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Modelling Geophysical Fields in Source Free Regions by Fourier Series and Rectangular Harmonic Analysis

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Abstract

In modelling geophysical fields in source free regions, the main interest is in representing data by means of a finite series, subject possibly to potential constraints, rather than in the analytical problem of finding the limit of an infinite series. Therefore, it is important that the series representing the field data be uniformly convergent, rather than merely convergent in mean square. Since these geophysical fields are continuous and have continuous derivatives of all orders, uniformly convergent series representations may be derived by the Sturm-Liouville theorem. The differential equation that governs potential fields (in three dimensions) is Laplace's Equation, which when solved by separation of variables also gives rise to Fourier series (in one and two dimensions). Some boundary conditions, such as the requirement of periodicity or the requirement of arbitrary values on the boundary, are self-adjoint and provide expansions in terms of orthogonal basis functions. Other boundary conditions, such as the requirement of both arbitrary values and arbitrary derivatives on the boundary, are not self-adjoint and orthogonal expansions cannot be found, although non-orthogonal expansions can be formed by superposition of basis functions from self-adjoint problems. In the case of single and double Fourier series, expansions can also be found by means of functional transformations. In cartesian geometry, the basis functions for the periodic boundary-value problem involve the familiar sine and cosine functions, and their harmonics, defined on a full period 2π. These will be referred to as "periodic" basis functions. The basis functions for arbitrary values on the boundary involve functions defined on a half-period π rather than on a full period 2π. These will be referred to as "half-periodic" basis functions, and give rise to the familiar cosine series when the interval is chosen appropriately. The basis functions that provide both arbitrary values and arbitrary derivatives on the boundary (a non-self-adjoint problem) are again "half-periodic", but now involve both cosine and sine functions. As a Fourier representation, this is a combination of the familiar cosine and sine series, and is referred to here as the "cosine+sine" series. Expansions that are based on "periodic" basis functions when they should in fact be based on "half-periodic" basis functions are convergent only in mean square and exhibit ringing at the boundaries. In the case of rectangular harmonic analysis, the "periodic" limit function does not even satisfy Laplace's Equation whereas the limit function from appropriately chosen "half-periodic" basis functions does. Furthermore, *the "periodic" expansions cannot then be differentiated term-wise, since the term-wise derivatives do not converge to the derivatives of the modelled field (even in mean square, let alone uniformly). Even when an expansion is uniformly convergent, its derivative may not be, unless the basis functions have been chosen accordingly. Similar remarks apply when half-periodic cosines are used when half-periodic cosines and sines should both be used, except that the ringing now takes place in the derivative. These matters are of vital consequence especially in potential field work where it is usually the derivatives that are of primary interest, but also in any work with Fourier series that requires differentiation. Various combinations of basis function expansions are possible, depending on which derivatives are required. The appropriate combinations are derived easily by applying the appropriate boundary conditions. Furthermore, when derivatives are correctly modelled, better extrapolation is possible beyond the data area.*

1. *Introduction*

Mathematical modelling of general fields by one and two dimensional Fourier series and of potential and potential-gradient fields by rectangular harmonic analysis has been carried out frequently. The modelling has usually been done with basis functions that are periodic over the given data interval. The convergence that is invoked is usually with respect to mean square, which permits the expansion of an extremely wide class of functions. With respect to uniform convergence, however, the expansion is restricted to those functions that are, at a very minimum, continuous over the interval and having equal values at the interval boundaries. Frequently, well behaved fields whose values at boundaries are not equal, but are instead arbitrary, have been expanded in terms of these periodic functions without regard to their non-uniform convergence and in the case of rectangular harmonic analysis without regard to the fact that the resulting expansion, in the limit, does not even satisfy Laplace's differential equation. Even more shocking, expansions that are convergent only in mean square have been differentiated term by term, leading to series which do not converge, even in mean square, to the derivatives of the expanded function. In a similar way, expansions that converge uniformly have been differentiated term by term, without regard for the fact that the differentiated series, although it converges in mean square, may not converge uniformly.

In attempts to reduce the ringing from these periodic expansions, terms in the cartesian coordinates x and y, and the cross-product xy, have been used by several authors. None of these coordinate terms are required when the basis functions are chosen to give a uniformly convergent model. Furthermore, these coordinate terms have been used in rectangular harmonic expansions, where they incorrectly give a non-zero potential when the vertical coordinate z is infinite. Terms involving z have also been used in rectangular harmonic expansions in order to combat the mathematical difficulties of extending rectangular geometry to spherical. However, these terms also violate the boundary condition of zero potential at infinite z. When the rectangular area becomes large, the analysis can no longer be done in a cartesian system.

Geophysical fields in source free regions are extremely well behaved. They and their derivatives are continuous on any closed domain, and have well defined values at the boundaries of those domains. Mathematical representations of such fields should therefore include these same properties. The very powerful theorems of Sturm-Liouville and Fourier analyses can be readily applied to, and provide appropriate basis functions for, the expansion of such fields.

Periodicity is a model constraint that is often required in coordinate systems other than cartesian. When the field is not periodic (or, more generally, when field values are not the same at opposite boundaries), it is pointless to constrain the model to be periodic, particularly when the correct model constraints can be easily applied and they lead to expansions that are uniformly convergent and can have, if required, uniformly convergent derivatives. The expansions then involve Fourier sine and cosine terms, the basis functions being "half-periodic" over the data interval (i.e., periodic over twice the interval). The cosine terms themselves provide a uniformly convergent expansion whereas both the cosine and sine terms are required if the derivatives are to be uniformly convergent also.

Some earlier uses of periodic basis functions in double Fourier series/rectangular harmonic analysis include *Tsuboi* (1938a; 1938b), *Tsuboi and Fuchida* (1938), and *Nagata* (1938a; 1938b). *Vestine and Davids* (1945) used periodic functions for a rectangular harmonic analysis of three-component magnetic anomalies and *Bhattacharyya* (1965) used periodic functions for modelling anomalous total field. *Lourenco and Morrison* (1973) used periodic rectangular basis functions to compute three-component anomaly data from total-field anomaly data. *Alldredge* (1981) continued the use of periodic basis functions for rectangular harmonic analysis of residual data, but added the cartesian coordinates x, y, and z as extra basis functions and excluded sine and cosine functions appearing individually in the expansion. These latter sine and cosine terms represent (in mean square) structure striking north-south and east-west, including the linear trends represented by the x and y terms. *Nakagawa and Yukutake* (1985) and *Nakagawa et al.* (1985) also used periodic functions, including the x, y, and z trend terms introduced by *Alldredge* (1981), but allowed the inclusion of the individually appearing sine and cosine terms. *Barton* (1987;1988) has also used periodic functions, as well as the x, y, and z terms, but included only individual sine and cosine terms of the fundamental period ($\sin x$, $\cos x$, $\sin y$, $\cos y$), excluding the higher harmonics.

In all of the above cases, the "half-periodic" basis functions would have been more appropriate, since differentiation was an essential aspect of the analyses. The expansions, being based on "periodic" basis functions, were not uniformly convergent and therefore did not necessarily provide derivatives that were convergent even in mean square. The practical problem of boundary ringing and the severity of any non-convergence evident at the truncation levels chosen were of course diminished by the use of anomaly data or by the use of x, y, and z trend terms with main field data. In the latter case, however, the addition of the coordinate basis functions x, y, and z to a potential expansion violates the condition of zero potential at infinite z.

In two later papers, *Alldredge* (1982; 1983) changed the fundamental wavelengths of the basis functions to twice the respective dimensions of the area under analysis, which effectively changed the basis functions from periodic to half-periodic. The x, y, and z terms were retained, and in the latter paper he finally allowed the inclusion of the individually appearing sine and cosine terms (which now represented structure striking north-south and east-west uniformly, rather than simply in mean square).

The trigonometric basis functions of the latter paper (*Alldredge*, 1983) are in fact appropriate for uniformly modelling differentiable functions with arbitrary values on the boundary, although of course various combinations of those basis functions may be chosen depending on which derivatives are required. Unfortunately, the addition of the coordinate basis functions x and y (no longer required for trend removal since the individual sine and cosine functions do that) and the coordinate basis function z violates, as before, the condition of zero potential at infinite z.

It should be emphasized that previous techniques of using basis functions that did not provide uniform convergence, of improperly differentiating these models, and of adding terms to the potential that do not fall to zero with increasing z, have nevertheless enabled useful results to be obtained. This is because the representations, over their domains of applicability, provided approximations to the mathematically correct formulations, and as such would have provided results that hopefully were not grossly in error.

The primary purpose of this paper is to derive basis functions for modelling potential fields in three-dimensional cartesian space, subject to various "boundary conditions" dictated by the mathematical properties required in the model. The solution of the relevant (Laplace's) differential equation is determined by the usual method of separation of variables, and involves, for the different boundary conditions, different combinations of trigonometric functions. Since the separated differential eigenequations are precisely the eigenequations that give rise to single and double Fourier series, the mathematical properties that apply to each of these will be discussed in turn. In this way, certain aspects of the full harmonic solution can be seen to apply also to modelling general fields (functions in one and two variables unconstrained by any differential equation) by the method of Fourier analysis. Of course, expansions other than Fourier series are possible in modelling these general fields. Because the Fourier technique is used so frequently, however, separate discussions of this technique, which falls out so easily from the harmonic analysis, will be useful.

