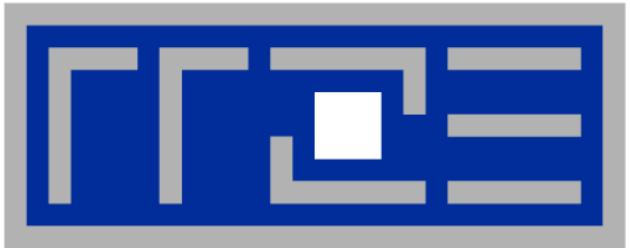


# Elementary Numerical Mathematics

Supporting material for

Interpolation and Polynomial Approximation

Lagrange Polynomial

Divided Differences

Hermite Interpolation

Cubic Splines

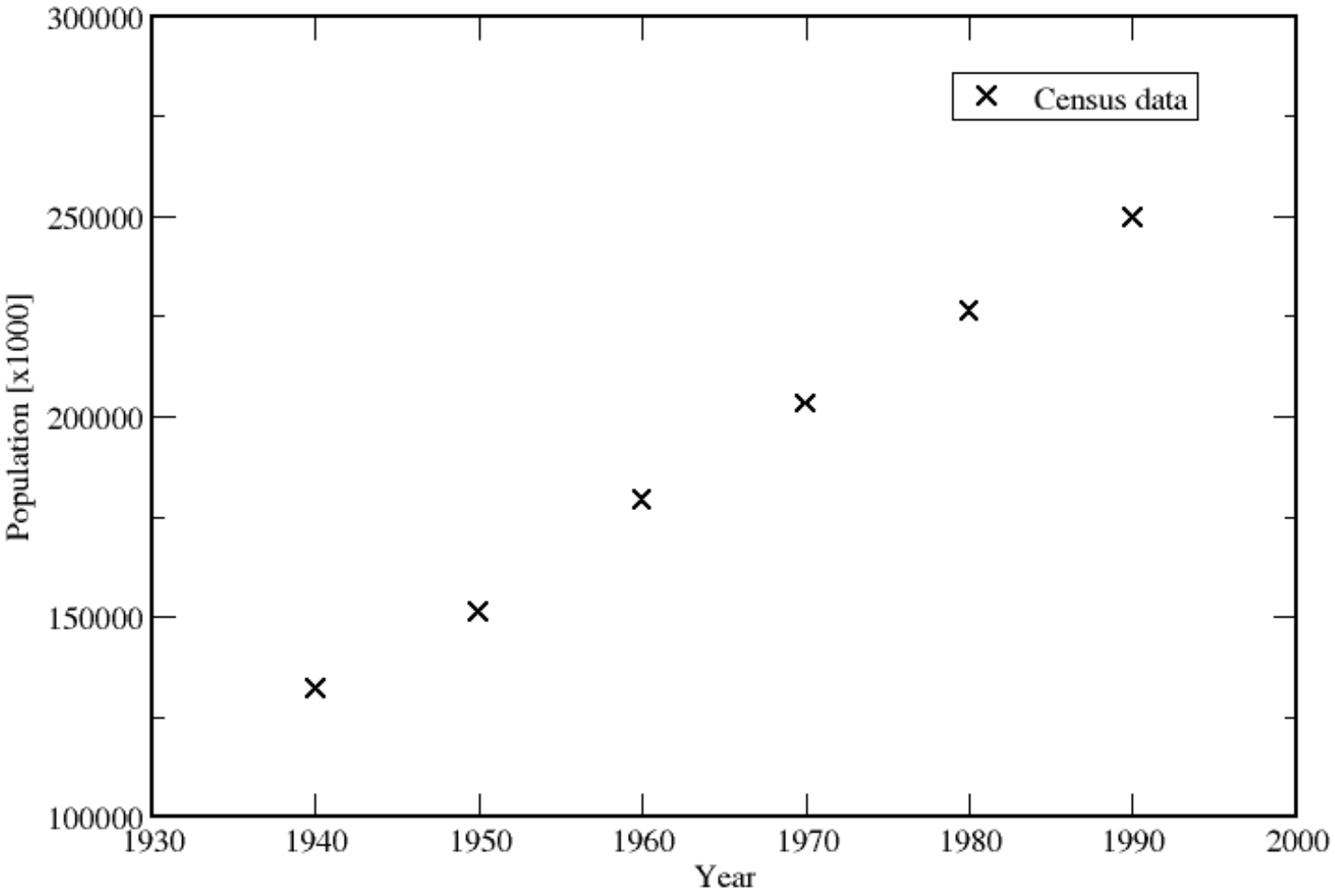
Winter Term 2019/20

Gerhard Wellein

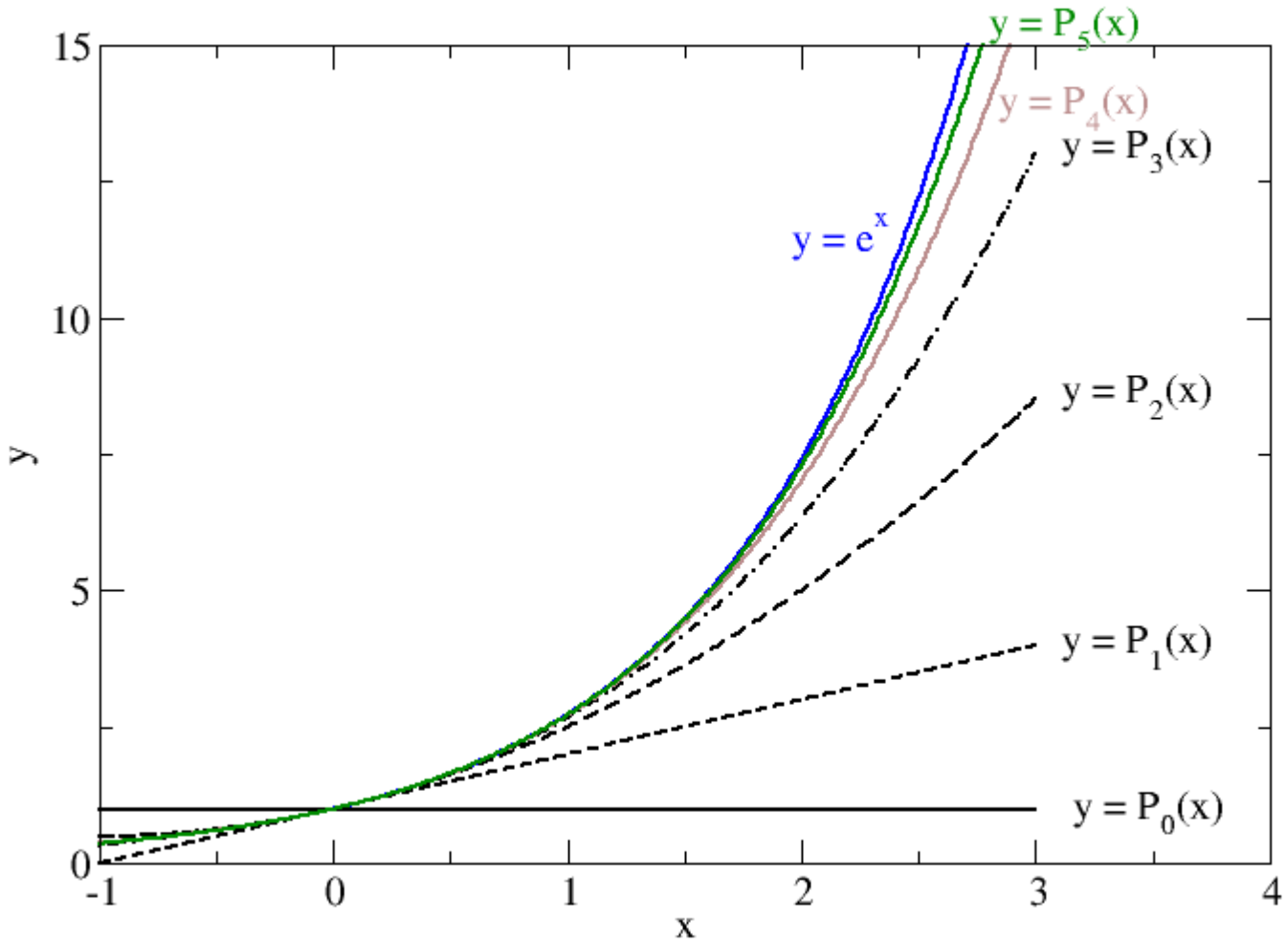
Department for Computer Science

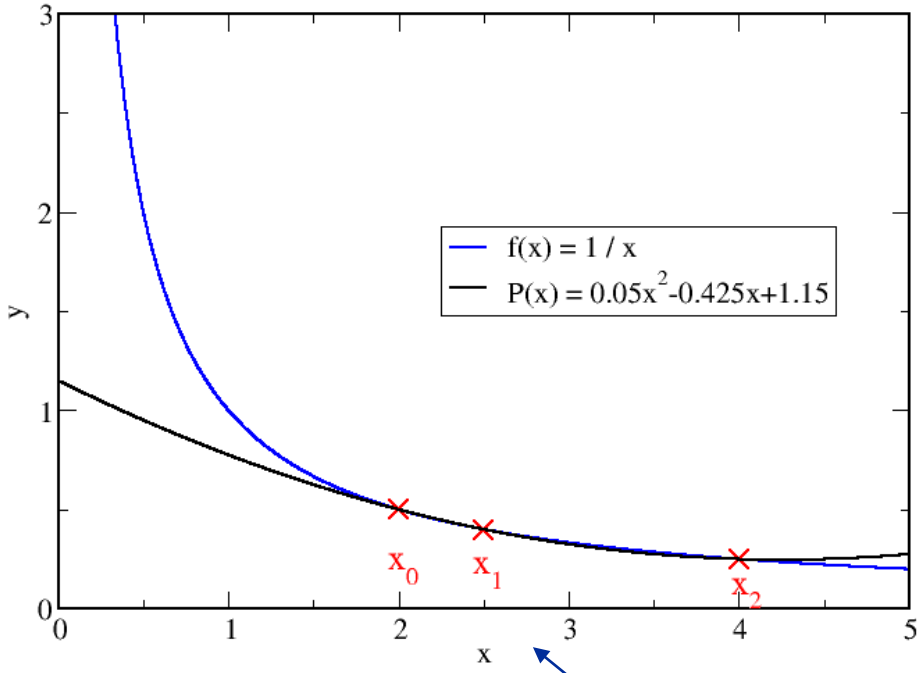
HPC Services, Regionales Rechenzentrum Erlangen (RRZE)

