PHY604 Lecture 10

October 5, 2023

Review: Bulirsch-Stoer Method and Richardson extrapolation

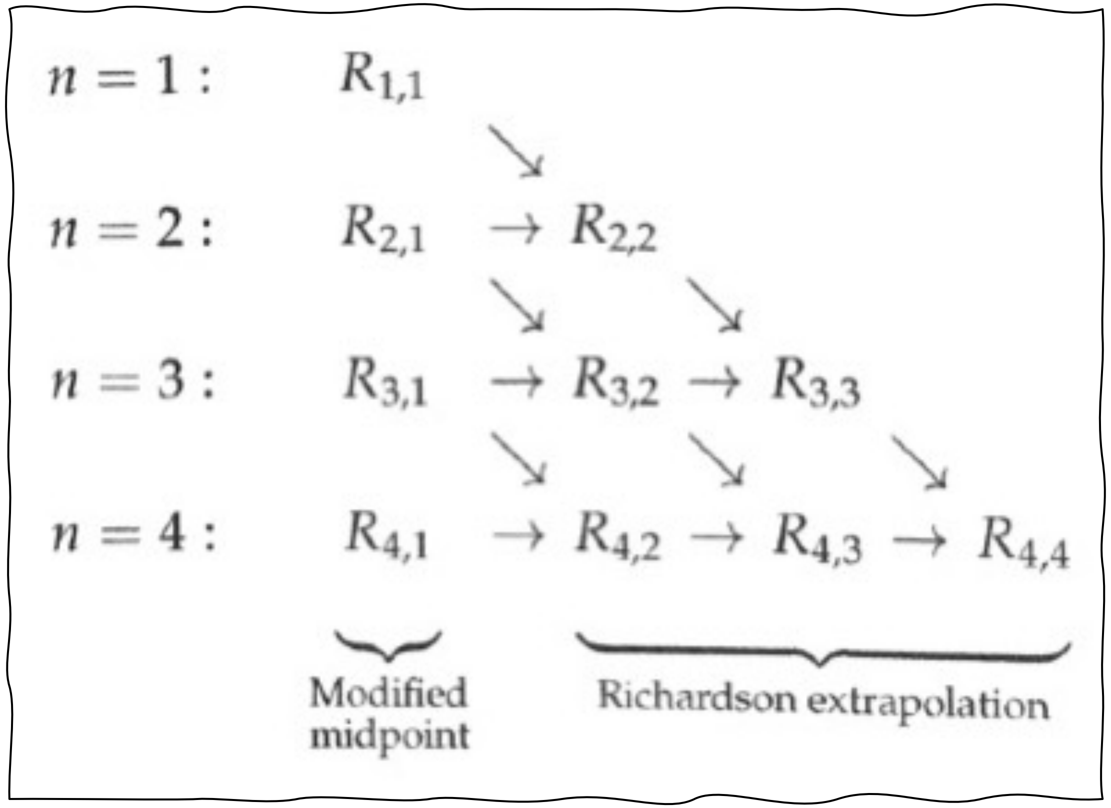
- n is the number of modified midpoint steps, which gives us $R_{n,1}$
  - Can obtain $R_{n,m}$ for $m < n$

$$R_{n,m+1} = R_{n,m} + \frac{R_{n,m} - R_{n-1,m}}{[n/(n-1)]^{2m} - 1}$$

  - See Newman Sec. 8.5

- Which gives an estimate of the result:

