Notes on Separation of Variables

Steven G. Johnson, MIT course 18.303

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1 Overview

Separation of variables is a technique to *reduce the dimensionality* of PDEs by writing their solutions $u(\vec{x}, t)$ as a *product of lower-dimensional functions*—or, more commonly, as a *superposition* of such functions. Two key points:

- It is only applicable in a *handful* of cases, usually from **symmetry**: time invariance, translation invariance, and/or rotational invariance.
- Most of the analytically solvable PDEs are such **separable** cases, and therefore they are extremely useful in gaining insight and as (usually) *idealized* models.

I will divide them into two main categories, which we will handle separately. **Separation in time** separates the time-dependence of the problem, and is essentially something we have been doing already via eigensolution expansions, under a different name. **Separation in space** separates the spatial dependence of the problem, and is mainly used to help us find the eigenfunctions of linear operators $\hat{A}$.

2 Separation in time

If we have a *time-invariant* linear PDE of the form

$$\frac{\partial u}{\partial t} = \hat{A}u,$$

that is where $\hat{A}$ is independent of time, we have approached this by solving for the eigenfunctions u_n ($\hat{A}u_n = \lambda_n u_n$) and then expanding the solution as

$$u(\vec{x}, t) = \sum_n \alpha_n e^{\lambda_n t} u_n(\vec{x}),$$

assuming that the u_n form a basis for the solutions of interest, where α_n are constant coefficients determined by the initial conditions. This, in fact, is a sum of *separable* solutions: $e^{\lambda_n t} u_n(\vec{x})$ is the product of two *lower-dimensional* functions, a function of time only ($e^{\lambda_n t}$) and a function of space only (u_n). This is **separation of variables** in *time*. If we know algebraic properties of $\hat{A}$, e.g. whether it is self-adjoint, definite, etcetera, we can often then conclude many properties of $u(\vec{x}, t)$ even if we cannot solve analytically for the eigenfunctions u_n. We have also used a similar technique for

$$\frac{\partial^2 u}{\partial t^2} = \hat{A}u,$$

in which case we obtained an expansion of the form

$$u(\vec{x}, t) = \sum_n [\alpha_n \cos(\omega_n t) + \beta_n \sin(\omega_n]\, t) u_n(\vec{x}),$$

where $\omega_n = \sqrt{-\lambda_n}$ and the coefficients α_n and β_n are determined by the (two) initial conditions on u.

More generally, assuming that we have a complete basis of eigenfunctions of $\hat{A}$, we could write any $u(\vec{x}, t)$ in the form

$$u(\vec{x}, t) = \sum_n c_n(t) u_n(\vec{x}) \tag{1}$$

for some time-dependent coefficients c_n. This is called a sum of **separable solutions** *if the $c_n(t)$ are determined by ODEs that are* ***independent*** *for different n,* so that each term $c_n u_n$ is a solution of the PDE *by itself* (for some initial conditions). Such independence occurs when the u terms in the PDE are *time-invariant* in the sense that it is the same equation, with the same coefficients, at every t. For example, PDEs of the form

$$\left(\sum_{m=1}^{d} a_m \frac{\partial^m}{\partial t^m}\right) u = \hat{A}u + f(\vec{x}, t)$$

have separable solutions if the coefficients a_m are constants and $\hat{A}$ is time-independent, even though the source term f may depend on time, because one can expand f in the u_n basis and still obtain a separate (inhomogeneous) ODE for each c_n.

2.1 "Generalization"

One often sees separation in time posed in a "general" form as looking for solutions $u(\vec{x}, t)$ of the form $T(t)S(\vec{x})$ where T is an unknown function of time and S is an uknown function of space. In practice, however, this inevitably reduces to finding that S must be an eigenfunction of $\hat{A}$ in equations like those above (and otherwise you find that separation of time doesn't work), so I prefer the linear-algebra perspective of *starting* with an eigenfunction basis.