## Census data of US population are available on a 10 year basis



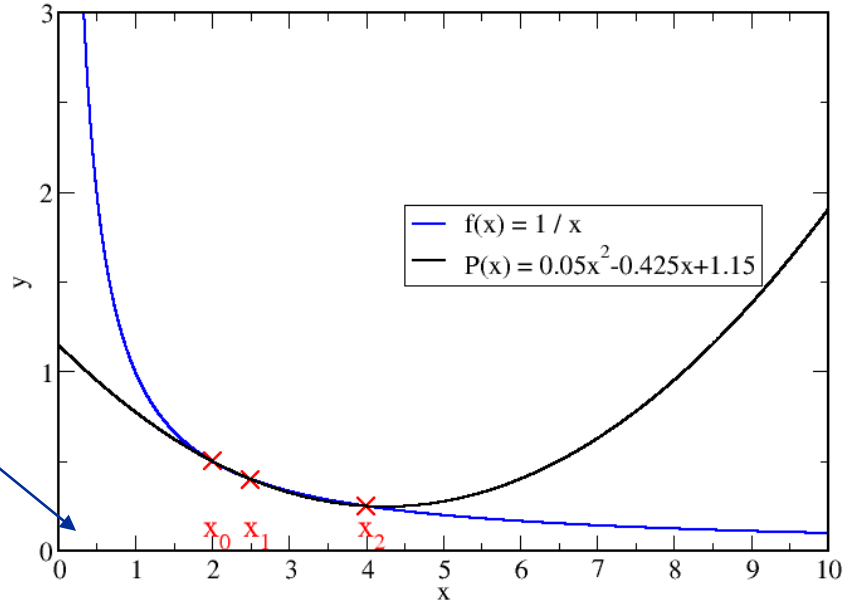
## Taylor polynomials $P_0(x),\ldots,P_5(x)$ for $f(x)=\exp(x)$ evaluated at $x_0=0$



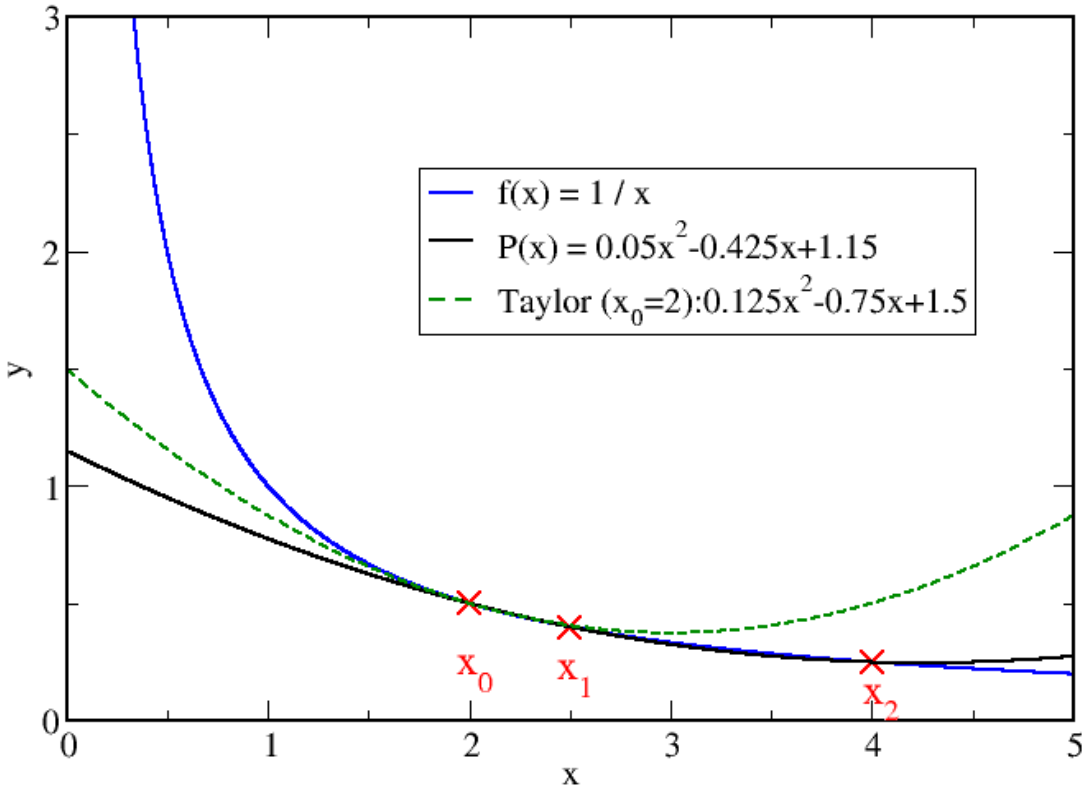



**Determine Lagrange interpolating polynomial of degree 2 polynomial (parabola) for `f(x) = 1/x` at $x_0, x_1, x_2$.**

**Different x-axis intervals!**



## Determine Lagrange interpolating polynomial of degree 2 polynomial (parabola) for $f(x) = 1/x$ at $x_0, x_1, x_2$ and Taylor at $x_0$



