Kimball-Shortley Iterative method for eigenvalue problems

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### Kimbal-Shortley method for the eigenvalue problem of 2nd-order ODEs[[1]](#footnote-20)

Le’t assume the a 2nd-order ODE in normal form and fixed boundary conditions:

formally being a Sturm-Liouville problem with kernel:

Upon a grid discretization the SL eigenvalue equations translates to the below set of algebraic difference equations:

where, ideally, in a universe of exact computations, it is assumed that

For such wavefunctions (for the given grid) we assume the following value for the inner product (overlap):

Introduction of this quadrature rule for the inner product allows to define the norm of a function as:

and the following quantity (in numerical analysis known as Rayleigh quotient (RQ), in quantum mechanics, the hamiltonian’s expectation value for the quantum state ):

The above expression for the RQ (or energy) is essentially a functional rather than a function, as it depends on the entire via the discretized values . We wish to examine its variation upon the variation of the values ; performing the relevant algebra and pointing that,

we find the below expression:

We know that,

minimum, or maximum; this is possible (again following standard calculus of variations algebra) when all partial derivatives of with respect to vanish, namely,

But the last equation is exactly the FD equation for the unknown solution, , which simply says that the solution gives the minimum/maximum value for the RQ (or energy).

As our concern is to produce an iterative scheme for the solution we re-write the above condition as,

So, now we can write down few remarks for this central (iterative) equation of the present discussion:

* For the above expression it was assumed
* the weight coefficients, appear in the updating formula via the expression and possibly in the coefficients
* when constant for all then disappear from the expression for and could be introduced via the constants only.

## Example

Let’s consider the below 2nd-order DE:

Then upon discretization with a step , and a three-point stencil for the 2nd derivative, we have the following rule holding for the values of the wavefunction on the grid points:

So the updating formula for the radial functions is as:

For a grid in the range we assume the fixed boundary conditions .

1. ‘*The Numerical Solution in Schrodinger’s Equation*’, G.E. Kimball and G.H. Shortley, Phys. Rev., **45,** 815, (1934) [↑](#footnote-ref-20)