Kimball-Shortley Iterative method for eigenvalue problems

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Kimball-Shortley method for the eigenvalue problem of 2nd-order ODEs[1]

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

$$\psi''(x) + U_0(x)\psi(x) = \lambda\psi(x), \qquad y(a) = y(b) = 0,$$

formally being a Sturm-Liouville problem with kernel:

$$\hat{L} = -\frac{d^2}{dx^2} + U_0(x)$$

Upon a grid discretization $[x_1, x_2, \cdots, x_N]$ the SL eigenvalue equations translates to the below set of algebraic difference equations:

$$\sum_{i=1}^{N} b_{jj} y_j = E y_i, \qquad y_0 = y_{N+1} = 0, \qquad i = 1(1)N$$

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

$$y_i \quad \rightarrow \quad \psi(x_i), \qquad \text{for} \qquad N \rightarrow \infty$$

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

$$N_{\psi\phi} = \langle \psi | \phi \rangle := \int_a^b dx \psi(x)\phi(x) = \sum_i c_i \psi_i \phi_i$$

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[1] '*The Numerical Solution in Schrodinger's Equation*', G.E. Kimball and G.H. Shortley, Phys. Rev., **45,** 815, (1934)

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

$$N_\phi := \sqrt{\langle\phi|\phi\rangle}$$

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

$$E[\phi] := \frac{\langle\phi|B|\phi\rangle}{\langle\phi|\phi\rangle} = \frac{\sum_{ij} c_i b_{ij} \phi_i \phi_j}{\sum_i c_i \phi_i^2}$$

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

$$\begin{aligned} \frac{\partial}{\partial\phi_i}(\langle\phi|B\phi\rangle) &= 2c_i \sum_j b_{ij}\phi_j, \qquad \text{when} \qquad c_i b_{ij} = c_j b_{ji} \\ \frac{\partial}{\partial\phi_i}(\langle\phi|\phi\rangle) &= 2c_i\phi_i \end{aligned}$$

we find the below expression:

$$\frac{\partial E[\phi]}{\partial\phi_i} = -c_i \frac{2}{N_\phi^2}\left[E[\phi]\phi - \sum_j b_{ij}\phi_j\right]$$

We know that,

$$\frac{\delta E[\psi]}{\delta\phi_i} = 0, \qquad \rightarrow \qquad \text{when } E[\psi] \text{ is a stationary value,}$$

minimum, or maximum; this is possible (again following standard calculus of variations algebra) when all partial derivatives of $E[\phi]$ with respect to ϕ_i vanish, namely,

$$\frac{\partial}{\partial\phi_i}E[\phi] = 0 \quad \rightarrow \quad \sum_j b_{ij}\phi_j = E[\phi]\phi_i$$

But the last equation is exactly the FD equation for the unknown solution, ψ, 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,

$$
(b_{ii} - E[\phi])\phi_i = -\sum_{j\neq i} b_{ij}\phi_j \quad \rightarrow \quad \boxed{\phi_i = \frac{\sum_{j\neq i} b_{ij}\phi_j}{E[\phi] - b_{ii}}, \qquad i = 1(1)N}
$$

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

- For the above expression it was assumed $\boxed{c_i b_{ij} = c_j bji}$
- the weight coefficients, c_i appear in the updating formula via the $E[\phi]$ expression and possibly in the $b_[ij]$ coefficients
- when $c_i =$ constant for all $i = 1(1)N$ then disappear from the expression for $E[\phi]$ and could be introduced via the b_{ij} constants only.

Example

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

$$
-\frac{1}{2}\frac{dy^2}{dx^2} + V(x)y(x) = Ey(x)
$$

Then upon discretization with a step h, 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:

$$
-\frac{1}{2h^2}(y_{i-1} - 2y_i + y_{i+1}) + V_i y_i = E y_i, \qquad i = 1(1)N.
$$
$$
y_0 = y_{N+1} = 0
$$

So the updating formula for the radial functions is as:

$$
y_i = -\frac{y_{i+1}/h^2 + y_{i-1}/h^2}{2E - (\frac{2}{h^2} + 2V_i)}, \qquad i = 1(1)N
$$

For a grid in the range $[a, b] = [0, b]$ we assume the fixed boundary conditions $y_0 = y_{N+1} = 0$.

> **ℹ Numerical**
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> In practice the above update equation is implemented as
>
> $$
> y_i = \frac{1}{2}\frac{y_{i+1} + y_{i-1}}{1 - h^2(V_i - E)}, \qquad i = 1(1)N
> $$