| i | $x_i$ | $f(x_i)$ |
|---|---|---|
| 0 | 1.0 | 0.7651977 |
| 1 | 1.3 | 0.6200860 |
| 2 | 1.6 | 0.4554022 |
| 3 | 1.9 | 0.2818186 |
| 4 | 2.2 | 0.1103623 |

| | | |
|---|---|---|
| $P_{1,2}$ | 0.5102968 | $1.5 * 10^{-3}$ |
| $P_{1,2,3}$ | 0.5112857 | $5.4 * 10^{-4}$ |
| $P_{0,1,2}$ | 0.5124715 | $6.4 * 10^{-4}$ |
| $P_{0,1,2,3}$ | 0.5118127 | $1.5 * 10^{-5}$ |
| $P_{1,2,3,4}$ | 0.5118302 | $2.5 * 10^{-6}$ |
| $P_{0,1,2,3,4}$ | 0.5118200 | $7.7 * 10^{-6}$ |

## Determine approximations to f(1.5)

- Use $x_1$, $x_2$ (linear, degree 1):
  $P_{1,2}$ =(1.5-1.6) / (1.3-1.6)*f(1.3) + (1.5-1.3) / (1.6-1.3) *f(1.6)
  $P_{1,2}$ = 0.5102968
- Use $x_1$, $x_2$ , $x_3$ (degree 2):
  $P_{1,2,3}$ = {(1.5-1.6)*(1.5-1.9)} / {(1.3-1.6)*(1.3-1.9)} * f(1.3) +
  {(1.5-1.3)*(1.5-1.9)} / {(1.6-1.3)*(1.6-1.9)} * f(1.6) +
  {(1.5-1.3)*(1.5-1.6)} / {(1.9-1.3)*(1.9-1.6)} * f(1.9)
  $P_{1,2,3}$ = 0.5112857
- Use $x_0$, $x_1$ , $x_2$ (degree 2):
  $P_{0,1,2}$ = 0.5124715
- Use $x_0$, $x_1$ , $x_2$ , $x_3$ (degree 3):
  $P_{0,1,2,3}$ = 0.5118127
- …

**Exact value: 0.5118277! (Bessel function of first kind of order zero)**

| | | $Q_{i,0}$ | $Q_{i,1}$ | $Q_{i,2}$ | $Q_{i,3}$ | $Q_{i,4}$ |
|---|---|---|---|---|---|---|
| i | $x_i$ | $f(x_i)$ | | | | |
| 0 | 1.0 | 0.7651977 | | | | |
| 1 | 1.3 | 0.6200860 | 0.5233449 | | | |
| 2 | 1.6 | 0.4554022 | 0.5102968 | 0.5124715 | | |
| 3 | 1.9 | 0.2818186 | 0.5132634 | 0.5112857 | 0.5118127 | |
| 4 | 2.2 | 0.1103623 | 0.5104270 | 0.5137361 | 0.5118302 | 0.5118200 |

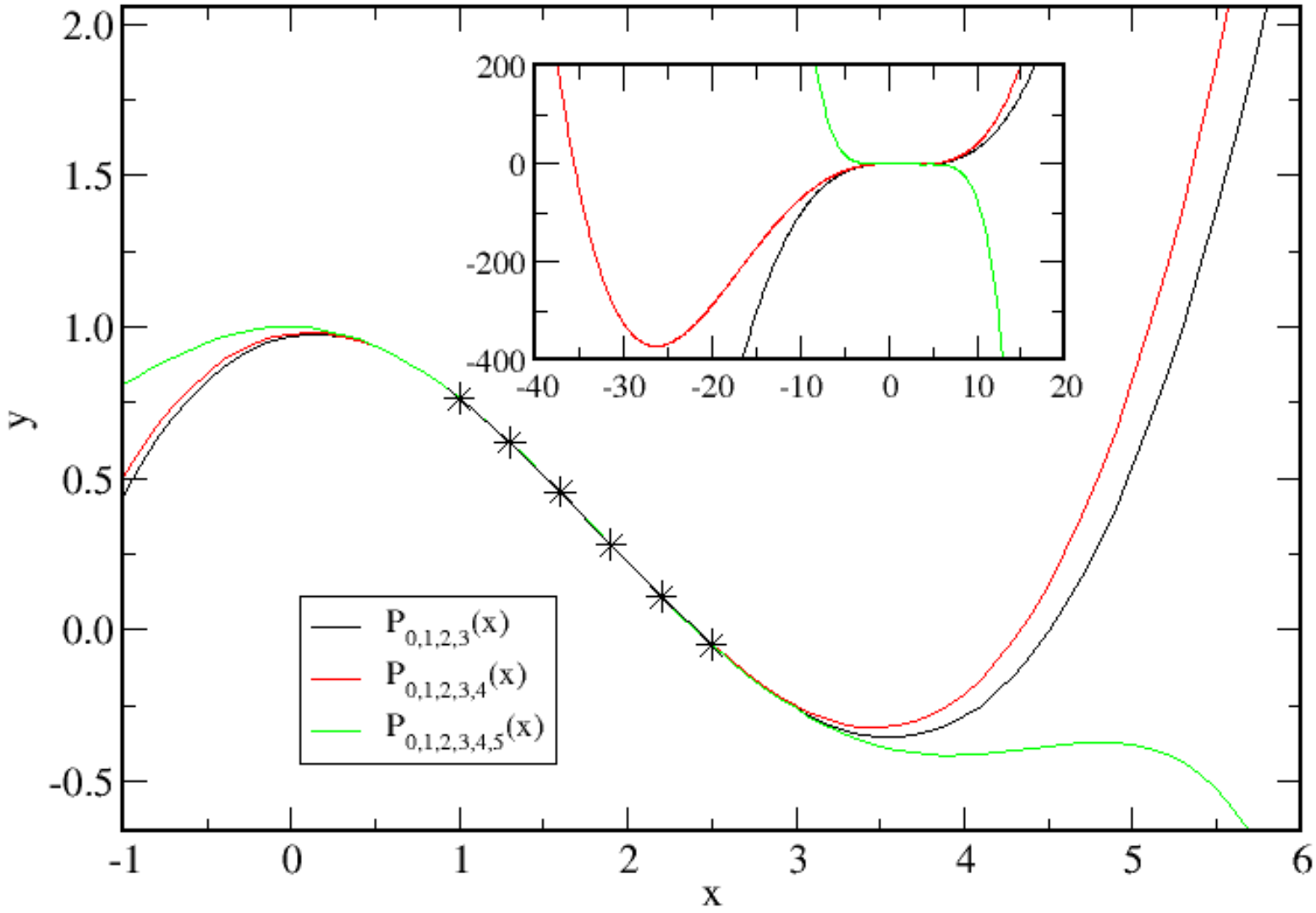
Potential stopping criterion for adding new nodes: $|Q_{i,i} - Q_{i-1,i-1}| < TOL$