Just for fun, however, we can do it that way. Consider $\hat{A}u = \frac{\partial u}{\partial t}$, for example, and suppose we pretend to be ignorant of eigenfunctions. Instead, we "guess" a solution of the form $u = T(t)S(\vec{x})$ and plug this in to obtain: $T\hat{A}S = T'S$, then divide by TS to obtain

$$\frac{\hat{A}S}{S} = \frac{T'}{T}.$$

Since the left-hand side is a function of $\vec{x}$ only, and the right-hand side is a function of t only, in order for them to be equal to one another for all $\vec{x}$ and for all t they must both equal a constant. Call that constant λ. Then $T' = \lambda T$ and hence $T(t) = T(0)e^{\lambda t}$, while $\hat{A}S = \lambda S$ is the usual eigenproblem.

2.2 Similar "coupled-mode" equations (eigenbasis, but *not* separable)

On the other, one does *not* usually have separable solutions if $\hat{A}(t)$ depends on time. In that case, one could of course solve the eigenequation $\hat{A}u = \lambda u$ at each time t to obtain eigenfunctions $u_n(\vec{x}, t)$ and eigenvalues $\lambda_n(t)$ that vary with time. One can still expand the solution $u(\vec{x}, t)$ in this basis at each t, in the form of eq. (1), but it obviously no longer separable because u_n now depends on t. Less obviously, if one substitutes eq. (1) back into the PDE, one will find that the c_n equations are now coupled together inextricably in general. The resulting equations for the c_n are called *coupled-mode equations*, and their study is of great interest, but it does not fall under the category of separation of variables.

3 Separation in space

Spatial separation of variables is most commonly applied to eigenproblems $\hat{A}u_n = \lambda_n u_n$, and we reduce this to an eigenproblem in fewer spatial dimensions by writing the $u_n(\vec{x})$ as a product of functions in lower dimensions. Almost always, spatial separation of variables is applied in one of only four cases, as depicted in figure 1:

- A "box" domain Ω (or higher-dimensional analogues), within which the PDE coefficients are *constant*, and with boundary conditions that are invariant within each wall of the box. We can then usually find separable solutions of the form $u_n(\vec{x}) = X(x)Y(y)\cdots$ for some univariate functions X, Y, etc.

- A rotationally invariant $\hat{A}$ and domain Ω (e.g. a circle in 2d or a spherical ball in 3d), with rotationally invariant boundary conditions and rotationally invariant coefficients [although we *can* have coefficients varying with r]. In this case, as a consequence of symmetry, it turns out that we can always find separable eigenfunctions $u_n(\vec{x}) = R(r)P(\text{angle})$ for some functions R and P. In fact, it turns out that the angular dependence P is always of the same form—for scalar u, one always obtains $P(\phi) = e^{im\phi}$ in 2d (where m is an integer) and $P(\theta, \phi) = Y_{\ell,m}(\theta, \phi)$ in 3d [where ℓ is a positive integer, m is an integer with $|m| \leq \ell$, and $Y_{\ell,m}$ is a "spherical harmonic" function $\sim P_{\ell,m}(\cos\theta)e^{im\phi}$ for Legendre polynomials $P_{\ell,m}$].