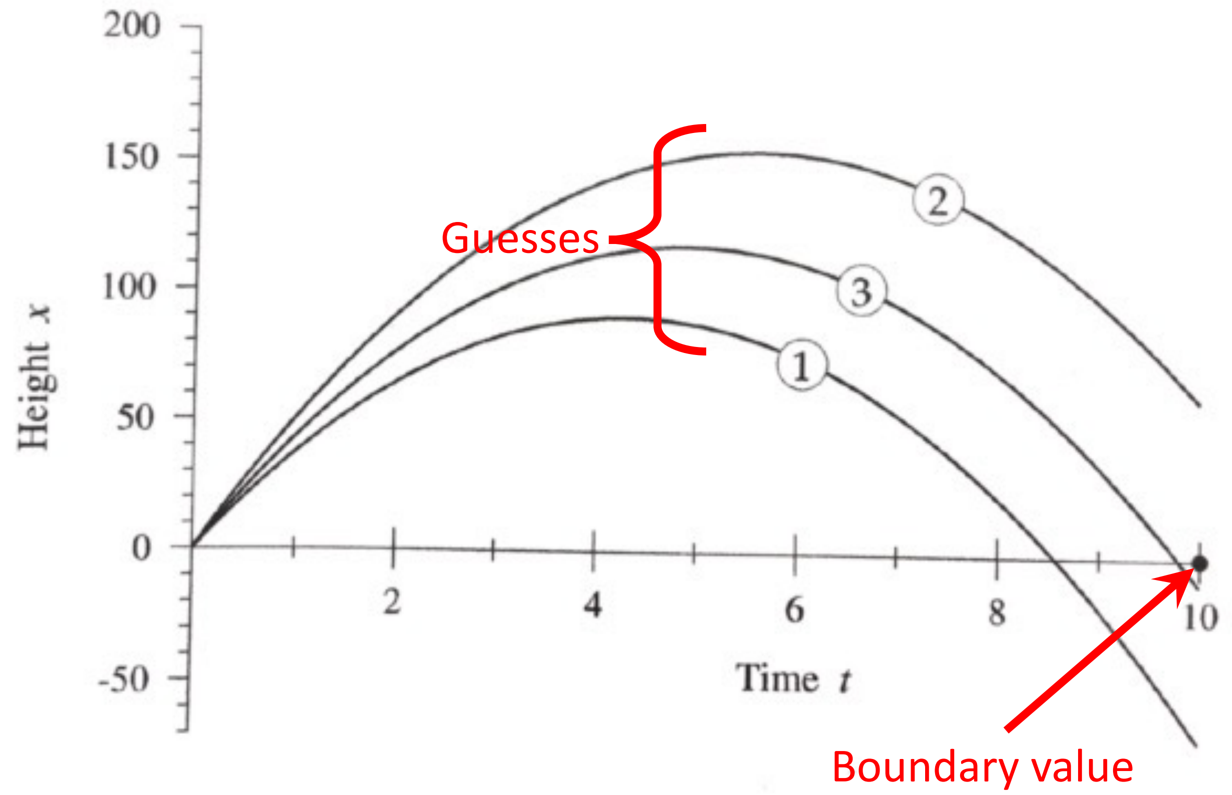
$$x(t+t_f) = R_{n,m+1} + \mathcal{O}(\Delta_n^{2m+2})$$



(Newman)

Review: Shooting method for boundary value problems

- Write the height of the ball at the boundary t_1 as $x = f(v)$ where v is the initial velocity
- If we want the ball to be at $x = 0$ at t_1, we need to solve $f(v) = 0$
- Reformulated the problem as finding a root of a function
- The function is "evaluated" by solving the differential equation