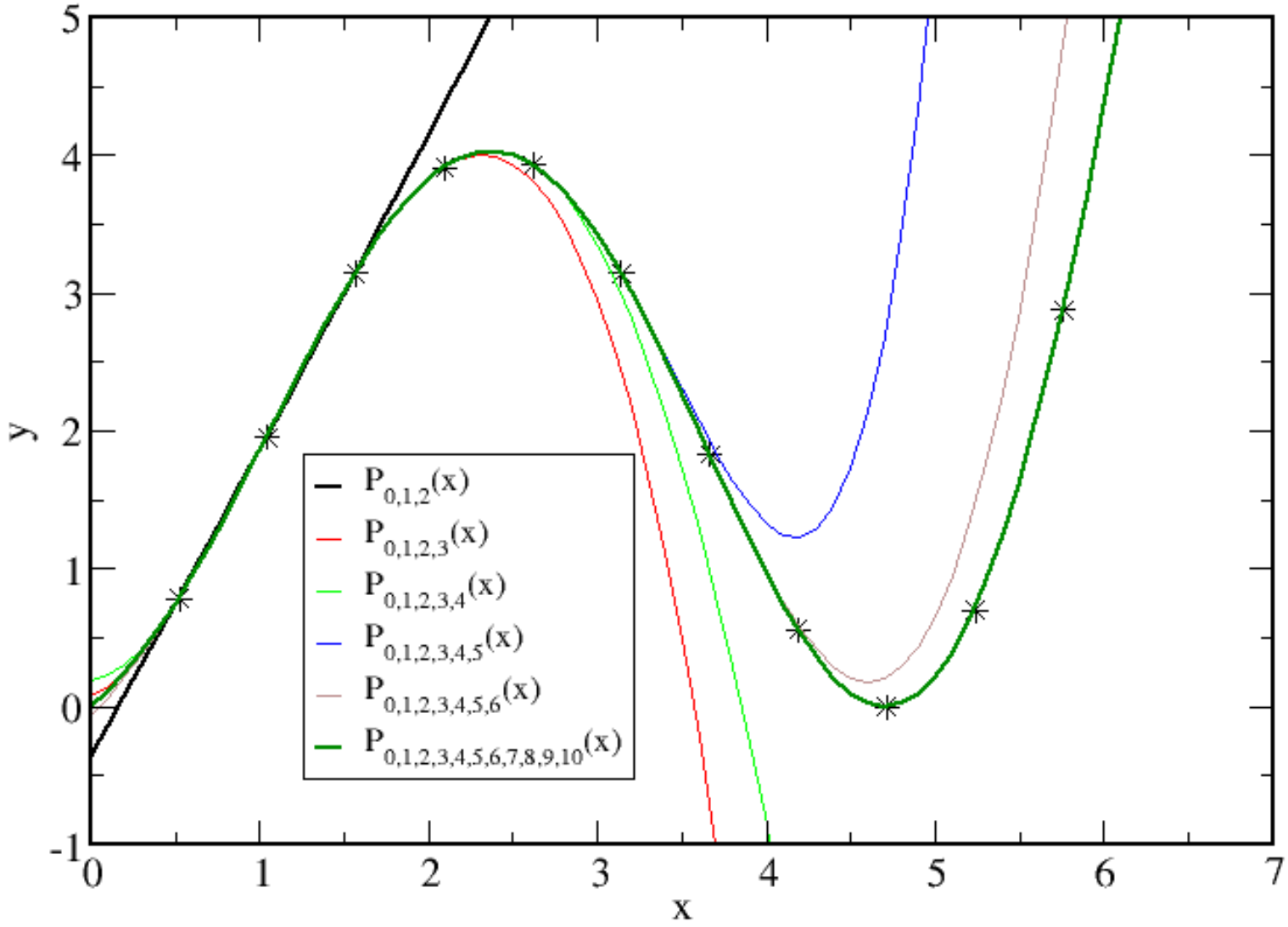
Adding the node $x_5$=2.5 results in the following new row:

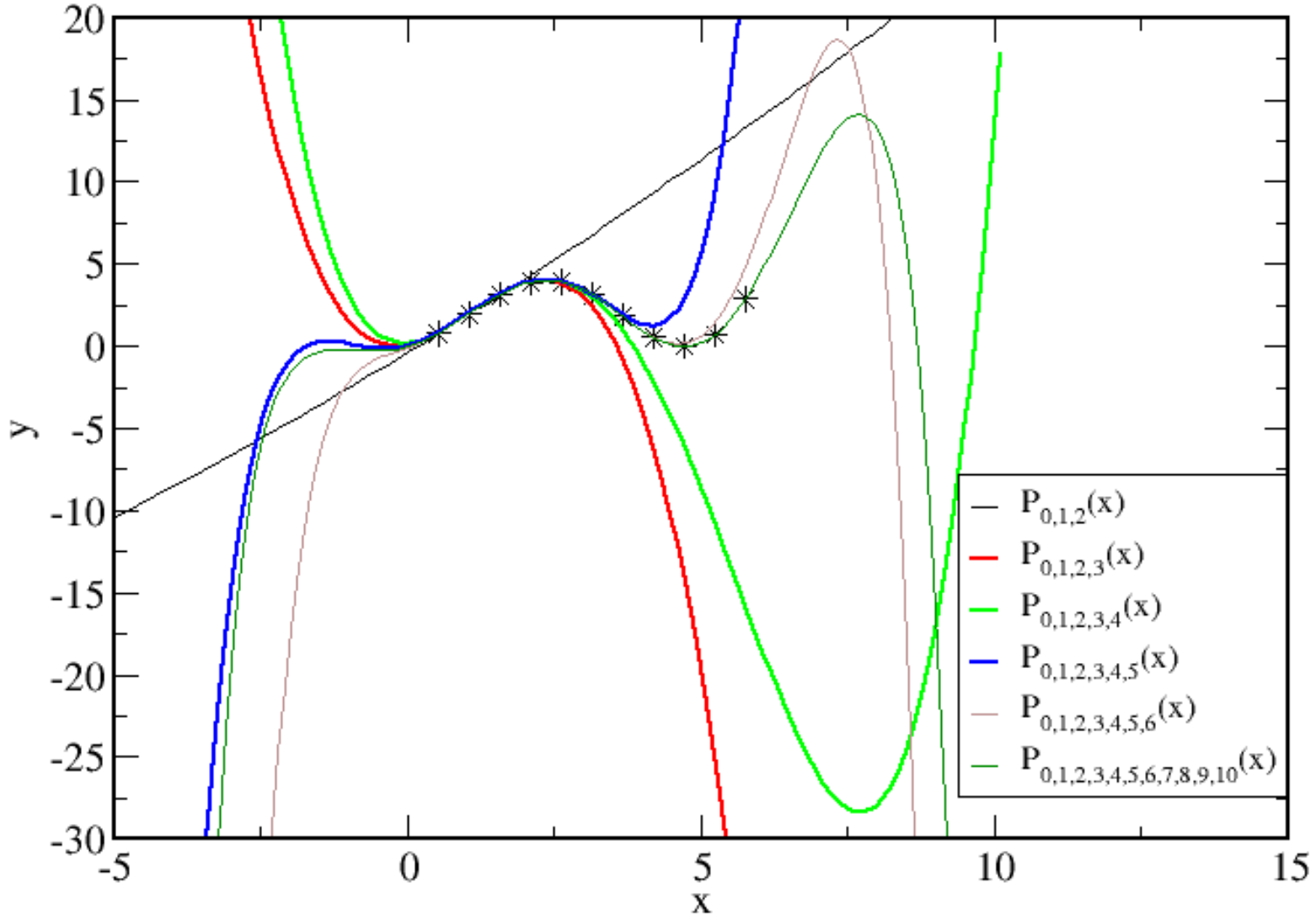
$Q_{5,0}$= -0.0483838
$Q_{5,1}$=0.4807699
$Q_{5,2}$=0.5301984
$Q_{5,3}$=0.5119070
$Q_{5,4}$=0.5118430
$Q_{5,5}$=0.5118277

