# PHY 342/442

Computational Physics

Syllabus—PHY 342

- Homework—much of the homework will be started in class (45% of final grade)
- Warm up exercises—reading assignment required *before* each lecture. There will be quiz for each reading. The quiz will be done on the course *D2L* page (5% of final grade)
- In class Exam—one mid term exam to take place on the 5th or 6th week (20% of final grade)
- Final Exam—cumulative final to take place Nov. 20 (30 % of grade)

Syllabus—PHY 442

- Homework—30%
- Warm up exercises—5%
- Project—15%
- In class exam—20%
- Final—30%

Topics

- Numerical Interpolation and Curve Fitting
- Monte Carlo Techniques
- Numerical solutions to ordinary differential equations
- Numerical Fourier Analysis
- Numerical Solutions to PDEs

Text

- *Course Notes,* by Jesús Pando. You should be getting this soon if you haven't yet gotten it already.
- *Matlab: A Practical Introduction to Programming and Problem Solving,* Attaway. *Suggested* if you have no experience with MatLab

MatLab

- Student version starts at $99.00.
- For this course the basic version is all you need.
- No need to purchase, you can use DePaul's virtual lab software that can be accessed here: https://depaul.apporto.com

Programming:

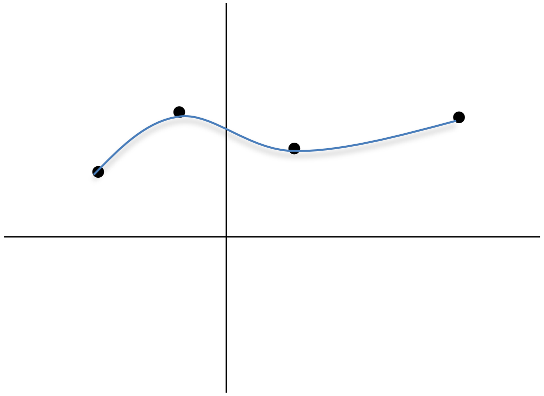
1. Write programs for people, not computers.
   a) Make names consistent, distinctive, and meaningful.
   b) Make code style and formatting consistent.
2. Make incremental changes.
   a) Work in small steps with frequent feedback and course correction
   b) Modularize code rather than copying and pasting.
3. Plan for mistakes.
   a) Use known cases to check code produces correct results
4. Optimize software only after it works correctly.
5. Document design and purpose, not mechanics.

Learning goals:

- Be able explain what *cubic spline interpolation* is and what is necessary to implement the algorithm
- Recognize what a *tridiagonal system* is and be able to solve these systems efficiently

When dealing with experimental or computer generated data, one often has to *approximate* the data with a function. These approximations come in two general types

- *Interpolation* is finding an approximating polynomial that exactly matches the data at specified points
- *Curve fitting* finds a set a parameters that *best fits* the data to a pre-specified function.
- We begin with *interpolation.*

