















# What is a good approximation? What can we consider as a good approximation to the original data if we do not know the original function? Data points may be interpolated by an infinite

number of functions







#### Some ideas for selecting g(x)

 Most interpolation methods are grounded on 'smoothness' of interpolated functions. However, it does not work all the time



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 Practical approach, i.e. what physics lies beneath the data

### Linear combination is the most common form of g(x)

linear combination of elementary functions, or trigonometric, or exponential functions, or rational functions, ...

 $g(x) = a_1 h_1(x) + a_2 h_2(x) + a_3 h_3(x) + \dots$ 

Three of most common approximating functions

- Polynomials
- Trigonometric functions
- Exponential functions

## Approximating functions should have following properties

- It should be easy to determine
- It should be easy to evaluate
- It should be easy to differentiate
- It should be easy to integrate

#### Linear Interpolation: Idea

The idea of linear interpolation is to approximate data at a point x by a straight line passing through two data points  $x_j$  and  $x_{j+1}$  closest to x.

$$g(x) = a_0 + a_1 x$$
 (4.1)

where  $a_0$  and  $a_1$  are coefficients of the linear functions. The coefficients can be found from a system of equations

$$g(x_j) = f_j = a_0 + a_1 x_j$$
(4.2)  

$$g(x_{j+1}) = f_{j+1} = a_0 + a_1 x_{j+1}$$
(4.3)

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# Linear Interpolation: coefficients Solving this system for $a_0$ and $a_1$ one have that the function g(x) takes the form $g(x) = f_j + \frac{x - x_j}{x_{j+1} - x_j} (f_{j+1} - f_j) \qquad (4.4)$ or $[x_j, x_{j+1}]$ interval. $g(x) = f_j \frac{x - x_{j+1}}{x_j - x_{j+1}} + f_{j+1} \frac{x - x_j}{x_{j+1} - x_j} \qquad (4.5)$





#### Linear interpolation: conclusions

- The linear interpolation may work well for very smooth functions when the second and higher derivatives are small.
- It is worthwhile to note that for the each data interval one has a different set of coefficients a<sub>0</sub> and a<sub>1</sub>.
- This is the principal difference from data fitting where the same function, with the same coefficients, is used to fit the data points on the whole interval [x<sub>1</sub>,x<sub>n</sub>].
- We may improve quality of linear interpolation by increasing number of data points x<sub>i</sub> on the interval.
- HOWEVER!!! It is much better to use higher-odrder interpolations. 20

#### Linear vs. Quadratic interpolations

example from F.S.Acton "Numerical methods that work"

"A table of sin(x) covering the first quadrant, for example, requires 541 pages if it is to be linearly interpolable to eight decimal places. If quadratic interpolation is used, the same table takes only one page having entries at one-degree intervals."

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#### **Polynomial Interpolation**

Polynomial interpolation is a very popular method due, in part, to simplicity

$$g(x) = a_0 + a_1 x + a_2 x^2 + \dots + a_n x^n.$$
(4.6)

The condition that the polynomial g(x) passes through sample points  $f_j(x_j)$ 

$$f_j(x_j) = g(x_j) = a_0 + a_1 x_j + a_2 x_j^2 + \dots + a_n x_j^n. \quad (4.7)$$

The number of data points minus one defines the order of interpolation. Thus, linear (or two-point interpolation) is the first order interpolation

#### Properties of polynomials

#### Weierstrass theorem:

If f(x) is a continuous function in the closed interval  $a \le x \le b$  then for every  $\varepsilon > 0$  there exists a polynomial  $P_n(x)$ , where the value on *n* depends on the value of  $\varepsilon$ , such that for all *x* in the closed interval  $a \le x \le b$ 

$$\left|P_n(x) - f(x)\right| < \varepsilon$$

System of equations for the second order  $f_{j} = a_{0} + a_{1}x_{j} + a_{2}x_{j}^{2}$   $f_{j+1} = a_{0} + a_{1}x_{j+1} + a_{2}x_{j+1}^{2}$   $f_{j+2} = a_{0} + a_{1}x_{j+2} + a_{2}x_{j+2}^{2}$   $\therefore$ We need three points for the second order interpolation  $\therefore$  Freedom to choose points?  $\therefore$  This system can be solved analytically











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#### Important!