The boundary conditions that are imposed on a model of course depend on what properties are required in the model. Uniform convergence is considered in this paper to be an essential property of a mathematical model. Differentiability may or may not be required, and if it is, only certain derivatives may be needed. Uniform convergence and differentiability together, however, lead to a "non-self-adjoint" boundary value problem, which is solved in this paper by a superposition of self-adjoint solutions, although for single and double Fourier series a second method of solution is also given. The paper will discuss some of the boundary conditions of use in mathematical modelling, and will derive basis functions that provide a uniformly convergent representation for a modelled field and also for various combinations of its derivatives. General scalar fields will be modelled by Fourier series, first in one and then in two variables, and finally scalar potential and vector potential-gradient fields will be modelled by rectangular harmonic analysis.

It will be shown that half-periodic cosine functions are appropriate for modelling uniformly, in source free regions, geophysical fields with arbitrary values on the boundaries. The basis functions are orthogonal, and require no trend removal. If the model is to be uniformly differentiable, with arbitrary derivatives on the boundaries, a second set of half-periodic sine functions is required, but some of these functions are not orthogonal to some of the cosine functions required merely for modelling the function. Using periodic basis functions results in ringing at the boundaries for both function and derivative because of the non-uniform convergence of the periodic expansion. Models that are able to provide correct slopes at the boundary are also able to provide better extrapolation beyond that boundary. An example will be given where the function $f(x) = x$ is modelled over the interval $(0, \pi)$ using various sets of basis functions.

By "Fourier series" in this paper is meant the familiar trigonometric series whose coefficients may be determined by the usual least-squares procedure. When the basis functions are orthogonal, of course, each coefficient may be simply expressed as a single Fourier integral (e.g., *Davis*, 1963, p.89). The same techniques presented in this paper could also be used for "generalized Fourier series" (*Churchill*, 1963, p.57), using differential equations other than Laplace's and coordinate systems other than cartesian, although these matters will not be discussed here. However, much of the discussion on modelling applies equally well to more generalized orthogonal expansions.

Throughout the paper, continuity of the modelled function and all its derivatives will be assumed. The emphasis will be on the boundary conditions that are satisfied by the function (or the derivative, if the derivative is being modelled), since continuity of function and derivative are not in themselves sufficient for the uniform convergence of a given expansion. That is, whereas usually in Fourier analysis the boundary condition is held fixed and the most general class of functions is obtained that provide mean square convergence, in this paper the class of functions is held fixed and the most general class of basis functions is obtained that provide uniform convergence for arbitrary boundary conditions.

2. *Uniform versus Ordinary and Mean Square Convergence*

If an infinite series of functions $s_n(x)$ converges to a limit function $S(x)$ over a closed interval, there is, at every point x in the interval, a number N such that $\sum_{n=1}^{N} s_n(x)$ differs from $S(x)$ by less than some predetermined error ϵ. With ordinary convergence, this truncation level N depends on both ϵ and x. Over certain parts of the interval, a small N may result in a sufficiently small ϵ, whereas in other parts a large value of N may be necessary to attain a reasonable accuracy and in fact no value of N will bring the error below a certain level. With uniform convergence, on the other hand, N depends only on ϵ. The same N will do for all points in the interval, and an N can be found to make ϵ as small as desired at all points within the closed interval. That is, a truncated series can be made to resemble the limit function, or the function being modelled, to any accuracy by choosing an appropriately large N.

Davis (1963, pp 114–115) gives a startling example of a non-uniformly convergent sequence, which for demonstration here could be written:

$$\sum_{n=1}^{N} s_n(x) = \frac{Nx}{1+N^2x^2}$$

As $N \to \infty$, this series tends to zero for every x, and yet there will always be a value of x for which a partial sum is equal to 1/2. A partial sum, for any value of N, will bear no resemblance to the limit function $S(x) = 0$.

The familiar Gibbs phenomenon of Fourier series, at a point of discontinuity, is another example where a non-uniformly converging series of functions does not resemble the limit function even at extremely large values of N. Over any interval that includes the point of discontinuity, no value of N will bring the error below a level of about 9% of the magnitude of the discontinuity (e.g., *Davis*, 1963, p.117). At the point of discontinuity, even the limit function differs from the function that the infinite series is intended to represent.

In contrast to both ordinary and uniform convergence, the series of functions $s_n(x)$ converges in mean square, over a given domain, to $S(x)$ when $\int \left(\sum_{n=1}^{N} s_n(x) - S(x)\right)^2 dx$ converges to zero as $N \to \infty$. This type of convergence (sometimes called convergence in the mean because the series converges to the mean of the right and left hand limits of $S(x)$) is very general, and applies to a wide class of functions. Even series that diverge may converge in mean square. Well-behaved functions do not require such a general definition for series convergence, the more restrictive uniform convergence being quite sufficient.

The importance of uniform convergence in geophysical modelling should be apparent. Although model representations, as derived mathematically, contain an infinite number of basis functions, in a practical problem only a finite number are used. That is, the infinite series is truncated so that the model is merely an approximation, rather than an exact representation, of a given function. Furthermore, the truncation level is a constant, the same number of terms being used for all points of the interval.

Thus, not only is it important that the mathematical representation converge to the appropriate limit function at all values of the functional argument, but also that the partial sums converge in a uniform way to the limit function so that, at every truncation level, they will resemble or "look like" the function they are intended to represent.

3. *Model Constraints*

If a field satisfies certain mathematical constraints throughout space, the mathematical model — the limit function, as well as any of the partial sums — must satisfy the same constraints. Similarly, if the field obeys constraints at one or more coordinate boundaries, the model must obey those constraints as well. For example, if the function or its derivative is specified at the boundaries, the basis functions must be such that the limit function attains those values on the boundaries. The basis functions themselves, however, may or may not satisfy the constraints. For example, if a function is zero on the boundary, all basis functions that have a zero boundary value will give a limit function with a zero boundary value. On the other hand, basis functions that are continuous may give a limit function that is not continuous. Similarly, basis functions that satisfy a certain differential equation may give a limit function that does not satisfy the same differential equation. A discontinuous limit function, for example, definitely does not satisfy Laplace's equation, even though the (continuous) basis functions may.

The basis functions may satisfy "modified" constraints that provide the proper model constraint in the limit. An example of a modified constraint is a zero derivative at the boundary. This constraint will be shown later to be a self-adjoint boundary condition and therefore gives basis functions for the orthogonal expansions of certain functions. If the basis functions satisfy this modified constraint, then the limit function can have an arbitrary value at the boundary. In this case, the limit function, even though it does not belong to the same class of functions as those with the modified constraint, can nevertheless be uniformly approximated by a series of functions from that class.

Another common "modified" constraint is that the basis functions be zero at a boundary. This self-adjoint constraint gives a limit function that can have an arbitrary derivative at the boundary (as well, of course, as constraining the limit function to have a zero boundary value). Here the derivative of the limit function, although it does not belong to the same class of functions as the basis function derivatives, can nevertheless be uniformly represented by function derivatives from that class.

4. *Differentiability of The Model*

Differentiability is really another constraint that must be imposed on the model if such is required. It is so frequently ignored, however, that it is useful to draw special attention to the fact that not only may differentiable basis functions not give a differentiable limit function, but even if they do, the corresponding series of basis function derivatives may not converge uniformly to the derivative of the limit function. This may be perfectly acceptable if the model need not be differentiated, but if the model is derivable from a derivative (as a potential field is usually derived from its gradient field) or if the derived model will subsequently be differentiated, then this differentiability must be imposed as a model constraint, and the basis functions must be such that the termwise derivative of the series gives the derivative of the limit function.

This relates, of course, to uniform convergence. An infinite series of derivatives does not necessarily converge to the derivative of the limit of the infinite series of functions, unless the series of derivatives is uniformly convergent and the series of functions converges in the given interval.

However, the main point is that the basis functions may come from a much more restricted class of functions than the limit function itself. The series of basis function derivatives may indeed converge, even uniformly, but only if the series of basis functions converges to a function of that restricted class. Otherwise, the derivative of the limit function will not be expressible in terms of the derivatives of the same restricted basis functions.

It may seem surprising that basis functions which satisfy a second-order differential equation may not provide a proper first derivative. The second derivative of a basis function $f_\lambda(x)$, however, is intimately related to the basis function itself through an equation such as

$$L\{f_\lambda(x)\} = \lambda f_\lambda(x)$$

where L is a second-order linear differential operator and λ is an eigenvalue. If L does not involve the first derivative, the eigenfunctions for modelling a function f and its second derivative f'' may not be appropriate for modelling the first derivative f'. For example, if $\cos(\lambda x)$ is an eigenfunction for $f(x)$, the first derivative $\sin(\lambda x)$ may not be an eigenfunction for $f'(x)$, even though the second derivative $\cos(\lambda x)$ is indeed an eigenfunction for $f''(x)$.

In addition to having the convenience of differentiability, models that contain information on derivatives also permit more accurate extrapolation beyond the data interval, provided of course that the regularity of the function continues into the extrapolated area. Basis functions that artificially introduce a discontinuity in a model at a data boundary give notoriously inaccurate extrapolations even at small distances beyond the boundary. But even uniformly convergent models that are not based on the differentiability constraint will not extrapolate particularly well outside the interval. If a model is derived for purposes of interpolation only, this is of no consequence. Frequently, however, some extrapolation is useful — the extrapolation over adjoining waters of a model derived from land-based data being one example.