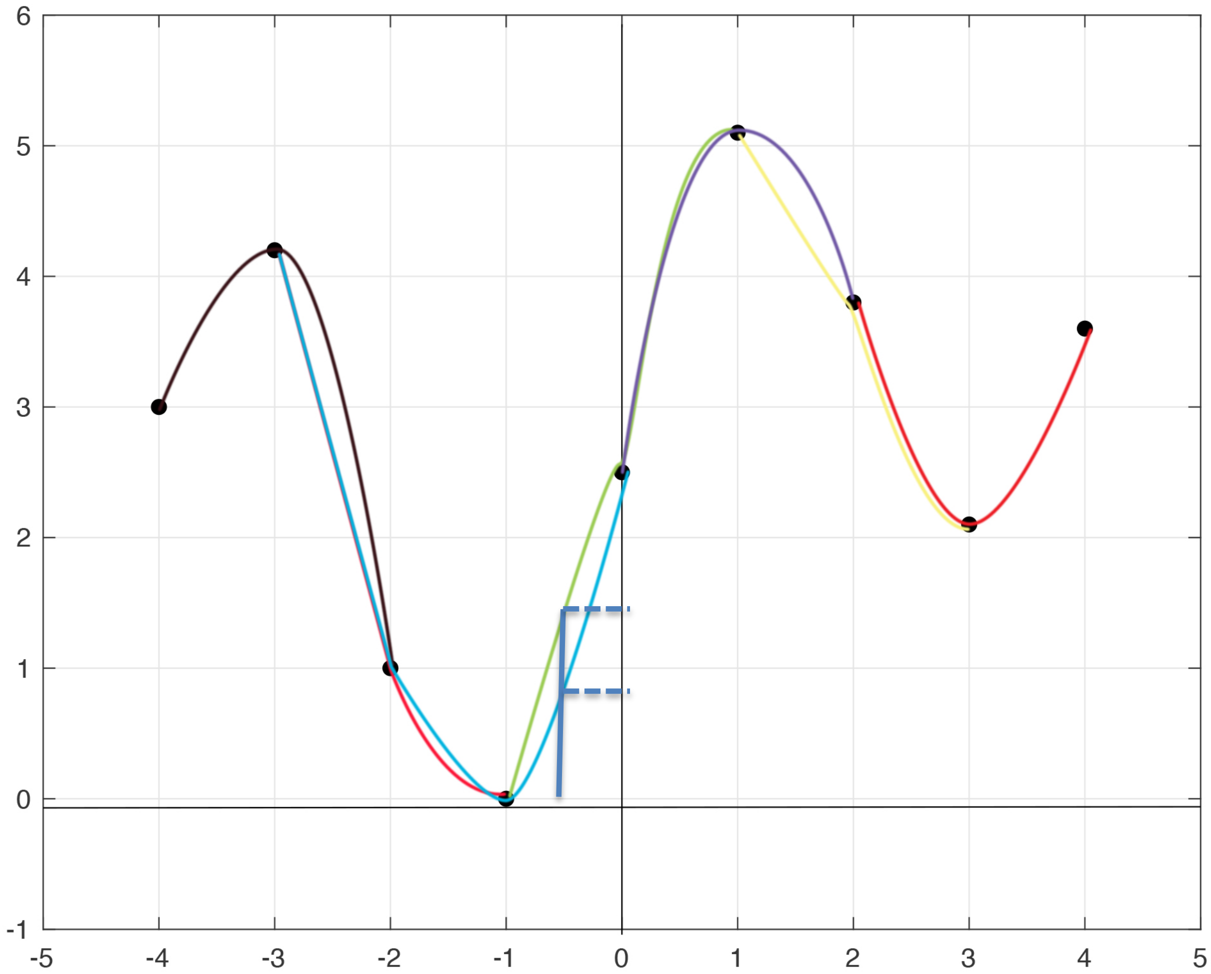


- We begin looking at interpolation by first looking at things graphically. Do questions (1) – (3) on the worksheet and S T O P.

