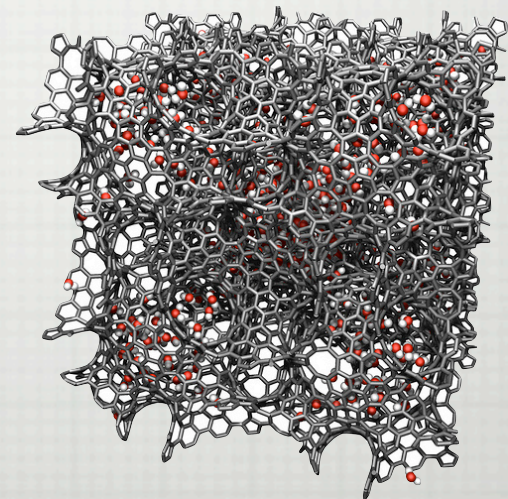
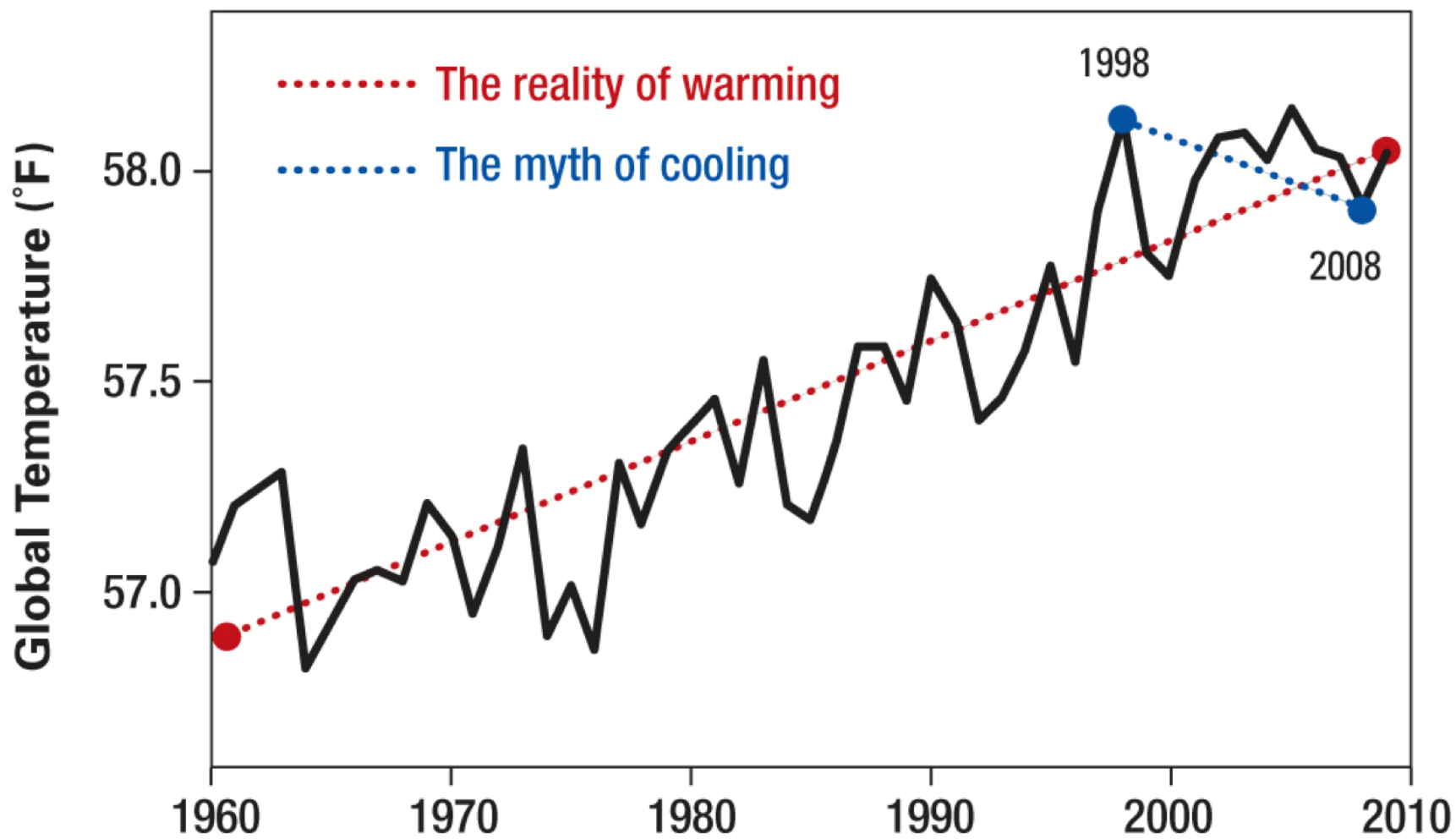


PHY-4810

COMPUTATIONAL PHYSICS

LECTURE 7: DATA FITTING





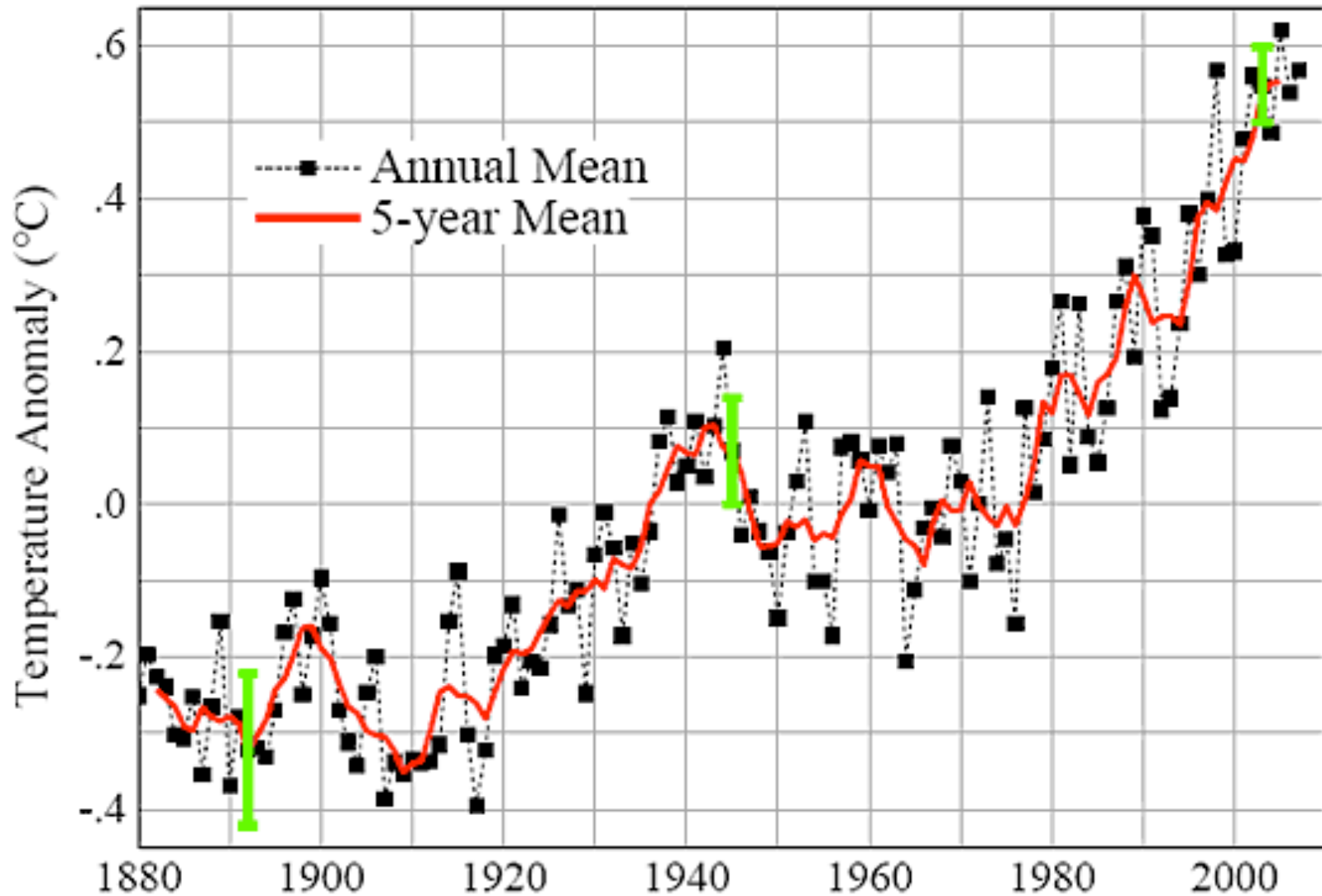
Global Surface Temperature Over the Last Fifty Years

HTTP://DATA.GISS.NASA.GOV/GISTEMP/TABLEDATA/GLB.TS+DSST.TXT

GLOBAL Land-Ocean Temperature Index in 0.01 degrees Celsius base period: 1951-1980																											
sources: GHDN 1880-01/2011 + SST: 1880-01/2011 HadISST1																											
using elimination of outliers and homogeneity adjustment																											
Notes: 1950 DJT = Dec 1949 - Feb 1950 ; ***** missing																											
AnnoMean																											
Year	Jan	Feb	Mar	Apr	May	Jun	Jul	Aug	Sep	Oct	Nov	Dec	J-DT	J-DT	J-DT	J-DT	J-DT	J-DT	J-DT	J-DT	J-DT	J-DT	J-DT	J-DT	J-DT	J-DT	J-DT
1880	-47	-27	-25	-31	-11	-39	-25	-15	-30	-27	-21	-25	-24****	-24	-26	-26	-26	-26	-26	-26	-26	-26	-26	-26	-26	-26	-26
1881	-21	-27	-2	-6	-10	-32	-13	-12	-27	-30	-38	-29	-21	-20	-24	-6	-19	-32	-1881								
1882	-11	-10	-10	-31	-36	-24	-15	-25	-27	-35	-35	-26	-14	-22	-26	-10	-32	-1882									
1883	-45	-40	-17	-22	-26	-10	-10	-24	-34	-34	-28	-27	-29	-46	-22	-16	-34	-1883									
1884	-26	-19	-37	-40	-38	-36	-28	-20	-32	-33	-36	-35	-32	-31	-24	-38	-28	-34	-1884								
1885	-41	-35	-24	-42	-35	-42	-29	-26	-25	-27	-34	-9	-32	-34	-44	-34	-33	-35	-1885								
1886	-39	-45	-36	-42	-30	-22	-9	-27	-26	-41	-35	-40	-35	-35	-50	-36	-19	-34	-1886								
1887	-65	-54	-36	-42	-30	-22	-9	-27	-26	-41	-35	-40	-35	-35	-50	-36	-19	-34	-1887								
1888	-43	-49	-46	-35	-28	-25	-19	-23	-19	-11	-5	-21	-27	-28	-44	-36	-22	-11	-1888								
1889	-22	-7	-2	-4	-7	-13	-17	-25	-21	-32	-37	-32	-17	-16	-12	-16	-18	-30	-1889								
1890	-49	-42	-35	-36	-51	-39	-31	-37	-39	-51	-34	-39	-39	-41	-40	-36	-39	-39	-1890								
1891	-49	-53	-18	-31	-22	-23	-24	-20	-18	-25	-38	-9	-27	-30	-45	-24	-22	-27	-1891								
1892	-37	-12	-24	-44	-33	-20	-29	-21	-28	-43	-46	-32	-29	-19	-37	-27	-11	-1892									
1893	-62	-59	-20	-36	-38	-28	-10	-27	-26	-17	-19	-33	-33	-34	-42	-31	-22	-21	-1893								
1894	-49	-20	-24	-45	-35	-43	-19	-24	-35	-27	-27	-28	-32	-33	-38	-34	-20	-23	-1894								
1895	-54	-49	-30	-26	-29	-21	-18	-18	-11	-16	-12	-19	-25	-26	-44	-28	-19	-13	-1895								
1896	-23	-17	-37	-14	-11	-5	-8	-3	-10	-10	-14	-15	-20	-27	-8	-6	-1896										
1897	-17	-16	-16	-6	-2	-11	-4	-7	-12	-11	-20	-13	-11	-14	-8	-7	-14	-1897									
1898	0	-24	-47	-27	-34	-17	-21	-22	-21	-29	-39	-27	-26	-24	-12	-36	-20	-29	-1898								
1899	-21	-28	-28	-16	-15	-26	-10	-7	-6	-2	-13	-27	-15	-15	-20	-20	-14	-1	-1899								
1900	-34	5	-2	-10	-7	-6	-8	-1	-14	-7	-8	-10	-19	-6	-8	-6	-6	-1900									
Year	Jan	Feb	Mar	Apr	May	Jun	Jul	Aug	Sep	Oct	Nov	Dec	J-DT	J-DT	J-DT	J-DT	J-DT	J-DT	J-DT	J-DT	J-DT	J-DT	J-DT	J-DT	J-DT	J-DT	J-DT
1901	-20	-2	2	-2	-14	-13	-14	-17	-21	-26	-22	-26	-15	-13	-9	-5	-15	-23	1901								
1902	-14	5	-22	-24	-27	-17	-26	-24	-32	-42	-44	-24	-23	-12	-12	-24	-23	-12	1902								
1903	-25	8	-13	-36	-32	-42	-27	-38	-40	-41	-31	-42	-30	-31	-21	-27	-36	-38	1903								
1904	-54	-46	-16	-15	-16	-18	-7	-11	-16	-25	-35	-44	-33	-30	-43	-30	-26	-40	1904								
1905	-29	-53	-19	-31	-28	-24	-20	-17	-16	-24	-8	-20	-24	-24	-35	-26	-20	-16	1905								
1906	-26	-30	-18	-20	-20	-14	-21	-11	-20	-14	-36	-12	-19	-19	-25	-13	-15	-23	1906								
1907	-42	-40	-26	-39	-28	-25	-37	-39	-28	-25	-41	-39	-27	-34	-40	-40	-32	-30	1907								
1908	-29	-26	-46	-40	-33	-25	-23	-33	-21	-30	-39	-39	-33	-33	-36	-39	-27	-30	1908								
1909	xx	xx	xx	xx	xx	xx	xx	xx	xx	xx	xx	xx	xx	xx	xx	xx	xx	xx	1909								

Year	Jan	Feb	Mar	Apr	May	Jun	Jul	Aug	Sep	Oct	Nov	Dec	J-D	J-D	J-D	J-D	J-D	J-D	J-D	J-D	J-D	J-D	J-D	J-D	J-D	J-D	J-D
1961	5	21	10	11	22	12	1	3	5	7	5	-15	7	10	15	14	5	7	1961								
1962	5	18	12	11	-10	7	-3	-5	2	1	8	0	4	3	3	5	0	4	1962								
1963	1	19	-13	-7	-2	6	14	26	25	9	14	3	8	8	7	-8	15	16	1963								
1964	-5	-8	-26	-33	-28	-2	-5	-24	-37	-30	-20	-30	-21	-18	-3	-29	-11	-29	1964								
1965	-10	-18	-10	-19	-6	-11	-20	-6	-16	-6	-6	-5	-11	-13	-19	-12	-13	-10	1965								
1966	-16	-1	11	-11	-7	-1	11	-5	1	-15	0	-4	-3	-3	-8	-3	2	-5	1966								
1967	-7	-23	7	-2	11	-6	6	1	0	10	-2	-1	-1	-1	-11	6	0	3	1967								
1968	-22	-14	24	-5	-9	0	-8	-5	-14	13	-3	-12	-4	-4	-12	4	-4	-1	1968								
1969	-7	-8	-2	20	13	11	-4	0	9	14	16	30	8	4	-9	10	3	13	1969								
1970	10	23	9	4	-5	-2	-1	-12	13	3	4	-12	3	6	21	3	-5	7	1970								
1971	-2	-20	-21	-11	-12	-22	-11	-2	-2	-5	-7	-11	-10	-11	-11	-15	-12	-5	1971								
1972	-26	-20	-2	-1	-2	6	0	20	5	4	-2	18	0	-2	-19	-2	9	2	1972								
1973	26	28	26	24	22	16	9	1	7	13	4	-8	14	16	24	9	8	9	1973								
1974	-14	-27	-5	-12	-5	-5	-2	10	-9	-7	-10	-11	-8	-8	-16	-7	1	-9	1974								
1975	1	1	11	-3	18	-3	-5	-21	-6	-11	-17	-22	-5	-4	-3	9	-10	-11	1975								
1976	-8	-12	-28	-16	-29	-15	-13	-20	-12	-29	-11	0	-16	-18	-14	-24	-16	-17	1976								
1977	10	15	15	19	29	22	19	17	-5	-5	12	2	12	12	8	21	19	1	1977								
1978	3	8	11	9	1	-8	4	-21	5	-4	6	1	1	1	4	7	-9	3	1978								
1979	6	-18	8	10	-6	4	-7	9	18	18	19	39	8	5	-4	4	2	18	1979								
1980	21	28	23	26	29	9	22	17	12	8	22	8	19	21	29	26	16	14	1980								
Year	Jan	Feb	Mar	Apr	May	Jun	Jul	Aug	Sep	Oct	Nov	Dec	J-D	J-D	J-D	J-D	J-D	J-D	J-D	J-D	J-D	J-D	J-D	J-D	J-D	J-D	J-D
1981	47	35	44	23	14	21	29	31	11	6	18	28	26	24	30	27	27	12	1981								
1982	0	7	-12	-3	10	1	11	-3	1	2	3	34	4	4	12	-2	3	2	1982								
1983	42	34	36	27	30	14	11	27	34	9	23	10	25	27	37	31	18	22	1983								
1984	22	7	22	3	29	-2	11	11	16	4	-5	-15	9	11	13	18	7	5	1984								
1985	15	-14	11	5	5	12	-8	10	6	4	-1	7	4	2	-5	7	5	3	1985								
1986	19	37	24	18	16	4	5	7	5	1	6	12	12	21	20	6	2	1986									
1987	25	38	11	17	17	32	41	19	30	26	21	42	27	24	23	15	31	26	1987								
1988	51	35	45	35	38	40	26	31	30	29	-3	19	31	33	43	39	33	19	1988								
1989	3	28	27	17	4	5	28	26	31	25	8	26	19	19	17	16	20	22	1989								