5. *Non-Orthogonal Basis Functions*

The convenience of having orthogonal basis functions is well known. Analytically, coefficients of an infinite series can be determined quickly and easily by multiplying the terms of the series by the relevant basis function and integrating over the interval. Because of the orthogonality, all terms disappear except the one involving the desired coefficient, and so that coefficient can be expressed simply in terms of the integral of the cross-product of the function and the relevant basis function. Numerically, orthogonal basis functions are convenient in that the least-squares matrix is better conditioned and so gives a more accurate solution than one from non-orthogonal basis functions. Thus it is convenient, both analytically and numerically, to have basis functions that are orthogonal.

On the other hand, non-self-adjoint boundary conditions are not compatible with basis function orthogonality. Such is the case when both a function and its derivative are to be arbitrary on their boundaries. If there is a relationship between the function and its derivative, such as $f(x)/f'(x)$ = constant, or sometimes if the function and its derivative are periodic over the interval, it is possible to find orthogonal basis functions whose limit function and limit function derivative satisfy the given constraints. But if the function and its derivative are to be independent and arbitrary, there will be two separate sets of basis functions. Within each set the functions will be mutually orthogonal, but some functions in the one set will not be orthogonal to some in the other. Such is the price to be paid for model differentiability.

The inherent ill-conditioning in such non-orthogonal problems is not a practical difficulty because the rate of convergence of an expansion depends on the order of the highest derivative that is modelled uniformly (*Davis*, 1963, 180–181; *Lanczos*, 1966, 98–100). Since the non-orthogonal series by design models both the function and its derivative uniformly, it will converge faster than an orthogonal series that models only the function uniformly, and much faster than one that does not even model the function uniformly. This will be demonstrated later by an example.

The choice, basically, is between orthogonal basis functions that give mean-square convergence only and non-orthogonal basis functions that give uniform convergence.

6. *Sturm-Liouville Expansions*

A theorem relevant to modelling a given field as a series expansion of basis functions is the Sturm-Liouville Theorem (e.g., *Churchill*, 1941,§24–25; 1963, §32–34; *Morse and Feshbach*, 1953, §6.3; *Davis*, 1963, §2.4). The theorem applies to a wide class of self-adjoint linear differential operators, subject to self-adjoint linear boundary conditions. If a separated differential equation and its boundary conditions over a closed interval are of the Sturm-Liouville type, the theorem states that any field satisfying the same equation and boundary conditions can be expanded in an infinite series of orthogonal basis functions that converge uniformly to the given field throughout the closed interval.

For the eigenfunction problem relevant to this paper (see Equation (1) below) the boundary conditions on two eigenfunctions $f_{\lambda_1}(x)$ and $f_{\lambda_2}(x)$ are self-adjoint (e.g., *Davis*, 1963, p.65, eq.16) from $x = 0$ to $x = L$ whenever

$$f'_{\lambda_1}(0)f_{\lambda_2}(0) - f'_{\lambda_2}(0)f_{\lambda_1}(0) = f'_{\lambda_1}(L)f_{\lambda_2}(L) - f'_{\lambda_2}(L)f_{\lambda_1}(L)$$

For example, the periodicity conditions $f(0) = f(L); f'(0) = f'(L)$ taken together are self-adjoint boundary conditions (i.e., they give rise to a class of self-adjoint eigenfunctions $f_\lambda(x)$). A set of functions each of which is a solution of the given Sturm-Liouville differential eigenequation and each of which satisfies the given self-adjoint boundary conditions will serve as a set of basis functions for the expansion of a wide class of functions. In general, the expansion will only converge in mean square, but if the function being expanded is continuous, has continuous derivatives, and satisfies the given self-adjoint boundary conditions (that the basis functions satisfy), the expansion will converge uniformly.

Of course, continuity of a function and its derivative is not necessary for the uniform convergence of a Sturm-Liouville expansion of that function, but together with satisfying the appropriate boundary conditions it is more than sufficient. Several theorems of Fourier analysis give minimal sufficiency conditions. These will not be discussed here, since geophysical fields in regions that are free of sources (i.e., fields which are continuous and have continuous derivatives of all orders) easily qualify as candidates for series expansions that are uniformly convergent, provided the basis functions are chosen to satisfy the appropriate Sturm-Liouville boundary conditions.

Two other boundary conditions that are each of the self-adjoint type are $f'(0) = f'(L) = 0$ and $f(0) = f(L) = 0$. This is the reason for using these conditions to model fields or derivatives of fields, respectively, with arbitrary values at the boundary. Termed "modified" constraints in a previous section, they give basis functions satisfying the given constraints but a limit function that is not so constrained but that in fact satisfies the model constraints.

Boundary value problems that are not self-adjoint are more difficult to solve than the self-adjoint ones (*Coddington and Levinson*, 1955, chap.12) and result in basis functions that are not orthogonal. The boundary problem that specifies, independently, both arbitrary values and arbitrary derivatives on boundaries is a non-self-adjoint problem. It may be solved by a simple superposition of the solution sets from each of the relevant self-adjoint modified constraints.

In the case of double Fourier series, a second method of solutionis given for the non-self-adjoint problem. The method, believed introduced here for the first time, is to find the general solution (rather than the eigensolution) of the differential equation that results when the eigenvalue is put to zero in the eigenequation. This general solution represents arbitrary values around the boundary of the domain. Then subtracting this solution from the data and solving the resulting (transformed, and now self-adjoint) boundary value problem gives the final non-self-adjoint solution for the original (untransformed) variables.

7. *Fourier Series*

The differential eigenvalue equation which gives rise to Fourier series is

$$\frac{d^2 f_\lambda(x)}{dx^2} + \lambda f_\lambda(x) = 0 \tag{1}$$

which has the solution

$$f_\lambda(x) = \begin{cases} A_0 + B_0 x, & \text{when } \lambda = 0 \\ A_\mu \cos(\mu x) + B_\mu \sin(\mu x), & \text{when } \lambda = \mu^2 > 0 \\ C_\mu \cosh(\mu x) + D_\mu \sinh(\mu x) & \\ \quad\text{or} & \text{when } \lambda = -\mu^2 < 0 \\ C_\mu \exp(\mu x) + D_\mu \exp(-\mu x) & \end{cases} \tag{2}$$

The eigenvalue λ, or the parameter μ, need only be real; under certain boundary conditions they may be integral.

A function $f(x)$ that is to be modelled is expressed by superimposing all the eigensolutions (2) that satisfy the given boundary conditions.

Consider first the Sturm-Liouville "periodic" boundary conditions: $f(0) = f(L)$ and $f'(0) = f'(L)$. These are required if the function $f(x)$ and its derivative $f'(x)$, defined on $-\infty < x < \infty$, are to be periodic with period L. However, they also obviously apply to any function, defined only on $0 \leq x \leq L$, whose values and slopes are equal at opposite boundaries, regardless of whether the function is periodic outside the interval or not. The solution is

$$f(x) = A_0 + \sum_{m=1}^{\infty} A_m \cos(2m\pi x/L) + B_m \sin(2m\pi x/L) \tag{3}$$

Although the basis functions in (3) are all continuous, with continuous derivatives, the limit function is not so restricted, and even discontinuous functions can be represented by the limit function. Similarly, functions can be represented by (3) that are continuous within the interval $0 < x < L$ but are such that $f(0) \neq f(L)$. This is the rationale for the use of periodic Fourier series even when the function being modelled does not satisfy the periodic conditions. Such periodic representations of non-periodic functions converge only in mean square, however. Modelling a discontinuous function or a continuous function with $f(0) \neq f(L)$ in this way results in a "ringing", and in the limit a Gibbs effect, at the point of discontinuity or at the boundary, respectively, since the series of basis functions is not in those cases uniformly convergent.

The derivative of the limit function in those cases is not given by the infinite sum of the derivatives of the periodic basis functions. Forming the derivative of a non-uniformly convergent series is not, in general, a straightforward matter. A case that does happen to be tractable, however, and is relevant to modelling, is that in which the function and its derivatives are continuous in the interval $0 \leq x \leq L$, but do not satisfy the given boundary conditions. Then the derivative can be shown (e.g., *Churchill*, 1941, §36; 1963, §45; *Tolstov*, 1962, chap.5, §9) to be

$$f'(x) = \frac{f(L) - f(0)}{L} + \frac{2}{L} \sum_{m=1}^{\infty} [f(L) - f(0) + m\pi B_m] \cos(\frac{2m\pi x}{L}) - m\pi A_m \sin(\frac{2m\pi x}{L}) \tag{4}$$

which reduces to the termwise derivative of (3) only when $f(0) = f(L)$. The summation in (4) will converge uniformly only when $f'(0) = f'(L)$. The termwise derivative of (3), when $f(0) \neq f(L)$, diverges.

Equation (4) is only useful in an analytical problem, where a given function is being expressed, or has already been expressed, as a Fourier series. In a modelling problem that involves differentiation during the modelling process, the boundary values of the function being modelled are not usually known or if they are may contain observational errors, and so the equation cannot generally be used to give $f'(x)$, even in mean square.

Of course, if the function and its derivatives really are continuous and satisfy the "periodic" boundary conditions, the series (3) is a uniformly convergent representation for the function, and the series obtained by differentiating under the summation sign is a uniformly convergent representation of the derivative of the function.

