

# DATA ANALYSIS ON BOUNDARY VALUE PROBLEM (SPHERICAL BODY)

*Rajurkar Ravindra Kawadu*

*Research Scholar, Dept. of Mathematics Cmj University, Shillong, Meghalaya*

## INTRODUCTION

In mathematics, in the field of differential equations, a boundary value problem is a differential equation together with a set of additional restraints, called the boundary conditions. A solution to a boundary value problem is a solution to the differential equation which also satisfies the boundary conditions.

Boundary value problems arise in several branches of physics as any physical differential equation will have them. Problems involving the wave equation, such as the determination of normal modes, are often stated as boundary value problems. A large class of important boundary value problems are the Sturm–Liouville problems. The analysis of these problems involves the Eigen functions of a differential operator.

To be useful in applications, a boundary value problem should be well posed. This means that given the input to the problem there exists a unique solution, which depends continuously on the input. Much theoretical work in the field of partial differential equations is devoted to proving that boundary value problems arising from scientific and engineering applications are in fact well-posed.

Among the earliest boundary value problems to be studied is the Dirichlet problem, of finding the harmonic functions (solutions to Laplace's equation); the solution was given by the Dirichlet's principle.

## DEFINITIONS OF MATHEMATICS

Aristotle defined mathematics as "the science of quantity", and this definition prevailed until the 18th century. Starting in the 19th century, when the study of mathematics increased in rigor and began to address abstract topics such as group theory and projective geometry, which have no clear-cut relation to quantity and measurement, mathematicians and philosophers began to propose a variety of new definitions. Some of these definitions emphasize the deductive character of much of mathematics, some emphasize its abstractness, some emphasize certain topics within mathematics. Today, no consensus on the definition of mathematics prevails, even among professionals. There is not even consensus on whether mathematics is an art or a science. A great many professional mathematicians take no interest in a definition of mathematics, or consider it undefinable. Some just say, "Mathematics is what mathematicians do."

Three leading types of definition of mathematics are called logicist, intuitionist, and formalist, each reflecting a different philosophical school of thought. All have severe problems, none has widespread acceptance, and no reconciliation seems possible.

An early definition of mathematics in terms of logic was Benjamin Peirce's "the science that draws necessary conclusions" (1870). In the Principia Mathematica, Bertrand Russell and

Alfred North Whitehead advanced the philosophical program known as logicism, and attempted to prove that all mathematical concepts, statements, and principles can be defined and proven entirely in terms of symbolic logic. A logicist definition of mathematics is Russell's "All Mathematics is Symbolic Logic" (1903).

Intuitionist definitions, developing from the philosophy of mathematician L.E.J. Brouwer, identify mathematics with certain mental phenomena. An example of an intuitionist definition is "Mathematics is the mental activity which consists in carrying out constructs one after the other." A peculiarity of intuitionism is that it rejects some mathematical ideas considered valid according to other definitions. In particular, while other philosophies of mathematics allow objects that can be proven to exist even though they cannot be constructed, intuitionism allows only mathematical objects that one can actually construct.