Global Temperature Land-Ocean Index



ON THE MENU

- ☐ **Lagrange multipliers**
- ☐ **Spline**
- ☐ **Fit to theory**
- ☐ **How to use Numerical Recipes**

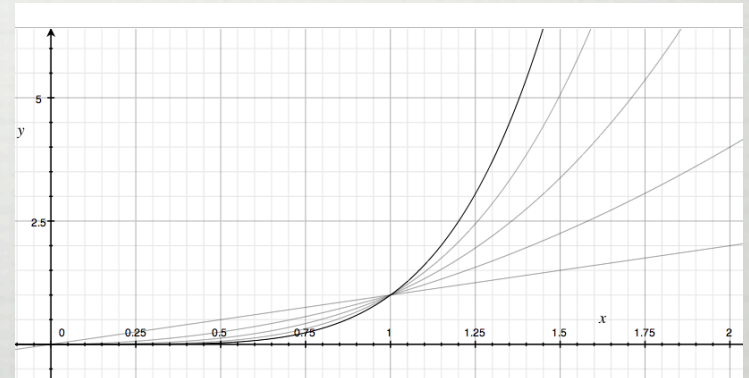
PART I: LAGRANGE INTERPOLATION

METHOD AND ALGORITHM

- Any function $g(x)$ can be approximated as a polynomial of degree $(n - 1)$ in each interval i for a sufficiently high n :

$$g_i(x) \simeq a_0 + a_1x + a_2x^2 + \cdots + a_{n-1}x^{n-1}$$

- Because our fit is local, we do not assume that one $g(x)$ can fit all the data in a list, but instead will use a different polynomial, that is, a different set of $\underline{a_i}$ values, for each region of the list.



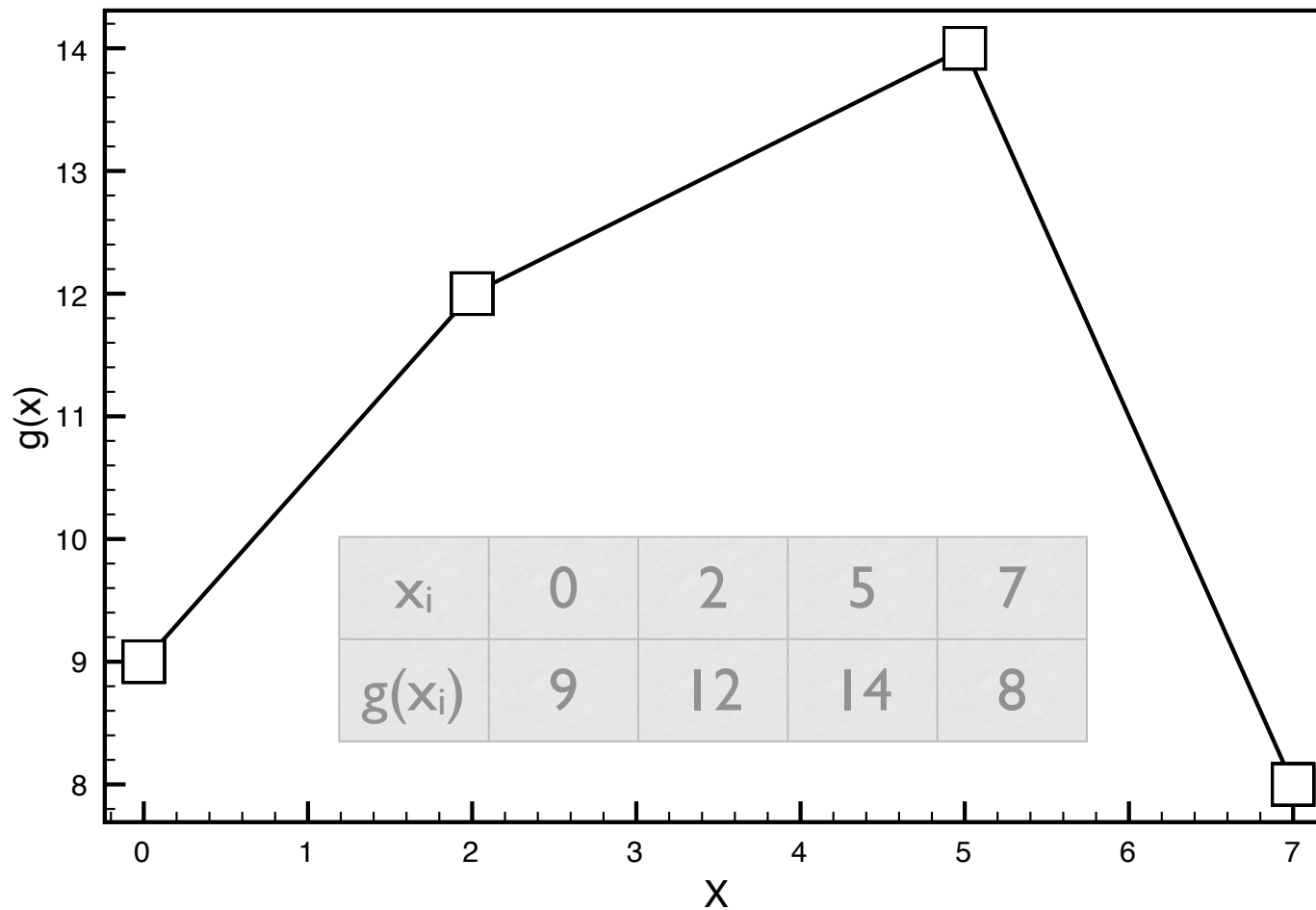
LAGRANGE INTERPOLATION FORMULA

- Lagrange figured out a closed-form approach that directly fits the $(n - 1)$ -order polynomial to n values of the function $g(x)$ evaluated at the points x_i . The formula is written as the sum of polynomials:

$$g(x) \simeq g_1\lambda_1(x) + g_2\lambda_2(x) + \cdots + g_n\lambda_n(x)$$
$$\lambda_i(x) = \prod_{j(\neq i)=1}^n \frac{x - x_j}{x_i - x_j} = \frac{x - x_1}{x_i - x_1} \frac{x - x_2}{x_i - x_2} \cdots \frac{x - x_n}{x_i - x_n}$$

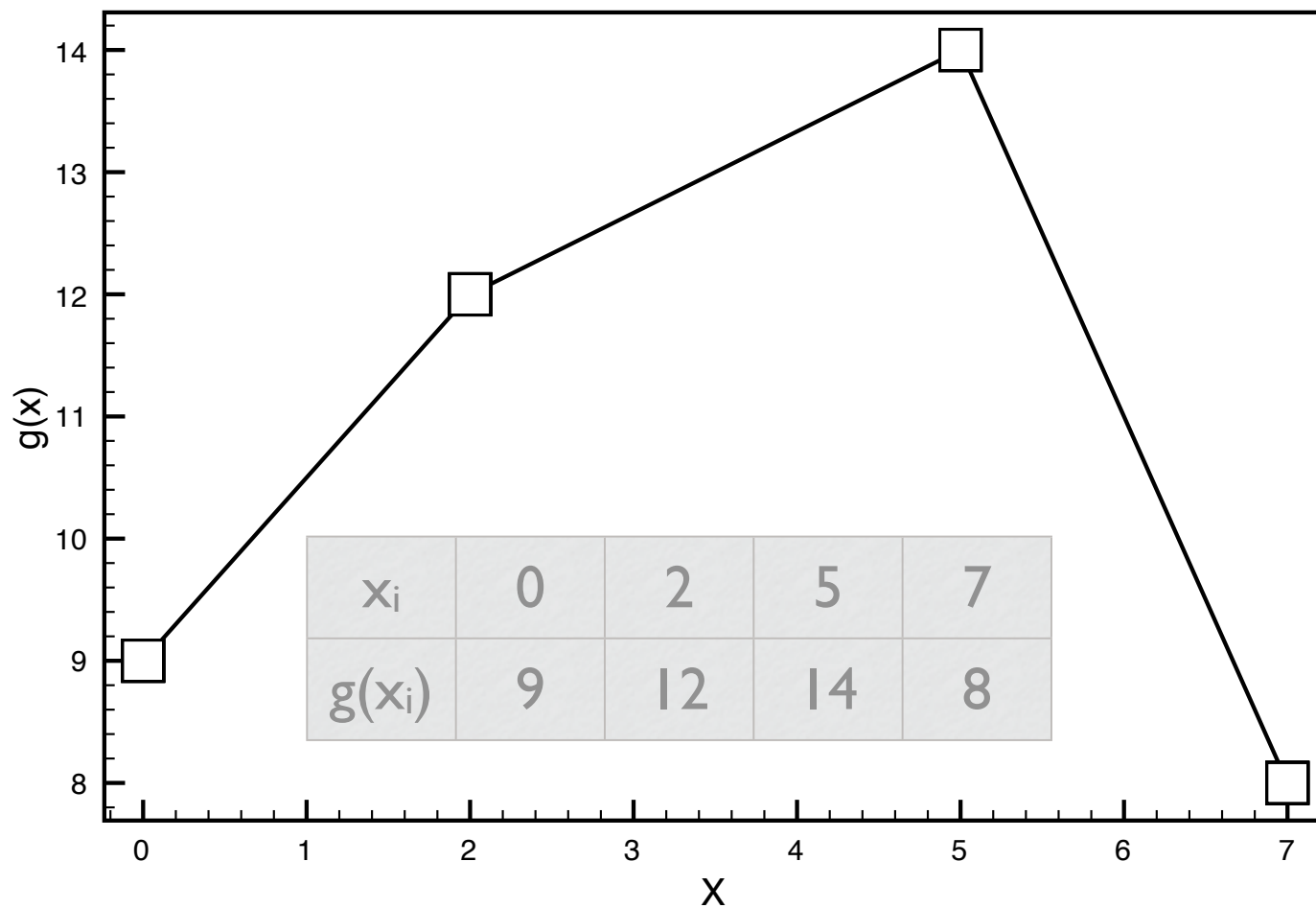
- For three points, this formula provides a second-degree polynomial, while for eight points it gives a seventh-degree polynomial.

EXAMPLE: POLYNOMIAL OF ORDER 3



$$g(x) \simeq g_1\lambda_1(x) + g_2\lambda_2(x) + \cdots + g_n\lambda_n(x)$$

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



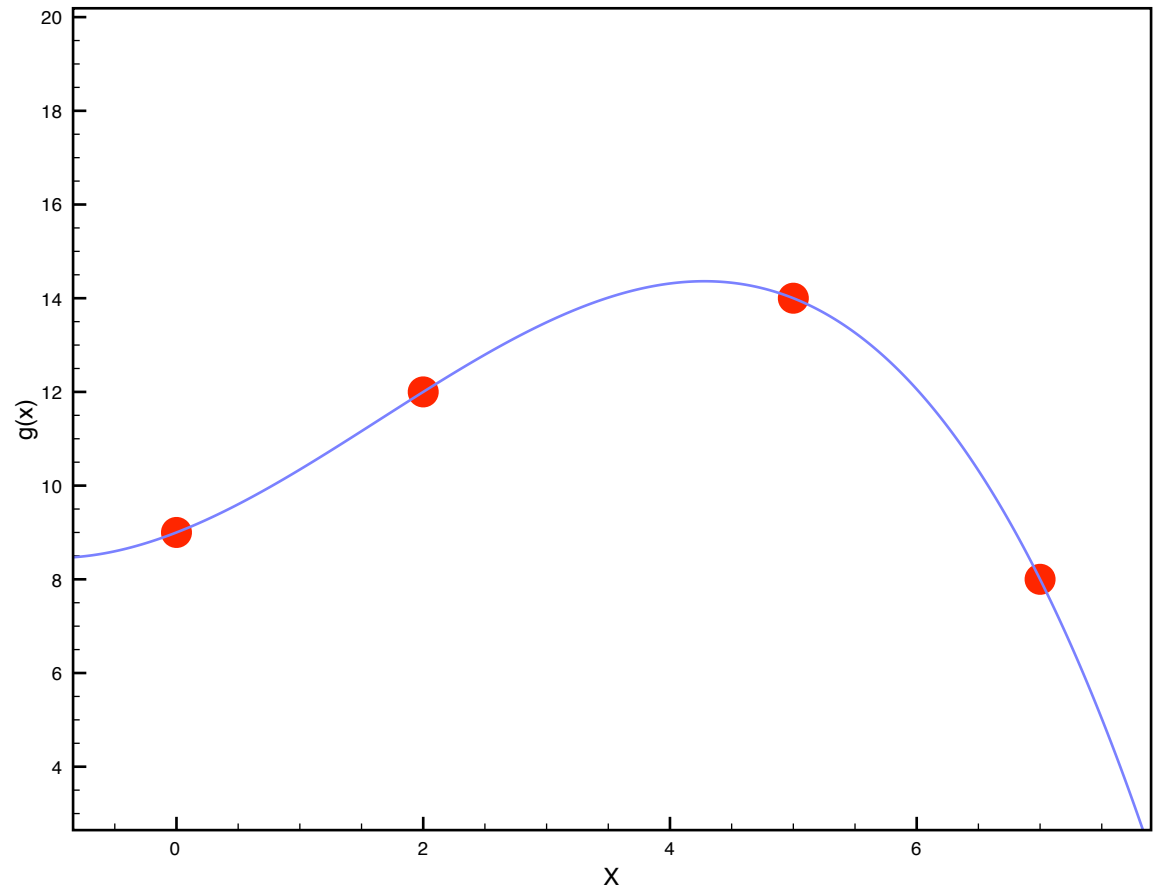
$$g(x) = g_1\lambda_1(x) + g_2\lambda_2(x) + g_3\lambda_3(x) + g_4\lambda_4(x)$$