- Moving from the first -order to the third and 5th order improves interpolated values to the original function.
- However, the 7th order interpolation instead being closer to the function f(x) produces wild oscillations.
- This situation is not uncommon for high-order polynomial interpolation.
- Rule of thumb: do not use high order interpolation.
   Fifth order may be considered as a practical limit.
- If you believe that the accuracy of the 5th order interpolation is not sufficient for you, then you should rather consider some other method of interpolation.

#### Cubic Spline

- The idea of spline interpolation is reminiscent of very old mechanical devices used by draftsmen to get a smooth shape.
- ➡ It is like securing a strip of elastic material (metal or plastic ruler) between knots (or nails).
- ⇒ The final shape is quite smooth.
- Cubic spline interpolation is used in most plotting software. (cubic spline gives most smooth result)

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#### Spline vs. Polynomials

- One of the principal drawbacks of the polynomial interpolation is related to discontinuity of derivatives at data points x<sub>j</sub>.
- The procedure for deriving coefficients of spline interpolations uses information from all data points, i.e. nonlocal information to guarantee global smoothness in the interpolated function up to some order of derivatives.

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#### Equations

the interpolated function on  $[x_{j},x_{j+1}]$  interval is presented in a cubic spline form

$$g(x) = f_j + b_j(x - x_j) + c_j(x - x_j)^2 + d_j(x - x_j)^3$$

What is different from polynomial interpolation? ... the way we are looking for the coefficients! Polynomial interpolation: 3 coefficient for 4 data points Spline interpolation: 3 coefficients for the each interval

#### Coefficients for spline interpolation

- For the each interval we need to have a set of three parameters b<sub>j</sub>, c<sub>j</sub> and d<sub>j</sub>.
   Since there are (n-1) intervals, one has to have 3n-3 equations for deriving the coefficients for j=1,n-1.
- The fact that  $g_j(x_j)=f_j(x_j)$  imposes (n-1) equations.





#### Cubic spline boundary conditions

Possibilities to fix two more conditions

- Natural spline the second order derivatives are zero on boundaries.
- Input values for the first order  $f^{(1)}(\boldsymbol{x})$  derivates at boundaries
- Input values for the second order  $f^{(2)}(\boldsymbol{x})$  derivates at boundaries

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a little math ...  $s_i(x) = a_i + b_i(x - x_i) + \frac{c_i}{2}(x - x_i)^2 + \frac{d_i}{6}(x - x_i)^3$ (1)  $x_{i-1} \leq x \leq x_i \qquad i = 1, 2, \dots N.$ Need to find  $a_i, b_i, c_i, d_i$ .  $s_i'(x) = b_i + c_i(x - x_i) + \frac{d_i}{2}(x - x_i)^2$  $s_i^{\prime\prime}(x) = c_i + d_i(x - x_i)$  $s_i^{\prime\prime\prime}(x) = d_i$ by the definition (interpolation)  $a_i = f(x_i)$ 1) s(x) must be continuous at  $x_i$ ,  $s_i(x_i) = s_{i+1}(x_i)$  $a_i = a_{i+1} + b_{i+1}(x_i - x_{i+1}) + \frac{c_{i+1}}{2}(x_i - x_{i+1})^2 + \frac{d_{i+1}}{6}(x_i - x_{i+1})^3$ 38

using  $h_i = x_i - x_{i-1}$   $h_i b_i - \frac{h_i^2}{2} c_i + \frac{h_i^3}{6} d_i = f_i - f_{i-1}$  (2) 2)  $s_i'(x_i) = s_{i+1}'(x_i)$  i = 1, 2, ..., N - 1  $c_i h_i - \frac{d_i}{2} h_i^2 = b_i - b_{i-1}$  i = 2, 3, ..., N (3) 3)  $s_i''(x_i) = s_{i+1}''(x_i)$   $d_i h_i = c_i - c_{i-1}$  i = 2, 3, ..., N (4) additional equations (conditions at the ends) s''(a) = s''(b) = 0 $s_1''(x_0) = 0$ ,  $s_N''(x_N) = 0$   $c_1 - d_1 h_1 = 0$ ,  $c_N = 0$ 