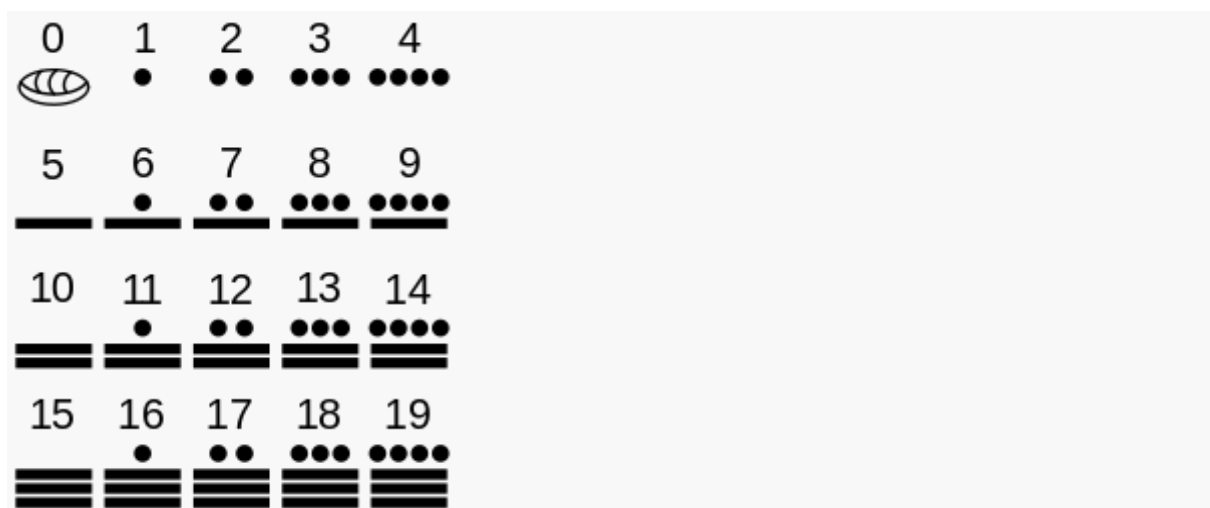
Formalist definitions identify mathematics with its symbols and the rules for operating on them. Haskell Curry defined mathematics simply as "the science of formal systems". A formal system is a set of symbols, or tokens, and some rules telling how the tokens may be combined into formulas. In formal systems, the word axiom has a special meaning, different from the ordinary meaning of "a self-evident truth". In formal systems, an axiom is a combination of tokens that is included in a given formal system without needing to be derived using the rules of the system.

Greek mathematician Pythagoras (c. 570 – c. 495 BC), commonly credited with discovering the Pythagorean Theorem.

The evolution of mathematics might be seen as an ever-increasing series of abstractions, or alternatively an expansion of subject matter. The first abstraction, which is shared by many animals, was probably that of numbers: the realization that a collection of two apples and a collection of two oranges (for example) have something in common, namely quantity of their members.

In addition to recognizing how to count physical objects, prehistoric peoples also recognized how to count abstract quantities, like time – days, seasons, years. Elementary arithmetic (addition, subtraction, multiplication and division) naturally followed.

Since numeracy pre-dated writing, further steps were needed for recording numbers such as tallies or the knotted strings called quipu used by the Inca to store numerical data. Numeral systems have been many and diverse, with the first known written numerals created by Egyptians in Middle Kingdom texts such as the Rhind Mathematical Papyrus.



## MAYAN NUMERALS

The earliest uses of mathematics were in trading, land measurement, painting and weaving patterns and the recording of time. More complex mathematics did not appear until around 3000 BC, when the Babylonians and Egyptians began using arithmetic, algebra and geometry for taxation and other financial calculations, for building and construction, and for astronomy. The systematic study of mathematics in its own right began with the Ancient Greeks between 600 and 300 BC.

Mathematics has since been greatly extended, and there has been a fruitful interaction between mathematics and science, to the benefit of both. Mathematical discoveries continue to be made today. According to Mikhail B. Sevryuk, in the January 2006 issue of the Bulletin of the American Mathematical Society, "The number of papers and books included in the Mathematical Reviews database since 1940 (the first year of operation of MR) is now more than 1.9 million, and more than 75 thousand items are added to the database each year. The overwhelming majority of works in this ocean contain new mathematical theorems and their proofs."

## SPHERICAL HARMONICS

In mathematics, spherical harmonics are the angular portion of a set of solutions to Laplace's equation. Represented in a system of spherical coordinates, Laplace's spherical harmonics  $Y_\ell^m$  are a specific set of spherical harmonics that forms an orthogonal system, first introduced by Pierre Simon de Laplace in 1782. Spherical harmonics are important in many theoretical and practical applications, particularly in the computation of atomic orbital electron configurations, representation of gravitational fields, geoids, and the magnetic fields of planetary bodies and stars, and characterization of the cosmic microwave background radiation. In 3D computer graphics, spherical harmonics play a special role in a wide variety of topics including indirect lighting (ambient occlusion, global illumination, precomputed radiance transfer, etc.) and recognition of 3D shapes.

