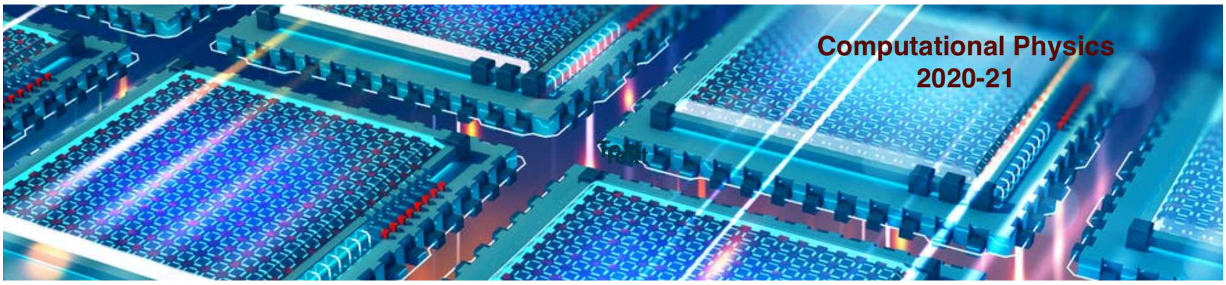
Computational Physics

numerical methods with C++ (and UNIX)

2020-21



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Numerical methods

- ✔ System of linear equations
  - Gauss elimination
  - LU decomposition
  - Gauss-Seidel method
- ✔ Interpolation
  - Lagrange interpolation
  - Newton method
  - Neville method
  - Cubic spline
- ✔ Numerical derivatives
  - First derivative $\mathcal{O}(h^2)$, $\mathcal{O}(h^4)$
  - Second derivative $\mathcal{O}(h^2)$, $\mathcal{O}(h^4)$
  - Derivative by interpolation
- ✔ Numerical integration
  - Newton-Cotes: trapezoidal and Simpson rules
  - Gaussian quadrature
- ✔ Monte-Carlo methods

Computational Physics

Data interpolation and

Data fitting

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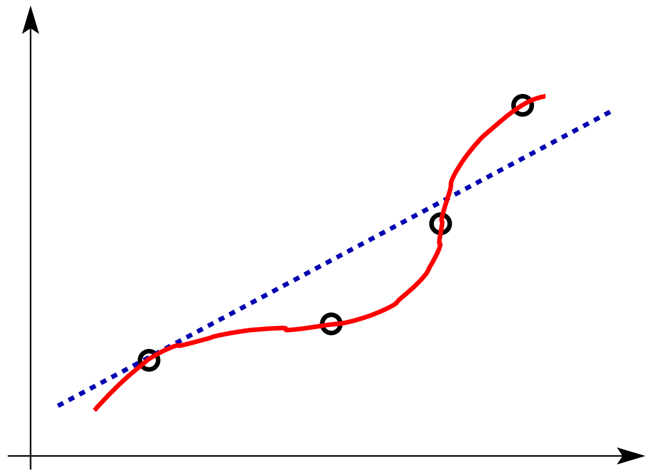
Data interpolation

- Having a set of discrete data points (x_i, y_i), **data interpolation** is the way of getting a continuous description passing through the data points



Lagrange interpolation

- Lagrange interpolation relies on the fact that in a finite interval a function $\mathbf{f}(\mathbf{x})$ can allways be represented by a polynomial $\mathbf{P}(\mathbf{x})$
- **Linear interpolation:** polynomial of **degree one** passing through data points $(\mathbf{x_1}, \mathbf{y_1})$ and $(\mathbf{x_2}, \mathbf{y_2})$

$$\boxed{P(x) = P_0 + P_1 x}$$

System to be solved:

$$\begin{cases} y_1 = & P_0 + P_1 x_1 \\ y_2 = & P_0 + P_1 x_2 \end{cases} \Rightarrow \begin{pmatrix} 1 & x_1 \\ 1 & x_2 \end{pmatrix} \begin{pmatrix} P_0 \\ P_1 \end{pmatrix} = \begin{pmatrix} y_1 \\ y_2 \end{pmatrix}$$

$$\boxed{\begin{cases} P_1 = \frac{y_2 - y_1}{x_2 - x_1} \\ P_0 = y_2 - P_1 x_1 \end{cases} \qquad P(x) = P_0 + P_1 x = y_1 \frac{x - x_2}{x_1 - x_2} + y_2 \frac{x - x_1}{x_2 - x_1}}$$

Lagrange interpolation (cont.)