Interpolation 1

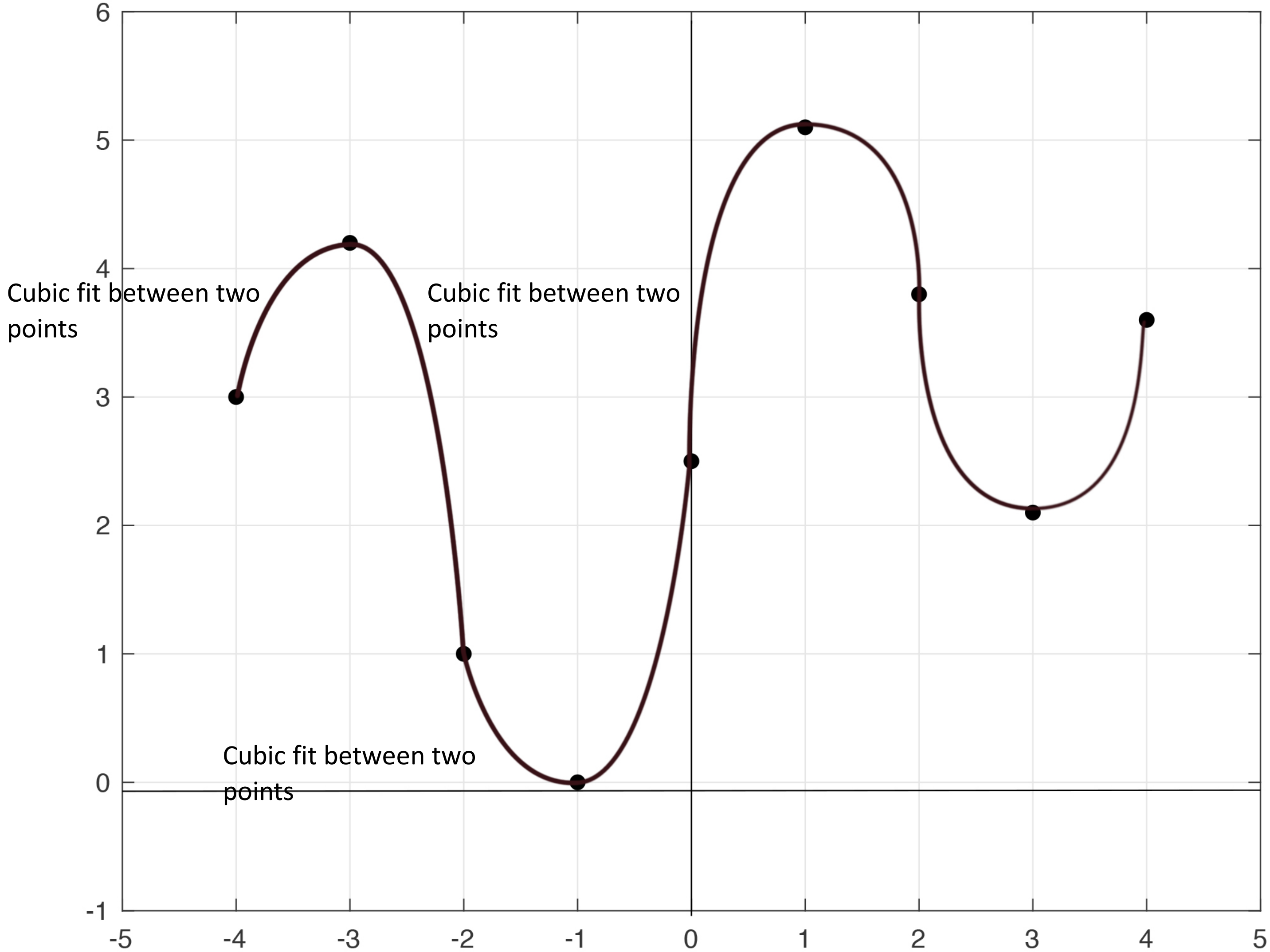
(1)

(2)




(3) The cubic is smoother, but is still discontinuous and not *smooth* at the data points

Interpolation 1



In a cubic spline, we fit a *cubic* between *each* set of points subject to the constraints that the first and second derivatives *match* at the end points

Let's focus now on two consecutive points, $x_j$ and $x_{j+1}$ A general cubic function, $p(x)$, in this interval has the form

$$p(x) = a_j(x - x_j)^3 + b_j(x - x_j)^2 + c_j(x - x_j) + d_j. \qquad (1)$$

The *j's* here represent the data points to which we are trying to fit a cubic. In order for us to find the interpolating cubic, we must solve for the constants $a_j$, $b_j$, $c_j$ and $d_j$

$d_j$ is relatively straightforward to find. Making the substitution in (1) , $x = x_j$ gives

$$p(x_j) = d_j$$

Do question (4) on the worksheet and S T O P

(4)

$$\begin{aligned}
p(x) &= a_j(x - x_j)^3 + b_j(x - x_j)^2 + c_j(x - x_j) + d_j \\
&\quad \text{letting } x = x_{j+1} \text{ and substituting above gives} \\
p(x_{j+1}) &= a_j(x_{j+1} - x_j)^3 + b_j(x_{j+1} - x_j)^2 + c_j(x_{j+1} - x_j) + d_j \\
&\quad \text{defining } h_j = x_{j+1} - x_j \text{ and } p_j = p(x_j) \text{ gives} \\
p_{j+1} &= a_j h_j^3 + b_j h_j^2 + c_j h_j + p_j
\end{aligned}$$

Recall we are going to demand that the first and second derivatives exist and match. Lets use this to see if we can solve for another constant.