Spherical harmonics were first investigated in connection with the Newtonian potential of Newton's law of universal gravitation in three dimensions. In 1782, Pierre-Simon de Laplace had, in his *Mécanique Céleste*, determined that the gravitational potential at a point  $\mathbf{x}$  associated to a set of point masses  $m_i$  located at points  $\mathbf{x}_i$  was given by

$$V(\mathbf{x}) = \sum_i \frac{m_i}{|\mathbf{x}_i - \mathbf{x}|}.$$

Each term in the above summation is an individual Newtonian potential for a point mass. Just prior to that time, Adrien-Marie Legendre had investigated the expansion of the Newtonian potential in powers of  $r = |\mathbf{x}|$  and  $r_1 = |\mathbf{x}_1|$ . He discovered that if  $r \leq r_1$  then

$$\frac{1}{|\mathbf{x}_1 - \mathbf{x}|} = P_0(\cos \gamma) \frac{1}{r_1} + P_1(\cos \gamma) \frac{r}{r_1^2} + P_2(\cos \gamma) \frac{r^2}{r_1^3} + \dots$$

Where  $\gamma$  is the angle between the vectors  $\mathbf{x}$  and  $\mathbf{x}_1$ . The functions  $P_i$  are the Legendre polynomials, and they are a special case of spherical harmonics. Subsequently, in his 1782 memoir, Laplace investigated these coefficients using spherical coordinates to represent the angle  $\gamma$  between  $\mathbf{x}_1$  and  $\mathbf{x}$ . (See Applications of Legendre polynomials in physics for a more detailed analysis.)

In 1867, William Thomson (Lord Kelvin) and Peter Guthrie Tait introduced the solid spherical harmonics in their Treatise on Natural Philosophy, and also first introduced the name of "spherical harmonics" for these functions. The solid harmonics were homogeneous solutions of Laplace's equation

$$\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} + \frac{\partial^2 u}{\partial z^2} = 0.$$

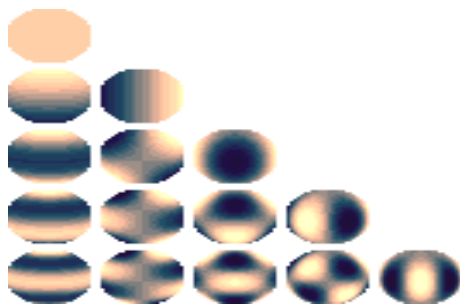
By examining Laplace's equation in spherical coordinates, Thomson and Tait recovered Laplace's spherical harmonics. The term "Laplace's coefficients" was employed by William Whewell to describe the particular system of solutions introduced along these lines, whereas others reserved this designation for the zonal spherical harmonics that had properly been introduced by Laplace and Legendre.

The 19th century development of Fourier series made possible the solution of a wide variety of physical problems in rectangular domains, such as the solution of the heat equation and wave equation. This could be achieved by expansion of functions in series of trigonometric functions. Whereas the trigonometric functions in a Fourier series represent the fundamental modes of vibration in a string, the spherical harmonics represent the fundamental modes of vibration of a sphere in much the same way. Many aspects of the theory of Fourier series could be generalized by taking expansions in spherical harmonics rather than trigonometric functions. This was a boon for problems possessing spherical symmetry, such as those of celestial mechanics originally studied by Laplace and Legendre.

The prevalence of spherical harmonics already in physics set the stage for their later importance in the 20th century birth of quantum mechanics. The spherical harmonics are Eigen functions of the square of the orbital angular momentum operator and therefore they represent the different quantized configurations of atomic orbitals.

$$-i\hbar \mathbf{r} \times \nabla,$$

## LAPLACE'S SPHERICAL HARMONICS



Real (Laplace) spherical harmonics  $Y_\ell^m$  for  $\ell = 0$  to  $4$  (top to bottom) and  $m = 0$  to  $4$  (left to right). The negative order harmonics  $Y_\ell^{-m}$  are rotated about the  $z$ -axis by  $90^\circ/m$  with respect to the positive order ones.

Laplace's equation imposes that the divergence of the gradient of a scalar field  $f$  is zero. In spherical coordinates this is:

$$\nabla^2 f = \frac{1}{r^2} \frac{\partial}{\partial r} \left( r^2 \frac{\partial f}{\partial r} \right) + \frac{1}{r^2 \sin \theta} \frac{\partial}{\partial \theta} \left( \sin \theta \frac{\partial f}{\partial \theta} \right) + \frac{1}{r^2 \sin^2 \theta} \frac{\partial^2 f}{\partial \varphi^2} = 0.$$