**Exact value: 0.5118277!**

```
Input:      xv; x(0:n), f(0:n)     % x(i)=x_i; f(i)=f(x_i)
Output:     Q := matrix(0:n,0:n);  % P(xv) = Q(n,n);
                                   % polynomila of degree n

for i=0 to n do Q(i,0) = f(i);

for i=1 to n do

    for j=1 to i do

        Q(i,j) = ((xv-x(i-j))*Q(i,j-1)-(xv-x(i))*Q(i-1,j-1)) / (x(i) - x(i-j))

    end for

end for
```


2.0
1.5
1.0
0.5
0.0
-0.5
y
-1
0
1
2
3
4
5
6
x
200
0
-200
-400
-40
-30
-20
-10
0
10
20
$P_{0,1,2,3}(x)$
$P_{0,1,2,3,4}(x)$
$P_{0,1,2,3,4,5}(x)$


5
4
3
2
1
0
-1
y
0
1
2
3
4
5
6
7
x
$P_{0,1,2}(x)$
$P_{0,1,2,3}(x)$
$P_{0,1,2,3,4}(x)$
$P_{0,1,2,3,4,5}(x)$
$P_{0,1,2,3,4,5,6}(x)$
$P_{0,1,2,3,4,5,6,7,8,9,10}(x)$


20
15
10
5
0
-5
-10
-15
-20
-25
-30
y
-5
0
5
10
15
x
$P_{0,1,2}(x)$
$P_{0,1,2,3}(x)$
$P_{0,1,2,3,4}(x)$
$P_{0,1,2,3,4,5}(x)$
$P_{0,1,2,3,4,5,6}(x)$
$P_{0,1,2,3,4,5,6,7,8,9,10}(x)$

```
Input:      x(0:n), f(0:n)          % x(i)=x_i; f(i)=f(x_i)
Output:     F := matrix(0:n,0:n); % Use diagonal entries of
                                    to determine polynomial

for i=0 to n do F(i,0) = f(i);

for i=1 to n do

    for j=1 to i do

        F(i,j) = (F(i,j-1) - F(i-1,j-1)) / (x(i) - x(i-j))

    end for

end for
```

| | | $f[x_i]$ | $f[x_{i-1},x_i]$ | $f[x_{i-2},x_{i-1},x_i]$ | $f[x_{i-3},\ldots,x_i]$ | $f[x_{i-4},\ldots,x_i]$ |
|---|---|---|---|---|---|---|
| i | $x_i$ | $f(x_i)$ | | | | |
| 0 | 1.0 | **0.7651977** | | | | |
| | | | **-0.4837057** | | | |
| 1 | 1.3 | 0.6200860 | | **-0.1087399** | | |
| | | | -0.5489460 | | **0.0658784** | |
| 2 | 1.6 | 0.4554022 | | -0.0494433 | | **0.0018251** |
| | | | -0.5786120 | | 0.0680685 | |
| 3 | 1.9 | 0.2818186 | | 0.0118183 | | |
| | | | -0.5715210 | | | |
| 4 | 2.2 | 0.1103623 | | | | |

$f[x_0,x_1]$ = (0.6200860 - 0.7651977) / 0.3  $f[x_1,x_2,x_3]$ = (-0.5786120+ 0.5489460) / 0.6

$$P_4(x) = 0.7651977 - 0.4837057\,(x-1.0) - 0.1087399*(x-1.0)*(x-1.3) + 0.0658784*(x-1.0)*(x-1.3)*(x-1.6) + 0.0018251*(x-1.0)*(x-1.3)*(x-1.6)*(x-1.9) \rightarrow P_4(1.5)=0.5118200$$

- **Reorder nodes $x_n, x_{n-1}, \dots, x_0$ to compute $P_n(x)$**
- **In general:**

$$\begin{aligned} P_n(x) = \quad & f[x_n] + \\ & f[x_n, x_{n-1}]\,(x - x_n) + \\ & f[x_n, x_{n-1}, x_{n-2}]\,(x - x_n)(x - x_{n-1}) + \\ & \dots + \\ & f[x_n, x_{n-1}, \dots, x_0]\,(x - x_n)(x - x_{n-1})\ \dots\ (x - x_0) \end{aligned}$$

- **For equally spaced nodes and $x = x_n + sh = x_i + (s + n - i)h$ we have**

$$\begin{aligned} P_n(x) = \quad & f[x_n] + \\ & s\,h \qquad\qquad\qquad\quad f[x_n, x_{n-1}] + \\ & s\,(s+1)\,h^2 \qquad\quad f[x_n, x_{n-1}, x_{n-2}] + \\ & \dots + \\ & s(s+1)\dots(s+n-1)h^n\, f[x_n, x_{n-1}, \dots, x_0] \end{aligned}$$

$$= f[x_n] + \sum_{k=1}^{n} s(s+1)\dots(s+k-1)h^k\, f[x_n, x_{n-1}, \dots, x_{n-k}]$$

| | | $f[x_i]$ | $f[x_{i-1}, x_i]$ | $f[x_{i-2}, x_{i-1}, x_i]$ | $f[x_{i-3}, \ldots, x_i]$ | $f[x_{i-4}, \ldots, x_i]$ |
|---|---|---|---|---|---|---|
| i | $x_i$ | $f(x_i)$ | | | | |
| 0 | 1.0 | ***0.7651977*** | | | | |
| | | | ***-0.4837057*** | | | |
| 1 | 1.3 | 0.6200860 | | ***-0.1087399*** | | |
| | | | -0.5489460 | | ***0.0658784*** | |
| 2 | 1.6 | 0.4554022 | | -0.0494433 | | ***0.0018251*** |
| | | | -0.5786120 | | *0.0680685* | |
| 3 | 1.9 | 0.2818186 | | *0.0118183* | | |
| | | | *-0.5715210* | | | |
| 4 | 2.2 | *0.1103623* | | | | |

$P_4(2.0) = P_4(2.2 - (2/3)*0.3) =$

$= 0.1103623 - (2/3) * 0.3 * (-0.5715210) - (2/3)*(1/3) * 0.3^2 * 0.0118183 -$

$(2/3)*(1/3)*(4/3)* 0.3^3 * 0.0680685 - (2/3)*(1/3)*(4/3)*(7/3)* 0.3^4 * (0.0018251) = 0.2238754$

Determine P(x=2.0)

| | | | |
|---|---|---|---|
| | s= | 3,3333333 | -0,6666667 |

**$P_i(x)$**

| i | xi | Forward Difference | Backward Difference |
|---|---|---|---|
| 0 | 1.0 | 0,7651977 | 0,1103623 |
| 1 | 1.3 | 0,2814920 | 0,2246665 |
| 2 | 1.6 | 0,2053741 | 0,2244301 |
| 3 | 1.9 | 0,2238200 | 0,2238856 |
| 4 | 2.2 | 0,2238711 ⟷ | 0,2238754 |