It may be instructive to consider the periodic boundary condition $f(0) = f(L)$, with no constraint on the first derivative. This would result, for example, from removing a linear trend from a function without regard to what it does to the derivative. It turns out that the same basis functions are required as in (3) — i.e., the artificial condition $f'(0) = f'(L)$ is imposed on the basis functions as well as the given condition $f(0) = f(L)$ — but of course the derivative of the limit function is not uniformly representable by the derivatives of the basis functions, although from (4) it can be represented in a non-uniform way by them. If $f'(x)$ were merely continuous in the interval, the series of basis function derivatives would exhibit ringing at the boundaries unless $f'(0) = f'(L)$.

Now, instead of imposing the self-adjoint periodic conditions, the self-adjoint conditions of zero slope and zero function will be imposed in order to represent uniformly a function or a function derivative, respectively, with arbitrary values on the boundaries (assuming as always in this paper that the function and all its derivatives are continuous). As discussed earlier, these conditions separately give uniformly convergent expansions for their respective classes of functions.

Consider first that $f(x)$ is to be uniformly convergent and arbitrary at the boundaries. The Sturm-Liouville conditions to make this so are $f'(0) = f'(L) = 0$ and the solution is

$$f(x) = \sum_{m=0}^{\infty} A_m \cos(m\pi x/L) \tag{5}$$

The basis functions here are not the same as the (periodic) basis functions of (3), since the periodicity constraint has not been imposed.

Consider next that $f'(x)$ is to be uniformly convergent and arbitrary at each boundary. This can be accomplished, as in the previous case, by setting $f''(0) = f''(L) = 0$, but from (1) these conditions are precisely equivalent, for $\lambda \neq 0$, to the Sturm-Liouville conditions $f(0) = f(L) = 0$. The solution is

$$f(x) = \sum_{m=1}^{\infty} B_m \sin(m\pi x/L) \tag{6}$$

Again, the basis functions are not the same as those of (3).

Now, if the function being modelled belongs to the appropriate Sturm-Liouville class of functions to which the basis functions belong, the series of basis functions as well as the series of basis function derivatives will be uniformly convergent. But if the function being modelled belongs to a wider or more general class of functions, this will not necessarily be the case. For example, if the function being modelled has arbitrary values at the boundaries (it and its derivatives being continuous), equation (5) will be uniformly convergent (indeed, that is why the particular Sturm-Liouville condition $f'(0) = f'(L) = 0$ was chosen) but the series formed from the derivatives of the basis functions in (5) will not converge uniformly to the derivative of the function being modelled. The latter series converges to zero at the boundaries by construction and so cannot converge uniformly to any function that has a non-zero derivative there.

Similarly, the series in equation (6) is uniformly convergent and has a uniformly convergent derivative for all functions (continuous with continuous derivatives) satisfying the Sturm-Liouville condition $f(0) = f(L) = 0$. The series for other functions, in particular those with arbitrary values at the boundaries, will be convergent only in mean square.

Series (5) and (6) are known as the Fourier cosine and sine series, respectively. The cosine series (5) is of course uniformly convergent even when its boundary condition is not satisfied, and so it may be differentiated term by term. The resulting derivative converges in mean square, and converges uniformly when the boundary condition $f'(0) = f'(L) = 0$ is satisfied. The sine series (6), on the other hand, is not uniformly convergent when its boundary condition $f(0) = f(L) = 0$ is not satisfied, and cannot be differentiated term by term. The derivative of the sine series (6), in fact, is

$$\begin{aligned} f'(x) =& \frac{f(L) - f(0)}{L} + \\ &+ \frac{1}{L}\sum_{m=1}^{\infty}\left[m\pi B_m - \begin{cases} 2\big(f(L) + f(0)\big), & \text{when } m \text{ is odd} \\ -2\big(f(L) - f(0)\big), & \text{when } m \text{ is even} \end{cases}\right]\cos(m\pi x/L) \end{aligned} \tag{7}$$

which reduces to the termwise derivative of (6) only when $f(0) = f(L) = 0$. This series is uniformly convergent even when its boundary condition is not satisfied. The termwise derivative of (6), when the boundary condition is not satisfied, diverges.

As in the comments relating to Equation (4), Equation (7) is of no use when differentiation must take place during the modelling process itself. In that case, it is imperative to choose basis functions that allow termwise differentiation.

Note that equivalently to (6), a cosine series expression like (5) could be chosen for $f'(x)$ as the solution to the self-adjoint problem $f''(0) = f''(L) = 0$. If the only interest is in modelling this derivative, then that cosine series would be all that is relevant. Here the interest is in modelling a function, like (6), that may be differentiated.

Thus, the cosine series in (5) may be used to represent uniformly a function that has arbitrary values on the boundary. Its derivative (found by termwise differentiation) converges in mean square generally, and converges uniformly if $f'(0) = f'(L) = 0$. Similarly, the sine series in (6) may be used to represent uniformly a derivative with arbitrary values on the boundaries through the cosine series in (7). The series in (6) for the non-differentiated function converges in mean square generally, and converges uniformly when $f(0) = f(L) = 0$. Each of these two problems is, separately, a self-adjoint problem and the basis functions for each series representation are orthogonal. If this is all that is required in the model, the mathematical problem is solved, equations (5) or (6)/(7) being sufficient. However, if either of the cosine series has to be differentiated with arbitrary derivatives at the boundaries, or if a uniform representation of the undifferentiated function (6) is required with arbitrary values at the boundaries, the resulting problem is not self-adjoint and must be solved either by a superposition of self-adjoint solutions or by an appropriate functional transformation. The resulting basis functions are then not orthogonal.

When uniform convergence is required in both the function and its derivative, the two solutions (5) and (6) may be superimposed because the Sturm-Liouville equation and boundary conditions are linear. For arbitrary function-values and derivative-values on the boundaries, the superposition solution is given by

$$f(x) = A_0 + \sum_{m=1}^{\infty} A_m \cos(m\pi x/L) + B_m \sin(m\pi x/L) \tag{8}$$

The basis functions are not completely orthogonal, since $\int_0^\pi \sin(mx)\cos(nx)\,dx \neq 0$ when $m - n$ is an odd integer. Equation (8) is referred to in this paper as the "cosine + sine" series.

The expansion (8) for uniformly convergent modelling of differentiable functions can be thought of as a decomposition of the function into two separate functions: one which is zero at each boundary but which has the same slopes there as the modelled function, and another which has a zero slope at each boundary but the same values there as the modelled function. The first is uniformly representable by the sine series, the second by the cosine series. Since each satisfies the boundary conditions of the basis functions, each one is uniformly termwise differentiable.

Alternatively, uniform convergence can be obtained in both function and derivative by transforming $f(x)$ to $f(x) - A_0 - B_0 x$. The transforming function, $A_0 + B_0 x$, is the solution of (1) when $\lambda = 0$. Then

$$f(x) = A_0 + B_0 x + \sum_{m=1}^{\infty} B_m \sin(m\pi x/L) \tag{9}$$

since the transformed function satisfies the Sturm-Liouville conditions leading to (6). The boundary conditions on $f(x)$ are not self-adjoint and technically the solution (9) applies to the case when A_0 and B_0 are known. Nevertheless, equation (9) is an acceptable solution to the non-self-adjoint problem, and in fact the term-wise series derivative converges uniformly to $f'(x)$ even when $f'(x)$ is arbitrary at the boundaries. Thus the non-orthogonal basis functions in (9) can be used in modelling uniformly both a function and its derivative. The choice between (5) and (9), or between (8) and (9) for differentiable functions, is based on how quickly each converges.

It is evident that the ringing brought about by modelling functions with arbitrary boundary values by means of the periodic basis functions of (3) is not necessary. The proper basis functions for such a case are given in (5), (8), or (9). Those in (5) are orthogonal but those in (8) and (9) will provide the proper slope at the boundaries and furthermore lead to a uniformly convergent derivative. That is, modelling continuous functions with continuous derivatives, having arbitrary values and derivatives on the boundaries, can be done either by (8) or (9), rather than (3), thus avoiding the ringing in the representation of the derivative as well as the ringing in the functional representation.

The convergence results of this section are summarized in Table 1. Note that in the three cases where $f'(0) = f'(L) = 0$, the "cosine + sine" series is actually the same as the "cosine" series, the coefficients of the sine terms being zero. An indication of the speed of convergence for the various boundary conditions is given in the table by how many UC's appear for the particular expansion; the more UC's the faster is the convergence. The last boundary condition of the table represents the most general case, and is the motivation of this paper. Only the "cosine + sine" basis functions give uniformly convergent expansions of both function and termwise derivative.

8. *Double Fourier Series*

The procedure for solving boundary value problems in two variables, x and y, is similar to that for one variable. The differential eigenequation is

$$\frac{\partial^2 f_\lambda(x,y)}{\partial x^2} + \frac{\partial^2 f_\lambda(x,y)}{\partial y^2} + \lambda f_\lambda(x,y) = 0 \tag{10}$$

Equation (10) is solved by separation of variables and functions $f(x,y)$ to be modelled are expanded by superimposing all possible combinations of eigenfunctions.

Table. 1. Convergence of the Fourier series discussed in this paper, for various boundary conditions. Continuity of function and all derivatives is assumed. The "sine", "cosine", and "cosine + sine" series are based on "half-periodic" sine and cosine functions. UC = uniformly convergent, MS = convergent in mean square, DV = divergent. For each boundary condition, the first line gives the type of convergence for the function f, the second line that for the first termwise derivative f', and the third line that for the second termwise derivative f''.

