

Fitting: Interpolation

"data fitting" in some sense
interpolate table of data
later: "best" fit to data

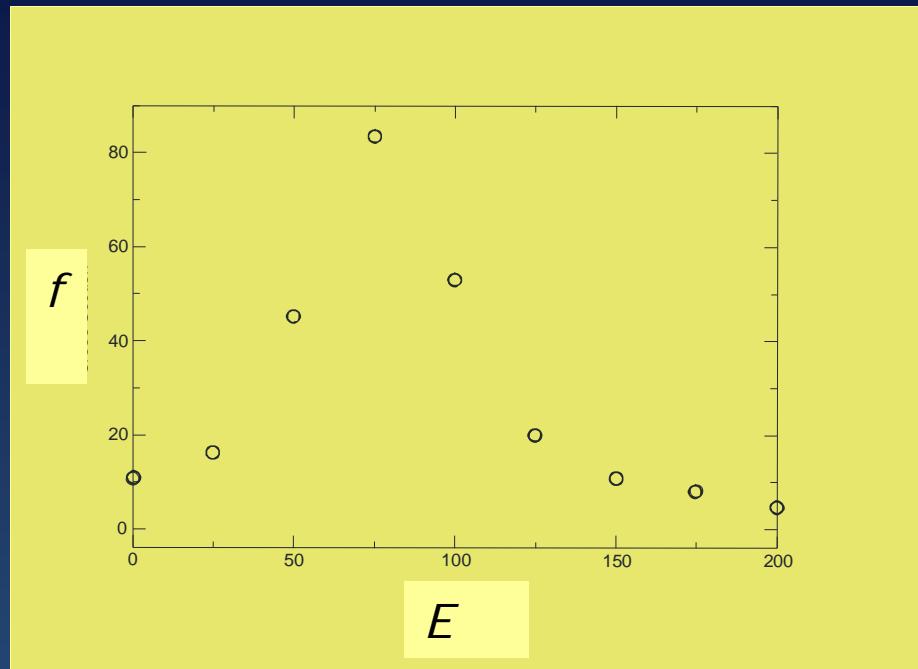
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Computational Physics for Undergraduates
BS Degree Program: Oregon State University

"Engaging People in Cyber Infrastructure"
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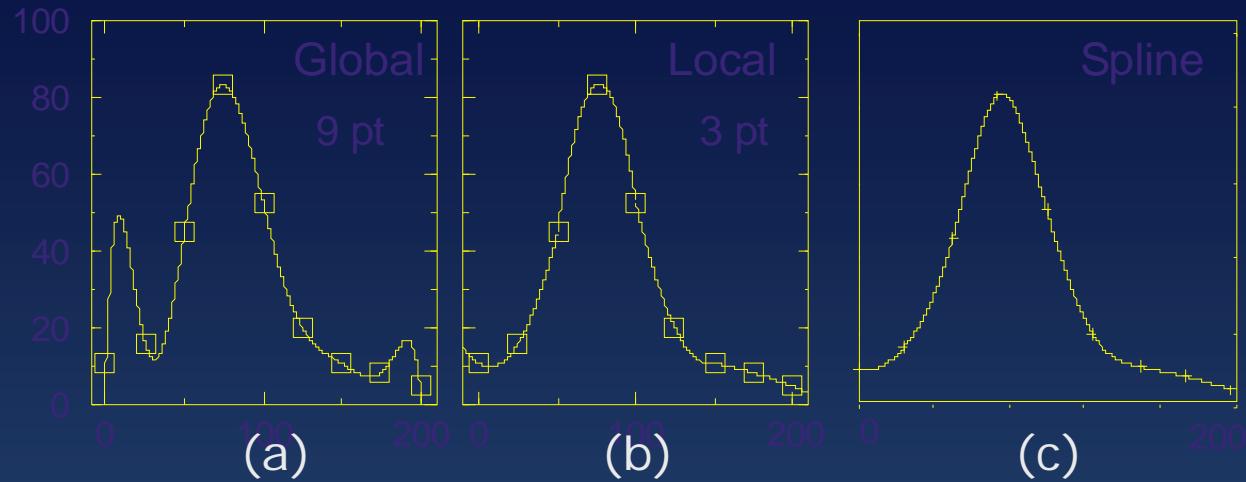
Problem: Interpolate Data

E	$f(E)$
0	10.6
25	16.0
50	45.0
75	83.5
100	52.8
125	19.9
150	10.8
175	8.25
200	4.7



- Tables = hard
- Look at data
- Determine $f(E)$ for E 's between entries
- Make table of numbers into a function
- Determine full width at half maximum

Method 1: Fit polynomial to Small Region



$$f(x) \simeq a_0 + a_1 x + a_2 x^2 + \cdots + a_{n-1} x^{n-1}, \quad (x \simeq x_i) \quad (1)$$