$$\lambda_1(x) = \frac{(x-2)(x-5)(x-7)}{-2 \times -5 \times -7}$$

$$\lambda_2(x) = \frac{x(x-5)(x-7)}{2 \times -3 \times -5}$$

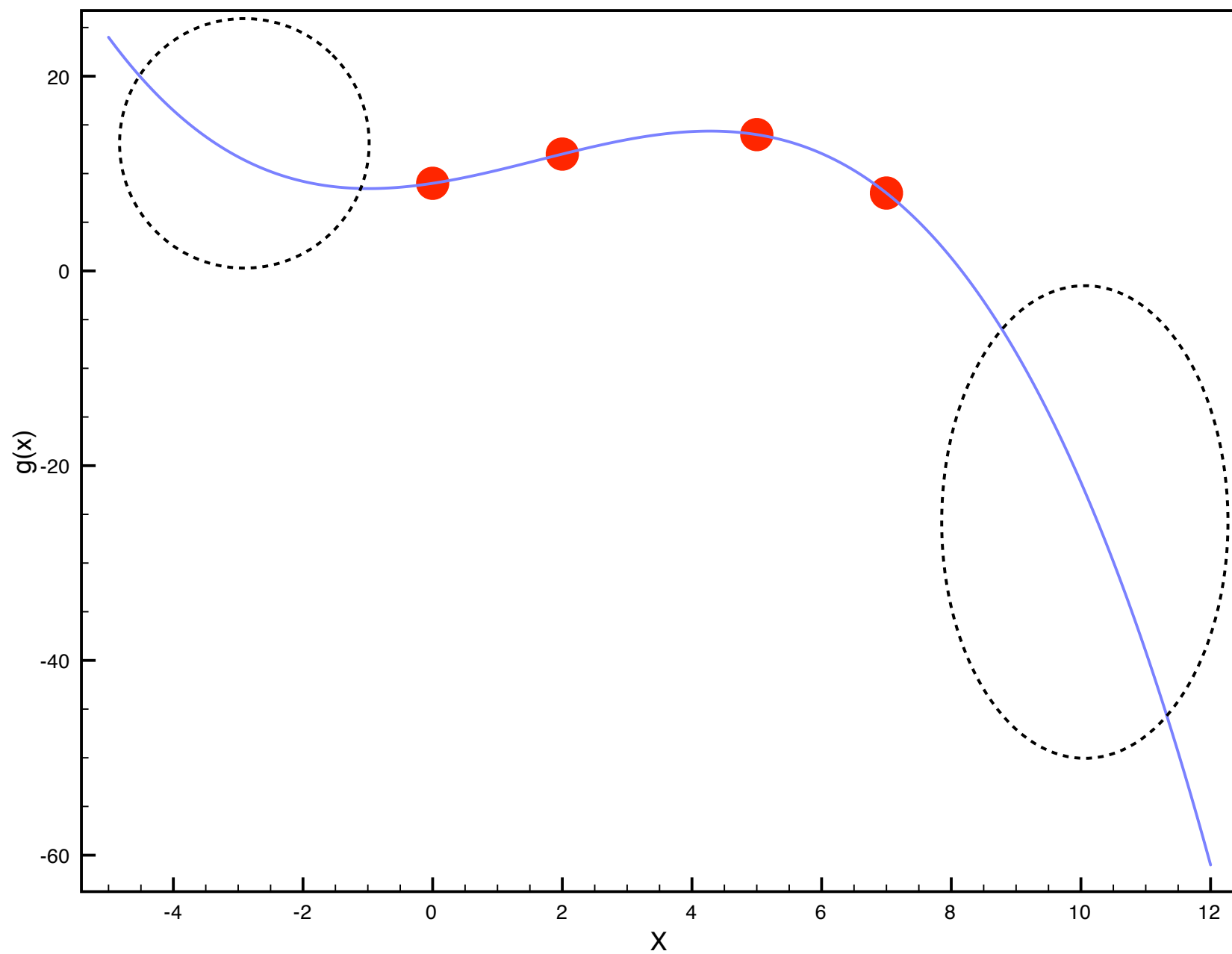
$$\lambda_3(x) = \frac{x(x-2)(x-7)}{5 \times 3 \times -2}$$

$$\lambda_4(x) = \frac{x(x-2)(x-5)}{7 \times 5 \times 2}$$

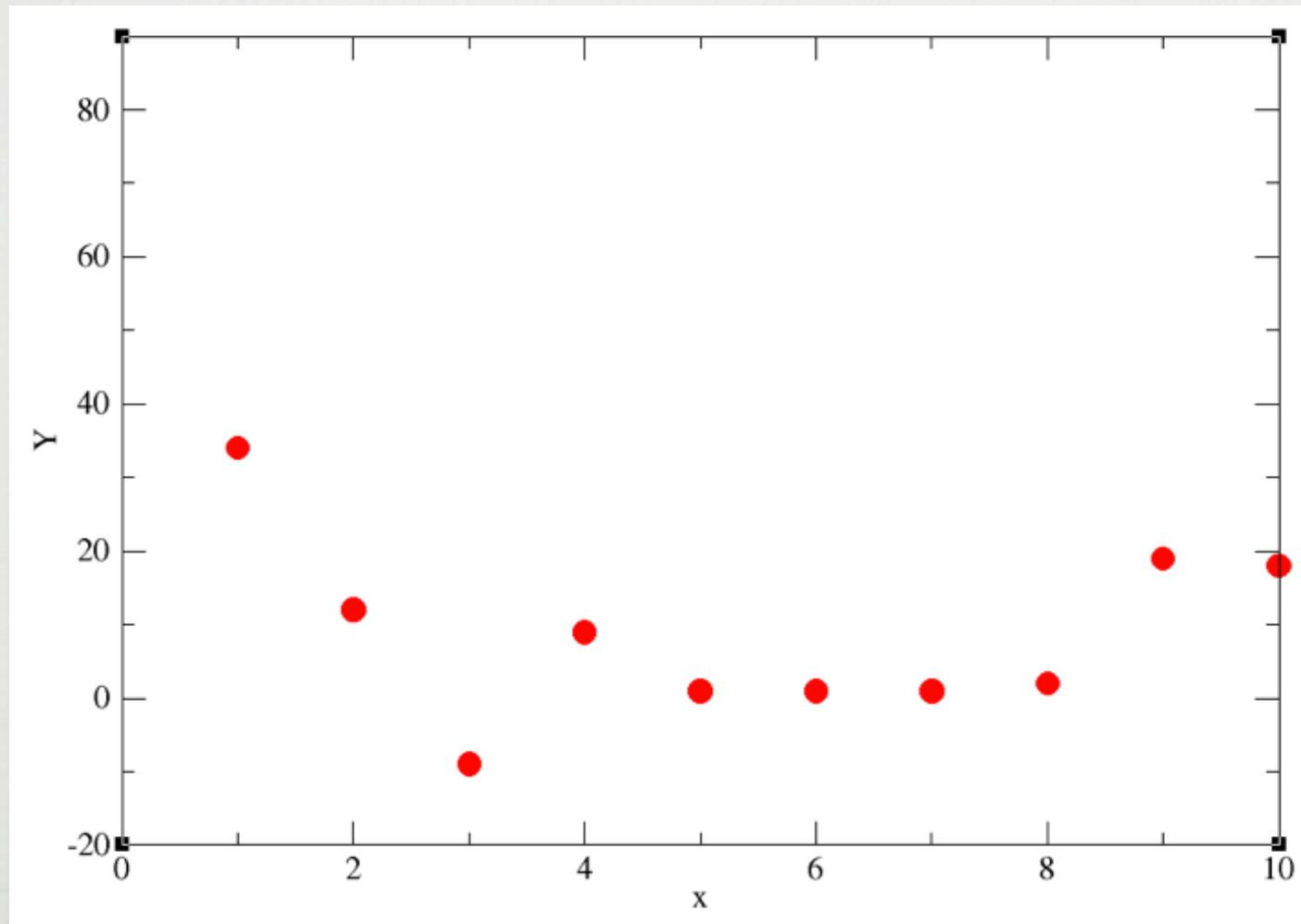


$$g(x) = \frac{-9}{70}(x-2)(x-5)(x-7) + \frac{2}{5}x(x-5)(x-7) + \frac{-7}{15}x(x-2)(x-7) + \frac{4}{35}x(x-2)(x-5)$$