Boundary Conditions		periodic	sine	cosine	cosine+sine
$f(0) = f(L) \neq 0$	f	UC	MS	UC	UC
$f'(0) = f'(L) \neq 0$	f'	UC	DV	MS	UC
	f''	MS*	DV	DV	UC
$f(0) = f(L) = 0$	f	UC	UC	UC	UC
$f'(0) = f'(L) \neq 0$	f'	UC	UC	MS	UC
	f''	MS*	MS**	DV	UC
$f(0) = f(L) \neq 0$	f	UC	MS	UC	UC
$f'(0) = f'(L) = 0$	f'	UC	DV	UC	UC
	f''	MS*	DV	UC	UC
$f(0) = f(L) = 0$	f	UC	UC	UC	UC
$f'(0) = f'(L) = 0$	f'	UC	UC	UC	UC
	f''	MS*	MS**	UC	UC
$f(0) = f(L) \neq 0$	f	UC	MS	UC	UC
$f'(0) \neq f'(L)$	f'	MS	DV	MS	UC
	f''	DV	DV	DV	UC
$f(0) = f(L) = 0$	f	UC	UC	UC	UC
$f'(0) \neq f'(L)$	f'	MS	UC	MS	UC
	f''	DV	MS**	DV	UC
$f(0) \neq f(L)$	f	MS	MS	UC	UC
$f'(0) = f'(L) \neq 0$	f'	DV	DV	MS	UC
	f''	DV	DV	DV	UC
$f(0) \neq f(L)$	f	MS	MS	UC	UC
$f'(0) = f'(L) = 0$	f'	DV	DV	UC	UC
	f''	DV	DV	UC	UC
$f(0) \neq f(L)$	f	MS	MS	UC	UC
$f'(0) \neq f'(L)$	f'	DV	DV	MS	UC
	f''	DV	DV	DV	UC

* UC if $f''(0) = f''(L)$

** UC if $f''(0) = f''(L) = 0$

A function f and its partial derivatives $\partial f/\partial y$ and $\partial f/\partial y$ satisfy the Sturm-Liouville "periodic" boundary conditions when

$$
\begin{aligned}
f(0,y) &= f(L_x,y)\\
f(x,0) &= f(x,L_y)\\
\partial f(0,y)/\partial x &= \partial f(L_x,y)/\partial x\\
\partial f(x,0)/\partial y &= \partial f(x,L_y)/\partial y
\end{aligned}
$$

As before, these may refer to a function defined on $-\infty < x < \infty; -\infty < y < \infty$ and periodic with period L_x in the x-direction and period L_y in the y-direction, or simply to a function defined on $0 \leq x \leq L_x$, $0 \leq y \leq L_y$ and whose values and slopes are equal at opposite boundaries. The solution is

$$
\begin{aligned}
f(x,y) = A_0^0 &+ \sum_{m=1}^{\infty} A_0^m \cos(\frac{2m\pi x}{L_x}) + B_0^m \sin(\frac{2m\pi x}{L_x})\\
&+ \sum_{n=1}^{\infty} A_n^0 \cos(\frac{2n\pi y}{L_y}) + C_n^0 \sin(\frac{2n\pi y}{L_y})\\
&+ \sum_{m=1}^{\infty}\sum_{n=1}^{\infty} A_n^m \cos(\frac{2m\pi x}{L_x})\cos(\frac{2n\pi y}{L_y}) + B_n^m \sin(\frac{2m\pi x}{L_x})\cos(\frac{2n\pi y}{L_y})\\
&\quad + C_n^m \cos(\frac{2m\pi x}{L_x})\sin(\frac{2n\pi y}{L_y}) + D_n^m \sin(\frac{2m\pi x}{L_x})\sin(\frac{2n\pi y}{L_y})
\end{aligned}
\tag{11}
$$

where

$$
\lambda = \left(\frac{2m\pi}{L_x}\right)^2 + \left(\frac{2n\pi}{L_y}\right)^2
$$

As in the case of single-variable Fourier series, this limit function belongs to a much wider class of functions than the restricted class of functions to which the basis functions belong. For modelling functions that belong to the restricted class, i.e., functions that satisfy the given boundary constraints (and that are continuous and have continuous first and second derivatives), the series in (11) will be uniformly convergent, as will its termwise derivative. However, if the function has equal values but non-equal derivatives at opposite boundaries, the series itself will be uniformly convergent but its derivative will converge only in mean square. A series (11) representation of a function whose values at opposite boundary points are not equal is not even uniformly convergent itself, and its termwise derivative diverges.

Double Fourier series corresponding to functions that are continuous over the rectangle, and have continuous derivatives, can be differentiated in the same way that (3) was differentiated to give (4). The coefficients of the differentiated series involve integrals over the boundary of the various cosine and sine functions in addition to the coefficients of the undifferentiated series, in the same way that the coefficients of (4) involve values at the boundaries in addition to the coefficients resulting from simple termwise differentiation. The series (11) can be differentiated term by term only when $f(0,y) = f(L_x,y)$ and $f(x,0) = f(x,L_y)$, in which case the resulting series will be uniformly convergent.

Now it will be shown, as in the case of single Fourier series, that self-adjoint boundary conditions other than those of periodicity may be imposed in order to represent, uniformly, continuous functions or function derivatives having arbitrary values on the boundary. Again it will be assumed that $f(x,y)$ is only defined or available on $0 \leq x \leq L_x$; $0 \leq y \leq L_y$.

For f to be uniformly convergent and arbitrary on the boundaries of this rectangle, the basis functions are chosen to satisfy

$$\partial f(0,y)/\partial x = \partial f(L_x,y)/\partial x = 0$$
$$\partial f(x,0)/\partial y = \partial f(x,L_y)/\partial y = 0$$

which gives the solution

$$f(x,y) = \sum_{m=0}^{\infty}\sum_{n=0}^{\infty} A_n^m \cos(m\pi x/L_x)\cos(n\pi y/L_y) \tag{12}$$

with the eigenvalues

$$\lambda = \left(\frac{m\pi}{L_x}\right)^2 + \left(\frac{n\pi}{L_y}\right)^2$$

For $\partial f/\partial x$ to be uniformly convergent and arbitrary on the boundaries, the Sturm-Liouville conditions are

$$f(0,y) = f(L_x,y) = 0$$
$$\partial f(x,0)/\partial y = \partial f(x,L_y)/\partial y = 0$$

which result in the solution

$$f(x,y) = \sum_{m=1}^{\infty}\sum_{n=0}^{\infty} B_n^m \sin(m\pi x/L_x)\cos(n\pi y/L_y) \tag{13}$$

For $\partial f/\partial y$ to be uniformly convergent and arbitrary on the boundaries, the Sturm-Liouville conditions are

$$\partial f(0,y)/\partial x = \partial f(L_x,y)/\partial x = 0$$
$$f(x,0) = f(x,L_y) = 0$$

giving the solution

$$f(x,y) = \sum_{m=0}^{\infty} \sum_{n=1}^{\infty} C_n^m \cos(m\pi x/L_x) \sin(n\pi y/L_y) \tag{14}$$

For the second partial derivative $\partial^2 f/\partial x \partial y$ to be uniformly convergent and arbitrary on the boundaries, the Sturm-Liouville conditions are

$$f(0,y) = f(L_x, y) = 0$$
$$f(x,0) = f(x, L_y) = 0$$

and the solution is

$$f(x,y) = \sum_{m=1}^{\infty} \sum_{n=1}^{\infty} D_n^m \sin(m\pi x/L_x) \sin(n\pi y/L_y) \tag{15}$$

The eigenvalues for (13) – (15) are as those for (12).

As for the one-dimensional series (5) and (6), the series in (12) – (15) are uniformly convergent whenever the function being modelled satisfies the given Sturm-Liouville conditions. Otherwise, they will merely converge in mean square.

Functions that satisfy any combination of the Sturm-Liouville conditions leading to (12) – (15) may be modelled by superimposing the appropriate eigenfunction solutions. For example, to model functions that have arbitrary values and arbitrary first derivatives on the rectangular boundaries, the solutions (12) – (14) are superimposed:

$$\begin{aligned} f(x,y) = A_0^0 &+ \sum_{m=1}^{\infty} A_0^m \cos(\frac{m\pi x}{L_x}) + B_0^m \sin(\frac{m\pi x}{L_x}) \\ &+ \sum_{n=1}^{\infty} A_n^0 \cos(\frac{n\pi y}{L_y}) + C_n^0 \sin(\frac{n\pi y}{L_y}) \\ &+ \sum_{m=1}^{\infty} \sum_{n=1}^{\infty} A_n^m \cos(\frac{m\pi x}{L_x}) \cos(\frac{n\pi y}{L_y}) + B_n^m \sin(\frac{m\pi x}{L_x}) \cos(\frac{n\pi y}{L_y}) \\ &+ C_n^m \cos(\frac{m\pi x}{L_x}) \sin(\frac{n\pi y}{L_y}) \end{aligned} \tag{16}$$