✔ **second-degree polynomial interpolation:** polynomial of **degree two** passing through data points $(\mathbf{x_1}, \mathbf{y_1})$, $(\mathbf{x_2}, \mathbf{y_2})$ and $(\mathbf{x_3}, \mathbf{y_3})$

$$\boxed{P(x) = P_0 + P_1 x + P_2 x^2}$$

System to be solved:

$$\begin{cases} y_1 = & P_0 + P_1 x_1 + P_2 x_1^2 \\ y_2 = & P_0 + P_1 x_2 + P_2 x_2^2 \\ y_3 = & P_0 + P_1 x_3 + P_2 x_3^2 \end{cases} \Rightarrow \begin{pmatrix} 1 & x_1 & x_1^2 \\ 1 & x_2 & x_2^2 \\ 1 & x_3 & x_3^2 \end{pmatrix} \begin{pmatrix} P_0 \\ P_1 \\ P_2 \end{pmatrix} = \begin{pmatrix} y_1 \\ y_2 \\ y_3 \end{pmatrix}$$

$$P(x) = y_1 \frac{(x-x_2)(x-x_3)}{(x_1-x_2)(x_1-x_3)} + y_2 \frac{(x-x_1)(x-x_3)}{(x_2-x_1)(x_2-x_3)} + y_3 \frac{(x-x_1)(x-x_2)}{(x_3-x_1)(x_3-x_2)}$$

Lagrange interpolation (cont.)

✔ **n polynomial interpolation:** polynomial of **degree n** passing through $(\mathbf{n+1})$ data points $(\mathbf{x_0}, \mathbf{y_0})$, $(\mathbf{x_1}, \mathbf{y_1})$, $\cdots$, $(\mathbf{x_n}, \mathbf{y_n})$

$$\boxed{P(x) = P_0 + P_1 x + P_2 x^2 + \cdots + P_n x^n}$$

$$\begin{aligned} P_n(x) &= \textstyle\sum_{i=0}^{n} y_i \; \ell_i(x) \\ &= y_0 \; \ell_0(x) + y_1 \; \ell_1(x) + \\ &\quad \cdots + y_n \; \ell_n(x) \end{aligned}$$

$$\ell_i(x) = \prod_{\substack{j=0 \\ j \neq i}}^{n} \frac{x - x_j}{x_i - x_j} \qquad (i = 0, 1, 2, \cdots, n)$$

algorithm

```
// n = polynomial degree

// n+1 = nb of data points

// x,y = abcissa and values

   double x[n+1], y[n+1];

// loop on data points (0...n)

   for (int i=0; i<n+1; i++) {

// we need a second loop for
// the product

      for (...) {

      }

   }
}
```

Interpolation: C++ class scheme

```
----------------------
|  class DataPoints  |
----------------------    class DataPoints {
   / \      / \             public:
    |        |                   ...
    |        |                   virtual double Interpolate(double x);
    |        |                   virtual void Draw();
    |        |                   virtual void Print();
    |        |              protected:
    |        |                   int N; //nb data points
    |        |                   double *x, *y; //x and y values
    |        |            };
    |        |
    |        |
    |        |
    |        |
    |    ----------------------------
    |    |  class LagrangeInterpol  |
    |    ----------------------------   class LagrangeInterpol : public DataPoints {
    |                                     public:
    .                                          ...
    .                                          double Interpolate(double x);
    .                                          void Draw();
 (other interpolation                          void Print();
  classes)                                private:
                                               ? //specific data to class
                                        };
```


Newton method

- ✔ The Newton method provides a better computational procedure to get an interpolating polynomial of degree n passing through $(n+1)$ data points

$$x_i = x_0, x_1, \cdots, x_n$$

$$y_i = y_0, y_1, \cdots, y_n$$

$$a_i = a_0, a_1, \cdots, a_n$$

$$\boxed{P(x) = a_0 + a_1(x - x_0) + a_2(x - x_0)(x - x_1) + \cdots + a_n(x - x_0)(x - x_1)\cdots(x - x_{n-1})}$$

- ✔ This polynomial can be written in an efficient computational way:

$$\boxed{P(x) = a_0 + (x - x_0)\ [a_1 + (x - x_1)\ [a_2 + (x - x_2)\,[\cdots[a_{n-1} + (x - x_{n-1})a_n]\ldots]}$$