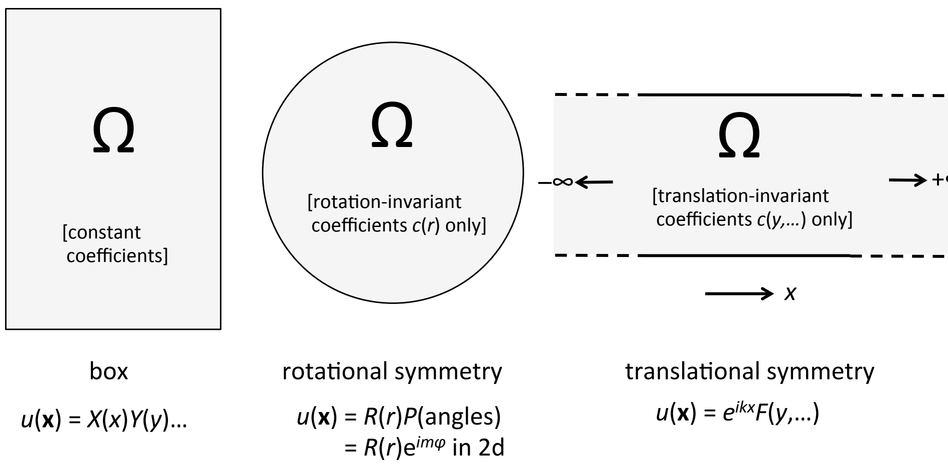

Figure 1: Most common cases where spatial separation of variables works: a box, a ball (rotational invariance), and an infinite tube (translational invariance).

- A translationally invariant problem, e.g. invariant (hence infinite) Ω in the x direction with x-invariant boundary conditions and coefficients. In this case, as a consequence of symmetry, it turns out that we can always find separable eigenfunctions $u_n(\vec{x}) = X(x)F(y,\ldots)$, and in fact it turns out that X always has the same form $X(x) = e^{ikx}$ for real k (if we are restricting ourselves to solutions that do not blow up at infinity).

- Combinations of the above cases. e.g. an infinite circular cylinder in 3d with corresponding symmetry in $\hat{A}$ has separable solutions $R(r)e^{im\phi+ikz}$.

The fact that symmetry leads to separable solutions is an instance of a much deeper connection between symmetry and solutions of linear PDEs, which is described by a different sort of algebraic structure that we won't really get to in 18.303: symmetries are described by a symmetry "group," and the relationship between the structure of this group and the eigensolutions is described in general terms of *group representation theory*.[1] In the case of rotational symmetry, expanding in the basis of eigenfunctions leads to a *Fourier series* in the ϕ direction (a sum of terms $\sim e^{im\phi}$), while in the case of translational symmetry one obtains a *Fourier transform* (a sum, or rather an integral, of terms $\sim e^{ikx}$). In 18.303, we will obtain the separable solutions by the simpler expedient of "guessing" a certain form of u_n, plugging it in, and showing that it works, but it is good to be aware that there is a deeper reason why this works in the cases above (and *doesn't work* in almost all other cases) and that if you encounter one of these cases you can just look up the form of the solution in a textbook.

In addition to the above situations, there are a few other cases in which separable solutions are obtained, but for the most part they aren't cases that one would encounter by accident; they are usually somewhat contrived situations that have been explicitly constructed to be separable.[2]

[1] See, for example, *Group Theory and Its Applications in Physics* by Inui *et al.*, or *Group Theory and Quantum Mechanics* by Michael Tinkham.

[2] For example, the separable cases of the Schrödinger operator $\hat{A} = -\nabla^2 + V(\vec{x})$ were enumerated by Eisenhart, *Phys. Rev.* **74**, pp. 87–89 (1948). An interesting nonsymmetric separable construction for the Maxwell equations was described in, for example, Watts *et al.*, Opt. Lett. **27**, pp. 1785–1787 (2002).

3.1 Example: ∇^2 in a 2d box

As an example, consider the operator $\hat{A} = \nabla^2$ in a 2d "box" domain $\Omega = [0, L_x] \times [0, L_y]$, with Dirichlet boundaries $u|_{\partial\Omega} = 0$. Even before we solve it, we should remind ourselves of the algebra properties we already know. This $\hat{A}$ is self-adjoint and negative-definite under the inner product $\langle u, v \rangle = \int_\Omega \bar{u}v = \int_0^{L_x} dx \int_0^{L_y} dy\, \overline{u(x,y)}v(x,y)$, so we should expect real eigenvalues $\lambda < 0$ and orthogonal eigenfunctions.