To model arbitrary differentiable functions, i.e., arbitrary functions with arbitrary derivatives of all orders, the solution (15) would be superimposed on the other solutions as well:

$$
\begin{aligned}
f(x,y) = A_0^0 &+ \sum_{m=1}^{\infty} A_0^m \cos(\frac{m\pi x}{L_x}) + B_0^m \sin(\frac{m\pi x}{L_x}) \\
&+ \sum_{n=1}^{\infty} A_n^0 \cos(\frac{n\pi y}{L_y}) + C_n^0 \sin(\frac{n\pi y}{L_y}) \\
&+ \sum_{m=1}^{\infty}\sum_{n=1}^{\infty} A_n^m \cos(\frac{m\pi x}{L_x})\cos(\frac{n\pi y}{L_y}) + B_n^m \sin(\frac{m\pi x}{L_x})\cos(\frac{n\pi y}{L_y}) \\
&\qquad + C_n^m \cos(\frac{m\pi x}{L_x})\sin(\frac{n\pi y}{L_y}) + D_n^m \sin(\frac{m\pi x}{L_x})\sin(\frac{n\pi y}{L_y})
\end{aligned}
\tag{17}
$$

It may be of interest to consider the problem of linear boundary conditions. The function $f(x,y)$ is transformed to $f(x,y) - A_0 - B_0x - C_0y - D_0xy$. Setting the transformed function to zero at the boundaries, as in the boundary problem leading to (15), gives the solution

$$
f(x,y) = A_0 + B_0\,x + C_0\,y + D_0\,xy + \sum_{m=1}^{\infty}\sum_{n=1}^{\infty} E_n^m \sin(\frac{m\pi x}{L_x})\sin(\frac{n\pi y}{L_y}) \tag{18}
$$

The polynomial in x and y represents the combination of separated eigensolutions of (10) for $\lambda = 0$. It may seem, since x, y, and xy are low order terms of a second degree polynomial, that higher order terms like x^2 and y^2 could be included to give arbitrary boundary values. It would be incorrect to do this (without imposing a complicated set of constraints on the polynomial coefficients) since these terms do not satisfy the linear differential equation. They represent non-linear boundary conditions on a linear system.

The basis functions for the transformed function are orthogonal over the rectangle; those for the original function are not. When the modelled function satisfies linear boundary conditions, (18) is uniformly convergent and has a uniformly convergent derivative. However, when the modelled function is arbitrary on the boundary, the solution (18) cannot be substituted for the more general solution (12), as (9) could be substituted for the alternate solution (5). In the two dimensional problem here, the series would not be uniformly convergent and there would be boundary ringing from such a fit.

For an alternate expression to (12), appropriate to arbitrary values on the boundary, the function may be transformed by subtracting the general solution of $\partial^2 f/\partial x^2 + \partial^2 f/\partial y^2 = 0$, just as the general solution of $d^2 f/dx^2 = 0$ was subtracted in the one-dimensional case leading to (9), although in that case the solution was the same as the corresponding eigensolution of (1) for $\lambda = 0$. Here, the transforming function is not merely the product of eigensolutions in x and y of (10) for $\lambda = 0$ (which was used for the linear boundary conditions leading to (18)), although it does satisfy (10) when $\lambda = 0$. In fact, it is the superposition of all products of eigenfunctions of the separated eigenequations in x and y whose eigenvalues, for the problem of arbitrary boundary values, add up to zero. The result is

$$\begin{aligned} f(x,y) =& A_0 + B_0\, x + C_0\, y + D_0\, xy + \\ &+ \sum_{m=1}^{\infty} \{[A_m \cosh(\frac{m\pi y}{L_x}) + B_m \sinh(\frac{m\pi y}{L_x})] \sin(\frac{m\pi x}{L_x}) + \\ &+ [C_m \cosh(\frac{m\pi x}{L_y}) + D_m \sinh(\frac{m\pi x}{L_y})] \sin(\frac{m\pi y}{L_y})\} + \\ &+ \sum_{m=1}^{\infty}\sum_{n=1}^{\infty} E_n^m \sin(\frac{m\pi x}{L_x}) \sin(\frac{n\pi y}{L_y}) \end{aligned} \tag{19}$$

The transforming function is analogous to the height of an elastic membrane over the rectangle, constrained to have given values (or heights) around the boundary. The sine-sine functions then provide additional height throughout the rectangular region according to additional (non-zero) values of λ in (10). This solution, like (9), is uniformly convergent and has a uniformly convergent derivative. The basis functions are not orthogonal over the rectangle.

Equation (19) is useful analytically, since the coefficients may all be determined individually, unaffected by the other coefficients. The coefficients A_0, B_0, C_0, and D_0 are determined by the values of $f(x,y)$ in the four corners, the A_m, B_m, C_m, and D_m may then be found by multiplying by a sine function and integrating over the appropriate boundary, and finally the E_n^m by a sine-sine multiplication and an integration over the rectangle. There is no such simple analytical solution for a type of equation like (17), whose least-squares coefficients must be determined from a system of interrelated linear algebraic equations.

Once again it is evident that the boundary ringing may be avoided, both in the fit of a function and in the fit of a function's derivatives, that results from using the periodic basis functions of (11). For a uniformly convergent fit of a function with arbitrary values on the boundary, the orthogonal basis functions of (12) are sufficient. For a uniformly convergent derivative as well, either (16) or (17) may be used, depending on whether the second derivative $\partial^2 f/\partial x \partial y$ is required, or else (19). In these latter (non-self-adjoint) cases, the basis functions are not orthogonal.

Notice that simply adding x and y terms to the periodic series (11) does not make it uniformly convergent. Furthermore, adding them to the "half-periodic" series (16) or (17) is unnecessary since these expansions are already uniformly convergent for their respective functions. To obtain an alternative representation to (16) or (17), for a uniformly convergent representation of a function and derivatives with arbitrary values on the boundaries, the hyperbolic sine and cosine terms have to be added as well, and then not to the periodic series (11) but to the half-periodic sine series (15).

9. *Rectangular Harmonic Analysis*

Rectangular harmonic analysis is a method of modelling a potential field, and usually its derivatives, over and on a rectangular area in cartesian coordinates x, y, and z. The method is important in that it allows a reasonably simple representation of potential and potential-gradient fields (such as magnetic and gravity fields) and satisfies automatically the physical constraints that the curl and divergence of potential-gradient fields be identically zero. It derives from the solution of Laplace's equation, in cartesian coordinates, subject to appropriate boundary conditions.

The equation is

$$\frac{\partial^2 f(x,y,z)}{\partial x^2} + \frac{\partial^2 f(x,y,z)}{\partial y^2} + \frac{\partial^2 f(x,y,z)}{\partial z^2} = 0 \qquad (20)$$

which is again solved by separation of variables and including all possible combinations of eigenfunctions. The eigenfunctions for the z-separation are multiplied by the eigenfunctions of the double Fourier series of the last section.

The range of z is $-\infty < z < +\infty$ and the boundary conditions at infinity are

$$f(x,y,\infty) = 0 \qquad \text{for "internal" sources}$$
$$f(x,y,-\infty) = 0 \qquad \text{for "external" sources}$$

and for these conditions only the exponential or hyperbolic trigonometric functions are involved (see equation (2) for $\lambda \leq 0$). It is more convenient here to choose exponential eigenfunctions, those for "internal" sources (those below the $z = 0$ plane) being $\exp(-\sqrt{\lambda}z)$ and those for "external" sources (those above the $z = 0$ plane) being $\exp(+\sqrt{\lambda}z)$ where λ is the eigenvalue in (10). The linear terms in z are prohibited since they do not satisfy the boundary conditions. In the same way as before, the solutions for these two boundary value problems may be superimposed to give the solution for both internal and external sources combined.

The boundary conditions on the four planes $x = 0$, $x = L_x$, $y = 0$, and $y = L_y$ are the same as the conditions leading to the respective solutions (12) to (15) at $z = 0$. For those solutions, however, the function $f(x,y,0)$, or perhaps $f'(x,y,0)$, was considered known (values of which were the "data") and the coefficients of the expansions were determined accordingly (by a least-squares procedure). If the function being modelled did not satisfy a boundary condition precisely (for example, if its slope was not zero at the boundary) the fitted solution was nevertheless a valid and uniform representation of that function. The data, in a sense, allowed the solution (in the limit) to transcend the restrictive boundary conditions. In the three-dimensional case here, the lack of data on the four planes will clearly restrict the final solution. The result of this is a restriction on how far the modelled field may be continued beyond the domain of the data. If the continuation distance is small relative to the dimensions L_x and L_y, there will be little error in the continuation field. Obviously, this error results from the influence of the field beyond the rectangular area, or volume. For instance, a large crustal anomaly just outside the area of analysis would affect the continued "internal" field close to the boundary at small continuation distances but throughout the whole area at large continuation distances. In most cases, of course, models are used for interpolative purposes and this continuation error is irrelevant.