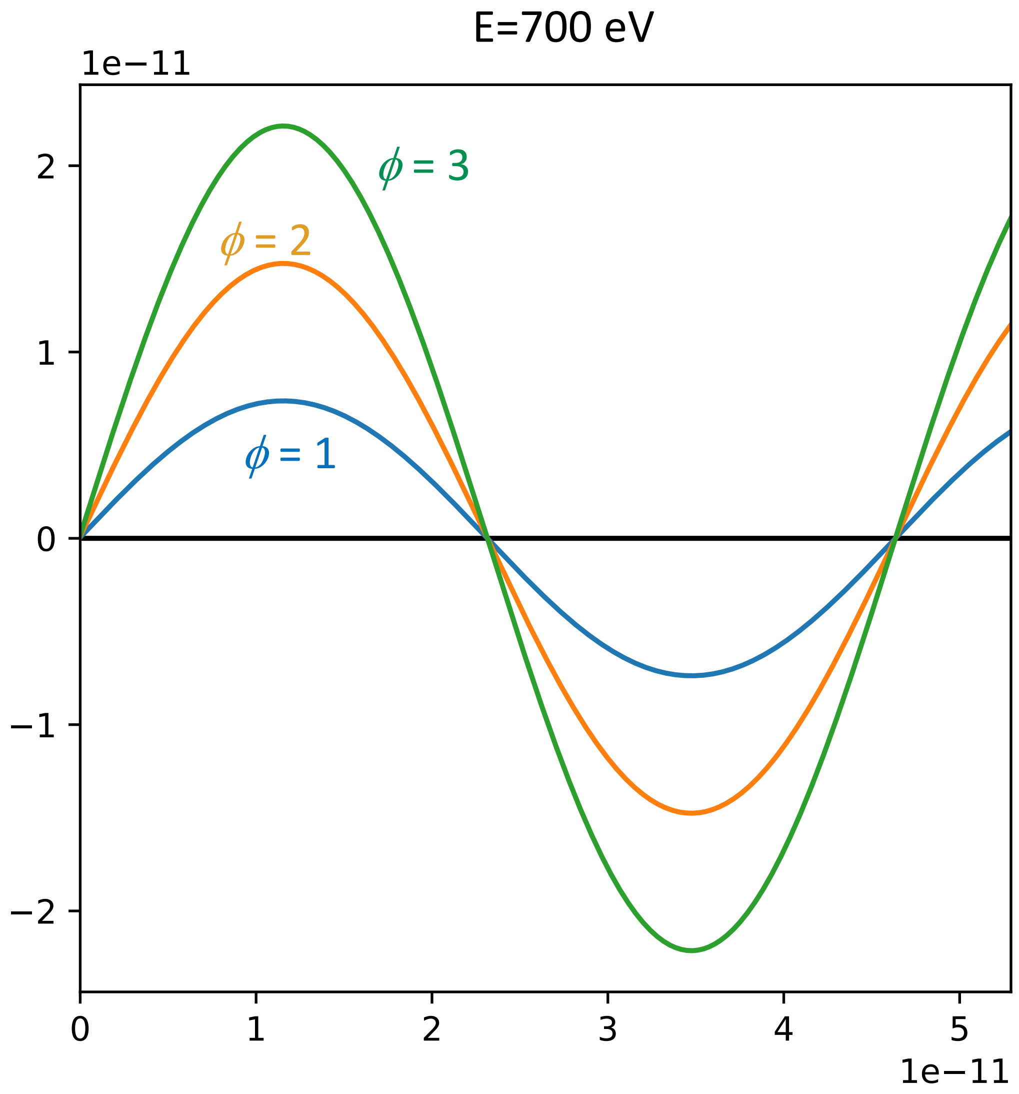
Review: Schrodinger equation in 1D well

- As usual, make into system of 1D ODEs:

$$\frac{d\psi}{dx} = \phi, \quad \frac{d\phi}{dx} = \frac{2m}{\hbar^2}[V(x) - E]\psi$$

- Know that $\psi = 0$ at $x = 0$ and $x = L$, but don't know ϕ
- Let's choose a value of E and solve using some choices for ϕ:
- Since the equation is linear, scaling the initial conditions exactly scales the $\psi(x)$

- **No matter what ϕ, we will never get a valid solution!** (only affects overall magnitude, not shape)



Today’s lecture: Linear Algebra

- Matrix manipulations
- Gaussian elimination

Numerical linear algebra (Garcia Ch. 4)

- Basic problem to solve: **A x** = **b**

- We have already seen many cases where we need to solve linear systems of equations
  - E.g., ODE integration, cubic spline interpolation

- More that we will come across:
  - Solving the diffusion PDE
  - Multivariable root-finding
  - Curve fitting

- We will explore some key methods to understand what they do
  - Mostly, efficient and robust libraries exist, so no need to reprogram

- Often it is illustrative to compare between how we would solve linear algebra by hand and (efficiently) on the computer

