - 1\right) = \frac{1}{3} \left(1 - \frac{r^2}{a^2}\right) + \frac{r^2}{a^2} \cos^2\theta. \tag{284}$$

This formula is simple so we can actually check that it solves the equation and also satisfies the boundary condition.