**Finite precision arithmetic**

**Correct value: 0,2238908**

- **Choose $x_0$ close to $x$ in the middle of the $(n+1)$ nodes and relabel nodes: $\ldots, x_{-3}, x_{-2}, x_{-1}, x_0, x_1, x_2, x_3, \ldots$**
- **If $n = 2m+1$ odd then determine polynomial approximation as follows with $x = x_0 + sh$ (i.e. $x - x_i = (s-i)h$ ):**

$$
\begin{aligned}
P_n(x) = P_{2m+1}(x) = \quad & f[x_0] + \\
& {}^1/_2 \; s\,h\,(f[x_{-1}, x_0] + f[x_0, x_1]) + \\
& s^2 h^2 \quad f[x_{-1}, x_0, x_1] + \\
& \tfrac{s(s^2-1)}{2} h^3 (f[x_{-2}, x_{-1}, x_0, x_1] + f[x_{-1}, x_0, x_1, x_2]) + \\
& \ldots + \\
& s^2 (s^2-1)(s^2-4) \ldots (s^2-(m-1)^2) h^{2m} f[x_{-m}, \ldots, x_m] + \\
& {}^1/_2 \; s (s^2-1) \ldots (s^2-m^2) h^{2m+1} (f[x_{-m-1}, \ldots, x_m] + f[x_{-m}, \ldots, x_{m+1}])
\end{aligned}
$$

- **If $n = 2m$ even then the $h^{2m+1}$ term is omitted**

| | | $f[x_i]$ | $f[x_{i-1}, x_i]$ | $f[x_{i-2}, x_{i-1}, x_i]$ | $f[x_{i-3}, \ldots, x_i]$ | $f[x_{i-4}, \ldots, x_i]$ |
|---|---|---|---|---|---|---|
| i | $x_i$ | $f(x_i)$ | | | | |
| 0 | 1.0 | 0.7651977 | | | | |
| | | | -0.4837057 | | | |
| 1 | 1.3 | 0.6200860 | | -0.1087399 | | |
| | | | **-0.5489460** | | **0.0658784** | |
| 2 | 1.6 | **0.4554022** | | **-0.0494433** | | **0.0018251** |
| | | | **-0.5786120** | | **0.0680685** | |
| 3 | 1.9 | 0.2818186 | | 0.0118183 | | |
| | | | -0.5715210 | | | |
| 4 | 2.2 | 0.1103623 | | | | |

$P_4(1.5) = P4\ (1.6 - (1/3)*0.3) =$

$= 0.4554022 + (-1/3) * (0.3/2) * \{(-0.5489460)+(-0.5715210)\} + (-1/3)^2 * 0.3^2 * (-0.0494433) +$

$(1/2)*(-1/3)*\{(-1/3)^2-1\}* 0.3^3 * (0.0658784+0.0680685) + (-1/3)^2*\{(-1/3)^2-1\} * 0.3^4 * (0.0018251)$

$= 0.5118200$

# Interpolation and Polynomial Approximation

*Hermite polynomial via Divided differences*

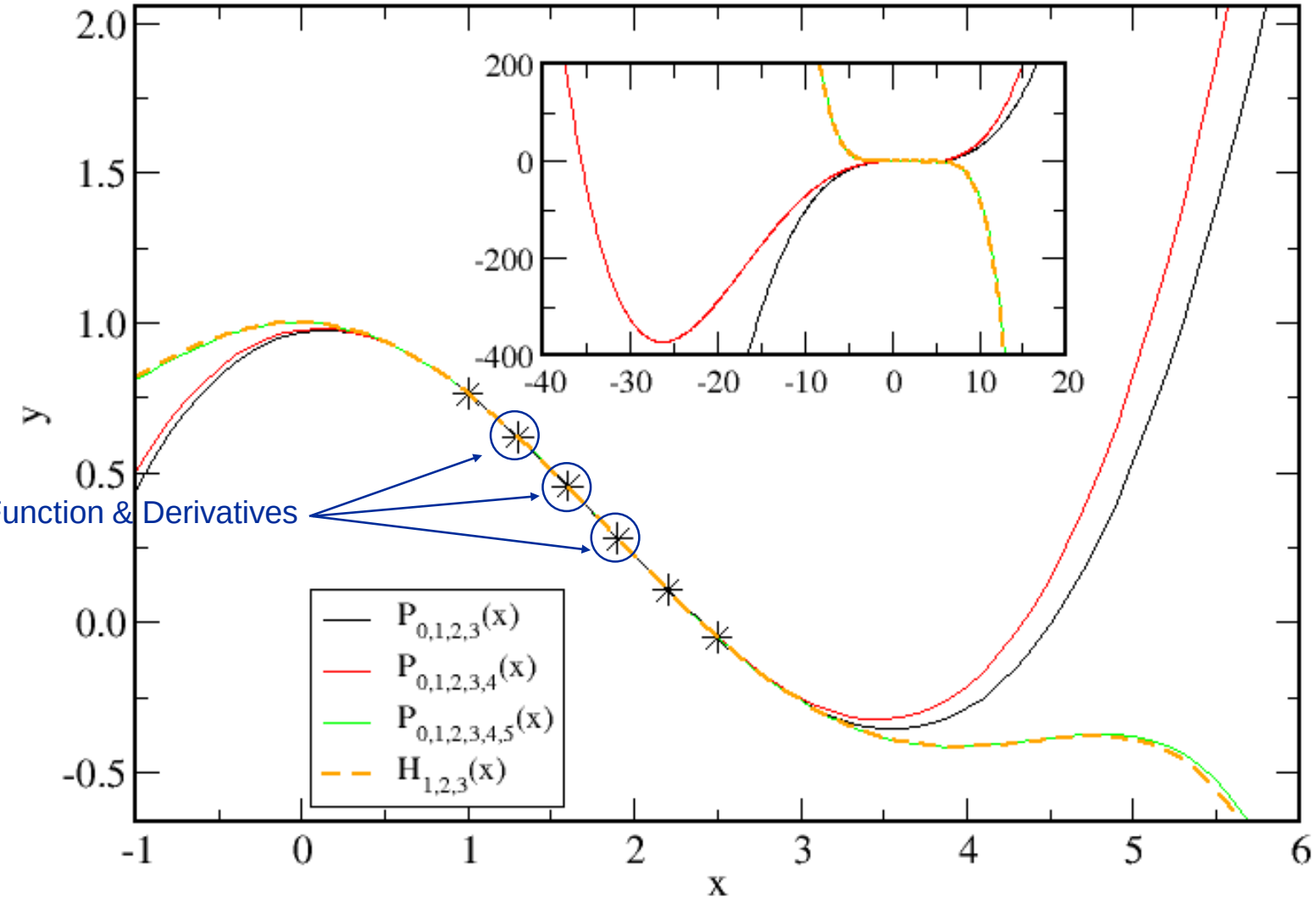
| i | $x_i$ | $f(x_i)$ | $f'(x_i)$ |
|---|---|---|---|
| 0 | 1.3 | **0.6200860** | **-0.5220232** |
| 1 | 1.6 | **0.4554022** | **-0.5698959** |
| 2 | 1.9 | **0.2818186** | **-0.5811571** |

| i | $z_i$ | $f[z_i]$ | $f[z_{i-1}, z_i]$ | $f[z_{i-2}, z_{i-1}, z_i]$ | $f[z_{i-3}, \ldots, z_i]$ | $f[z_{i-4}, \ldots, z_i]$ | $f[z_{i-5}, \ldots, z_i]$ |
|---|---|---|---|---|---|---|---|
| 0 | 1.3 | **0.6200860** | | | | | |
| | | | **-0.5220232** | | | | |
| 1 | 1.3 | **0.6200860** | | ***-0.0897427*** | | | |
| | | | **-0.5489460** | | ***0.0663657*** | | |
| 2 | 1.6 | **0.4554022** | | ***-0.0698330*** | | ***0.0026663*** | |
| | | | **-0.5698959** | | ***0.0679655*** | | ***-0.0027738*** |
| 3 | 1.6 | **0.4554022** | | ***-0.0290537*** | | ***0.0010020*** | |
| | | | **-0.5786120** | | ***0.0685667*** | | |
| 4 | 1.9 | **0.2818186** | | ***-0.00884837*** | | | |
| | | | **-0.5811571** | | | | |
| 5 | 1.9 | **0.2818186** | | | | | |