- ✔ The coefficients are determined by imposing the polynomial to pass through the data points:

$$(x_0, y_0):\quad y_0 = a_0$$

$$(x_1, y_1):\quad y_1 = a_0 + a_1\ (x_1 - x_0)$$

$$(x_2, y_2):\quad y_2 = a_0 + a_1\ (x_2 - x_0) + a_2\ (x_2 - x_0)(x_2 - x_1)$$

$$(x_3, y_3):\quad y_3 = a_0 + a_1\ (x_3 - x_0) + a_2\ (x_3 - x_0)(x_3 - x_1) + a_3\ (x_3 - x_0)(x_3 - x_1)(x_3 - x_2)$$

$$\vdots$$

$$(x_n, y_n):\quad y_n = a_0 + a_1\ (x_n - x_0) + \cdots + a_n\ (x_n + x_0)(x_n - x_1)\cdots(x_n - x_{n-1})$$

$$a_0 = y_0$$

$$a_1 = \frac{y_1 - y_0}{x_1 - x_0}$$

$$y_2 - y_0 = a_1(x_2 - x_0) + a_2(x_2 - x_0)(x_2 - x_1)$$

$$\frac{y_2 - y_0}{x_2 - x_0} = a_1 + a_2(x_2 - x_1)$$

$$a_2 = \frac{1}{x_2 - x_1}\left[\underbrace{\frac{y_2 - y_0}{x_2 - x_0}}_{\Delta y_2} - \underbrace{\frac{y_1 - y_0}{x_1 - x_0}}_{\Delta y_1}\right]$$

Newton method

✔ **Coefficients:**

$$
\begin{aligned}
a_0 &= y_0 \\
a_1 &= \frac{y_1-y_0}{x_1-x_0} \equiv \nabla y_1 \\
a_2 &= \frac{1}{x_2-x_1}\left(\frac{y_2-y_0}{x_2-x_0} - \frac{y_1-y_0}{x_1-x_0}\right) \\
&= \frac{\nabla y_2 - \nabla y_1}{x_2-x_1} \equiv \nabla^2 y_2 \\
a_3 &= \nabla^3 y_3 \\
a_4 &= \nabla^4 y_4 \\
\vdots &= \vdots \\
a_n &= \nabla^n y_n
\end{aligned}
$$

	0th	1st	2nd	3rd	4th
x_0	y_0				
x_1	y_1	∇y_1			
x_2	y_2	∇y_2	$\nabla^2 y_2$		
x_3	y_3	∇y_3	$\nabla^2 y_3$	$\nabla^3 y_3$	
x_4	y_4	∇y_4	$\nabla^2 y_4$	$\nabla^3 y_4$	$\nabla^4 y_4$

The diagonal terms of the table are the coefficients of the polynomial

Divided diferences:
n degree polynomial
n+1 data points

$$
\begin{aligned}
\nabla y_i &= \frac{y_i-y_0}{x_i-x_0} && (i=1,2,..,n) \\
\nabla^2 y_i &= \frac{\nabla y_i-\nabla y_1}{x_i-x_1} && (i=2,3,..,n) \\
\nabla^3 y_i &= \frac{\nabla^2 y_i-\nabla^2 y_2}{x_i-x_2} && (i=3,4,..,n) \\
&\vdots
\end{aligned}
$$

k iteration

$$
\begin{aligned}
\nabla^k y_i &= \frac{\nabla^{(k-1)} y_i-\nabla^{(k-1)} y_{k-1}}{x_i-x_{k-1}} && (i=k+1,...,n) \\
&\vdots \\
\nabla^n y_n &= \frac{\nabla^{n-1} y_n-\nabla^{n-1} y_{n-1}}{x_n-x_{n-1}}
\end{aligned}
$$

k index: 0, 1, 2, ..., n

0 iteration is just a copy of Y values

Newton method: interpolating polynomial

✔ Suppose four data points $\Rightarrow$ $n = 3$ polynomial degree

$(x_0, y_0)\ (x_1, y_1)\ (x_2, y_2)\ (x_3, y_3)$

✔ The polynomial

$$
\begin{aligned}
P_3(x) &= a_0 + (x-x_0)\,a_1 + (x-x_0)(x-x_1)\,a_2 + (x-x_0)(x-x_1)(x-x_2)\,a_3 \\
&= a_0 + (x-x_0)\,[a_1 + (x-x_1)\,[a_2 + (x-x_2)\,a_3]]
\end{aligned}
$$