- Local: different poly each interval
- Low O polynomial (small n), but many: (b) (c)
- Full region: global fit higher poly (large n)
 - probably bad representation (a)
 - even if perfect fit!
- Do not extrapolate

n Point Lagrange Interpolation = $n-1^{\text{th}}$ O Poly

$$f(x) \simeq f_1 \lambda_1(x) + f_2 \lambda_2(x) + \cdots + f_n \lambda_n(x) \quad (1)$$

i	f_i
1	-12
2	-12
3	-24
4	-60

$$\lambda_i(x) = \prod_{j(\neq i)=1}^n \frac{x - x_j}{x_i - x_j} = \frac{x - x_1}{x_i - x_1} \frac{x - x_2}{x_i - x_2} \cdots \frac{x - x_n}{x_i - x_n} \quad (2)$$

- E.g. 4-points, 3rd degree polynomial to table:

$$f(x) = (-12) \frac{(x-1)(x-2)(x-4)}{(0-1)(0-2)(0-4)} + (-12) \frac{x(x-2)(x-4)}{(1-0)(1-2)(1-4)} \quad (3)$$

$$+ (-24) \frac{x(x-1)(x-4)}{(2-0)(2-1)(2-4)} + (-60) \frac{x(x-1)(x-2)}{(4-0)(4-1)(4-2)}$$

$$\Rightarrow f(x) = x^3 - 9x^2 + 8x - 12 \quad (4)$$

$$\bullet \text{ Check: } f(4) = 4^3 - 94^2 + 32 - 12 = -60 \quad (5)$$

Method 2: Cubic Splines

$$f(x) \simeq f_i(x) = f_i + f_i^{(1)}(x - x_i) + \frac{1}{2}f_i^{(2)}(x - x_i)^2 + \frac{1}{6}f_i^{(3)}(x - x_i)^3$$

- 3rd degree polynomial in each interval: most eye-pleasing
- Continuous 1st, 2nd derivatives
- Spline: flexible drafting tool
- Guaranteed: integrable, differentiable ($F = -dV/dx$)
- Complex procedure: easy for computers
- Popular for graphics



Try out Applet

[Spline.html](#)

Cubic Splines Implementation

$$f(x) \simeq f_i(x) = f_i + f_i^{(1)}(x - x_i) + \frac{1}{2}f_i^{(2)}(x - x_i)^2 + \frac{1}{6}f_i^{(3)}(x - x_i)^3 \quad (1)$$

1. Match f_i adjoining intervals Eq(2)
2. Match $f^{(1)}, f^{(2)}$ adjoining intervals Eq(3)
3. Match $f^{(3)}$ (forward difference) Eq(4)
4. Boundary Conditions: input $f^{(1)}$
 - natural spline: $f^{(2)}(a) = f^{(2)}(b) = 0$

$$f_i(x_{i+1}) = f_{i+1}(x_{i+1}), \quad i = 1, N - 1 \quad (2)$$

$$f_{i-1}^{(1)}(x_i) = f_i^{(1)}(x_i), \quad f_{i-1}^{(2)}(x_i) = f_i^{(2)}(x_i) \quad (3)$$

$$f_i^{(3)} \simeq \frac{f_{i+1}^{(2)} - f_i^{(2)}}{x_{i+1} - x_i} \quad (4)$$

Implementation: SplineAppl.java

```
public class SplineAppl {  
    public static void main( {  
        double x[] = { 0., 1.2, 2.5, 3.7, 5., 6.2, 7.5, 8.7, 9.9 };           // input  
        double y[] = { 0., 0.93, .6, -0.53, -0.96, -0.08, 0.94, 0.66, -0.46 };  
        yp1 = (y[1] - y[0]) / (x[1] - x[0]) - (y[2] - y[1]) / (x[2] - x[1])  
            + (y[2] - y[0]) / (x[2]-x[0]);  
        ypn = (y[n-1] - y[n-2]) / (x[n-1]-x[n-2]) - (y[n-2]-y[n-3])  
            / (x[n-2] - x[n-3]) + (y[n-1] - y[n-3]) / (x[n-1] - x[n-3]);  
        y2[0] = u[0] = 0.;                                              // Natural  
        for ( i=1; i <= n-2; i++ ) { ... }                            // Decomposition loop  
        qn = un = 0.;                                              // Natural  
        y2[n-1] = (un-qn*u[n-2]) / (qn*y2[n-2] + 1.);  
        for ( k = n-2; k>= 0; k--) y2[k] = y2[k] * y2[k + 1] + u[k];  
        for ( i=1; i <= Nfit; i++ ) { } // initialization  
        xout = x[0] + ( x[n-1] - x[0] ) * (i - 1) / (Nfit);  
        ...  
        yout = ( a*y[klo] + b*y[khi] + ( (a*a*a-a)*y2[klo]  
            + ( b*b*b - b ) * y2[khi] ) * (h*h)/6. );  
    } } }
```

Go try these out!