The first and second derivatives of eq.(1) are

$$\begin{aligned} p'(x) &= 3a_j(x-x_j)^2 + 2b_j(x-x_j) + c_j \\ p''(x) &= 6a_j(x-x_j) + 2b_j \end{aligned}$$

Setting $x = x_j$ in the second derivative gives

$$\begin{aligned} p''_j &= 2b_j \\ b_j &= \frac{p''_j}{2} \end{aligned}$$

Do question (5) on the worksheet and S T O P

(5)

The first and second derivatives of Eq. (1) are

$$\begin{aligned} p'(x) &= 3a_j(x-x_j)^2 + 2b_j(x-x_j) + c_j \\ p''(x) &= 6a_j(x-x_j) + 2b_j \end{aligned}$$

Setting $x = x_{j+1}$ in the second derivative gives

$$\begin{aligned} p''_{j+1} &= 6a_j h_j + 2b_j \\ a_j &= \frac{1}{6}\,\frac{p''_{j+1} - p''_j}{h_j} \end{aligned}$$

where $b_j = p''_j/2$ that we found earlier was used.

We now have values for $a_j$, $b_j$, and $d_j$. We can use Eq.(1) to solve for $c_j$ and the full cubic:

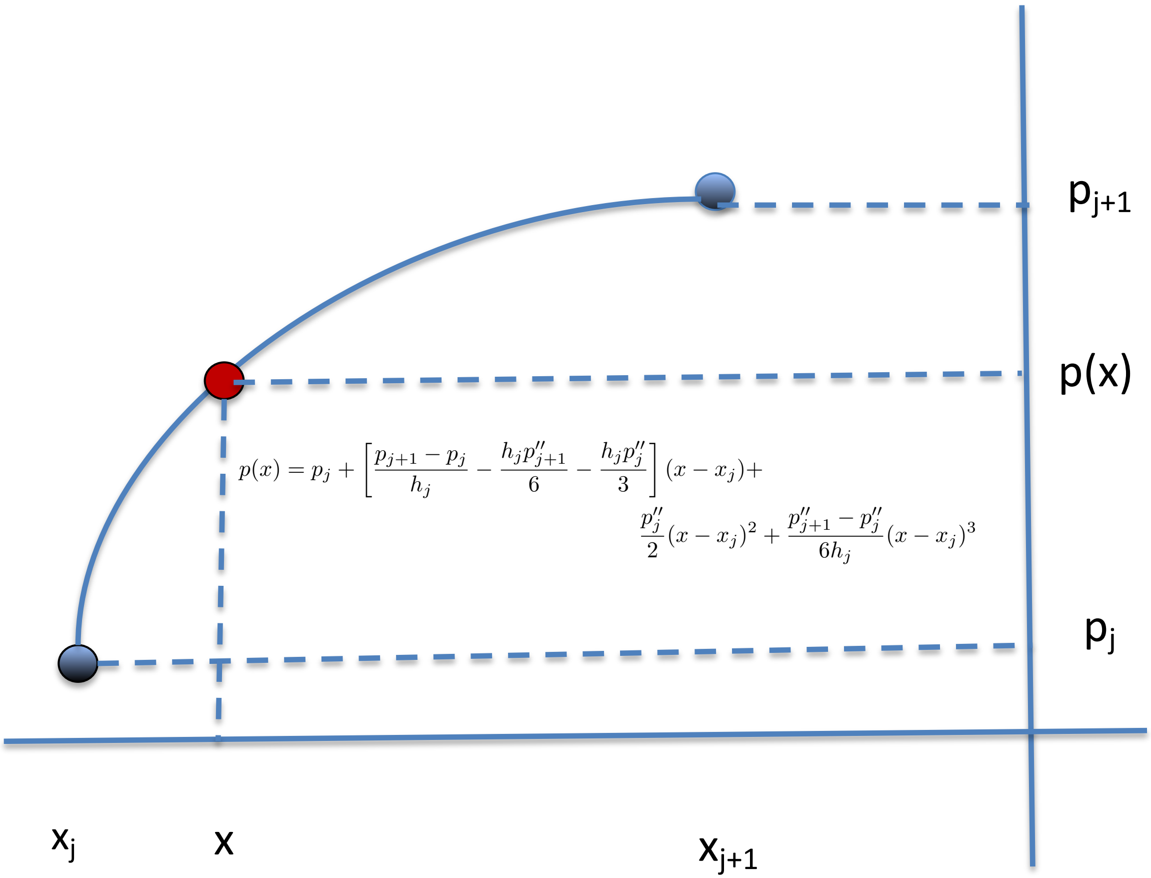
$$c_j = \frac{p_{j+1} - p_j}{h_j} - \frac{h_j p''_{j+1} + 2h_j p''_j}{6}$$