Consider the problem of finding solutions of the form  $f(r, \theta, \varphi) = R(r)Y(\theta, \varphi)$ . By separation of variables, two differential equations result by imposing Laplace's equation:

$$\frac{1}{R} \frac{d}{dr} \left( r^2 \frac{dR}{dr} \right) = \lambda, \quad \frac{1}{Y} \frac{1}{\sin \theta} \frac{\partial}{\partial \theta} \left( \sin \theta \frac{\partial Y}{\partial \theta} \right) + \frac{1}{Y} \frac{1}{\sin^2 \theta} \frac{\partial^2 Y}{\partial \varphi^2} = -\lambda.$$

The second equation can be simplified under the assumption that  $Y$  has the form  $Y(\theta, \varphi) = \Theta(\theta)\Phi(\varphi)$ . Applying separation of variables again to the second equation gives way to the pair of differential equations

$$\frac{1}{\Phi(\varphi)} \frac{d^2 \Phi(\varphi)}{d\varphi^2} = -m^2$$

$$\lambda \sin^2(\theta) + \frac{\sin(\theta)}{\Theta(\theta)} \frac{d}{d\theta} \left[ \sin(\theta) \frac{d\Theta}{d\theta} \right] = m^2$$

for some number  $m$ . A priori,  $m$  is a complex constant, but because  $\Phi$  must be a periodic function whose period evenly divides  $2\pi$ ,  $m$  is necessarily an integer and  $\Phi$  is a linear combination of the complex exponentials  $e^{\pm im\varphi}$ . The solution function  $Y(\theta, \varphi)$  is regular at the poles of the sphere, where  $\theta=0, \pi$ . Imposing this regularity in the solution  $\Theta$  of the second equation at the boundary points of the domain is a Sturm–Liouville problem that forces the parameter  $\lambda$  to be of the form  $\lambda = \ell(\ell+1)$  for some non-negative integer with  $\ell \geq |m|$ ; this is also explained below in terms of the orbital angular momentum. Furthermore, a change of variables  $t = \cos\theta$  transforms this equation into the Legendre equation, whose solution is a multiple of the associated Legendre polynomial  $P_\ell^m(\cos\theta)$ . Finally, the equation for  $R$  has solutions of the form  $R(r) = Ar^\ell + Br^{-\ell-1}$ ; requiring the solution to be regular throughout  $R^3$  forces  $B = 0$ .

Here the solution was assumed to have the special form  $Y(\theta, \varphi) = \Theta(\theta)\Phi(\varphi)$ . For a given value of  $\ell$ , there are  $2\ell+1$  independent solutions of this form, one for each integer  $m$  with  $-\ell \leq m \leq \ell$ . These angular solutions are a product of trigonometric functions, here represented as a complex exponential, and associated Legendre polynomials:

$$Y_\ell^m(\theta, \varphi) = N e^{im\varphi} P_\ell^m(\cos\theta)$$

which fulfill

$$r^2 \nabla^2 Y_\ell^m(\theta, \varphi) = -\ell(\ell+1) Y_\ell^m(\theta, \varphi).$$

Here  $Y_\ell^m$  is called a spherical harmonic function of degree  $\ell$  and order  $m$ ,  $P_\ell^m$  is an associated Legendre polynomial,  $N$  is a normalization constant, and  $\theta$  and  $\varphi$  represent colatitude and longitude, respectively. In particular, the colatitude  $\theta$ , or polar angle, ranges from 0 at the North Pole to  $\pi$  at the South Pole, assuming the value of  $\pi/2$  at the Equator, and the longitude  $\varphi$ , or azimuth, may assume all values with  $0 \leq \varphi < 2\pi$ . For a fixed integer  $\ell$ , every solution  $Y(\theta, \varphi)$  of the Eigen value problem.

$$r^2 \nabla^2 Y = -\ell(\ell + 1)Y$$

is a linear combination of  $Y_\ell^m$ . In fact, for any such solution,  $r^\ell Y(\theta, \varphi)$  is the expression in spherical coordinates of a homogeneous polynomial that is harmonic, and so counting dimensions shows that there are  $2\ell+1$  linearly independent such polynomials.