Review of matrices: Multiplication

- Matrix-vector multiplication:
  - **A** is *m* x *n* matrix
  - **x** is *n* x 1 (column) vector
  - Result: **b** is *m* x 1 (column vector)
  - Simple scaling: $O(N^2)$ operations

$$b_i = (Ax)_i = \sum_{j=1}^{n} A_{ij} x_j$$

- Matrix-matrix multiplication
  - **A** is *m* x *n* matrix
  - **B** is *n* x *p* matrix
  - Result: **AB** is *m* x *p* matrix
  - Direct multiplication: $O(N^3)$ operations
    - Some faster algorithms exist (make use of organization of sub-matrices for simplification)

$$(AB)_{ij} = \sum_{k=1}^{n} A_{ik} B_{kj}$$

Review of matrices: Determinant

- Encodes some information about a square matrix
  - Used in some linear systems algorithms
  - Solution to linear systems only exists if determinant is nonzero
- Simple algorithm for obtaining determinant is Laplace expansion
- For simple matrices, can be done by hand:

$$\begin{vmatrix} a & b \\ c & d \end{vmatrix} = ad - bc$$

$$\begin{vmatrix} a & b & c \\ d & e & f \\ g & h & i \end{vmatrix} = a \begin{vmatrix} e & f \\ h & i \end{vmatrix} - b \begin{vmatrix} d & f \\ g & i \end{vmatrix} + c \begin{vmatrix} d & e \\ g & h \end{vmatrix}$$

- What about big matrices?

Review of matrices: Determinant

- Encodes some information about a square matrix
  - Used in come linear systems algorithms
  - Solution to linear systems only exists if determinant is nonzero
- **By hand:** Simple algorithm for obtaining determinant is Laplace expansion
- For simple matrices, can be done by hand:

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- What about big matrices? **Will need a more efficient implementation!**

Review of matrices: Inverse

- $\mathbf{A}^{-1}\mathbf{A}=\mathbf{A}\mathbf{A}^{-1}=\mathbf{I}$
- Formally, the solution to a linear system $\mathbf{A}\,\mathbf{x} = \mathbf{b}$ is $\mathbf{x} = \mathbf{A}^{-1}\mathbf{b}$
  - Usually less expensive to get the solution without computing the inverse first
- Non-invertible (i.e., singular) if determinant is 0

By hand: Cramer's rule

- One simple way to solve **A x** = **b** is:

$$x_i = \frac{|\mathbf{A}_i|}{|\mathbf{A}|}$$

- Where $\mathbf{A}_i$ is **A** with the *i*th column replaced by **b**

- Comparable speed to calculating the inverse

By hand: Gaussian elimination

- Main general technique for solving **A x** = **b**
  - Does not involve matrix inversion
  - For “special” matrices, faster techniques may apply
- Involves forward-elimination and back-substitution

- Consider a simple example (from Garcia Ch. 4):

$$\begin{aligned} x_1 + x_2 \; + x_3 &= 6 \\ -x_1 + 2x_2 \quad\;\; &= 3 \\ 2x_1 \qquad\;\; + x_3 &= 5 \end{aligned}$$

By hand: Forward elimination

- 1. Eliminate x_1 from second and third equation. Add first equation to the second and subtract twice the first equation from the third:

$$\begin{aligned} x_1 + x_2 \quad + x_3 &= 6 \\ 3x_2 + x_3 &= 9 \\ -2x_2 - x_3 &= -7 \end{aligned}$$

- 2. Eliminate x_2 from third equation. Multiply the second equation by (-2/3) and subtract it from the third

$$\begin{aligned} x_1 + x_2 \quad + x_3 &= 6 \\ 3x_2 \quad + x_3 &= 9 \\ -\frac{1}{3}x_3 &= -1 \end{aligned}$$

By hand: Back substitution

$$
\begin{aligned}
x_1 + x_2 \quad + x_3 &= 6 \\
3x_2 \ + x_3 &= 9 \\
-\frac{1}{3}x_3 &= -1
\end{aligned}
$$

- 3. Solve for $x_3 = 3$.
- 4. Substitute x_3 into the second equation to get $x_2 = 2$
- 5. Substitute x_3 and x_2 into the first equation to get $x_1 = 1$

- In general, for N variables and N equations:
  - Use forward elimination make the last equation provide the solution for x_N
  - Back substitute from the Nth equation to the first
  - Scales like N^3 (can do better for "sparse" equations)