$$p(x) = p_j + \left[\frac{p_{j+1} - p_j}{h_j} - \frac{h_j p''_{j+1}}{6} - \frac{h_j p''_j}{3}\right](x - x_j) + \frac{p''_j}{2}(x - x_j)^2 + \frac{p''_{j+1} - p''_j}{6h_j}(x - x_j)^3, \quad x_j \leq x \leq x_{j+1} \quad (1)$$

**with first derivative**

$$p'(x) = \frac{p_{j+1} - p_j}{h_j} - \frac{h_j p''_{j+1}}{6} - \frac{h_j p''_j}{3} + p''_j(x - x_j) + \frac{p''_{j+1} - p''_j}{2h_j}(x - x_j)^2, \quad x_j \leq x \leq x_{j+1}. \quad (2)$$

Interpolation 1




$$p(x) = p_j + \left[\frac{p_{j+1}-p_j}{h_j} - \frac{h_j p''_{j+1}}{6} - \frac{h_j p''_j}{3}\right](x-x_j) + \frac{p''_j}{2}(x-x_j)^2 + \frac{p''_{j+1}-p''_j}{6h_j}(x-x_j)^3$$

Notice that all we need is the second derivatives, *p''*

Note that to apply our result, we need to find the unknown second derivatives.
We find the second derivatives by replacing *j* by *j -1.* Doing so and a bit of algebra gives:

$$h_{j-1}p''_{j-1} + (2h_j + 2h_{j-1})\, p''_j + h_j p''_{j+1}$$
$$= 6\left(\frac{p_{j+1}-p_j}{h_j} - \frac{p_j - p_{j-1}}{h_{j-1}}\right), \quad j = 2, \ldots, N-1$$

Notice that all the unknown $p_j''$ are on the left hand side and only known terms are on right hand side. Also note that there are $N-2$ equations for the $N$ unknown $p_j''$

The last two equations come from specifying the derivatives at the endpoints, $x_1$ and $x_N$ which yields

$$\begin{aligned} 2h_1p_1'' + h_1p_2'' &= 6\frac{p_2-p_1}{h_1} - 6p_1' \\ h_{N-1}p''_{N-1} + 2h_{N-1}p''_N &= -6\frac{p_N - p_{N-1}}{h_{N-1}} + 6p'_N \end{aligned}$$

There are a total of $N$ unknowns and $N$ equations. This can be written in matrix form as

$$\begin{bmatrix} 2h_1 & h_1 & & & & \\ h_1 & 2(h_1+h_2) & h_2 & & & \\ & h_2 & 2(h_2+h_3) & h_3 & & \\ & & & \ddots & & \\ & & & h_{N-2} & 2(h_{N-2}+h_{N-1}) & h_{N-1} \\ & & & & h_{N-1} & 2h_{N-1} \end{bmatrix} \begin{bmatrix} p_1'' \\ p_2'' \\ p_3'' \\ \vdots \\ p_{N-1}'' \\ p_N'' \end{bmatrix}$$