The system of equations	s to find coefficients						
$h_i d_i = c_i - c_{i-1}$	$i = 1, 2, \dots N$ $c_0 = c_N = 0$	(5)					
$h_i c_i - \frac{h_i^2}{2} d_i = b_i - b_{i-1}$	i = 2, 3, N	(6)					
$h_i b_i - \frac{h_i^2}{2} c_i + \frac{h_i^3}{6} d_i = f_i - f_{i-1}$	$i = 1, 2, \dots N$	(7)					
Solve the system for $c_i$ $i = 1, 2,, N - 1$							
Consider two equations (7) for points $i$ and $i-1$							
$b_i = \frac{h_i}{2}c_i + \frac{h_i^2}{6}d_i = \frac{f_i - f_{i-1}}{h_i}$							
$b_{i-1} = \frac{h_{i-1}}{2}c_{i-1} + \frac{h_{i-1}^2}{6}d_{i-1} = \frac{f_{i-1}}{6}$	$\frac{1-f_{i-2}}{h_{i-1}}$						
and sustract the second equation from the first							
$b_i - b_{i-1} = \frac{1}{2}(h_i c_i - h_{i-1} c_{i-1}) - \frac{1}{2}(h_i c_i - h_{i-1} c_{i$	$\frac{1}{6}(h_i^2d_i - h_{i-1}^2d_{i-1}) + \frac{f_i - f_{i-1}}{h_i} - \frac{1}{h_i}$	$\frac{f_{i-1} - f_{i-2}}{h_{i-1}}$					

Use the difference 
$$b_i - b_{i-1}$$
 in the right side of (6)  
 $h_i c_i + h_{i-1} c_{i-1} - \frac{h_{i-1}^2}{2} d_{i-1} - \frac{2h_i^2}{3} d_i = 2 \left( \frac{f_i - f_{i-1}}{h_i} - \frac{f_{i-1} - f_{i-2}}{h_{i-1}} \right)$  (8)  
Then from (5)  
 $h_i^2 d_i = h_i (c_i - c_{i-1}),$   
 $h_{i-1}^2 d_{i-1} = h_{i-1} (c_{i-1} - c_{i-2})$   
Substitute in (8)  
 $h_{i-1} c_{i-2} + 2(h_{i-1} + h_i) c_{i-1} + h_i c_i = 6 \left( \frac{f_{i+1} - f_i}{h_{i+1}} - \frac{f_i - f_{i-1}}{h_i} \right)$  (9)  
for  $i = 1, 2, \dots N - 1,$   $c_0 = c_N = 0$   
This is a tridiagonal system of equations (use Thomas method)  
then  $d_i = \frac{c_i - c_{i-1}}{h_i},$   $b_i = \frac{h_i}{2} c_i - \frac{h_i^2}{6} d_i + \frac{f_i - f_{i-1}}{h_i}$  for  $i = 1, 2, \dots N$ ,





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# **Divided Differences** the first divided difference at point i $f[x_i, x_{i+1}] = \frac{f_{i+1} - f_i}{x_{i+1} - x_i}$ the second divided difference

$$f[x_i, x_{i+1}, x_{i+2}] = \frac{f[x_{i+1}, x_{i+2}] - f[x_i, x_{i+1}]}{x_{i+2} - x_i}$$

in general

$$f[x_i, x_{i+1}, \dots, x_n] = \frac{f[x_{i+1}, x_{i+2}, \dots, x_n] - f[x_i, x_{i+1}, \dots, x_{n+i-1}]}{x_n - x_i}$$
other notations

 $f_i^{(0)} = f_i, \quad f_i^{(1)} = f[x_i, x_{i+1}], \quad f_i^{(2)} = f[x_i, x_{i+1}, x_{i+2}] \quad {}^{47}$ 

#### **Divided Difference Polynomials**

Let's define a polynomials  $P_n(x)$  where the coefficients are divided differences

$$P_n(x) = f_i^{(0)} + (x - x_i)f_i^{(1)} + (x - x_i)(x - x_{i+1})f_i^{(2)} + \dots + (x - x_i)(x - x_{i+1})\dots(x - x_{i+n-1})f_i^{(n)}$$

It is easy to show that  $P_n(x)$  passes exactly through the data points

$$P_n(x_i) = f_i, \quad P_n(x_{i+1}) = f_{i+1}...$$

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#### Comments

Polynomials satisfy a uniqueness theorem – a polynomial of degree n passing exactly through n+1 points is unique.