$H_5(1.5) = 0.5118277$

```
Input: x(0:n), f(0:n), fd(0:n)     % x(i)=x_i; f(i)=f(x_i)
                                   % fd(i): derivative of f at x_i
Output: Q := matrix(0:2n+1,0:2n+1) % Use diagonal entries of
                                   % to determine Hermite polynomial

for i=0 to n
    z(2*i)     = x(i); z(2*i+1)   = x(i)
    Q(2*i,0)   = f(i); Q(2*i+1,0) = f(i)

    Q(2*i+1,1) = fd(i)

    if(i>0) Q(2*i ,1) = ( Q(2*i,0) - Q(2*i-1,0) ) / ( z(2*i) - z(2*i-1) )
end for


for i=2 to 2*n+1 do

     for j= 2 to i do

          Q(i,j) = ( Q(i,j-1) - Q(i-1,j-1) ) / ( z(i) - z(i-j) )

     end for

end for
```

$H_{1,2,3}(x)$: Function & Derivatives



**Definiton (IV.10.): Given a function f defined on [a,b] and a set of nodes $a = x_0 < x_1 < \cdots < x_n = b$, a cubic spline interpolant S for f is a function that satisfies the following conditions:**

a. **S(x) is a cubic polynomial, denoted $S_j(x)$, on the subinterval $[x_j, x_{j+1}]$ for each j=0,1,…,n-1 ;**

b. $S_j(x_j) = f(x_j)$ **and** $S_j(x_{j+1}) = f(x_{j+1})$ **for each j=0,1,...n-1;**

c. $S_{j+1}(x_{j+1}) = S_j(x_{j+1})$ **for each j=0,1,...n-2;**

d. $S'_{j+1}(x_{j+1}) = S'_j(x_{j+1})$ **for each j=0,1,...n-2;**

e. $S''_{j+1}(x_{j+1}) = S''_j(x_{j+1})$ **for each j=0,1,...n-2;**

f. **One of the following sets of boundary condition is satisfied**
   1. $S''(x_0) = S''(x_n) = 0$ **(free or natural boundary conditions)**
   2. $S'(x_0) = f'(x_0)$ *and* $S'(x_n) = f'(x_n)$ **(clamped boundary)**

**Ansatz for cubic spline interpolant $S_j(x)$ for each j=0,1,...,n-1:**

$$S_j(x) = a_j + b_j(x - x_j) + c_j(x - x_j)^2 + d_j(x - x_j)^3$$

- Determine $\{a_j, b_j, c_j, d_j ; j = 0, \dots, n-1\}$ via conditions b. – e. of Def. (IV.10):

- $S_j(x_j) = f(x_j)$ (cond. b.) → $a_j = f(x_j)$
- Use: $x_{j+1} - x_j = h_j$

- From c.: $a_{j+1} = a_j + b_j\ h_j + c_j\ h_j^2 + d_j\ h_j^3$
- From d.: $b_{j+1} = b_j + 2\ c_j\ h_j + 3\ d_j\ h_j^2$
- From e.: $c_{j+1} = c_j + 3\ d_j\ h_j$

- These equations can be solved for $\{ b_j ; j = 0, \dots, n\}$ and $\{ d_j ; j = 0, \dots, n\}$

- Finally the values of $\{ c_j ; j = 0, \dots, n\}$ are determined by solving a LSE (see next slide)

# Cubic spline (natural boundary)

- The coefficients $\mathbf{c_j}$ can be obtained by solving the system **Ax=b** with: ( $\mathbf{a_j = f(x_j)}$ )

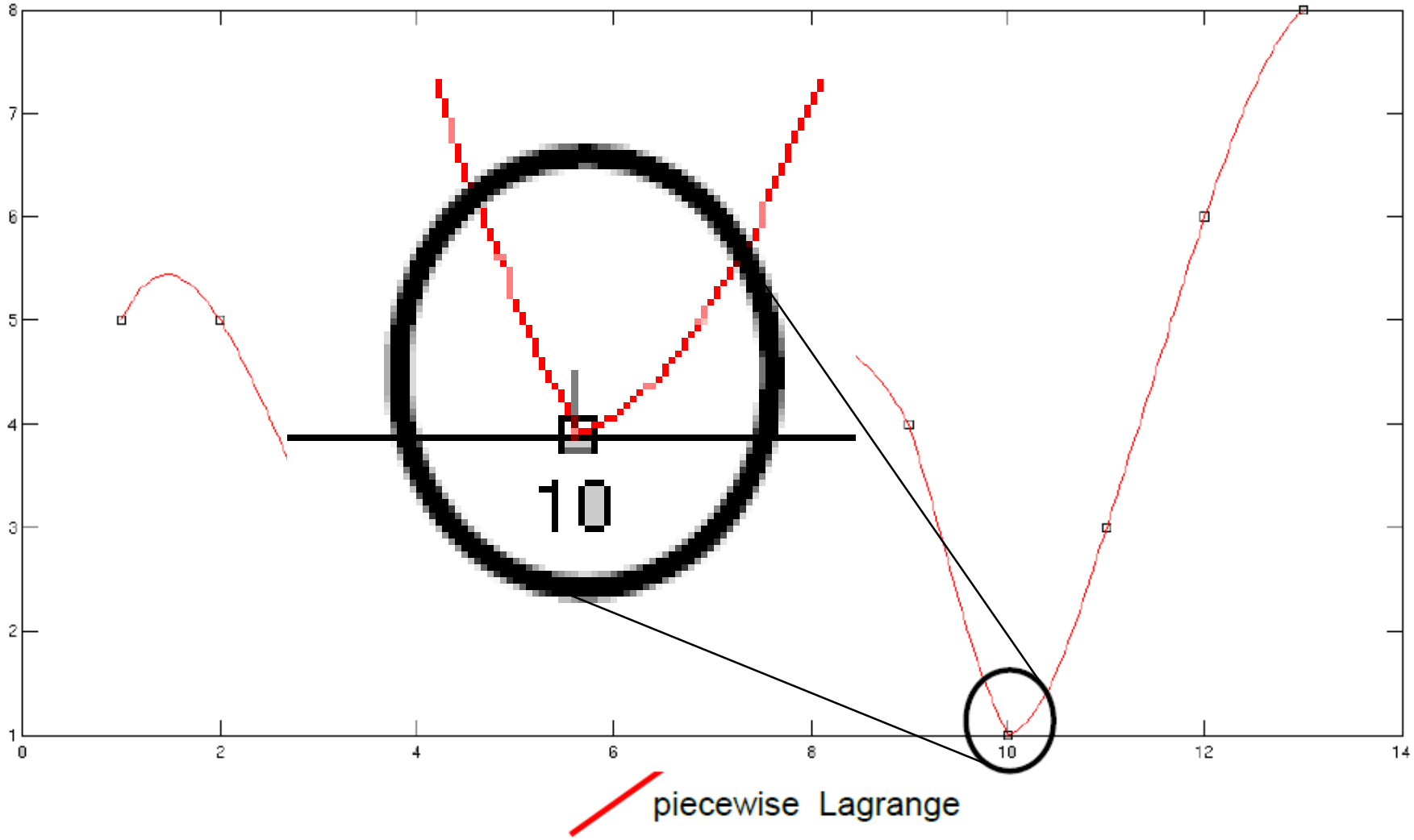
$$A = \begin{bmatrix} 1 & 0 & 0 & \cdots & 0 \\ h_0 & 2(h_0+h_1) & h_1 & & \vdots \\ 0 & h_1 & 2(h_1+h_2) & h_2 & 0 \\ \vdots & & \ddots & \ddots & h_{n-1} \\ 0 & \cdots & 0 & 0 & 1 \end{bmatrix} \quad \mathbf{b} = \begin{bmatrix} 0 \\ \frac{3}{h_1}(a_2-a_1) - \frac{3}{h_0}(a_1-a_0) \\ \vdots \\ \frac{3}{h_{n-1}}(a_n-a_{n-1}) - \frac{3}{h_{n-2}}(a_{n-1}-a_{n-2}) \\ 0 \end{bmatrix} \quad \mathbf{x} = \begin{bmatrix} c_0 \\ c_1 \\ \vdots \\ c_n \end{bmatrix}.$$