$$= \begin{bmatrix} 6\frac{p_2-p_1}{h_1} - 6p_1' \\ 6\frac{p_3-p_2}{h_2} - 6\frac{p_2-p_1}{h_1} \\ 6\frac{p_4-p_3}{h_3} - 6\frac{p_3-p_2}{h_2} \\ \vdots \\ 6\frac{p_n-p_{N-1}}{h_{N-1}} - 6\frac{p_{N-1}-p_{N-2}}{h_{N-2}} \\ -6\frac{p_N-p_{N-1}}{h_{N-1}} + 6p_N' \end{bmatrix} \quad (1)$$

Do questions 6—8 on the worksheet

(6) From the RHS of the matrix equation we see that we need the *first derivative at the end points*

(7) The matrix will look the same except the *first* and *last* entries on the RHS will be *zero*

(8)

1. We use Eq. (2) to find the cubic polynomial that lies between $x_j$ and $x_{j+1}$ However, the $p_j''$ are unknown.
2. Use Eq. (4) or its natural spline version to solve for the $p_j''$.
3. Repeat for the next $x_j$.

We see that what in order to use cubic one needs to solve the system of linear equations given by Eq. (4) in the worksheet. This type of system is called a *tridiagonal linear system*.

We now develop a numerically efficient way of solving these kinds of system.

## Tridiagonal systems

$$\begin{pmatrix} b_1 & c_1 & & & & \\ a_2 & b_2 & c_2 & & & \\ & a_3 & b_3 & c_3 & & \\ & & & \ddots & & \\ & & & a_{N-1} & b_{N-1} & c_{N-1} \\ & & & & a_N & b_N \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \\ x_3 \\ \vdots \\ x_{N-1} \\ x_N \end{pmatrix} = \begin{pmatrix} r_1 \\ r_2 \\ r_3 \\ \vdots \\ r_{N-1} \\ r_N \end{pmatrix} \tag{5}$$

To solve, we use *Gaussian elimination*. For example, multiplying first row by $a_2 / b_1$ and subtracting from second row gives a new equation. We can substitute this equation in for the second row and get

$$\begin{array}{llll} b_1 x_1 & +c_1 x_2 & = r_1 & \text{original first row} \\ & \left(b_2 - \frac{a_2}{b_1} c_1\right) x_2 + c_2 x_3 & = r_2 - \frac{a_2}{b_1} r_1 & \text{modified second row} \end{array}$$

The process continues *N – 1* times after which the system has the form

$$
\begin{array}{lllllll}
\beta_1 x_1 & +c_1 x_2 & & & & = & \rho_1 \\
& \beta_2 x_2 & +c_2 x_3 & & & = & \rho_2 \\
& & \beta_3 x_3 & +c_3 x_4 & & = & \rho_3 \\
& & & \ddots & & & \vdots \\
& & & & \beta_{N-1} x_{N-1} \quad +c_{N-1} x_N & = & \rho_{N-1} \\
& & & & \beta_N x_N & = & \rho_N
\end{array} \tag{6}
$$

**where**

$$\beta_1 = b_1, \quad \beta_j = b_j - \frac{a_j}{\beta_{j-1}} c_{j-1} \quad j = 2, \ldots, N \tag{7}$$

**and**

$$\rho_1 = r_1, \quad \rho_j = r_j - \frac{a_j}{\beta_{j-1}} \rho_{j-1} \quad j = 2, \ldots, N. \tag{8}$$

We can write the general form for the solution of $x_j$ as,

$$x_{N-j} = \frac{(\rho_{N-j} - c_{N-j} x_{N-j+1})}{\beta_{N-j}}, \quad j = 1, \ldots, N. \tag{9}$$

That's it! You now have everything you need to interpolate using *cubic splines*. You use Eqs (6) -(9) to find the second derivatives, which are then substituted into Eq. (2) to find the values of the spline.

Do question (9) on the worksheet

Learning goals:

- Be able explain what *cubic spline interpolation* is and what is necessary to implement the algorithm
- Recognize what a *tridiagonal system* is and be able to solve these systems efficiently