The data points in the divided difference polynomials do not have to be in any specific order. However, more accurate results are obtained for interpolation if the data are arranged in order of closeness to the interpolated point

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#### Divided Difference coefficients





Example: Fortran
double precision d(n,n), x(n), f(n)
integer i,j
d = 0.0
! initialization of d(n,1)
do i=1,n
d(i,1) = f(i)
end do
! calculations
do j=2,n
do i=1,n-j+1
d(i,j) = (d(i+1,j-1) - d(i,j-1)) / (x(i+1+j-2) - x(i))
end do
end do
! print results
do 1=1,n
write(*,200) (d(1,j),j=1,n-1+1)
ena ao
200 IOTMAT (SILU.6)

	Exc	am	ple	2:												
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	f:	f: 0.312500,0.303030,0.298507,0.294118,														
		0.265/14,0.2////8,0.2/59/5,0.2/02/0														
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	0.3125	00	-0.	.094	700	0.	0282	265	-0.	007	311	-0.	006	774	•••	
	0.3030	30	-0.	.090	460	0.	0268	302	-0.	009	343	0.	010	684	• • •	
	0.2985	07	-0.	. 087	780	0.	0249	934	-0.	006	138	-0.	001	741	• • •	
	0.2941	.18	-0.	.084	040	0.	0233	399	-0.	006	660	-0.	000	053		
	0.2857	14	-0.	079	360	Ο.	021	734	-0.	006	676					
	0.2777	78	-0.	076	100	Ο.	0203	399								
	0.2739	73	-0.	074	060											
	0.2702	70														
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Difference tables are useful for evaluating the quality of a set of tabular data smooth difference => "good" data not monotonic differences => possible errors in the original data, or the step in *x* is too large, or may be a singularity in f(x)









#### When using rational functions is a good idea?

Rational functions may well interpolate functions with poles

$$g(x) = \frac{a_0 + a_1 x + a_2 x^2 + \dots + a_n x^n}{b_0 + b_1 x + b_2 x^2 + \dots + b_m x^m}$$

that is with zeros of the denominator

$$b_0 + b_1 x + b_2 x^2 + \dots b_m x^m = 0$$

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#### The procedure has two principal steps

- On the first step we need to choose powers for the numerator and the denominator, i.e. n and m. You may need to attempt a few trials before coming to a conclusion.
- Once we know the number of parameters we need to find the coefficients

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#### Example for n=2 and m=1

$$g(x) = \frac{a_0 + a_1 x + a_2 x^2}{b_0 + b_1 x}$$

- We need five coefficients i.e. 5 data points
- We should fix one of the coefficients since only the ratio makes sense.
- If we choose, for example, b<sub>0</sub> as a fixed number c then we need 4 data points to solve a system of equations to find the coefficients









#### What is extrapolation?

- If you are interested in function values outside the range x<sub>1</sub>...x<sub>n</sub> then the problem is called extrapolation.
- Generally this procedure is much less accurate than interpolation.
- You know how it is difficult to extrapolate (foresee) the future, for example, for the stock market.

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#### What is data fitting?

- If data values f<sub>i</sub>(x<sub>i</sub>) are a result of experimental observation with some errors, then data fitting may be a better way to proceed.
- In data fitting we let g(x<sub>i</sub>) to differ from measured values f<sub>i</sub> at x<sub>i</sub> points having one function only to fit all data points; i.e. the function g(x) fits all the set of data.
- Data fitting may reproduce well the trend of the data, even correcting some experimental errors.

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