$$b_j = 1/h_j(a_{j+1} - a_j) - h_j/3(2c_j + c_{j+1})$$

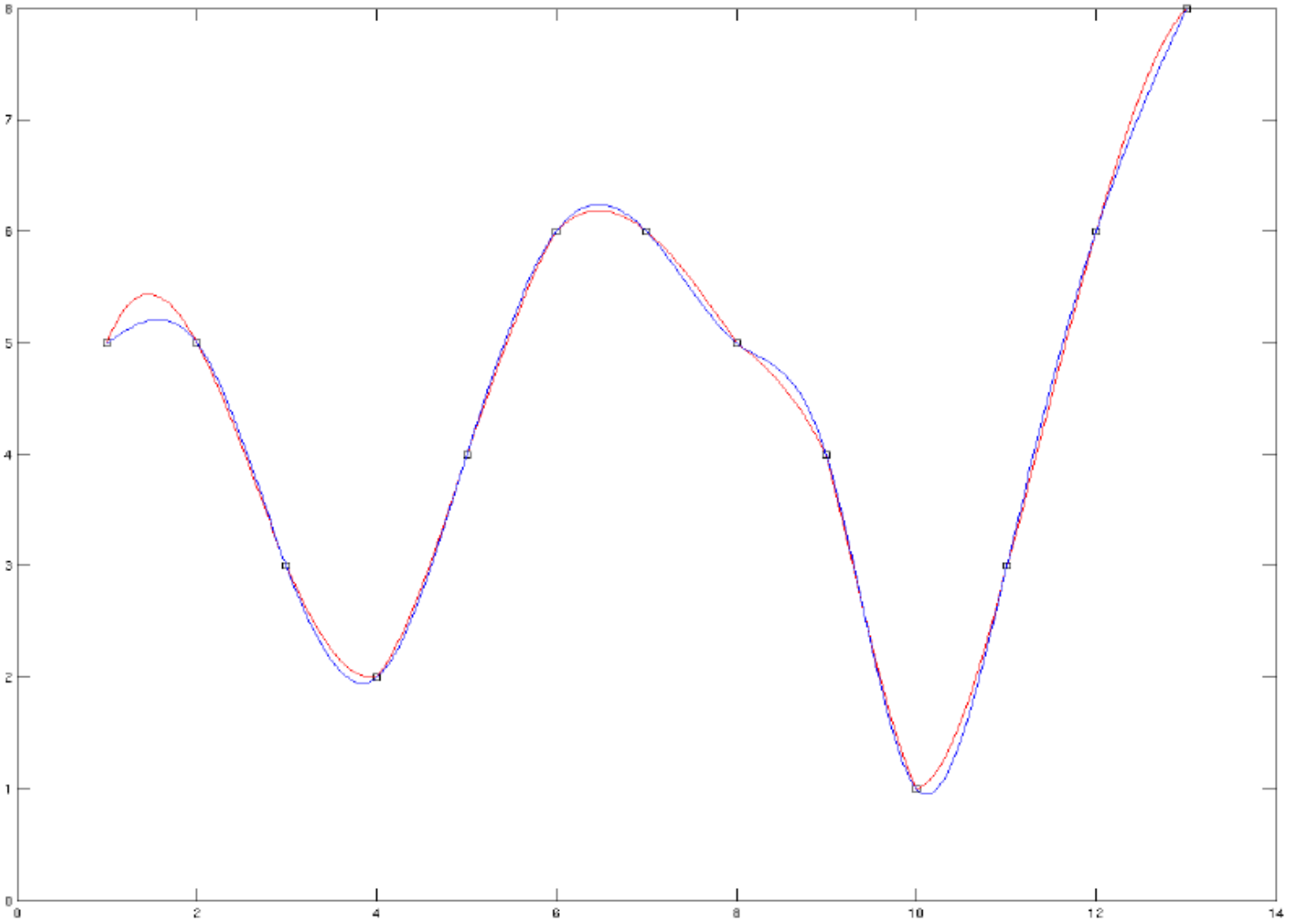
$$d_j = (c_{j+1} - c_j)/3h_j$$

with $h_j = x_{j+1} - x_j$

# Piecewise Lagrange



# Piecewise Lagrange vs. Cubic Spline



# Midterm Exam

- **Tuesday – Dezember 17th, 2019**
- **Location: H4**
- **Time: 18:00 – 19:00**
- **Please show up at 17:50 latest!**

# Midterm Exam: Topics

- **Binary FP number representation**
  - Basics, e.g. which number can be exactly represented)
- **Errors in FP operations – add/mult/div**
  - Basics, e.g. loss of (least) significant bits when adding large and small FP numbers
- **Computational Complexity**
  - Calculate FP operations counts & Complexity order for basic numeric schemes/kernels, e.g. matrix vector multiply
- **Features of DETERMINANT**

# Midterm Exam – Topics

- **LSE: Direct Methods**
  - Gaussian Elimination (GE) with permutation, e.g. solve given LSE with GE
  - Matrix Factorization
    - General idea/concept
    - LU factorization by GE
    - Other factorizations (basics only)
- **LSE: Iterative Methods**
  - Vector / Matrix norm – induced norm
  - Eigenvalues/vectors
  - Special Types of matrices
  - Jacobi / Gauss-Seidel / SOR
    - Basic Idea
    - Apply to a given problem
    - Convergenece (III.27. – III.33.)
  - CG – Basics:
    - Iterative or Direct?
    - III.38.

# Midterm Exam

- **Interpolation & Polynomial Approximation**
  - Taylor (IV.2.) !!!!
  - Lagrange Polynomial (IV.3.) / (IV.4.)
  - Neville's Method
  - Divided Differences!
  - Do not forget Error Terms and their meaning!!!!
- **Switch on brain and consider shortcuts!!!!**