Pitfalls of Gaussian substitution: Roundoff errors

- Consider a different example (also from Garcia):

$$\begin{aligned}\epsilon x_1 + x_2 + x_3 &= 5\\ x_1 + x_2 \quad\quad &= 3\\ x_1 + \quad + x_3 &= 4\end{aligned}$$

- First, lets take $\epsilon \to 0$ and solve:

Subtract second from third:

$$\begin{aligned}x_2 + x_3 &= 5\\ x_1 + x_2 \quad\quad &= 3\\ -x_2 + x_3 &= 1\end{aligned}$$

Add first to third:

$$\begin{aligned}x_2 + x_3 &= 5\\ x_1 + x_2 \quad\quad &= 3\\ 2x_3 &= 6\end{aligned}$$

Back substitute:

$$\begin{aligned}x_2 &= 2\\ x_1 &= 1\\ x_3 &= 3\end{aligned}$$

Roundoff error example: Now solve with ε

- Forward elimination starts by multiplying first equation by $1/\varepsilon$ and subtracting it from second and third:

$$
\begin{aligned}
\epsilon x_1 + \quad x_2 \quad &+ x_3 = 5 \\
(1 - 1/\epsilon)x_2 \quad &- (1/\epsilon)x_3 = 3 - 5/\epsilon \\
-(1/\epsilon)x_2 \quad &+ (1 - 1/\epsilon)x_3 = 4 - 5/\epsilon
\end{aligned}
$$

- Clearly have an issue if ε is near zero, e.g., if $C - 1/\epsilon \to -1/\epsilon$ for C order unity:

$$
\begin{aligned}
\epsilon x_1 + \quad x_2 \quad &+ x_3 = 5 \\
-(1/\epsilon)x_2 \quad &- (1/\epsilon)x_3 = -5/\epsilon \\
-(1/\epsilon)x_2 \quad &- (1/\epsilon)x_3 = -5/\epsilon
\end{aligned}
\left.\vphantom{\begin{aligned} a \\ b \end{aligned}}\right\}
$$

Cannot solve, now have two equations, three unknowns

Simple fix: Pivoting

- Interchange the order of the equations before performing the forward elimination

$$\begin{aligned} x_1 + x_2 &= 3 \\ \epsilon x_1 + x_2 + x_3 &= 5 \\ x_1 + + x_3 &= 4 \end{aligned}$$

- Now the first step of forward elimination gives us:

$$\begin{aligned} x_1 + x_2 &= 3 \\ (1-\epsilon)x_1 + x_3 &= 5 - 3\epsilon \\ -x_2 + x_3 &= 1 \end{aligned}$$

- Now we round off:

$$\left.\begin{aligned} x_1 + x_2 &= 3 \\ x_1 + x_3 &= 5 \\ -x_2 + x_3 &= 1 \end{aligned}\right\}$$

Same as when we initially took ε to 0.

Gaussian elimination with pivoting

- Partial-pivoting:
  - Interchange of rows to move the one with the largest element in the current column to the top
  - (Full pivoting would allow for row and column swaps—more complicated)

- Scaled pivoting
  - Consider largest element relative to all entries in its row
  - Further reduces roundoff when elements vary in magnitude greatly

- Row echelon form: This is the form that the matrix is in after forward elimination

Matrix determinants with Gaussian elimination

- Once we have done forward substitution and obtained a row echelon matrix it is trivial to calculate the determinant:

$$\det(\mathbf{A}) = (-1)^{N_{\mathrm{pivot}}} \prod_{i=1}^{N} A_{ii}^{\text{row-echelon}}$$

- Every time we pivoted in the forward substitution, we change the sign

Matrix inverse with Gaussian elimination

- We can also use Gaussian elimination to fin the inverse of a matrix
- We would like to find $\mathbf{A}\mathbf{A}^{-1} = \mathbf{I}$
- We can use Gaussian elimination to solve: $\mathbf{A}\,\mathbf{x}_i = \mathbf{e}_i$
  - $\mathbf{e}_i$ is a column of the identity:

$$\mathbf{e}_1 = \begin{bmatrix} 1 \\ 0 \\ 0 \\ \vdots \end{bmatrix}, \quad \mathbf{e}_2 = \begin{bmatrix} 0 \\ 1 \\ 0 \\ \vdots \end{bmatrix}, \quad \mathbf{e}_3 = \begin{bmatrix} 0 \\ 0 \\ 1 \\ \vdots \end{bmatrix}, \ldots, \ \mathbf{e}_N = \begin{bmatrix} \vdots \\ 0 \\ 0 \\ 1 \end{bmatrix}$$