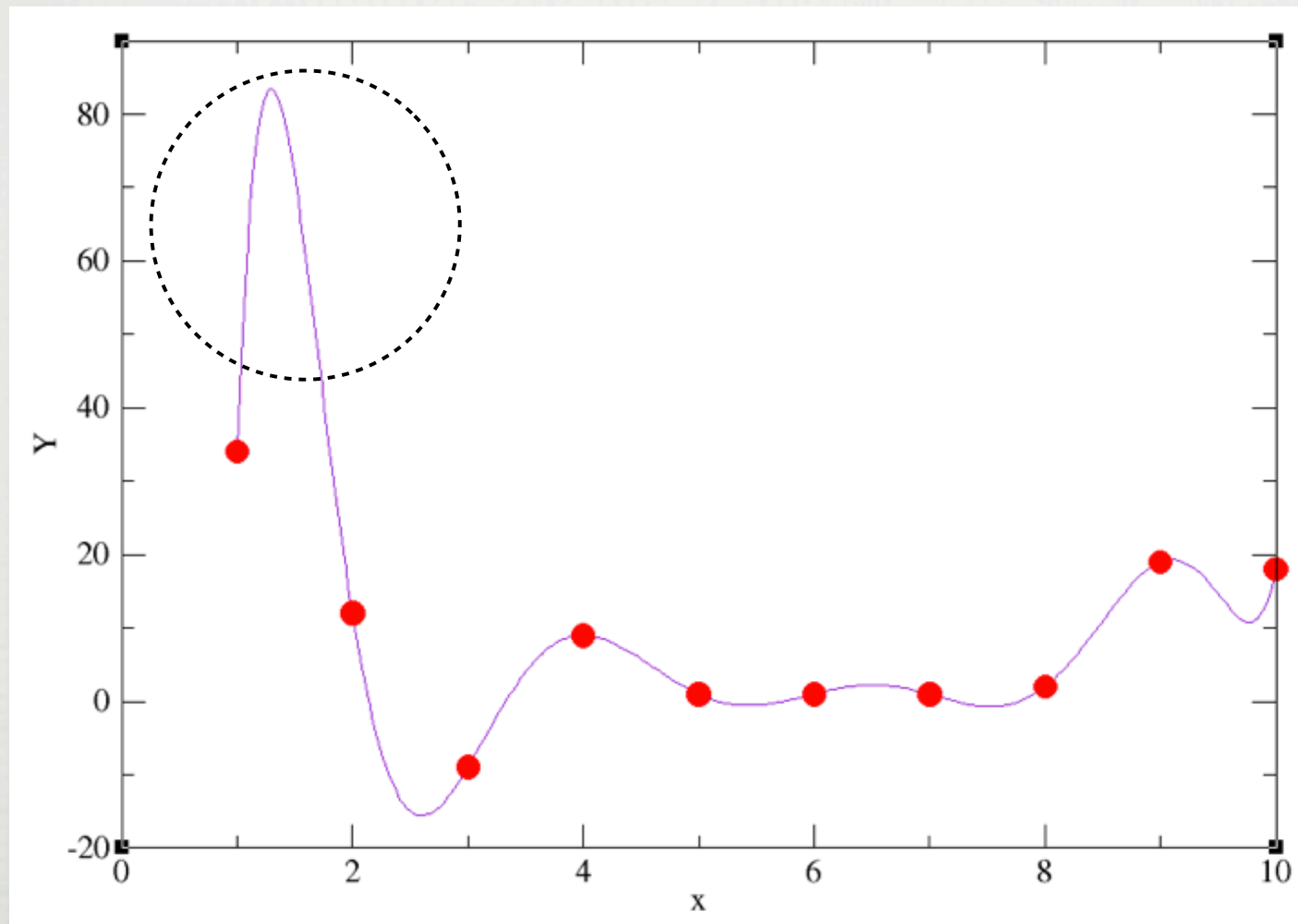
**...HOWEVER...RESIST THE TEMPTATION...
(INTERPOLATION VS. EXTRAPOLATION)**



10 DATA POINTS: POLYNOMIAL OF ORDER 9



POLYNOMIAL FIT



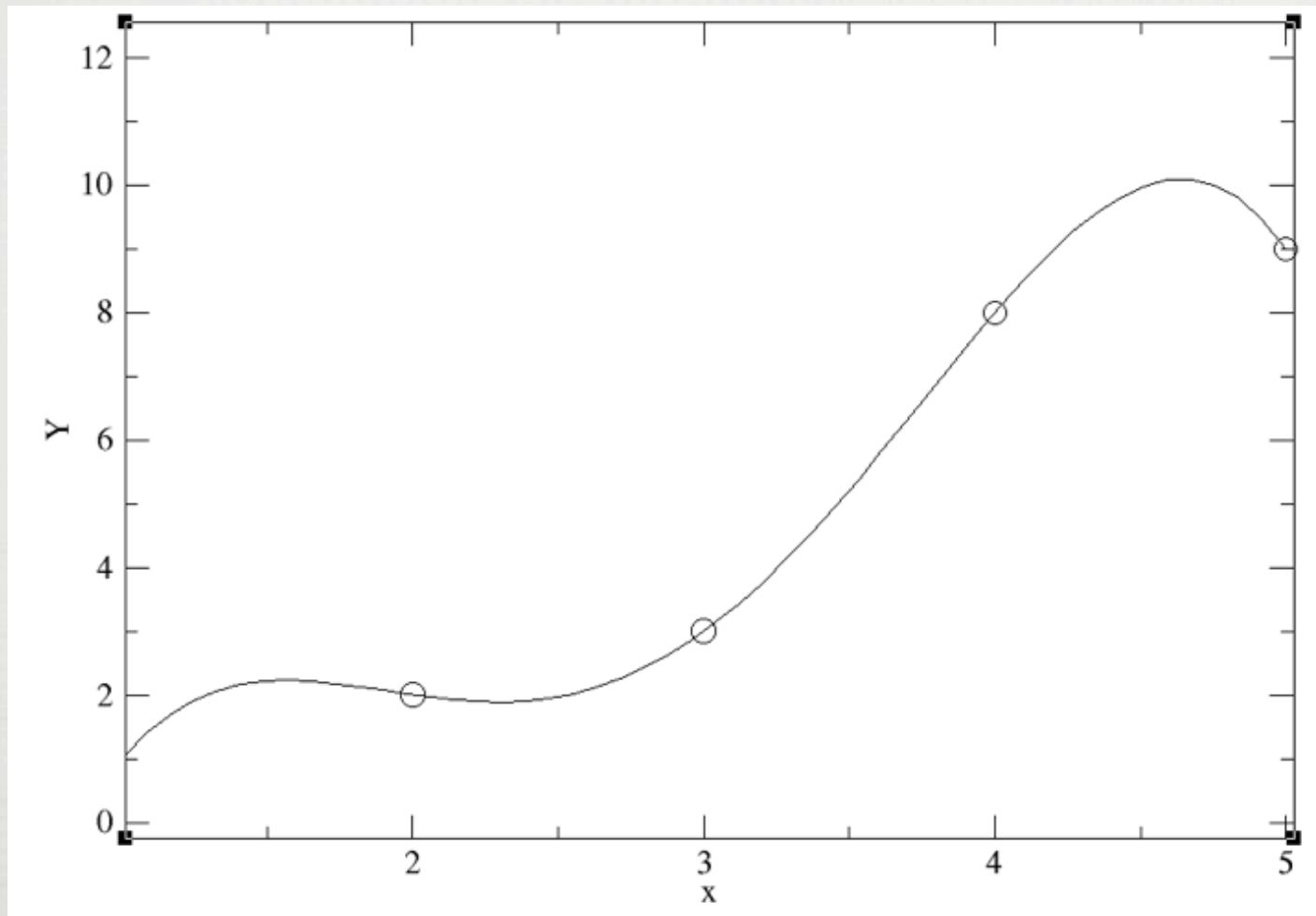
LET'S HAVE A LOOK AT THE C++ CODE

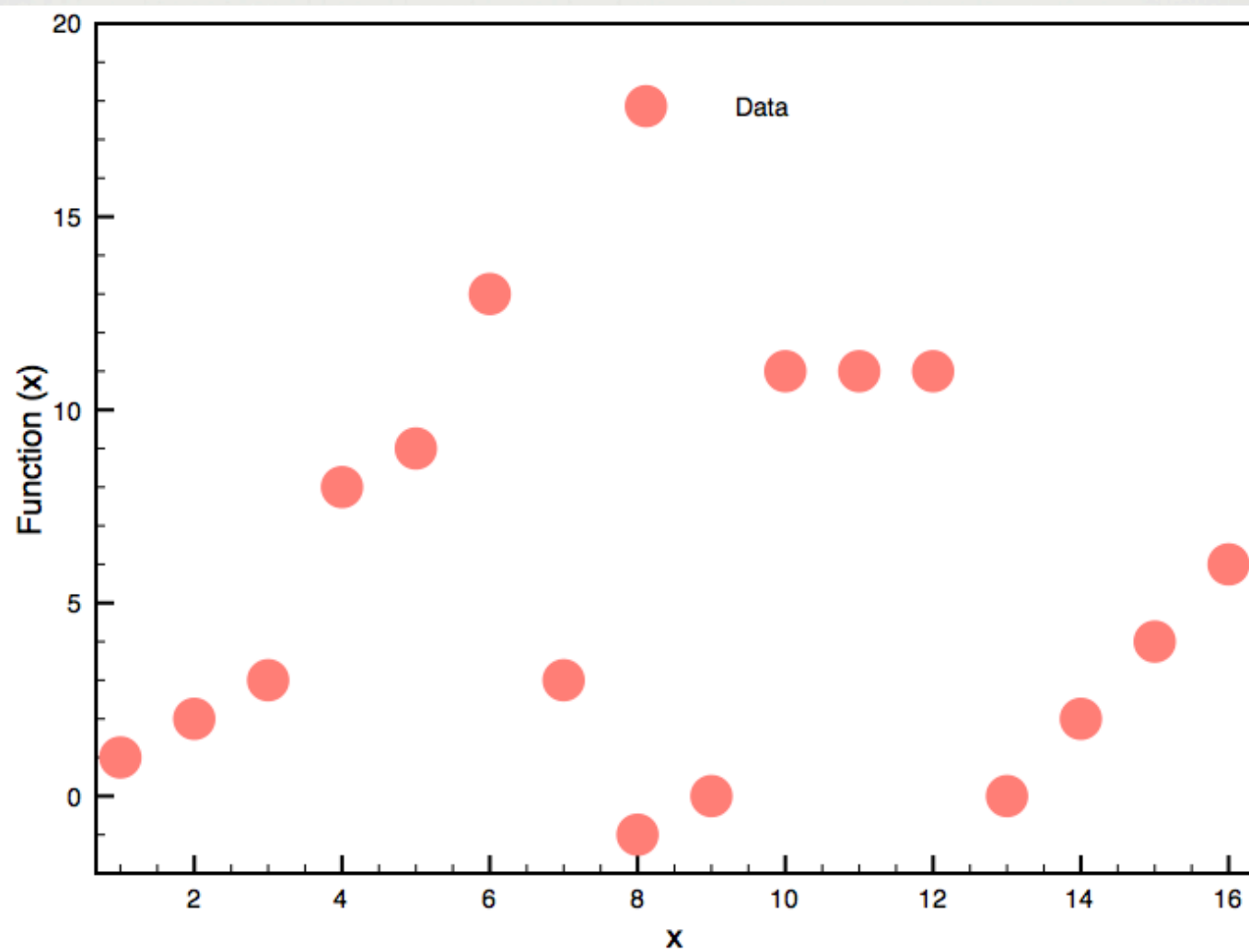
```
#INCLUDE <Iostream>
using namespace std;

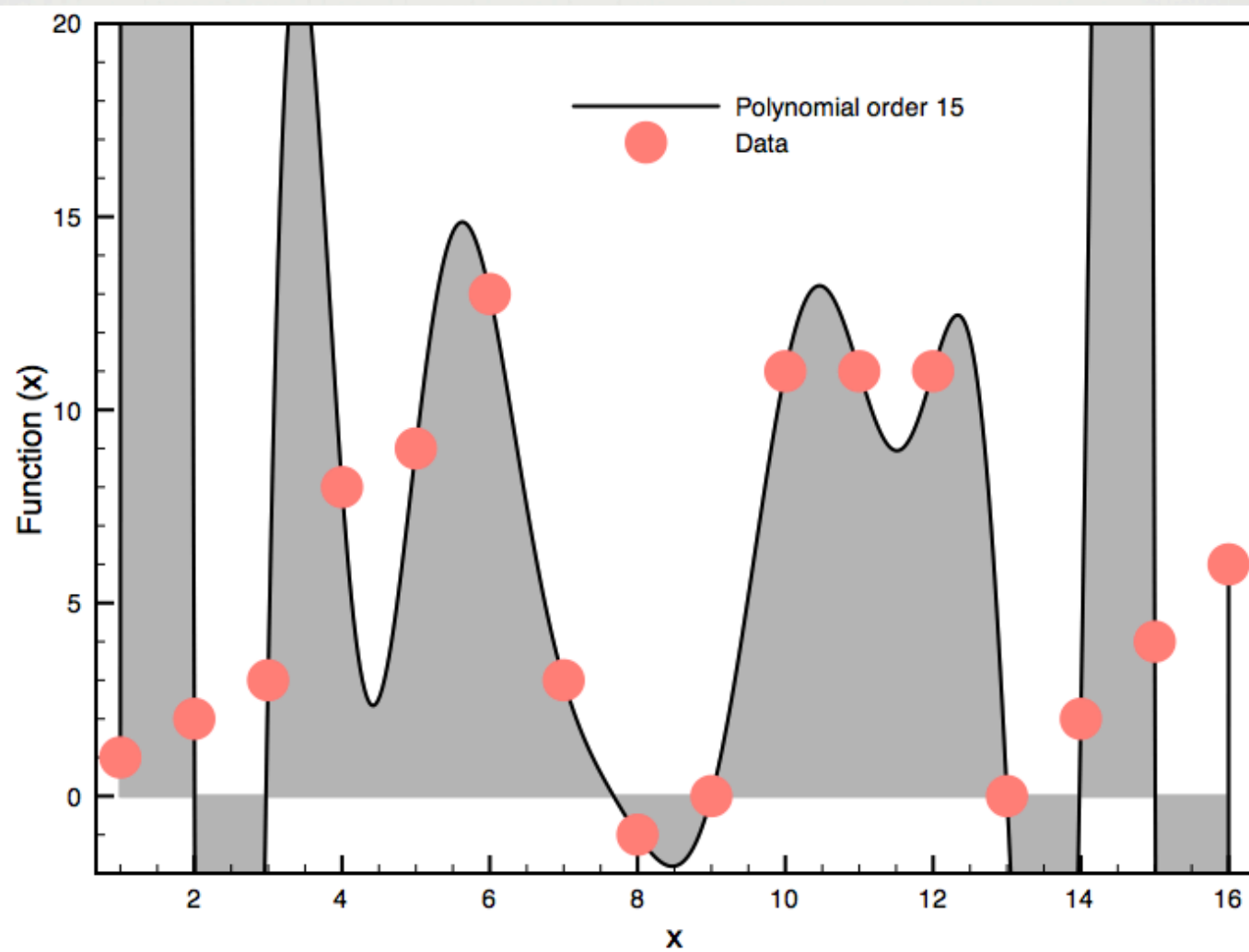
int main () {
    // INSERT CODE HERE...
    int I, J, K;
    int KMAX=393;
    double XX=0, GXX=0;
    double XXMIN, XXMAX;
    //
    int NPOINTS;
    cin >> NPOINTS;
    //
    double X[NPOINTS], G[NPOINTS];
    double LAMBDA[NPOINTS];

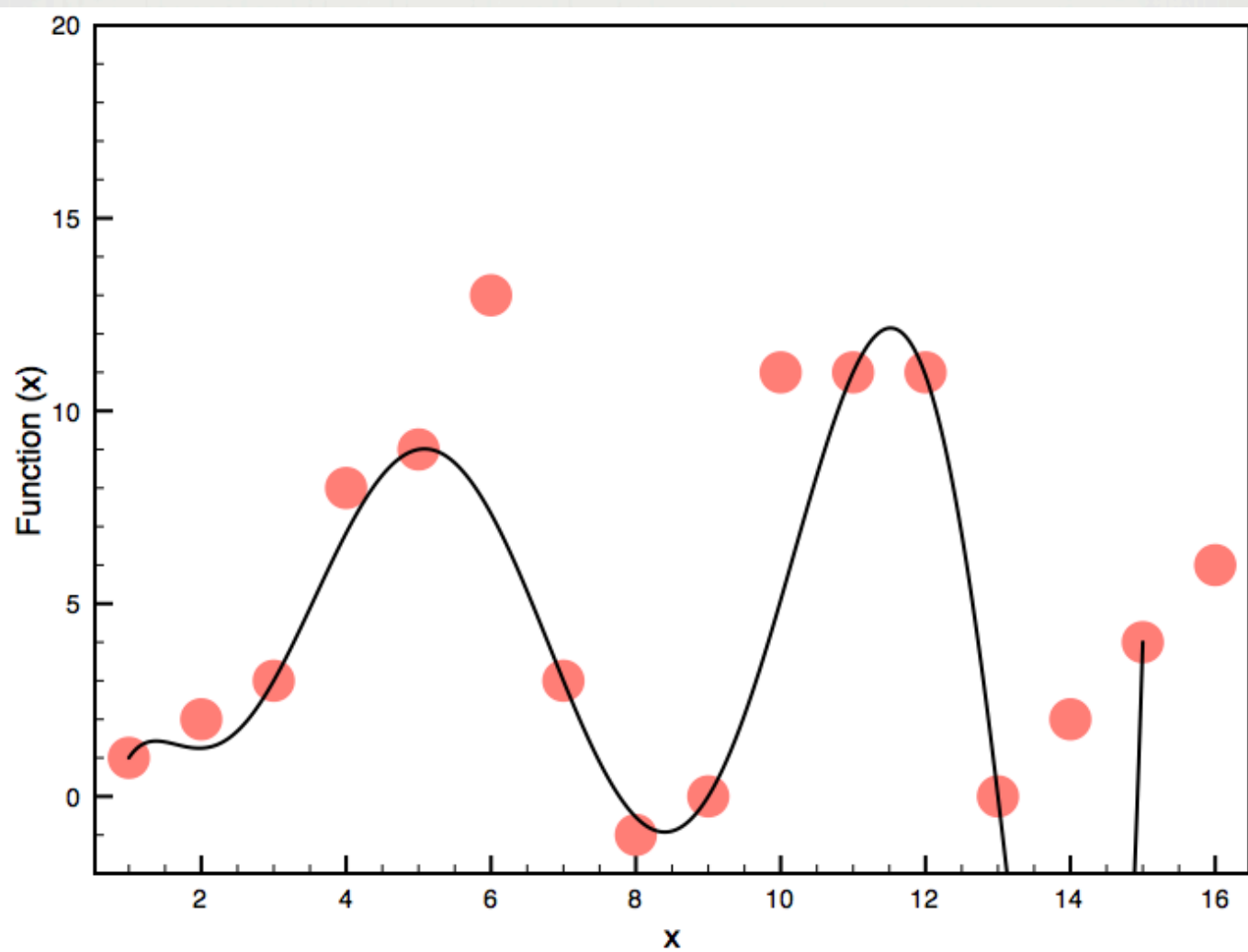
    //
    for (I=0; I<NPOINTS; I++){
        cin >> X[I] >> G[I];
    }
    //
    XXMIN=X[0];
    XXMAX=X[NPOINTS-1];
    //
    for(K=0; K<KMAX; K++){
        XX=XXMIN+(double)K*(XXMAX-XXMIN)/((double)KMAX-1);
        GXX=0.0;
        for (I=0; I<NPOINTS; I++){
            LAMBDA[I]=1.;
            for (J=0; J<NPOINTS; J++){
                if (J==I) continue;
                LAMBDA[I]*=(XX-X[J])/(X[I]-X[J]);
            }
            GXX+=LAMBDA[I]*G[I];
        }
        cout << XX << " " << GXX << endl;
    }
    return 0;
}
```

EXAMPLE OF POLYNOMIAL OBTAINED USING NEVILLE'S ALGORITHM









NEVILLE'S ALGORITHM

- A much better algorithm to construct the (unique) polynomial is called Neville's algorithm

```

//NEVILLE's ALGORITHM
#include <iostream>
using namespace std;

int main () {
    int i,k,m;
    int kmax=50;
    double xx=0, gxx=0;
    double xxmin, xxmax;
    double sum;
    //
    int npoints;
    cin >> npoints;
    //
    double x[npoints], g[npoints];
    double P0[npoints], P[npoints];

    //
    for (i=0;i<npoints;i++){
        cin >> x[i] >> g[i];
    }
    //
    xxmin=x[0];
    xxmax=x[npoints-1];
    //
    for(k=0;k<kmax;k++){
        xx=xxmin+(double)k*(xxmax-xxmin)/((double)kmax-1);
        gxx=0.0;
        sum=0;

        for(m=0;m<npoints;m++){

            if(m==0){
                for (i=0;i<npoints;i++){
                    P[i]=g[i];
                }
            }
            else {
                for (i=0;i<npoints-m;i++){
                    P[i]=((xx-x[i+m])*P0[i]+(x[i]-xx)*P0[i+1])/(x[i]-x[i+m]);
                }
            }
            for (i=0;i<npoints-m;i++){
                P0[i]=P[i];
            }

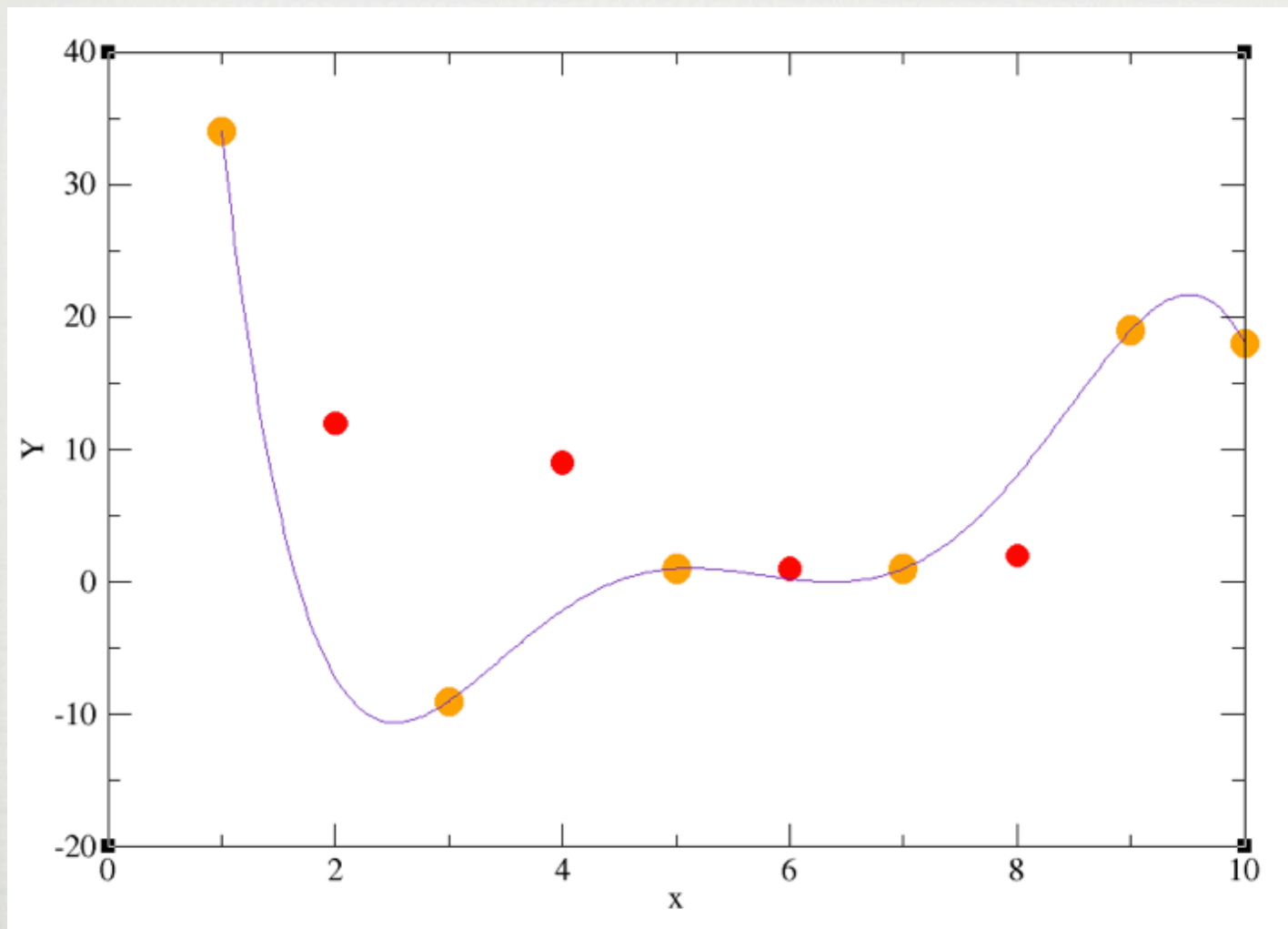
        }
        cout << xx << " " << P[0] << endl;
    }

    return 0;
}

