Derivation of Numerov’s Algorithm on a Non-Uniform Mesh

and Application to the Radial Schrödinger Equation

Matt Sieger

September 2007

Updated December 2009

Contents

[Finite Difference Estimates of Derivatives 2](#_Toc248052798)

[Discrete approximation for the first derivative: 2](#_Toc248052799)

[Taylor series expansions 2](#_Toc248052800)

[Non-uniform mesh 3](#_Toc248052801)

[Discrete approximation of the 2nd derivative: 3](#_Toc248052802)

[Non-uniform mesh 4](#_Toc248052803)

[Generalized Numerov’s Method 4](#_Toc248052804)

[Earlier results 8](#_Toc248052805)

[Calculating y1 8](#_Toc248052806)

[FE representation of the radial Schrodinger equation: 9](#_Toc248052807)

# Finite Difference Estimates of Derivatives

## Discrete approximation for the first derivative:

The definitions of the one-sided discrete derivatives are:

|  |  |  |
| --- | --- | --- |
|  |  |  |

|  |  |  |
| --- | --- | --- |
|  |  |  |

The “centered approximation” is the average of the one-sided derivatives:

|  |  |  |
| --- | --- | --- |
|  |  |  |

For a uniform mesh (*δx* is a constant = *h*), the centered approximation reduces to:

|  |  |  |
| --- | --- | --- |
|  |  |  |

### Taylor series expansions

In order to connect the finite-difference approximations of derivatives to analytical derivatives, we make use of the Taylor series expansion about the point *x*,

|  |  |  |
| --- | --- | --- |
|  |  |  |

|  |  |  |
| --- | --- | --- |
|  |  |  |

An estimate of the error in the finite difference approximation can be had by substituting the Taylor expansions of *u*(*x* ± *h*) into the expressions for *D±u*:

|  |  |  |
| --- | --- | --- |
|  |  |  |

|  |  |  |
| --- | --- | --- |
|  |  |  |

From these expressions, it can be seen that the expected deviation from the true value of the first derivative is dominated by the first term in *h*, meaning that the error is of first order in *h.*

The usefulness of the centered approximation is due to the alternating signs of the odd order terms in Eqs 7 and 8, which cause these terms to cancel out produce an estimate good to second order in *h*:

|  |  |  |
| --- | --- | --- |
|  |  |  |

### Non-uniform mesh

For the more general case of a non-uniform mesh, the cancellation of terms in the centered approximation does not occur:

|  |  |  |
| --- | --- | --- |
|  |  |  |

Here we have defined *h*+ = (*xi* + 1 – *xi*) and *h*– = (*xi* – *xi* – 1). In this case, the error is dominated by a term on the order of the difference in size of adjacent mesh points *h*+ – *h*– = *xi* + 1 – 2*xi* + *xi* – 1.

Rearranging terms to isolate the first derivative,

|  |  |  |
| --- | --- | --- |
|  |  |  |

Expanding out to higher orders in u,

|  |  |  |
| --- | --- | --- |
|  |  |  |

## Discrete approximation of the 2nd derivative:

The centered approximation for the second derivative is

|  |  |  |
| --- | --- | --- |
|  |  |  |

Here we have introduced the notation *u*+ = *ui* + 1, *u*– = *ui* – 1, and *u*0 = *ui*. In the case of a uniform mesh, this reduces to

|  |  |  |
| --- | --- | --- |
|  |  |  |

Substituting the Taylor expansions into the uniform mesh case, we arrive at the error estimate:

|  |  |  |
| --- | --- | --- |
|  |  |  |

showing that this estimate in the 2nd derivative is good to second order in *h*. Simple rearrangement of the expression gives

|  |  |  |
| --- | --- | --- |
|  |  |  |

### Non-uniform mesh

|  |  |  |
| --- | --- | --- |
|  |  |  |

In the limit of a symmetric mesh, Eq. 15 reduces to Eq, 13. Reducing Eq. 15 to an expression for the second derivative gives

|  |  |  |
| --- | --- | --- |
|  |  |  |

Showing that the error in the 2nd derivative for a non-symmetric mesh is on the order of the size of adjacent mesh points *h*+ – *h*– = *xi* + 1 – 2*xi* + *xi* – 1, the same as for the first derivative. In the limit of a symmetric mesh, Equation 16 reduces to Eq. 14.

# Generalized Numerov’s Method

Given a differential equation of the form:

|  |  |  |
| --- | --- | --- |
|  |  |  |

We wish to obtain a finite-difference solution of this equation that is usable on an arbitrary mesh. If we define and apply the finite-difference approximation for the second derivative, we obtain

|  |  |  |
| --- | --- | --- |
|  |  |  |

For the rest of this section, we will adopt the notation *a* = *h*+, *b* = *h*–.