Recurrence relations to evaluate polynomial:

$P_0(x) = a_3$
$P_1(x) = a_2 + (x-x_2)P_0(x)$
$P_2(x) = a_1 + (x-x_1)P_1(x)$
$P_3(x) = a_0 + (x-x_0)P_2(x)$

Computing the interpolated value at x with the polynomial computed in a recursive way:

$$\boxed{P_k(x) = a_{n-k} + (x-x_{n-k})P_{k-1}(x) \quad (k=1,2,...,n)}$$

Newton method: algorithm

Coefficients:

```
// degree n polynomial
// n+1 data points
//
// For computing the coefficients
// we can use a one-dimensional
// array a[n+1]
//
// X[n+1] array, contains x data values

 1) make array a[n+1];

 2) copy contents of Y[] data to array a[]

 3) compute divided differences and
    store them in the one dimensional
    array a[]

    loop on k=1; k<n+1; k++

       loop on i=k; i<n+1; i++

          a[i] = (a[i] - a[k-1]) /
                 (X[i] - X[k-1])
```

Polynomial:

```
// degree n polynomial
// n+1 data points
//
// For computing the polynomial at a point x
// we use the recurrence existing
// after factorizing the polynomial
//
// We assume having already the
// coefficients
// computed in the array a[n+1]
//
// X[n+1] array, contains x data values
//

 1) init the last polynomial P

    P = a[n];

 2) loop on k=1; k<n+1; k++

       P = a[n-k] + (x - X[n-k])*P
```


Neville method

✔ The Neville algorithm is still better by computing standards for finding the n degree polynomial because does not require a computation in two steps

✔ It uses linear interpolations between successive iterations: one point needed at $0th$ order, two points at $1st$ order, three points at $2nd$ order, ..., $n+1$ points at nth order

0th order: $P_0[x_0] = y_0, \cdots P_n[x_n] = y_n$

1st order (linear): $P_1[x_0, x_1] = C_0 + C_1 x = \frac{y_1(x-x_0)-y_0(x-x_1)}{x_1-x_0} = \frac{(x-x_0)\,P[x_1]-(x-x_1)\,P[x_0]}{x_1-x_0}$

2nd order: $P_2[x_0, x_1, x_2] = \frac{(x-x_2)\,P[x_0,x_1]-(x-x_0)\,P[x_1,x_2]}{x_0-x_2}$

3rd order: $P_3[x_0, x_1, x_2, x_3] = \frac{(x-x_3)\,P[x_0,x_1,x_2]-(x-x_0)\,P[x_1,x_2,x_3]}{x_0-x_3}$

$\ldots$ $\ldots$

x	0th order	1st order	2nd order	3rd order	k$order$
x_0	$P_0(x_0) = y_0$				
x_1	$P_0(x_1) = y_1$	$P_1[x_0, x_1]$			
x_2	$P_0(x_2) = y_2$	$P_1[x_1, x_2]$	$P_2[x_0, x_1, x_2]$		
x_3	$P_0(x_3) = y_3$	$P_1[x_2, x_3]$	$P_2[x_1, x_2, x_3]$	$P_3[x_0, x_1, x_2, x_3]$	
x_4	$P_0(x_4) = y_4$	$P_1[x_3, x_4]$	$P_2[x_2, x_3, x_4]$	$P_3[x_1, x_2, x_3, x_4]$	
$\ldots$	$\ldots$	$\ldots$	$\ldots$		
x_n	$P_0(x_n) = y_n$	$P_1[x_{n-1}, x_n]$	$P_2[x_{n-2}, x_{n-1}, x_n]$	$P_3[x_{n_3}, x_{n-2}, x_{n-1}, x_n]$	

Neville method: algorithm?

```
1) We can work with only one array (1-dim) y[]
   init y with  0th order polynomials (y0, y1, ..., yn)

2) loop on the order of the polynomials:
   k=1, k<n+1

3) loop on every column to compute the different polynomial
   i=k, i<n+1

   y[] array will be rewritten with new values

4) the interpolant calculated at the coordinate x,
   corresponds  to the last value
```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17-2