  - $\mathbf{x}_i$ is a column of the inverse:

$$\mathbf{A}^{-1} = \begin{bmatrix} \mathbf{x}_1 & \mathbf{x}_2 & \mathbf{x}_3 & \ldots & \mathbf{x}_N \end{bmatrix}$$

Singular matrix

- If a matrix has a vanishing determinant, then the system is not solvable
- Common way for this to enter, one equation in the system is a linear combination of some others
- Not always easy to detect from the start

Singular and close to singular matrices

- Condition number: Measures how close to singular we are
  - How much **x** would change with a small change in **b**

$$\mathrm{cond}(\mathbf{A}) = ||\mathbf{A}||\ ||\mathbf{A}^{-1}||$$

  - Requires defining a norm of **A**
    - https://en.wikipedia.org/wiki/Matrix_norm
  - See, e.g., numpy implementation:
    - https://numpy.org/doc/stable/reference/generated/numpy.linalg.cond.html

- Rule of thumb: $\dfrac{||\mathbf{x}^{\mathrm{exact}} - \mathbf{x}^{\mathrm{calc}}||}{||\mathbf{x}^{\mathrm{exact}}||} \simeq \mathrm{cond}(\mathbf{A}) \cdot \epsilon^{\mathrm{machine}}$

Tridiagonal and banded matrices

- We saw this type of matrix when solving for cubic spline coefficients:

$$\begin{pmatrix} 4\Delta x & \Delta x & & & & \\ \Delta x & 4\Delta x & \Delta x & & & \\ & \Delta x & 4\Delta x & \Delta x & & \\ & & \ddots & \ddots & \ddots & \\ & & & \Delta x & 4\Delta x & \Delta x \\ & & & & \Delta x & 4\Delta x \end{pmatrix} \begin{pmatrix} p''_1 \\ p''_2 \\ p''_3 \\ \vdots \\ p''_{n-2} \\ p''_{n-1} \end{pmatrix} = \frac{6}{\Delta x} \begin{pmatrix} f_0 - 2f_1 + f_2 \\ f_1 - 2f_2 + f_3 \\ f_2 - 2f_3 + f_4 \\ \vdots \\ f_{n-3} - 2f_{n-2} + f_{n-1} \\ f_{n-2} - 2f_{n-1} + f_n \end{pmatrix}$$

- Often come up in physical situations
- These types of matrices can be efficiently solved with Gaussian elimination

Gaussian elimination for banded matrices

- Only need to do Gaussian elimination steps for *m* nonzero elements below given row (*m* is less than the number of diagonal bands)
- Example:

$$\begin{pmatrix} 2 & 1 & 0 & 0 \\ 3 & 4 & -5 & 0 \\ 0 & -4 & 3 & 5 \\ 0 & 0 & 1 & 3 \end{pmatrix} \to \begin{pmatrix} 2 & 1 & 0 & 0 \\ 0 & 2.5 & -5 & 0 \\ 0 & -4 & 3 & 5 \\ 0 & 0 & 1 & 3 \end{pmatrix} \to \begin{pmatrix} 2 & 1 & 0 & 0 \\ 0 & 2.5 & -5 & 0 \\ 0 & 0 & -5 & 5 \\ 0 & 0 & 1 & 3 \end{pmatrix} \to \begin{pmatrix} 2 & 1 & 0 & 0 \\ 0 & 2.5 & -5 & 0 \\ 0 & 0 & -5 & 5 \\ 0 & 0 & 0 & 4 \end{pmatrix}$$

After class tasks

- Homework 1 graded, sees GRADES.md in your repo
- Homework 2 due today
- Homework 3 will be posted today or tomorrow

- Readings:
  - Newman Ch. 6
  - Garcia Ch. 4
  - Pang Sec. 5.3