|  |  |  |
| --- | --- | --- |
|  |  |  |

If we then replace the first and second derivatives of *F* with centered difference approximations, and *F* with its definition:

|  |  |  |
| --- | --- | --- |
|  |  |  |

|  |  |  |
| --- | --- | --- |
|  |  |  |

|  |  |  |
| --- | --- | --- |
|  |  |  |

Substituting for the first derivative and simplifying as we go,

|  |  |  |
| --- | --- | --- |
|  |  |  |

|  |  |  |
| --- | --- | --- |
|  |  |  |

|  |  |  |
| --- | --- | --- |
|  |  |  |

|  |  |  |
| --- | --- | --- |
|  |  |  |

|  |  |  |
| --- | --- | --- |
|  |  |  |

Substituting in for the second derivative:

|  |  |  |
| --- | --- | --- |
|  |  |  |

Gathering terms on *F*,

|  |  |  |
| --- | --- | --- |
|  |  |  |

Now substituting in the definitions of *F*:

|  |  |  |
| --- | --- | --- |
|  |  |  |

|  |  |  |
| --- | --- | --- |
|  |  |  |

To arrive at a recursion relation we gather terms on *y*+

|  |  |  |
| --- | --- | --- |
|  |  |  |

|  |  |  |
| --- | --- | --- |
|  |  |  |

|  |  |  |
| --- | --- | --- |
|  |  |  |

As a quick check, let’s see what this reduces to in the limit that *a* = *b*:

|  |  |  |
| --- | --- | --- |
|  |  |  |

Which is correct!

Let’s go back to Eq. 23.10 and further collect terms, we arrive at our final expression for Numerov’s algorithm on a generic mesh:

|  |  |  |
| --- | --- | --- |
|  |  |  |

In the special case where *u*(*x*) = 0 (as is true for the Schrodinger equation), this expression reduces to

|  |  |  |
| --- | --- | --- |
|  |  |  |

Again checking in the limit that *a* = *b* = *h*,

|  |  |  |
| --- | --- | --- |
|  |  |  |

Which again is correct.

What is very odd is that the earlier expression I derived for the non-uniform mesh is NOT equivalent to this expression, but does reduce to exactly the same thing in the limit that *a* = *b*.

## Earlier results





When *u*(*x*) = 0,

|  |  |  |
| --- | --- | --- |
|  |  |  |

Note that the expression in Eq. 25 is NOT the same.

## Calculating y1

In order to apply this recursion relation, it is necessary to know the values of *y*0 and *y*1. If *y*1 is not known *a priori*, it can be computed if the first derivative of *y* is known:

|  |  |  |
| --- | --- | --- |
|  |  |  |

In our case,

|  |  |  |
| --- | --- | --- |
|  |  |  |

Using the definition of F utilized in Eq. 19,

|  |  |  |
| --- | --- | --- |
|  |  |  |

Similarly,

|  |  |  |
| --- | --- | --- |
|  |  |  |

|  |  |  |
| --- | --- | --- |
|  |  |  |

Substituting Eq. 32 into Eq. 30 gives

|  |  |  |
| --- | --- | --- |
|  |  |  |

|  |  |  |
| --- | --- | --- |
|  |  |  |

Substituting for F,

|  |  |  |
| --- | --- | --- |
|  |  |  |

Collecting terms on *y*+,

|  |  |  |
| --- | --- | --- |
|  |  |  |

If *u* = 0,

|  |  |  |
| --- | --- | --- |
|  |  |  |

which matches Numerov’s result.

When y0 = 0,



I suggest starting with a guess for y’ and normalizing after-the-fact. Later on, I can look up what y’ is experimentally and optimize the guess.

### Starting backward integration

In order to apply this recursion relation, it is necessary to know the values of *y*N and *y*-. If *y*- is not known *a priori*, it can be computed if the first derivative of *y* is known:

|  |  |  |
| --- | --- | --- |
|  |  |  |

In our case,

|  |  |  |
| --- | --- | --- |
|  |  |  |

Using the definition of F utilized in Eq. 19,

|  |  |  |
| --- | --- | --- |
|  |  |  |

Similarly,

|  |  |  |
| --- | --- | --- |
|  |  |  |

|  |  |  |
| --- | --- | --- |
|  |  |  |

Substituting Eq. 42 into Eq. 40 gives

|  |  |  |
| --- | --- | --- |
|  |  |  |

|  |  |  |
| --- | --- | --- |
|  |  |  |

Substituting for F,

|  |  |  |
| --- | --- | --- |
|  |  |  |

Collecting terms on *y*-,

|  |  |  |
| --- | --- | --- |
|  |  |  |

If *u* = 0,

|  |  |  |
| --- | --- | --- |
|  |  |  |

|  |  |  |
| --- | --- | --- |
|  |  |  |

When *yN* = 0,

|  |  |  |
| --- | --- | --- |
|  |  |  |

I suggest starting with a guess for y’ and normalizing after-the-fact. Later on, I can look up what y’ is experimentally and optimize the guess.

# FE representation of the radial Schrodinger equation:

The radial equation that must be solved is:

 (19)

(in Rydberg units)

where ** is the reduced mass of the electron and *V*(*r*) is the potential given above. I’m thinking this equation only has solutions for quantized values of *E* < 0.

The *Pi* are the *r*-multiplied radial wave functions:

 (20)

and are normalized such that

 (21)

Cast in the form:



we can apply Numerov’s method with *u*(*r*) = 0, *v*(*r*) = *g*(*r*), and *Fn* = *gnPn* to solve numerically for *P*(*r*) on a generalized mesh:





The boundary conditions require that



The form of the spherically symmetric radial potential is:



The *r*-multiplied potential *U*(*r*) has the advantage of being finite everywhere.



**FE Solution to Radial Equation when E < V**

Assume the solution is of the form:





Substituting into the RSE produces an equation to solve for *f* (*r*):



***Discretizing on a uniform mesh,***



Using a similar finite difference for the first derivative produces



Further drilling into the third derivative,





Substituting,



Note that terms in *fi*+2 have been introduced, so we reorient ourselves on this point:



Now we substitue for the 4th order derivative











Since 