We will "guess" separable solutions to the eigenproblem $\hat{A}u = \lambda u$, of the form

$$u(\vec{x}) = X(x)Y(y),$$

and plug this into our eigenproblem. We need to check (i) that we can find solutions of this form and (ii) that solutions of this form are sufficient (i.e. we aren't missing anything—that all solutions can be expressed as superpositions of separable solutions). Of course this isn't really a guess, because in reality we would have immediately recognized that this is one of the handful of cases where separable solutions occur, but let's proceed as if we didn't know this. Plugging this u into the eigenequation, we obtain

$$\nabla^2 u = X''Y + XY'' = \lambda u = \lambda XY,$$

where primes denote derivatives as usual. In order to obtain such a separable solution, we must be able to separate all of the x and y dependence into separate equations, and the trick is (always) to divide both sides of the equation by u. We obtain:

$$\frac{X''}{X} + \frac{Y''}{Y} = \lambda.$$

Observe that we have a function X''/X of x alone plus a function Y''/Y of y alone, and their sum is a *constant* λ for *all* values of x and y. The only way this can happen is if X''/X and Y''/Y are themselves constants, say α and β respectively, so that we have two *separate* eigenequations

$$X'' = \alpha X,$$

$$Y'' = \beta Y,$$

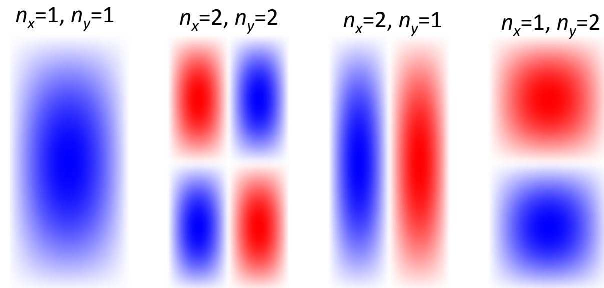

Figure 2: Example separable eigenfunctions u_{n_x,n_y} of ∇^2 in a 2d rectangular domain. (Blue/white/red = negative/zero/positive.)

with $\lambda = \alpha + \beta$. But we have already solved these equations, in one dimension, and we know that the solutions are sines/cosines/exponentials! More specifically, what are the boundary conditions on X and Y? To obtain $u(0, y) = X(0)Y(y) = 0 = u(L_x, y) = X(L_x)Y(y)$ for *all* values of y, we must have $X(0) = X(L_x) = 0$ (except for the trivial solution $Y = 0 \implies u = 0$). Similarly, $Y(0) = Y(L_y) = 0$. Hence, this is the familiar 1d Laplacian eigenproblem with Dirichlet boundary conditions, and we can quote our previous solution:

$$X_{n_x}(x) = \sin\left(\frac{n_x \pi x}{L_x}\right), \quad \alpha_{n_x} = -\left(\frac{n_x \pi}{L_x}\right)^2,$$

$$Y_{n_y}(x) = \sin\left(\frac{n_y \pi y}{L_y}\right), \quad \beta_{n_y} = -\left(\frac{n_y \pi}{L_y}\right)^2,$$

for positive integers $n_x = 1, 2, \ldots$ and $n_y = 1, 2, \ldots$, so that our final solution is

$$u_{n_x,n_y}(x, y) = \sin\left(\frac{n_x \pi x}{L_x}\right) \sin\left(\frac{n_y \pi y}{L_y}\right),$$

$$\lambda_{n_x,n_y} = -\pi^2 \left[\left(\frac{n_x}{L_x}\right)^2 + \left(\frac{n_y}{L_y}\right)^2\right].$$