```

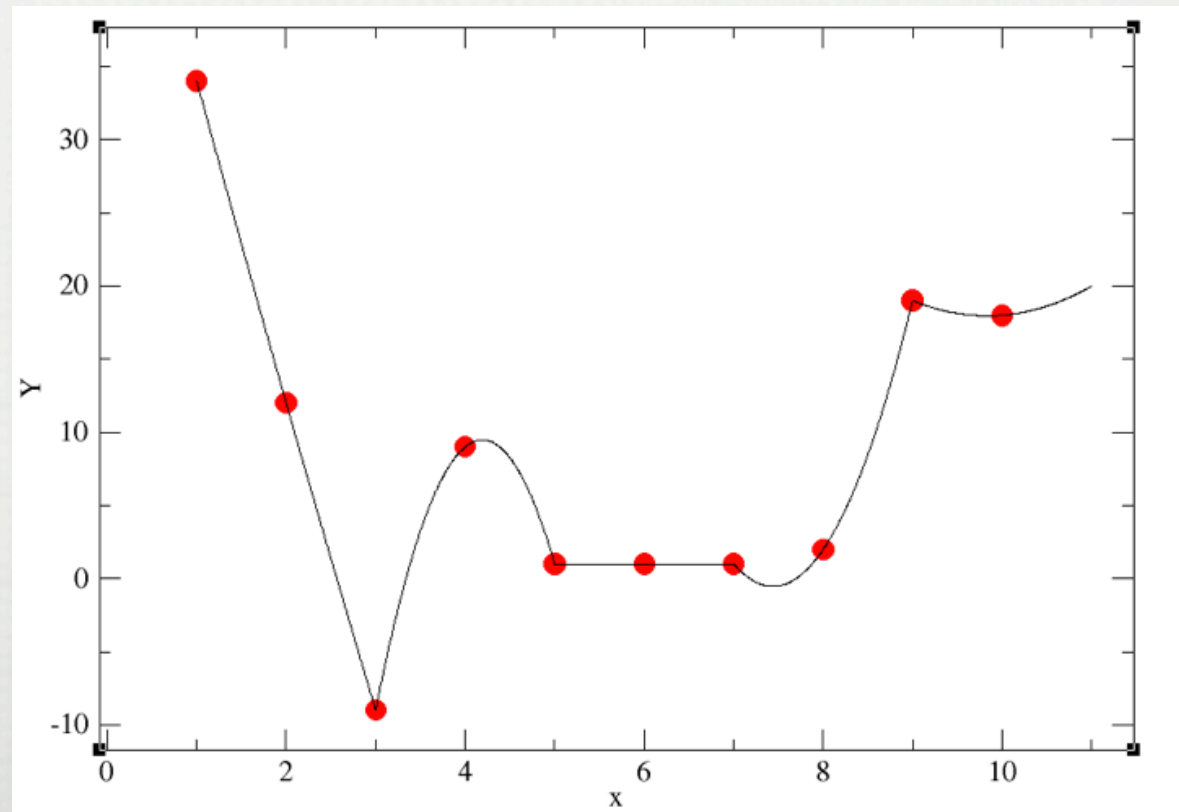

PRACTICAL CONSIDERATIONS

- ☐ If the data contain little noise, this polynomial can be used with some confidence within the range of data, but with risk beyond the range of data.
- ☐ Notice that Lagrange interpolation makes no restriction that the points in the table be evenly spaced.
- ☐ As a check, it is also worth noting that the sum of the Lagrange multipliers equals one, $\sum \lambda_i = 1$.
- ☐ Usually the Lagrange fit is made to only a small region of the table with a small value of n , even though the formula works perfectly well for fitting a high-degree polynomial to the entire table.

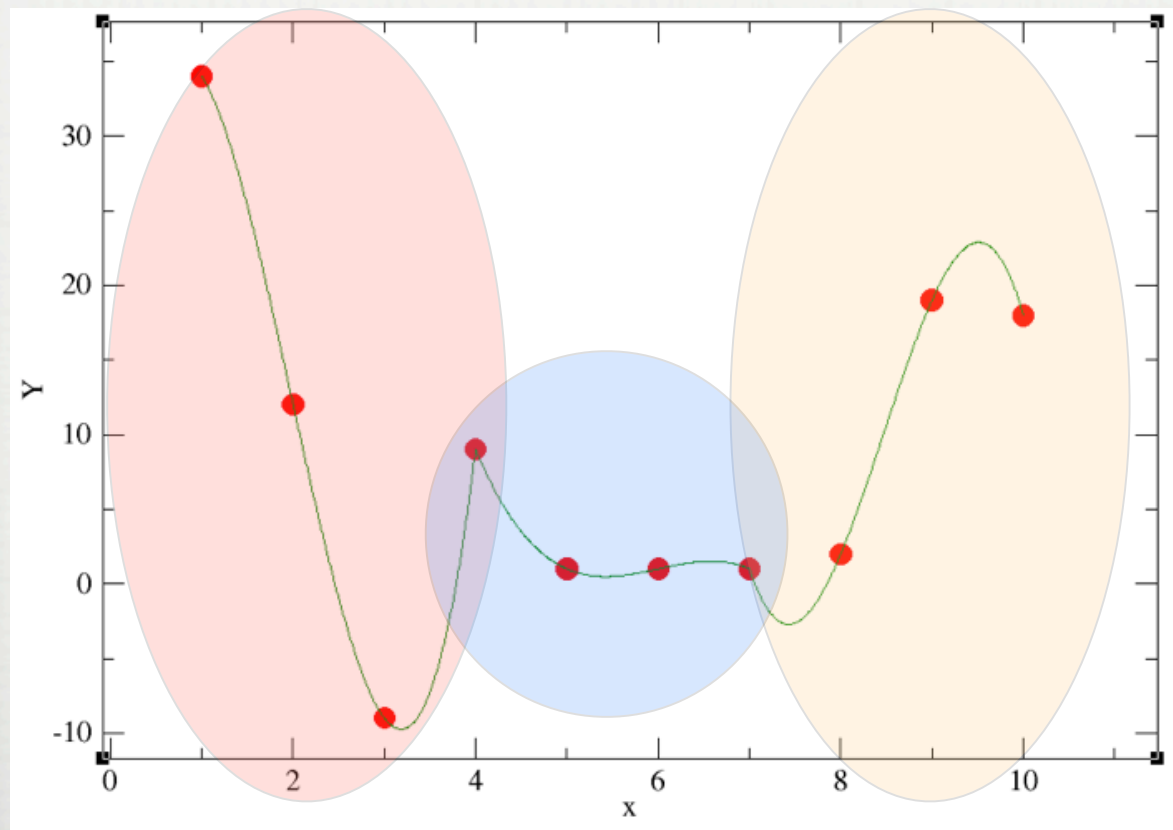


LOCAL INTERPOLATION

- Here, we interpolate the function, small interval by small interval, with a low order polynomial (here: 3-points or parabola)

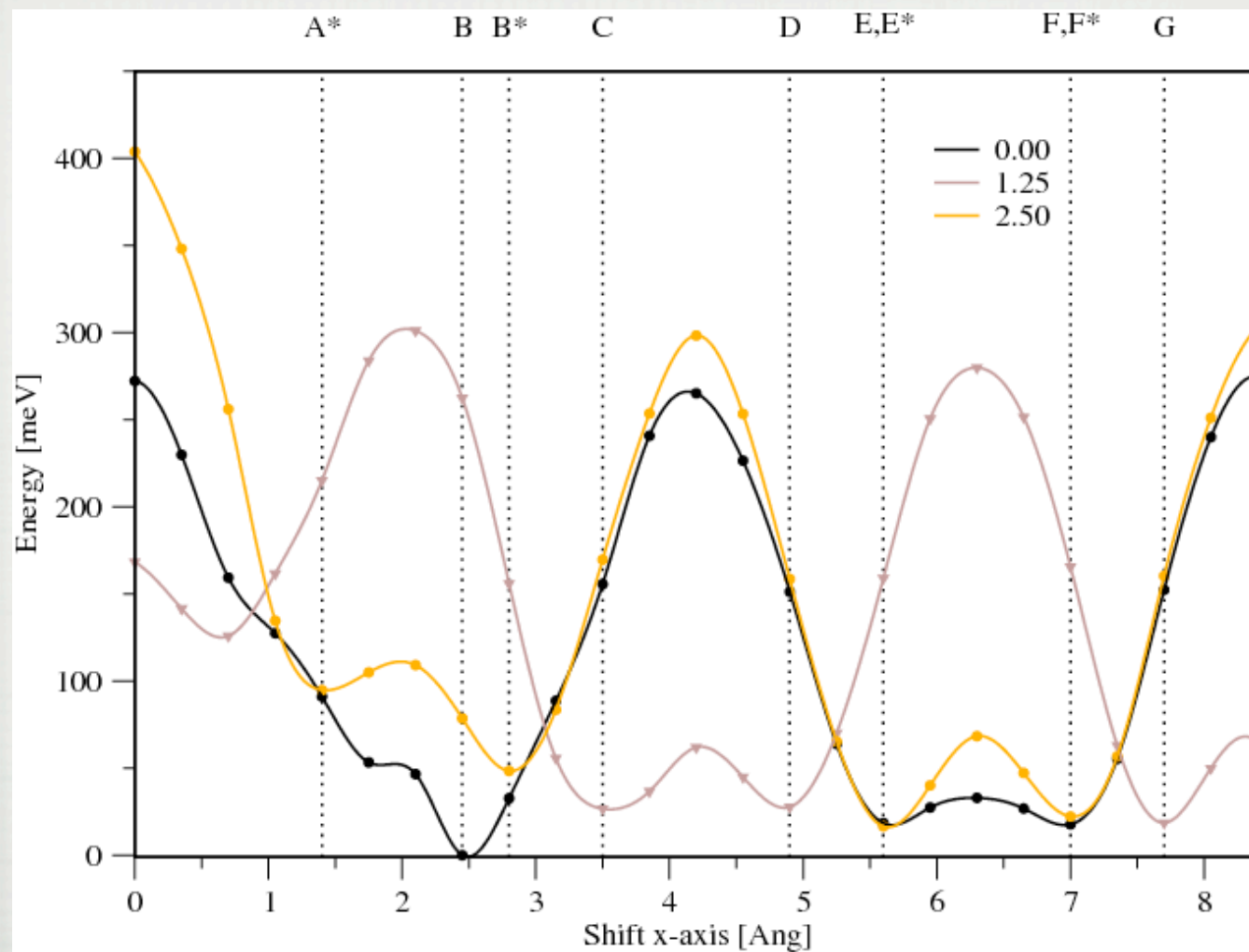


4-POINT SEGMENTATION (THIRD ORDER POLYNOMIAL)



PROBLEMS: DISCONTINUITY IN DERIVATIVE!

PART2: SPLINE



SPLINE: INTRODUCTION

- ☐ Fitting parabolas (three-point interpolation) within a table may avoid the erroneous and possibly catastrophic deviations of a high-order formula.
- ☐ (Two-point interpolation, which connects the points with straight lines, may not lead you far astray, but it is rarely pleasing to the eye or precise.)
- ☐ A sophisticated variation of $n = 4$ interpolation, known as cubic splines, often leads to surprisingly eye-pleasing fits.

SPLINE: INTRODUCTION (II)

- In this approach, cubic polynomials are fit to the function in each interval, **with the additional constraint that the first and second derivatives of the polynomials must be continuous from one interval to the next.** This continuity of slope and curvature is what makes the spline fit particularly **eye-pleasing**.

SPLINE: C'TD

- ☐ The series of cubic polynomials obtained by spline-fitting a table can be integrated and differentiated, and is guaranteed to have well-behaved derivatives.
- ☐ The complexity of simultaneously matching polynomials and their derivatives over all the interpolation points leads to many simultaneous, linear equations to be solved.
- ☐ This makes splines unattractive for hand calculations, yet easy for computers.

- ✧ The basic approximation of splines is the representation of the function $g(x)$ in the subinterval $[x_i, x_{i+1}]$ with a cubic polynomial:

$$g(x) \simeq g_i(x) \quad \text{for } x_i \leq x \leq x_{i+1}$$

$$g_i(x) = g_i + g'_i(x - x_i) + \frac{1}{2}g''_i(x - x_i)^2 + \frac{1}{6}g'''_i(x - x_i)^3$$

- ✧ This representation makes it clear that the coefficients in the polynomial equal the values of $g(x)$ and to its first, second, and third derivatives at the tabulated points x_i . Derivatives beyond the third vanish.

- ✧ The computational chore is to determine these derivatives in terms of the N tabulated values g_i .
- ✧ The matching of g_i from one interval to the next (at the nodes) provides the equations

$$g_i(x_{i+1}) = g_{i+1}(x_{i+1}) \quad i = 1, N - 1$$

- ✧ The matching of the first and second derivatives at each subinterval's boundary provides the equations

$$g'_{i-1}(x_i) = g'_i(x_i) \quad g''_{i-1}(x_i) = g''_i(x_i)$$

To provide the additional equations needed to determine all constants, the third derivatives at adjacent nodes are matched. Values for the third derivatives are found by approximating them in terms of the second derivatives (our old FD approximation):

$$g_i''' \simeq \frac{g_{i+1}'' - g_i''}{x_{i+1} - x_i}$$

It is straightforward though complicated to solve for all the parameters.

BOUNDARIES

Matching at the boundaries of the intervals results in only $N - 2$ linear equations for N unknowns. Further input is required.

It usually is taken to be the boundary conditions at the endpoints $a = x_1$ and $b = x_N$, specifically, the second derivatives $g''(a)$, and $g''(b)$.

- **Natural spline:** Set $g''(a) = g''(b) = 0$, (This is “natural” because the derivative vanishes for the flexible spline drafting tool (its ends being free).)
- **Input values for g' at boundaries:** The computer uses $g'(a)$ to approximate $g''(a)$. If you do not know the first derivatives, you can calculate them numerically from the table of g_i values.
- **Input values for g'' at boundaries:** Knowing values is of course better than assuming values, but it requires more input. If the values of g'' are not known, they can be approximated by applying a forward-difference approximation to the tabulated values