The general solution to Laplace's equation in a ball centered at the origin is a linear combination of the spherical harmonic functions multiplied by the appropriate scale factor  $r^\ell$ ,

$$f(r, \theta, \varphi) = \sum_{\ell=0}^{\infty} \sum_{m=-\ell}^{\ell} f_\ell^m r^\ell Y_\ell^m(\theta, \varphi),$$

where the  $f_\ell^m$  are constants and the factors  $r^\ell Y_\ell^m$  are known as solid harmonics. Such an expansion is valid in the ball

$$r < R = 1 / \limsup_{\ell \rightarrow \infty} |f_\ell^m|^{1/\ell}.$$

## ORBITAL ANGULAR MOMENTUM

In quantum mechanics, Laplace's spherical harmonics are understood in terms of the orbital angular momentum [4]

$$\mathbf{L} = -i\hbar \mathbf{x} \times \nabla = L_x \mathbf{i} + L_y \mathbf{j} + L_z \mathbf{k}.$$

The  $\hbar$  is conventional in quantum mechanics; it is convenient to work in units in which  $\hbar = 1$ . The spherical harmonics are Eigen functions of the square of the orbital angular momentum

$$\begin{aligned} \mathbf{L}^2 &= -r^2 \nabla^2 + \left( r \frac{\partial}{\partial r} + 1 \right) r \frac{\partial}{\partial r} \\ &= -\frac{1}{\sin \theta} \frac{\partial}{\partial \theta} \sin \theta \frac{\partial}{\partial \theta} - \frac{1}{\sin^2 \theta} \frac{\partial^2}{\partial \varphi^2}. \end{aligned}$$

Laplace's spherical harmonics are the joint Eigen functions of the square of the orbital angular momentum and the generator of rotations about the azimuthal axis:

$$\begin{aligned} L_z &= -i \left( x \frac{\partial}{\partial y} - y \frac{\partial}{\partial x} \right) \\ &= -i \frac{\partial}{\partial \varphi}. \end{aligned}$$

These operators commute, and are densely defined self-adjoint operators on the Hilbert space of functions  $f$  square-integrable with respect to the normal distribution on  $\mathbb{R}^3$ :

$$\frac{1}{(2\pi)^{3/2}} \int_{\mathbb{R}^3} |f(x)|^2 e^{-|x|^2/2} dx < \infty.$$

Furthermore,  $L^2$  is a positive operator.

If  $Y$  is a joint Eigen function of  $L^2$  and  $L_z$ , then by definition

$$\begin{aligned} L^2 Y &= \lambda Y \\ L_z Y &= m Y \end{aligned}$$

for some real numbers  $m$  and  $\lambda$ . Here  $m$  must in fact be an integer, for  $Y$  must be periodic in the coordinate  $\varphi$  with period a number that evenly divides  $2\pi$ . Furthermore, since

$$L^2 = L_x^2 + L_y^2 + L_z^2$$

and each of  $L_x, L_y, L_z$  are self-adjoint, it follows that  $\lambda \geq m^2$ .

Denote this joint eigenspace by  $E_{\lambda,m}$ , and define the raising and lowering operators by

$$\begin{aligned} L_+ &= L_x + iL_y \\ L_- &= L_x - iL_y \end{aligned}$$

Then  $L_+$  and  $L_-$  commute with  $L^2$ , and the Lie algebra generated by  $L_+, L_-, L_z$  is the special linear Lie algebra, with commutation relations

$$[L_z, L_+] = L_+, \quad [L_z, L_-] = -L_-, \quad [L_+, L_-] = 2L_z.$$

Thus  $L_+ : E_{\lambda,m} \rightarrow E_{\lambda,m+1}$  (it is a "raising operator") and  $L_- : E_{\lambda,m} \rightarrow E_{\lambda,m-1}$  (it is a "lowering operator"). In particular,  $L_+^k : E_{\lambda,m} \rightarrow E_{\lambda,m+k}$  must be zero for  $k$  sufficiently large, because the inequality  $\lambda \geq m^2$  must hold in each of the nontrivial joint Eigen spaces. Let  $Y \in E_{\lambda,m}$  be a nonzero joint Eigen function, and let  $k$  be the least integer such that

$$L_+^k Y = 0.$$

Then, since

$$L_- L_+ = L^2 - L_z^2 - L_z$$

it follows that

$$0 = L_- L_+^k Y = (\lambda - (m+k)^2 - (m+k))Y.$$

Thus  $\lambda = \ell(\ell+1)$  for the positive integer  $\ell = m+k$ .

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