Some examples of these eigenfunctions are plotted in figure 2. Note that λ is real and < 0 as expected. Furthermore, as expected the eigenfunctions are orthogonal:

$$\langle u_{n_x,n_y}, u_{n_x',n_y'} \rangle = 0 \text{ if } n_x \neq n_{x'} \text{ or } n_y \neq n_y'$$

because the $\langle u_{n_x,n_y}, u_{n'_x,n'_y}\rangle$ integral for separable u factors into two separate integrals over x and y,

$$\langle u_{n_x,n_y}, u_{n'_x,n'_y}\rangle = \left[\int_0^{L_x} X_{n_x}(x)X_{n'_x}(x)dx\right] \cdot \left[\int_0^{L_y} Y_{n_y}(y)Y_{n'_y}(y)dy\right],$$

and so the familiar orthogonality of the 1d Fourier sine series terms applies.

So, separable solutions exist. The next question is, are these enough? We need to be able to construct *every* function u in our Hilber (or Sobolev) space as a superposition of these separable functions. That is, can we write "any" $u(x,y)$ as

$$\begin{aligned} u(x,y) &= \sum_{n_x,n_y} c_{n_x,n_y} u_{n_x,n_y}(x,y) \\ &= \sum_{n_x=1}^{\infty}\sum_{n_y=1}^{\infty} c_{n_x,n_y} \sin\left(\frac{n_x\pi x}{L_x}\right)\sin\left(\frac{n_y\pi y}{L_y}\right) \end{aligned} \tag{2}$$

for some coefficients c_{n_x,n_y} [$= \langle u_{n_x,n_y}, u\rangle / \langle u_{n_x,n_y}, u_{n_x,n_y}\rangle$ because of the orthogonality of the basis]? The answer is *yes* (for any square-integrable u, i.e. finite $\langle u,u\rangle$) because we simply have a combination of two Fourier-sine series, one in x and one in y. For example, if we fix y and look as a function of x, we know we can write $u(x,y)$ as a 1d sine series in x:

$$u(x,y) = \sum_{n_x=1}^{\infty} c_{n_x}(y)\sin\left(\frac{n_x\pi x}{L_x}\right),$$

with different coefficients c_{n_x} for each y. Furthermore, we can write $c_{n_x}(y)$ itself as a sine series in y (noting that c_{n_x} must vanish at $y=0$ and $y=L_y$ by the boundary conditions on u):

$$c_{n_x}(y) = \sum_{n_y=1}^{\infty} c_{n_x,n_y}\sin\left(\frac{n_y\pi y}{L_y}\right)$$

for coefficients c_{n_x,n_y} that depend on n_x. The combination of these two 1d series is exactly equation (2)!

3.2 Non-separable examples

If the problem were not separable, something would have gone wrong in plugging in the separable form of $u(\vec{x})$ and trying to solve for the 1d functions individually. It is not hard to construct *non*-separable example problems, since *almost all* PDEs are *not* separable. However, let's start with the box problem above, and show how even a "small" change to the problem can spoil separability.

For example, suppose that we keep the same box domain Ω and the same boundary conditions, but we change our operator $\hat{A}$ to $\hat{A} = c(\vec{x})\nabla^2$ with some arbitrary $c(\vec{x}) > 0$. This operator is still self-adjoint and negative definite under the inner product $\langle u,v\rangle = \int_\Omega \bar{u}v/c$. But if we try to plug $u = X(x)Y(y)$ into the eigenequation $\hat{A}u = \lambda u$ and follow the same procedure as above to try to separate the x and y dependence, we obtain

$$\frac{X''}{X} + \frac{Y''}{Y} = \frac{\lambda}{c(x,y)}.$$

On the left-hand side, we still have a function of x alone plus a function of y alone, but on the right-hand side we now have a function of both x and y. So, we can no longer conclude that X''/X and Y''/Y are constants to obtain separate eigenequations for X and Y. Indeed, it is obvious that, for an arbitrary c, we cannot in general express λ/c as the sum of functions of x and y alone. (There are *some* c functions for which separability still works, but these cases need to be specially contrived.)