HARD WORK

NUMERICAL RECIPES

The Art of Scientific Computing

THIRD EDITION

William H. Press
Saul A. Teukolsky
William T. Vetterling
Brian P. Flannery



Includes
CD-ROM

```

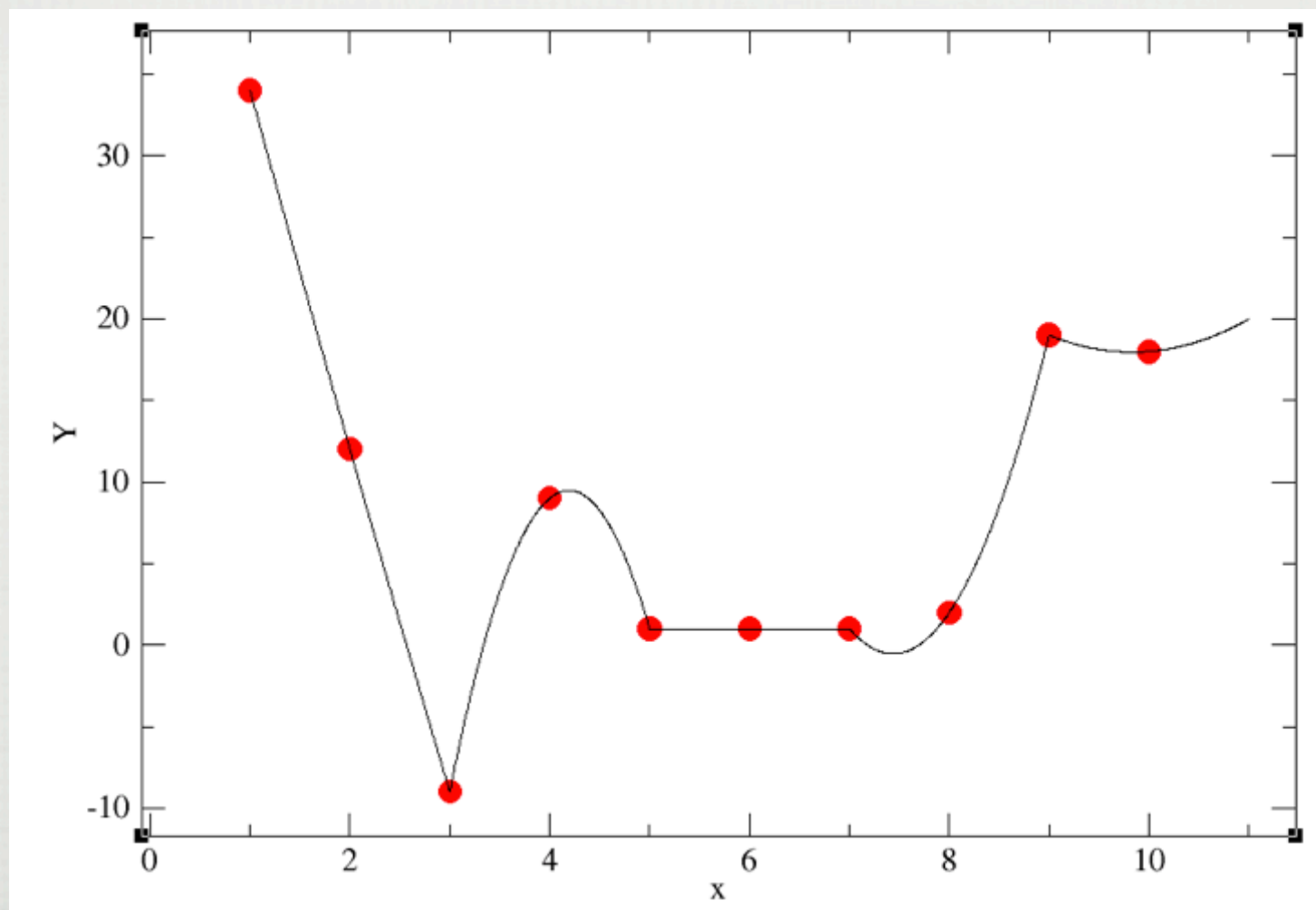
#include <iostream>
#include "nr3.h"
#include "interp_1d.h"
using namespace std;
int main () {
    int i,k;
    int kmax=50;
    double xx=0, gxx=0;
    double xxmin, xxmax;
    //
    int npoints;

    //GET INPUT
    cin >> npoints;
    //allocate memory
    VecDoub x(npoints), g(npoints);
    //read in data points
    for (i=0;i<npoints;i++){
        cin >> x[i] >> g[i];
    }
    //CREATE SPLINE OBJECT
    Spline_interp myspline (x,g);

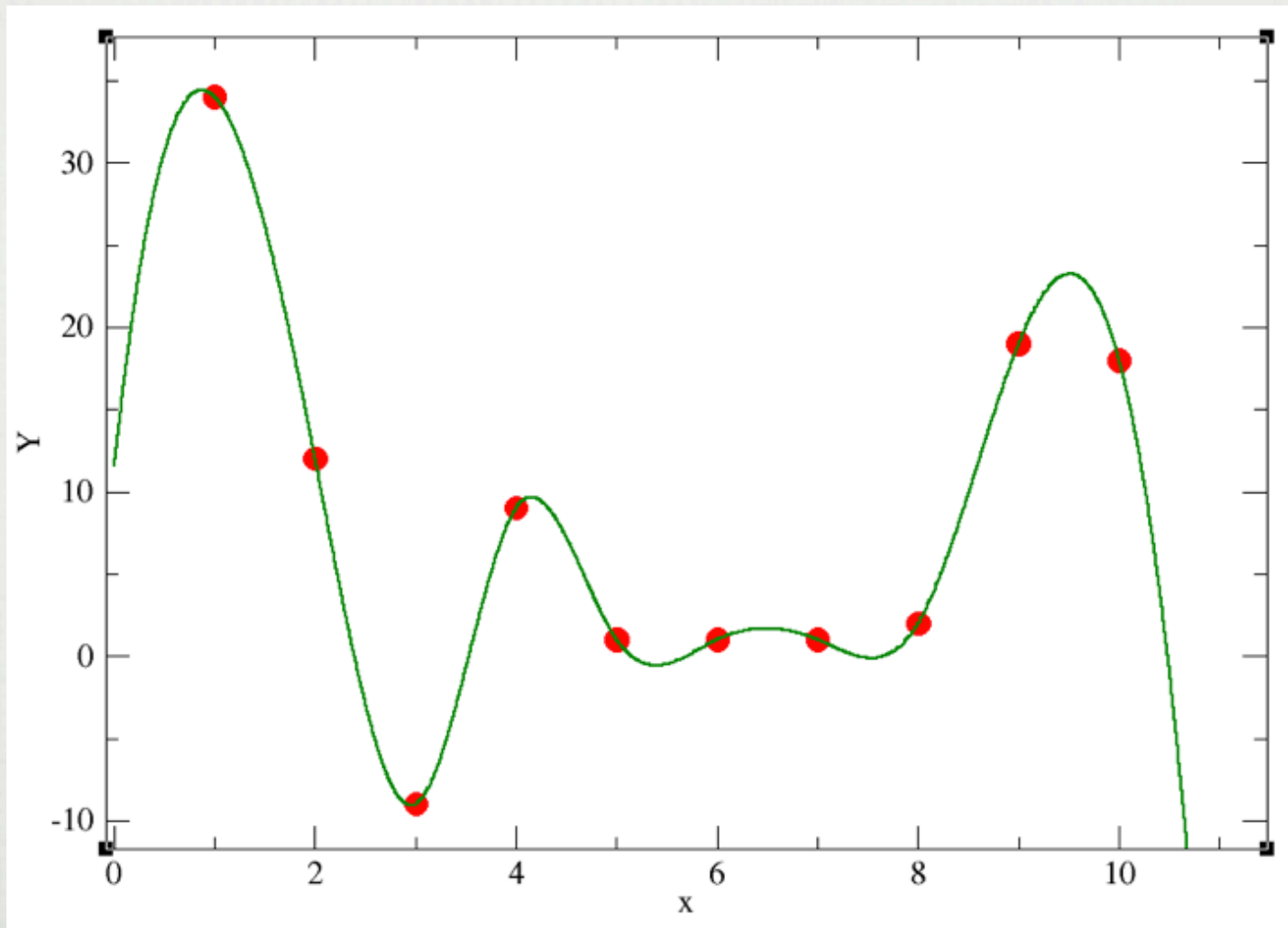
    //CREATE INTERPOLATION
    xxmin=x[0];
    xxmax=x[npoints-1];
    //
    for(k=0;k<kmax;k++){
        xx=xxmin+(double)k*(xxmax-xxmin)/((double)kmax-1);
        gxx= myspline.interp(xx);
        cout << xx << " " << gxx << endl;
    }
}

```

SPLINE WITH NUMREC



SPLINE!



USING SPLINES FOR INTEGRATION

- ☐ A powerful integration scheme is to fit an integrand with splines, and then integrate the cubic polynomials analytically.
- ☐ If you have the ability to actually calculate the function for arbitrary x , Gaussian quadrature may be preferable. We know that the spline fit to g in each interval is the cubic (9.8),

$$g(x) \simeq g_i + g'_i(x - x_i) + \frac{1}{2}g''_i(x - x_i)^2 + \frac{1}{6}g'''_i(x - x_i)^3$$

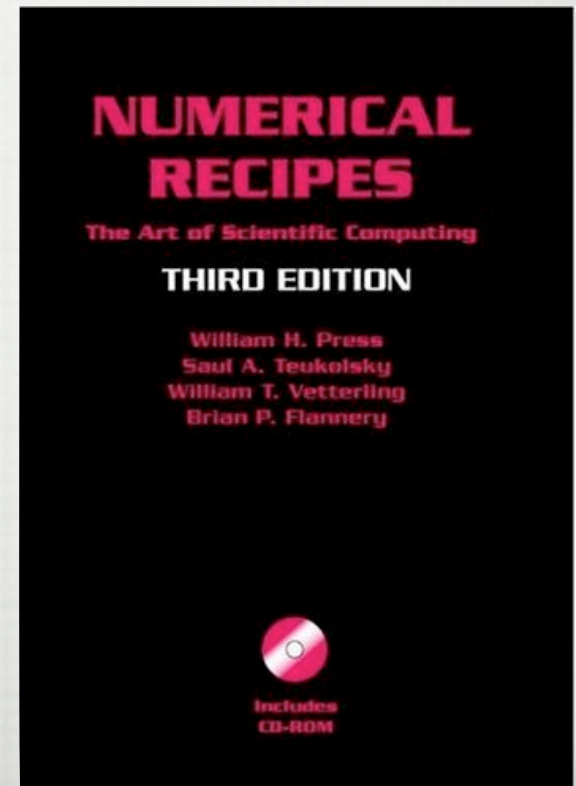
- ☐ It is easy to integrate this to obtain the integral of g for this interval, and then to sum over all intervals:

$$\int_{x_i}^{x_{i+1}} g(x) dx \simeq \left(g_i x + \frac{1}{2}g'_i x^2 + \frac{1}{6}g''_i x^3 + \frac{1}{24}g'''_i x^4 \right) \Big|_{x_i}^{x_{i+1}}$$
$$\int_{x_j}^{x_k} g(x) dx = \sum_{i=j}^k \int_{x_i}^{x_{i+1}} g(x) dx$$

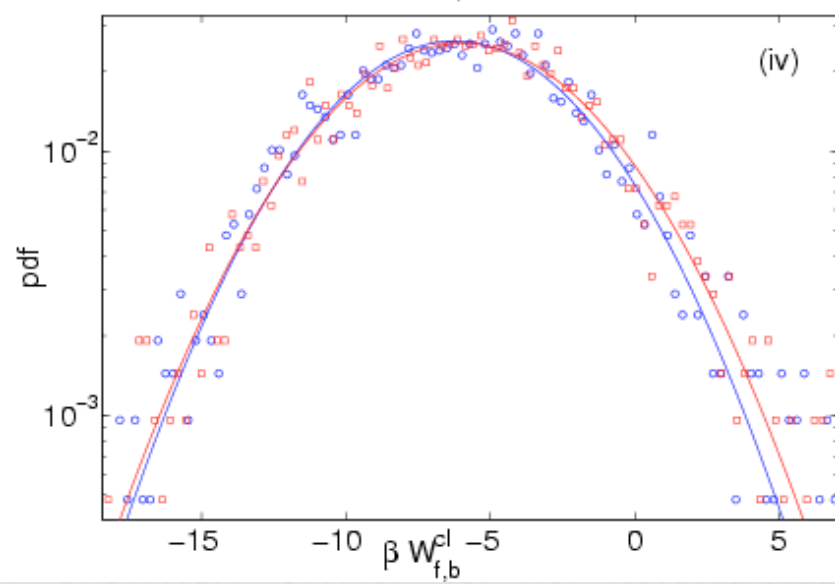
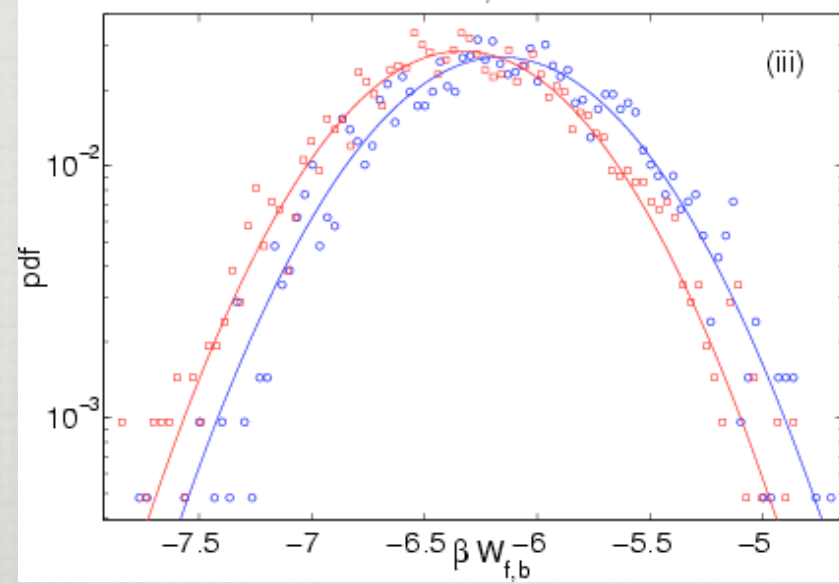
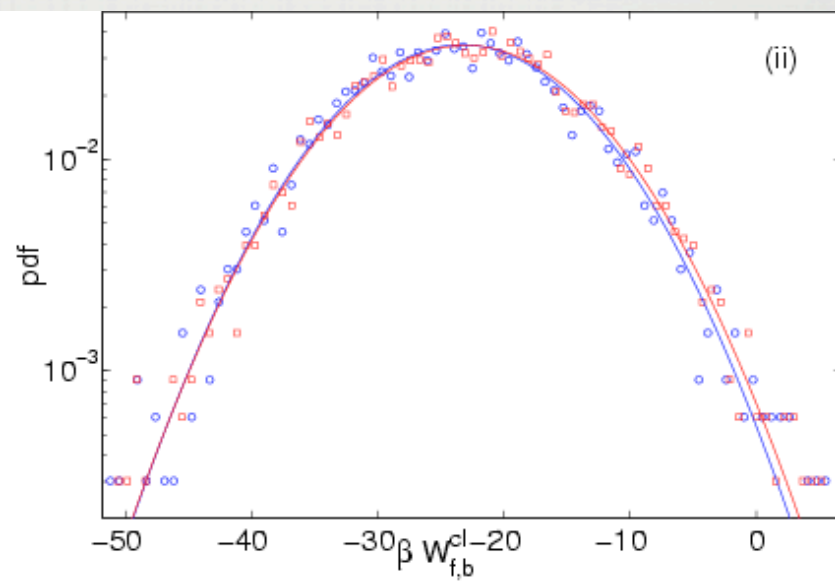
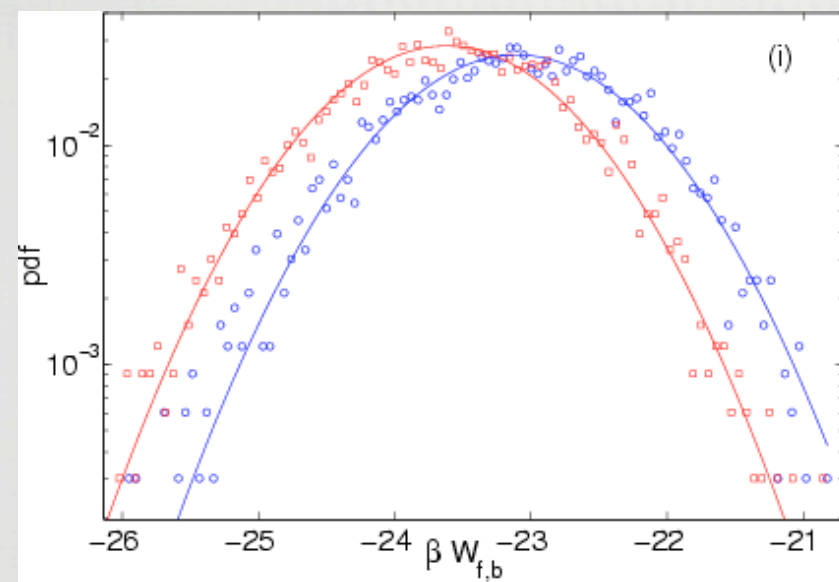
- ☐ Making the intervals smaller does not necessarily increase precision as subtractive cancellations may get large.

HOW DO WE USE THESE METHODS?

- ☐ Preferred method: using numerical libraries
- ☐ Go online to nr.com or look in a book...or download the routines...
- ☐ Example: spline
- ☐ <http://www.nr.com/dependencies/index.php>



PART 3:
FIT TO A FUNCTION (“FIT
TO THEORY”)



LEAST SQUARE FITTING: “GOODNESS OF A FIT”

- Imagine that you have measured N_D data values of the independent variable y as a function of the dependent variable x :

$$(x_i, y_i \pm \sigma_i) \quad i = 1, N_D$$

- where $\pm\sigma_i$ is the uncertainty in the i th value of y .
- Our goal is to determine how well a mathematical function $y = g(x)$ (also called theory or model) can describe these data.

$$g(x) = g(x; \{a_1, a_2, \dots, a_{M_P}\}) = g(x; \{a_m\})$$

- ❖ We assume that the model function $g(x)$ contains, in addition to the functional dependence on x , an additional dependence upon MP parameters $\{a_1, a_2, \dots, a_{M_P}\}$.
- ❖ The parameters $\{a_m\}$ are not variables, in the sense of numbers read from a meter, but rather are parts of the theoretical model such as the size of a box, the mass of a particle, or the depth of a potential well.

MINIMIZATION “CHI-SQUARE”

$$\chi^2 \quad \underline{\underline{\text{def}}} \quad \sum_{i=1}^{N_D} \left(\frac{y_i - g(x_i; \{a_m\})}{\sigma_i} \right)^2$$

- ✧ We use the chi-squared (χ^2) measure as a gauge of how well a theoretical function g reproduces data

$$\chi^2 \quad \stackrel{\text{def}}{=} \quad \sum_{i=1}^{N_D} \left(\frac{y_i - g(x_i; \{a_m\})}{\sigma_i} \right)^2$$

- ✧ The sum is over the N_D experimental points $(x_i, y_i \pm \sigma_i)$.
- ✧ The definition is such that smaller values of χ^2 are better fits, with $\chi^2 = 0$ occurring if the theoretical curve went through the center of every data point.
- ✧ Notice also that the $1/\sigma_i^2$ weighting means that measurements with larger errors contribute less to χ^2 .