For those functions that are defined over all space but which are periodic over the rectangle $0 \leq x \leq L_x,\ 0 \leq y \leq L_y$, or (more practically) for those functions defined only on $0 \leq x \leq L_x,\ 0 \leq y \leq L_y$ but satisfying the "periodic" boundary constraints, the combined (external and internal) solution, from (11), is

$$
\begin{aligned}
f(x,y,z) &= \sum_{m=1}^{\infty}\{A_0^m \cos(\frac{2m\pi x}{L_x}) + B_0^m \sin(\frac{2m\pi x}{L_x})\} \exp\big(-\frac{2\pi m z}{L_x}\big) \\
&+ \sum_{n=1}^{\infty}\{A_n^0 \cos(\frac{2n\pi y}{L_y}) + C_n^0 \sin(\frac{2n\pi y}{L_y})\} \exp\big(-\frac{2\pi n z}{L_y}\big) \\
&+ \sum_{m=1}^{\infty}\sum_{n=1}^{\infty}\{A_n^m \cos(\frac{2m\pi x}{L_x})\cos(\frac{2n\pi y}{L_y}) + B_n^m \sin(\frac{2m\pi x}{L_x})\cos(\frac{2n\pi y}{L_y}) \\
&+ C_n^m \cos(\frac{2m\pi x}{L_x})\sin(\frac{2n\pi y}{L_y}) + D_n^m \sin(\frac{2m\pi x}{L_x})\sin(\frac{2n\pi y}{L_y})\} \exp\left(-2\pi z\sqrt{(\frac{m}{L_x})^2+(\frac{n}{L_y})^2}\right) \\
&+ \sum_{m=1}^{\infty}\{E_0^m \cos(\frac{2m\pi x}{L_x}) + F_0^m \sin(\frac{2m\pi x}{L_x})\} \exp\big(+\frac{2\pi m z}{L_x}\big) \\
&+ \sum_{n=1}^{\infty}\{E_n^0 \cos(\frac{2n\pi y}{L_y}) + G_n^0 \sin(\frac{2n\pi y}{L_y})\} \exp\big(+\frac{2\pi n z}{L_y}\big) \\
&+ \sum_{m=1}^{\infty}\sum_{n=1}^{\infty}\{E_n^m \cos(\frac{2m\pi x}{L_x})\cos(\frac{2n\pi y}{L_y}) + F_n^m \sin(\frac{2m\pi x}{L_x})\cos(\frac{2n\pi y}{L_y}) \\
&+ G_n^m \cos(\frac{2m\pi x}{L_x})\sin(\frac{2n\pi y}{L_y}) + H_n^m \sin(\frac{2m\pi x}{L_x})\sin(\frac{2n\pi y}{L_y})\} \exp\left(+2\pi z\sqrt{(\frac{m}{L_x})^2+(\frac{n}{L_y})^2}\right)
\end{aligned}
\tag{21}
$$

The trigonometric terms occurring in the single summations are what was referred to in the introduction as "individually appearing" sine and cosine functions. As was mentioned earlier, if Equation (20) is used to model a function that is merely continuous over the rectangle but whose values are not the same at opposite boundaries, the limit function will be discontinuous (and therefore nondifferentiable) and so will not satisfy Laplace's Equation (20).

The solution for arbitrary values on the boundary, from (12), is

$$f(x,y,z) = \sum_{m=0}^{\infty}\sum_{n=0}^{\infty} \cos(\frac{m\pi x}{L_x})\cos(\frac{n\pi y}{L_y}) \cdot \left\{ A_n^m \exp\left(-\pi z\sqrt{(\frac{m}{L_x})^2+(\frac{n}{L_y})^2}\right) + B_n^m \exp\left(+\pi z\sqrt{(\frac{m}{L_x})^2+(\frac{n}{L_y})^2}\right) \right\} \tag{22}$$

This is the solution required to fit an arbitrary potential over the rectangle. If only "internal" sources are to be considered, only the negative exponential terms are included; if only the "external" sources are considered, only the positive exponentials are included.

The solution (22) is not uniformly differentiable — the term by term differentiation of the series in (22) will not converge uniformly to the derivative of the modelled function (unless the modelled function has zero slope at the boundaries). Of course, (22) is differentiable in mean square.

The uniformly convergent solution for a completely differentiable function — i.e., a function with arbitrary values and arbitrary derivatives of all orders — from (17) is,

$$\begin{aligned}
f(x,y,z) &= \sum_{m=1}^{\infty}\{A_0^m \cos(\frac{m\pi x}{L_x}) + B_0^m \sin(\frac{m\pi x}{L_x})\}\exp\left(-\frac{\pi m z}{L_x}\right) \\
&+ \sum_{n=1}^{\infty}\{A_n^0 \cos(\frac{n\pi y}{L_y}) + C_n^0 \sin(\frac{n\pi y}{L_y})\}\exp\left(-\frac{\pi n z}{L_y}\right) \\
&+ \sum_{m=1}^{\infty}\sum_{n=1}^{\infty}\{A_n^m \cos(\frac{m\pi x}{L_x})\cos(\frac{n\pi y}{L_y}) + B_n^m \sin(\frac{m\pi x}{L_x})\cos(\frac{n\pi y}{L_y}) \\
&+ C_n^m \cos(\frac{m\pi x}{L_x})\sin(\frac{n\pi y}{L_y}) + D_n^m \sin(\frac{m\pi x}{L_x})\sin(\frac{n\pi y}{L_y})\}\exp\left(-\pi z\sqrt{(\frac{m}{L_x})^2+(\frac{n}{L_y})^2}\right) \\
&+ \sum_{m=1}^{\infty}\{E_0^m \cos(\frac{m\pi x}{L_x}) + F_0^m \sin(\frac{m\pi x}{L_x})\}\exp\left(+\frac{\pi m z}{L_x}\right) \\
&+ \sum_{n=1}^{\infty}\{E_n^0 \cos(\frac{n\pi y}{L_y}) + G_n^0 \sin(\frac{n\pi y}{L_y})\}\exp\left(+\frac{\pi n z}{L_y}\right) +
\end{aligned}$$

$$+\sum_{m=1}^{\infty}\sum_{n=1}^{\infty}\{E_n^m\cos(\frac{m\pi x}{L_x})\cos(\frac{n\pi y}{L_y})+F_n^m\sin(\frac{m\pi x}{L_x})\cos(\frac{n\pi y}{L_y})$$

$$+G_n^m\cos(\frac{m\pi x}{L_x})\sin(\frac{n\pi y}{L_y})+H_n^m\sin(\frac{m\pi x}{L_x})\sin(\frac{n\pi y}{L_y})\}\exp\left(+\pi z\sqrt{(\frac{m}{L_x})^2+(\frac{n}{L_y})^2}\right) \quad (23)$$

The terms connected with the negative exponential are for modelling differentiable fields resulting from sources at $z=-\infty$, or "internal" sources. Those connected with the positive exponential are for modelling differentiable fields from sources at $z=+\infty$, or "external" sources.

To model fields with arbitrary values and arbitrary derivatives of first order only, the $\sin(m\pi x/L_x)\sin(n\pi y/L_y)$ functions of (15) may be excluded in the above formulation, in both the "internal" and "external" portions. In this case, the model, analogously to (16), will have its cross partial derivative $\partial^2 f/\partial x\partial y$ constrained to be zero in the four corners of the rectangle and an expansion of that derivative will not converge uniformly unless the function being modelled is also so constrained.

Which particular form is chosen for a given model is thus seen to depend on what boundary conditions the model is expected to fulfill. If only horizontal gradient fields ($\partial f/\partial x$ and $\partial f/\partial y$) are required, the mathematical model may be based on the superimposed series (13) and (14). If it is important that the other partial derivatives are also properly represented at the boundaries, the full representation (23) is required.

As mentioned earlier, if the periodic solution (21) is used to model a function whose values are not the same at opposite boundaries, the limit function will be discontinuous (and therefore non-differentiable) at the boundary and so cannot satisfy Laplace's Equation (20). The limit function of the differentiable solution (23), on the other hand, clearly satisfies Laplace's Equation. Similarly, other solutions like (22) are compatible with Laplace's Equation, since in these cases no differentiation of the series actually takes place. That is, the limit function is continuous and well-behaved, and could itself be differentiated, but no relationship is construed to exist between the derivative of the limit function and the derivative of the series. This is quite different from the case of having a discontinuous limit function, or actually forming a termwise derivative from a series like (22).

An alternative solution similar to (19) relevant to fitting both functions and their derivatives is not so straightforward. The solution (19), appropriate for $\lambda=0$, would have to be multiplied by the corresponding eigensolution in z, which by the boundary conditions on z must be zero. Any alternative solution based on the general solutions of (10) for non-zero values of λ would be inordinately complicated and of little use.

10. *Analytical Example*

To illustrate the effect of different sets of basis functions on the convergence of a model and on the convergence of derivatives of that model, the function $f(x) = x$ has been modelled by the four sets of trigonometric basis functions discussed in this paper. Putting $L = \pi$, and truncating the series at $m = M$, the periodic series of Equation (3) and the sine series of Equation (6) are used in Figures 1a and 1b, respectively, and the cosine series of Equation (5) and the "cosine + sine" series of Equation (8) are used in Figures 2a and 2b. The results for three truncation levels, $M = 3$, 5, and 7, are shown. Because the function x that is being modelled has different values at the ends of the interval, neither the periodic series nor the sine series of Figure 1 are uniformly