- ✧ **Least-squares fitting refers to adjusting the theory until a minimum in χ^2 is found**
- ✧ **The goal is to find a curve that produces the least value for the summed squares of the deviations of the data from the function $g(x)$.**
- ✧ **In general, this is the best fit possible or the best way to determine the parameters in a theory.**
- ✧ **The MP parameters $\{a_m, m = 1, M_P\}$ that make χ^2 an extremum are found by solving the MP equations:**

$$\frac{\partial \chi^2}{\partial a_m} = 0 \quad \Rightarrow \quad \sum_{i=1}^{N_D} \frac{[y_i - g(x_i)]}{\sigma_i^2} \frac{\partial g(x_i)}{\partial a_m} = 0 \quad (m = 1, M_P)$$

GOODNESS OF A FIT

- ☐ When the deviations from theory are due to random errors and when these errors are described by a Gaussian distribution, there are some useful rules of thumb to remember.
- ☐ You know that your fit is good if the value of χ^2 calculated via the definition is approximately equal to the number of degrees of freedom $\chi^2 \approx ND - MP$, where ND is the number of data points and MP the number of parameters in the theoretical function.
- ☐ If your χ^2 is much less than $ND - MP$, it does not mean that you have a “great” theory or a really precise measurement; instead, you probably have too many parameters or have assigned errors (σ_i values) that are too large. In fact, too small a χ^2 may indicate that you are fitting the random scatter in the data rather than missing ~ 1 of the error bars, as expected for Gaussian statistics.

FITTING TO A STRAIGHT LINE: LINEAR REGRESSION

- The MP simultaneous equations simplify considerably if the functions $g(x; \{a_i\})$ depend linearly on the parameter values a_i :

$$g(x; \{a_1, a_2\}) = a_1 + a_2 x$$

- In this case there are MP = 2 parameters, **the slope a_2 and the y intercept a_1** .
- A unique solution is not possible unless the number of data points is equal to or greater than the number of parameters.
- For this linear case, there are just two derivatives,

$$\frac{\partial g(x_i)}{\partial a_1} = 1 \qquad \frac{\partial g(x_i)}{\partial a_2} = x_i$$

- and after substitution, the χ^2 minimization equations can be solved

LINEAR REGRESSION (2)

$$a_1 = \frac{S_{xx}S_y - S_xS_{xy}}{\Delta}$$

$$a_2 = \frac{SS_{xy} - S_xS_y}{\Delta}$$

$$S = \sum_{i=1}^{N_D} \frac{1}{\sigma_i^2}$$

$$S_x = \sum_{i=1}^{N_D} \frac{x_i}{\sigma_i^2}$$

$$S_y = \sum_{i=1}^{N_D} \frac{y_i}{\sigma_i^2}$$

$$S_{xx} = \sum_{i=1}^{N_D} \frac{x_i^2}{\sigma_i^2}$$

$$S_{xy} = \sum_{i=1}^{N_D} \frac{x_i y_i}{\sigma_i^2}$$

$$\Delta = SS_{xx} - S_x^2$$

- Statistics also gives you an expression for the variance or uncertainty in the deduced parameters:

$$\sigma_{a_1}^2 = \frac{S_{xx}}{\Delta}$$

$$\sigma_{a_2}^2 = \frac{S}{\Delta}$$

```
#include <iostream>
#include "nr3.h"
#include "gamma.h"
#include "incgammabeta.h"
#include "fitab.h"
```

```
using namespace std;
```

```
int main () {
    int i,k;
    int kmax=500;
    double xx=0, gxx=0;
    double aa, bb, xxmin, xxmax;
    //
    int npoints;
    cin >> npoints;
    //
    VecDoub x(npoints), g(npoints);
    //
    for (i=0;i<npoints;i++){
        cin >> x[i] >> g[i];
    }
    Fitab myreg(x,g);
    //
    xxmin=x[0];
    xxmax=x[npoints-1];
    //
    aa=myreg.a;
    bb=myreg.b;
    cout << aa << " " << bb << " " << myreg.chi2<< endl;

    for(k=0;k<kmax;k++){
        xx=xxmin+(double)k*(xxmax-xxmin)/((double)kmax-1);
        gxx=bb*xx+aa;
        cout << xx << " " << gxx <<endl;
    }
}
```

LINEAR REGRESSION

sources: GHCN 1880-01/2011 + SST: 1880-11/1981 HadISST1
12/1981-01/2011 Reynolds v2
using elimination of outliers and homogeneity adjustment
Notes: 1950 DJF = Dec 1949 - Feb 1950 ; ***** = missing

Year	Jan	Feb	Mar	Apr	May	Jun	Jul	Aug	Sept	Oct	Nov	Dec	J-B	J-B	JMT	JSH	JRN	Year
1961	5	21	10	11	22	12	1	3	8	7	8	-15	7	15	14	8	7	1961
1962	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1962
1963	1	19	-13	-7	-2	-6	14	26	25	9	14	3	8	8	7	-8	15	16 1963
1964	-5	-8	-26	-33	-28	-2	-6	-24	-37	-30	-20	-21	-18	-3	-29	-11	-29	1964
1965	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1965
1966	-16	-11	-11	-11	-7	-1	11	-5	-1	-15	0	-4	-3	-3	-3	-2	-5	1966
1967	-7	-23	7	-2	-11	6	1	6	10	-2	-1	-1	-1	-1	-1	-1	-1	1967
1968	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1968
1969	-7	-8	-2	-20	13	-11	-4	0	9	14	16	30	8	4	-9	-10	3	13 1969
1970	10	23	9	5	-2	-1	-12	13	3	4	-12	-1	-11	-10	-11	6	21	3 1970
1971	-2	-27	-1	-22	-11	-2	-2	-2	-2	-2	-2	-2	-2	-2	-2	-2	-2	1971
1972	-26	-20	-2	-1	-2	0	20	5	4	-2	-18	0	-2	-19	-2	9	2	9 1972
1973	26	28	26	24	22	16	9	1	7	13	4	-8	14	16	24	9	8	1973
1974	14	-14	-14	-14	-14	-14	-14	-14	-14	-14	-14	-14	-14	-14	-14	-14	-14	1974
1975	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1975
1976	-8	-12	-28	-16	-29	-15	-10	-20	-12	-29	-11	0	-16	-18	-14	-24	-16	1976
1977	3	8	11	9	1	-6	4	-21	5	-4	6	1	1	1	4	7	-9	3 1977
1978	6	-18	8	10	1	-8	4	-7	9	18	18	19	39	8	5	-4	2	18 1978
1980	21	28	26	26	26	29	9	22	17	12	6	22	6	19	21	29	26	14 1980
Year	Jan	Feb	Mar	Apr	May	Jun	Jul	Aug	Sept	Oct	Nov	Dec	J-B	J-B	JMT	JSH	JRN	Year
1981	0	7	-12	-3	10	1	11	-3	2	3	34	4	4	12	-2	3	2	1981
1982	0	34	26	27	30	14	11	27	34	9	23	10	25	27	37	11	22	1982
1983	24	29	24	24	24	24	24	24	24	24	24	24	24	24	24	24	24	1983
1984	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1984
1985	15	-14	11	8	5	12	-8	0	6	-1	7	4	2	-5	-7	5	3	1985
1986	19	37	24	16	16	4	5	7	0	5	1	6	12	12	21	20	6	2 1986
1987	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1987
1988	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1988
1989	51	35	45	35	38	40	26	31	30	29	-3	19	31	33	33	33	33	1989
1990	3	28	27	17	4	5	28	26	31	25	8	26	19	19	17	16	20	1990

1928	9	-3	-19	-25	-25	-20	-11	-16	-11	-11	-1	-10	-15	-15	-10	-21	-18	0	1928
1929	10	-1	-19	-25	-25	-20	-11	-16	-11	-11	-1	-10	-15	-15	-10	-21	-18	0	1929
1930	-17	-15	-17	-17	-18	-15	-8	-8	-8	-8	-9	-7	-8	-12	-24	-13	-10	6	1930
1931	0	-12	-2	-14	-11	-11	-11	-8	-8	-2	-2	-2	-3	-6	-9	-6	-6	2	1931
1932	-12	-12	-12	-12	-12	-12	-12	-12	-12	-12	-12	-12	-12	-12	-12	-12	-12	-12	1932
1933	-22	-15	-16	-16	-16	-16	-7	-11	-15	-15	-28	-9	-19	-17	-19	-17	-12	-13	1933
1934	-22	-15	-16	-16	-16	-16	-7	-11	-15	-15	-28	-9	-19	-17	-19	-17	-12	-13	1934
1935	-26	-21	-4	-20	-23	-10	-11	-13	-14	0	-22	-12	-12	-11	0	-13	-12	-13	1935
1936	-26	-21	-4	-20	-23	-10	-11	-13	-14	0	-22	-12	-12	-11	0	-13	-12	-13	1936
1937	3	20	-7	-2	4	9	8	18	15	19	0	7	8	11	7	7	7	7	1937
1938	15	10	20	20	6	-3	8	6	12	16	16	10	10	11	8	16	4	6	1938
1939	-1	3	3	3	3	3	3	3	3	3	3	3	3	3	3	3	3	3	1939
1940	-17	-1	3	3	11	4	-1	19	-3	7	2	6	12	4	7	6	7	6	1940
Year	Jan	Feb	Mar	Apr	May	Jun	Jul	Aug	Sep	Oct	Nov	Dec	J-J-B-N	Jan	Feb	Mar	Apr	May	Jun
1942	21	-9	-1	0	8	5	-2	1	-2	1	1	1	1	1	1	1	1	1	1
1943	13	12	-8	0	16	12	0	15	0	23	19	25	19	25	19	25	19	25	19
1944	16	16	16	16	16	16	16	16	16	16	16	16	16	16	16	16	16	16	16
1945	11	11	11	11	11	11	11	11	11	11	11	11	11	11	11	11	11	11	11
1946	-3	-3	-3	-3	-3	-3	-3	-3	-3	-3	-3	-3	-3	-3	-3	-3	-3	-3	-3
1947	-3	-1	14	5	-7	-2	-7	-2	-7	-12	12	10	0	-1	10	-5	-5	6	1947
1948	-3	-1	14	5	-7	-2	-7	-2	-7	-12	12	10	0	-1	10	-5	-5	6	1948
1949	-14	-16	-4	-11	-8	-20	-10	-10	-5	-6	-10	-10	-7	-8	-7	-8	-12	-4	1949
1950	-25	-26	-2	-16	-14	-5	-10	-11	-16	-29	-10	-16	-16	-21	-12	-11	-11	-11	1950
1951	-25	-26	-2	-16	-14	-5	-10	-11	-16	-29	-10	-16	-16	-21	-12	-11	-11	-11	1951
1952	14	14	8	8	0	4	8	16	9	-3	-3	3	5	15	1	7	-2	1952	
1953	14	14	8	8	0	4	8	16	9	-3	-3	3	5	15	1	7	-2	1953	
1954	-7	-7	-7	-7	-12	-12	-12	-12	-12	-12	-12	-12	-10	-7	-2	-11	-17	1954	
1955	-7	-7	-7	-7	-12	-12	-12	-12	-12	-12	-12	-12	-10	-7	-2	-11	-17	1955	
1956																			

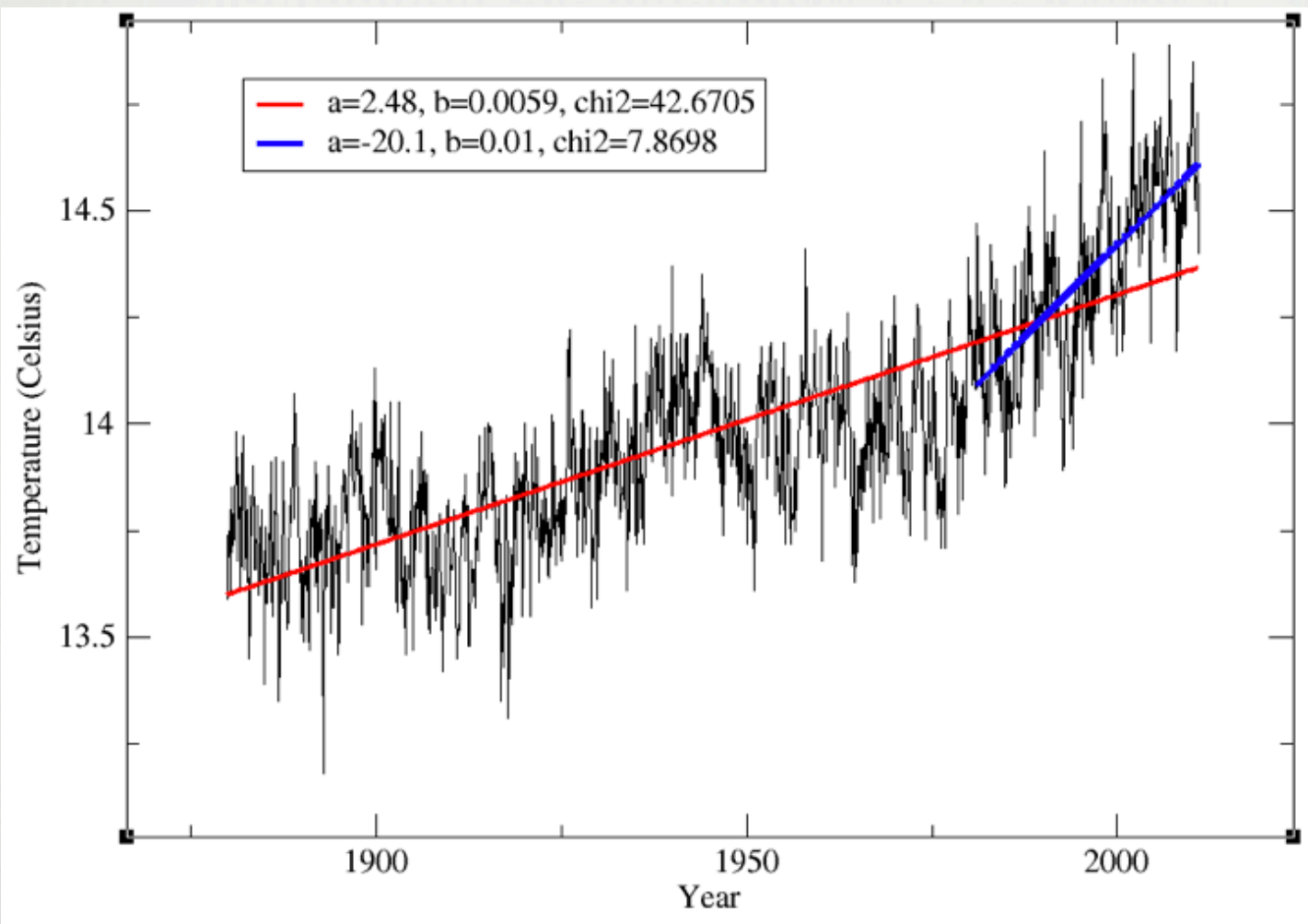
2006	46	61	58	42	38	55	42	65	57	59	64	71	55	54	56	46	54	60	2006
2007	89	63	64	68	60	52	55	54	50	54	47	40	58	61	74	64	54	50	2007
2008	17	26	66	45	41	34	52	34	53	55	58	47	44	43	28	50	40	55	2008
2009	85	46	47	50	54	61	66	57	65	61	68	60	55	56	49	50	61	64	2009
2010	70	75	85	75	64	55	50	54	54	62	73	40	63	65	69	75	53	63	2010
2011	46																		2011
Year	Jan	Feb	Mar	Apr	May	Jun	Jul	Aug	Sep	Oct	Nov	Dec	J-J	B-N	J-T	M-M	J-J	S-N	
Divide by 100 to get changes in degrees Celsius (deg-C).																			
Multiply that result by 1.8(=9/5) to get changes in degrees Fahrenheit (deg-F).																			
Best estimate for absolute global mean for 1951-1980 is 14.0 deg-C or 57.2 deg-F, so add that to the temperature change if you want to use an absolute scale (this note applies to global annual means only, J-J and B-N !)																			
Example	--	Table Value :		40				change :		0.40 deg-C or 0.72 deg-F				abs. scale if global annual mean :		14.0 deg-C or 57.92 deg-F			

Divide by 100 to get changes in degrees Celsius (deg-C).
Multiply that result by 1.8(=9/5) to get changes in degrees Fahrenheit (deg-F).

Best estimate for absolute global mean for 1951-1980 is 14.0 deg-C or 57.2 deg-F, so add that to the temperature change if you want to use an absolute scale (this note applies to global annual means only, J-D and D-N !)