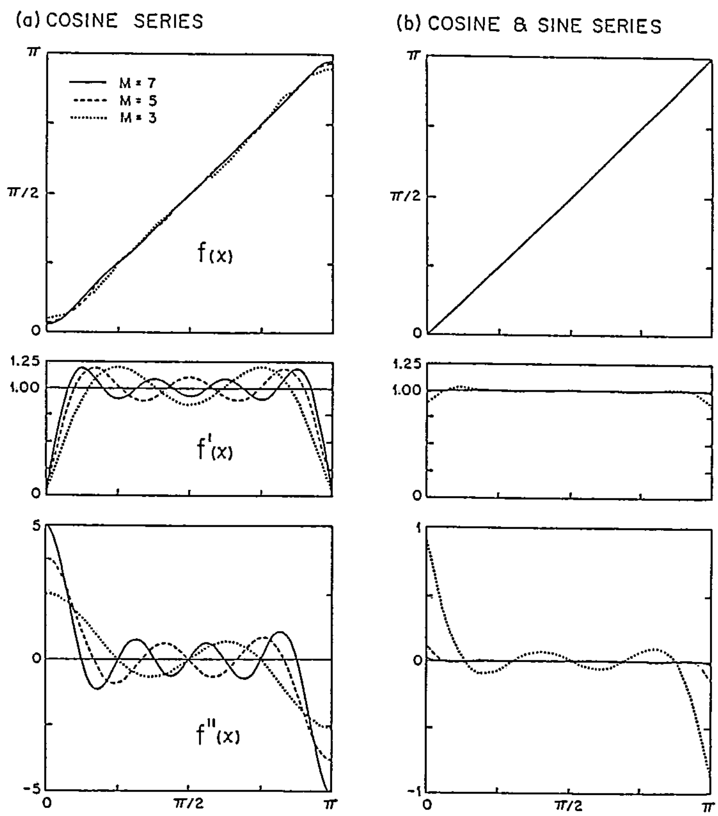

Fig. 1. Non-uniformly convergent models of the function $f(x) = x$ based on (a) the periodic (full Fourier) series and (b) the Fourier sine series. The termwise derivatives $f'(x)$ and $f''(x)$ of such series diverge.

convergent. Even the pointwise convergence of the models (on the open interval) is very slow, and the termwise derivatives diverge. Modelling x by either the cosine or the cosine + sine series, however, results in models (Figure 2) that are uniformly convergent. If the model need not be differentiated, the cosine series of Figure 2a is adequate. Its first derivative is not uniformly convergent, and of course the second derivative diverges. The cosine + sine series (Figure 2b), on the other hand, is designed not only to be uniformly convergent but to have uniformly convergent derivatives. Notice that the scale of the first derivative changes by a factor of 16 from Figure 1 to Figure 2, and the scale of the second derivative changes by factors of 2, 20, and 100 in progressing from the periodic models of Figure 1a to the cosine + sine models of Figure 2b.

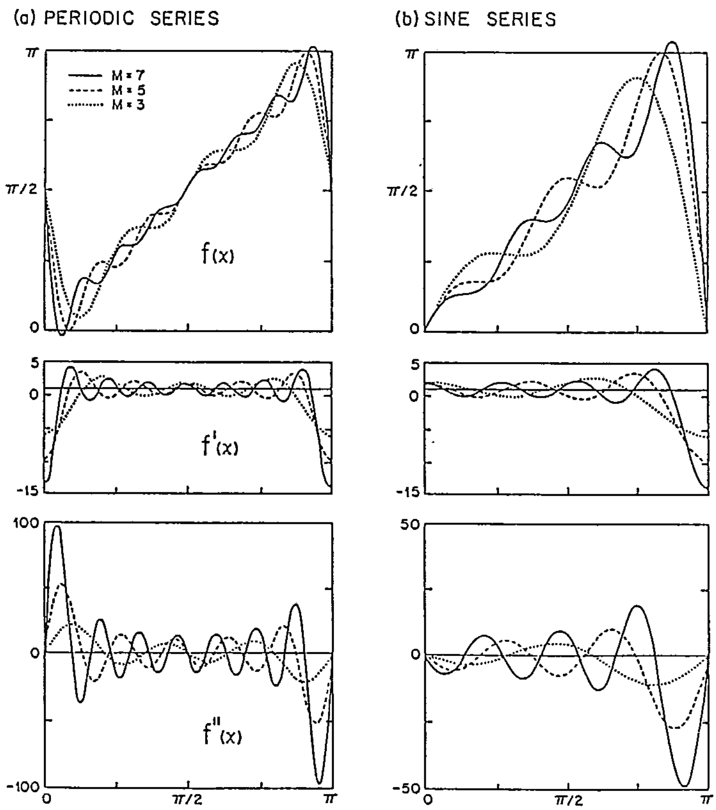

Fig. 2. Uniformly convergent models of the function $f(x) = x$ based on (a) the Fourier cosine series and (b) the "cosine + sine" series. The cosine series alone does not give a uniformly convergent derivative and is therefore inappropriate if the model must be differentiated. The second derivative diverges. The cosine + sine series, by design, has uniformly convergent derivatives. Note the scale changes in $f'(x)$ and $f''(x)$ relative to Figure 1.

Because the modelled function x is odd, or skew-symmetric, about the center of the interval, coefficients A_m of the cosine series, Equation (5), are zero when m is even and positive. For the same reason, the A_m of the cosine + sine series, Equation (8), are zero for even $m > 0$, and the B_m are zero for odd m. That is, for modelling the function x at a truncation level M, there are $M+1$ coefficients in the periodic series; M in the sine series; $(M+3)/2$ in the cosine series; and $M+1$ in the cosine + sine series.

Table. 2. Maximum absolute value of residuals of models of the function $f(x) = x$ and their first and second termwise derivatives, up to a truncation level $M = 9$

	M	periodic	sine	cosine	cosine+sine
$f(x) - x$	1	1.5708	3.1416	.2976	.2976
	2	1.5708	3.1416		.0523
	3	1.5708	3.1416	.1561	.0091
	4	1.5708	3.1416		.0016
	5	1.5708	3.1416	.1052	.00027
	6	1.5708	3.1416		.00005
	7	1.5708	3.1416	.0792	.000008
	8	1.5708	3.1416		.0000014
	9	1.5708	3.1416	.0635	.0000005
$f'(x) - 1$	1	3.00	3.00	1.00	1.000
	2	5.00	5.00		.422
	3	7.00	7.00	1.00	.134
	4	9.00	9.00		.037
	5	11.00	11.00	1.00	.009
	6	13.00	13.00		.0022
	7	15.00	15.00	1.00	.0005
	8	17.00	17.00		.00011
	9	19.00	19.00	1.00	.000023
$f''(x) - 0$	1	4.00	2.00	1.27	1.27
	2	10.94	5.47		1.52
	3	21.37	10.70	2.55	.93
	4	35.21	17.68		.41
	5	52.80	26.40	3.82	.15
	6	73.69	36.84		.05
	7	97.05	49.07	5.09	.015
	8	126.01	63.00		.0041
	9	153.75	78.74	6.37	.0011

Table 2 gives the maximum absolute value of the residuals for the models and their first and second derivatives, up to a truncation level of $M = 9$. The values are based on calculations at 101 equispaced points over the interval. Since the cosine series contain only odd terms, cosine values are left blank for even M. They would be the same as the values for $M - 1$.

Table 2 demonstrates how quickly the cosine + sine series converges to x, even relative to the (also uniformly convergent) cosine series. Both first and second derivatives of the cosine + sine series converge uniformly and rapidly. The first derivatives of the cosine series, on the other hand, like the functions themselves for the periodic and sine series, converge in mean square but not uniformly. Termwise derivatives of these all diverge.

Notice that in any extrapolation based on the periodic or sine series, the extrapolated values may be highly inaccurate. Values of x slightly higher than π will give errors of approximately π in the first case and 2π in the second. Extrapolations based on the cosine series is not as inaccurate, but (being reflected about $x = \pi$) gives an erroneous change in slope and does result in fairly large errors as the extrapolation distance increases. Because the slope of the "cosine + sine" series is modelled in addition to the function values, however, extrapolations for this series are very accurate. With $M = 7$, for example, the extrapolation error at $x = 5\pi/4$ is only 0.212.

11. *Conclusions*

This paper has emphasized the importance of uniform convergence in a mathematical model, and demonstrated the way in which boundary conditions affect the basis functions of the model. Choosing basis functions that apply to inappropriate boundary conditions may result in convergence in mean square but not uniform convergence. The practical result of this is ringing at the boundaries, poor extrapolation outside the domain of the data, a slower rate of convergence, and non-differentiability of the series expansion.

In particular, it has been shown that periodic basis functions (i.e., periodic over the data interval) are inappropriate for geophysical modelling in cartesian coordinates. They give non-uniformly convergent models, and cannot be differentiated term-wise. Periodic basis functions are essential in situations of circular symmetry, of course, where polar coordinates are used, but inappropriate in non-periodic situations in cartesian geometry.

Coordinate terms like x and y reduce ringing somewhat in periodic expansions of non-periodic functions but certainly do not eliminate it. These terms are unnecessary when the proper basis functions are chosen. In a rectangular harmonic representation, these terms, as well as coordinate terms like z, actually violate potential boundary conditions that that representation is supposed to satisfy.

The use of "half-periodic" basis functions (a combination of the familiar Fourier cosine and sine series), in contrast, provide uniformly convergent representations for geophysical fields in cartesian coordinates. These representations, like the geophysical fields themselves, may have arbitrary values at the boundary of the domain. They may be differentiated term by term, the derivatives also being uniformly convergent, and allowing arbitrary derivative-values at the boundary. Which representation is chosen in a particular problem clearly depends on which mathematical properties are required in the model. For example, if the cross partial derivative $\partial^2 f/\partial x\partial y$ is not required, then the sine-sine basis functions of the rectangular harmonic expansion (23) (or of the double Fourier series (17)) are not required. Similarly, if differentiation with respect to x and y is not required (when fitting only the vertical component of a potential-gradient field, for example), only the cosine-cosine basis functions (22 or 12) are required.

Because these expansions and their derivatives are uniformly convergent, problems of ringing do not exist and convergence is very rapid. Furthermore, when derivatives are modelled correctly, extrapolation outside the modelling area (but staying within source free regions) is obviously more accurate.

12. *Acknowledgments*

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