Example	--	Table Value :	40
		change :	0.40 deg-C or 0.72 deg-F
obs. scale if global annual mean :			14.40 deg-C or 57.92 deg-F

Year	Jan	Feb	Mar	Apr	May	Jun	Jul	Aug	Sep	Oct	Nov	Dec	J-J-10	D-JT	1946	1947	1948	1949	1950
1951	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1
1952	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1
1953	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1
1954	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1
1955	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1
1956	-10	-16	-10	-10	-10	-10	-10	-10	-10	-10	-10	-10	-10	-10	-10	-10	-10	-10	-10
1957	-7	-20	-10	-10	-10	-10	-10	-10	-10	-10	-10	-10	-10	-10	-10	-10	-10	-10	-10
1958	-7	-20	-10	-10	-10	-10	-10	-10	-10	-10	-10	-10	-10	-10	-10	-10	-10	-10	-10
1959	-7	-20	-10	-10	-10	-10	-10	-10	-10	-10	-10	-10	-10	-10	-10	-10	-10	-10	-10
1960	-7	-20	-10	-10	-10	-10	-10	-10	-10	-10	-10	-10	-10	-10	-10	-10	-10	-10	-10
1961	-7	-20	-10	-10	-10	-10	-10	-10	-10	-10	-10	-10	-10	-10	-10	-10	-10	-10	-10
1962	-7	-20	-10	-10	-10	-10	-10	-10	-10	-10	-10	-10	-10	-10	-10	-10	-10	-10	-10
1963	-7	-20	-10	-10	-10	-10	-10	-10	-10	-10	-10	-10	-10	-10	-10	-10	-10	-10	-10
1964	-7	-20	-10	-10	-10	-10	-10	-10	-10	-10	-10	-10	-10	-10	-10	-10	-10	-10	-10
1965	-7	-20	-10	-10	-10	-10	-10	-10	-10	-10	-10	-10	-10	-10	-10	-10	-10	-10	-10
1966	-7	-20	-10	-10	-10	-10	-10	-10	-10	-10	-10	-10	-10	-10	-10	-10	-10	-10	-10
1967	-7	-20	-10	-10	-10	-10	-10	-10	-10	-10	-10	-10	-10	-10	-10	-10	-10	-10	-10
1968	-7	-20	-10	-10	-10	-10	-10	-10	-10	-10	-10	-10	-10	-10	-10	-10	-10	-10	-10
1969	-7	-20	-10	-10	-10	-10	-10	-10	-10	-10	-10	-10	-10	-10	-10	-10	-10	-10	-10
1970	-7	-20	-10	-10	-10	-10	-10	-10	-10	-10	-10	-10	-10	-10	-10	-10	-10	-10	-10
1971	-7	-20	-10	-10	-10	-10	-10	-10	-10	-10	-10	-10	-10	-10	-10	-10	-10	-10	-10
1972	-7	-20	-10	-10	-10	-10	-10	-10	-10	-10	-10	-10	-10	-10	-10	-10	-10	-10	-10
1973	-7	-20	-10	-10	-10	-10	-10	-10	-10	-10	-10	-10	-10	-10	-10	-10	-10	-10	-10
1974	-7	-20	-10	-10	-10	-10	-10	-10	-10	-10	-10	-10	-10	-10	-10	-10	-10	-10	-10
1975	-7	-20	-10	-10	-10	-10	-10	-10	-10	-10	-10	-10	-10	-10	-10	-10	-10	-10	-10
1976	-7	-20	-10	-10	-10	-10	-10	-10	-10	-10	-10	-10	-10	-10	-10	-10	-10	-10	-10
1977	-7	-20	-10	-10	-10	-10	-10	-10	-10	-10	-10	-10	-10	-10	-10	-10	-10	-10	-10
1978	-7	-20	-10	-10	-10	-10	-10	-10	-10	-10	-10	-10	-10	-10	-10	-10	-10	-10	-10



WITH EXPERIMENTAL ERROR!

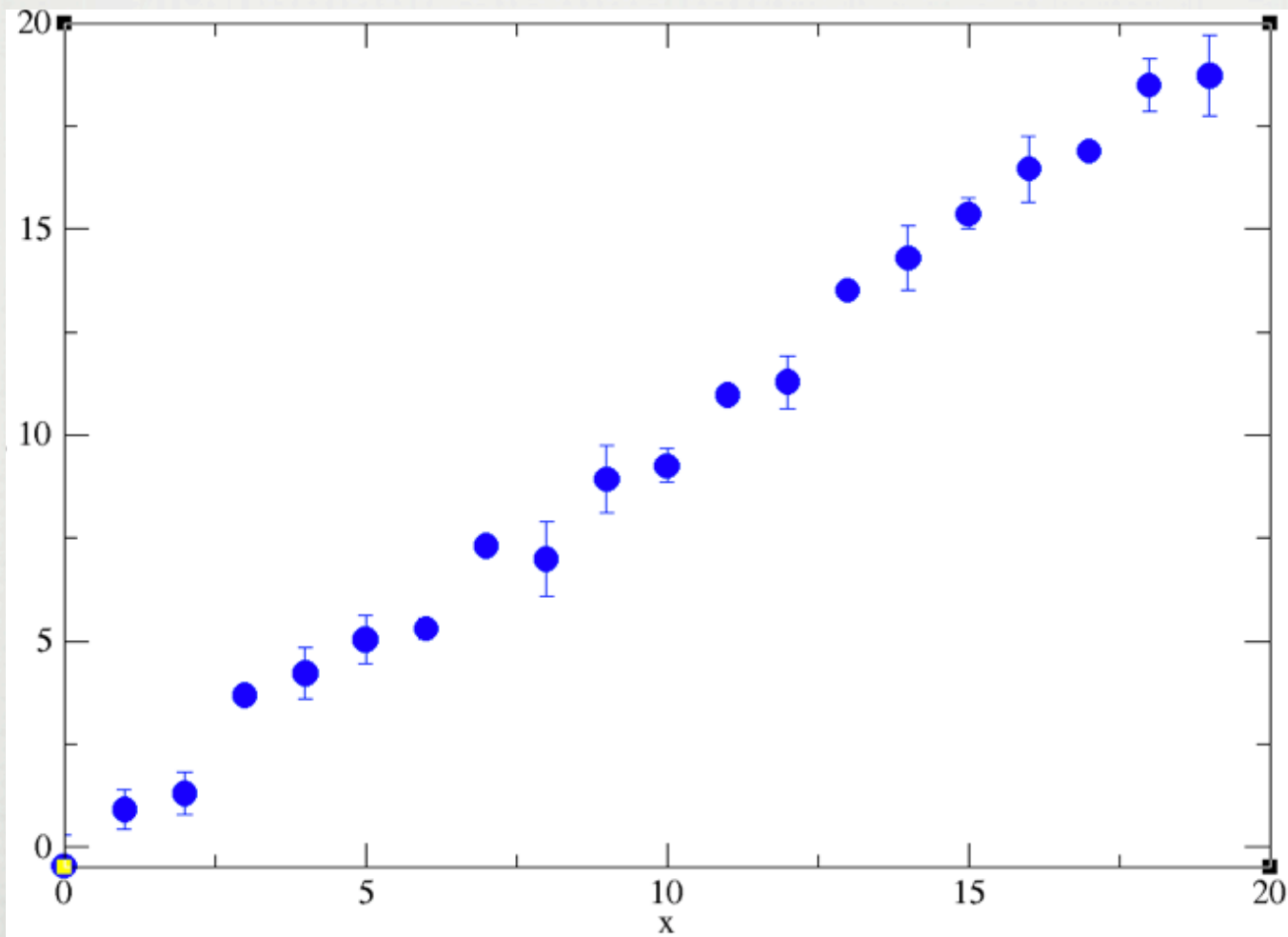
```
#include <iostream>
#include "nr3.h"
#include "gamma.h"
#include "incgammabeta.h"
#include "fitab.h"

using namespace std;
double randDouble(double low, double high)
{
    double temp;
    temp = ((double) rand() / (static_cast<double>(RAND_MAX) + 1.0)) * (high - low) + low;
    return temp;
}
int main () {
    int i,k;
    int kmax=500;
    double xx=0, gxx=0;
    double aa, bb, xxmin, xxmax;
    //
    int npoints=20;
    srand((unsigned) time(0));
    VecDoub x(npoints), g(npoints), sigma(npoints);

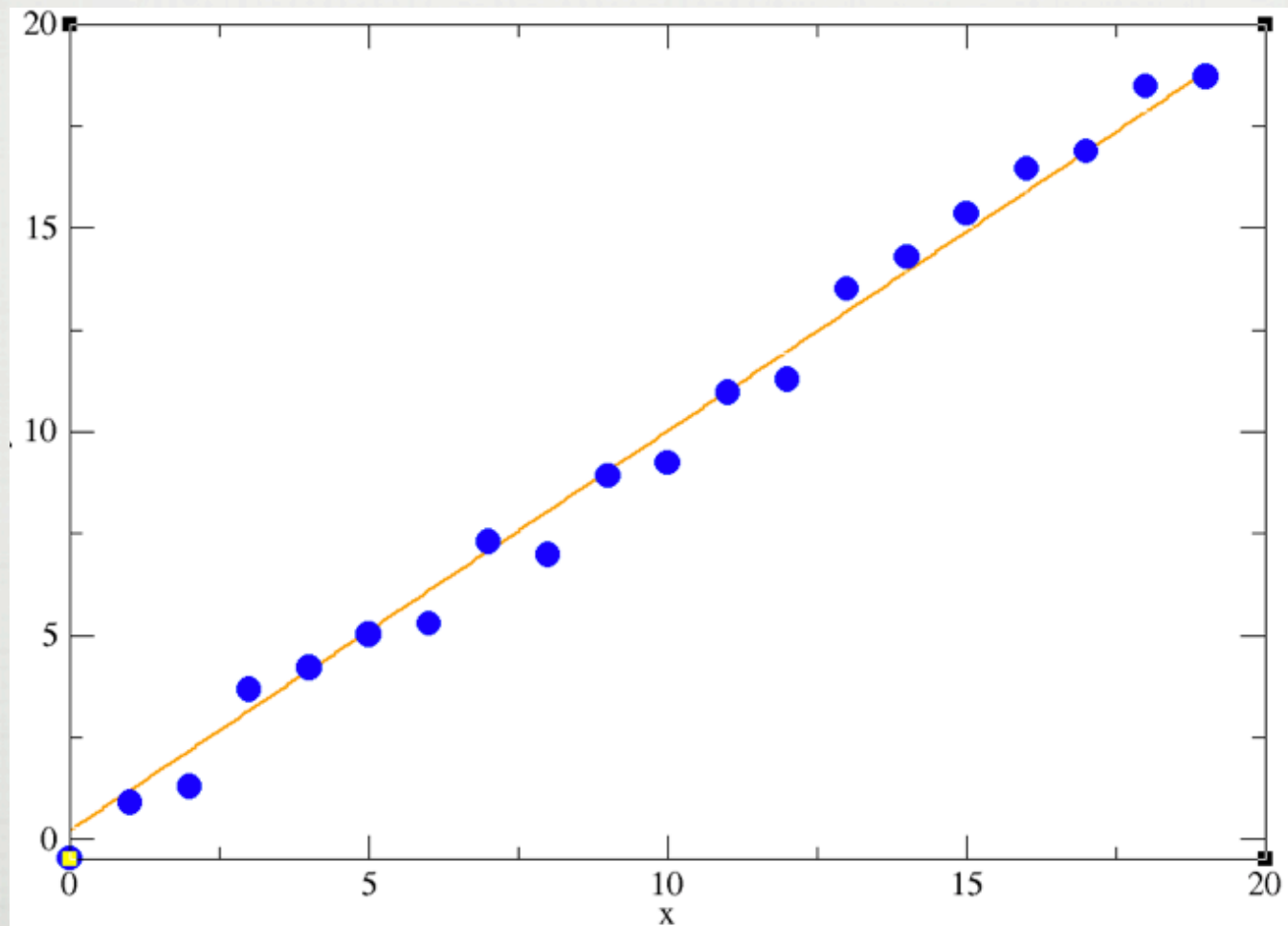
    for (i=0;i<npoints;i++){
        x[i]=double(i);
        g[i]=randDouble(-1.0,1.0)+x[i];
        sigma[i]=randDouble(-1.,1.0);
        cout << x[i] << " " << g[i] << " " << sigma[i]<< endl;
    }
    Fitab myreg(x,g,sigma);

    //
    xxmin=x[0];
    xxmax=x[npoints-1];
    //
    aa=myreg.a;
    bb=myreg.b;
    cout << aa << " " << bb << " " << myreg.chi2<< endl;
    for(k=0;k<kmax;k++){
        xx=xxmin+(double)k*(xxmax-xxmin)/((double)kmax-1);
        gxx=bb*xx+aa;
        cout << xx << " " << gxx <<endl;
    }
}
```

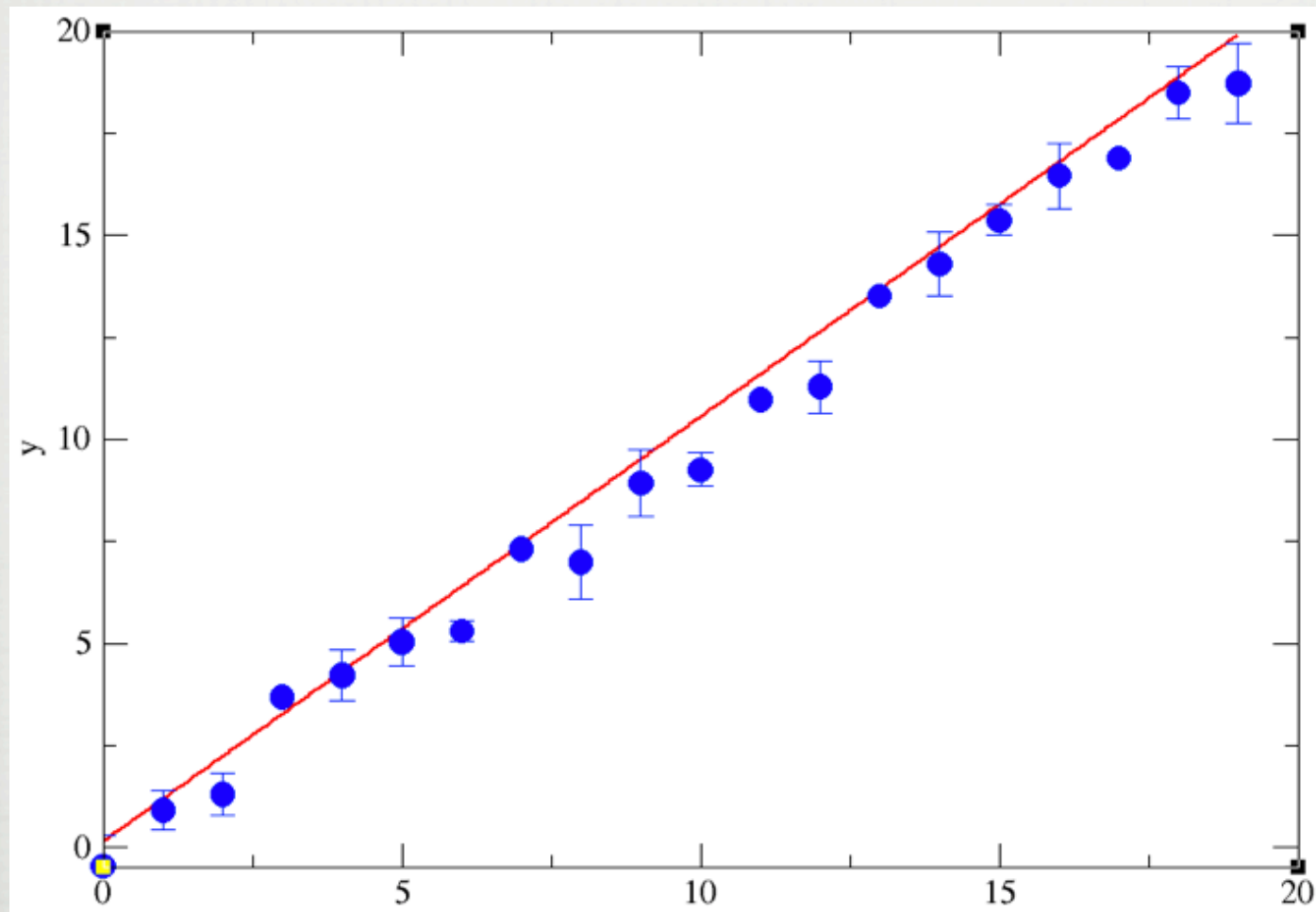
DATA SET



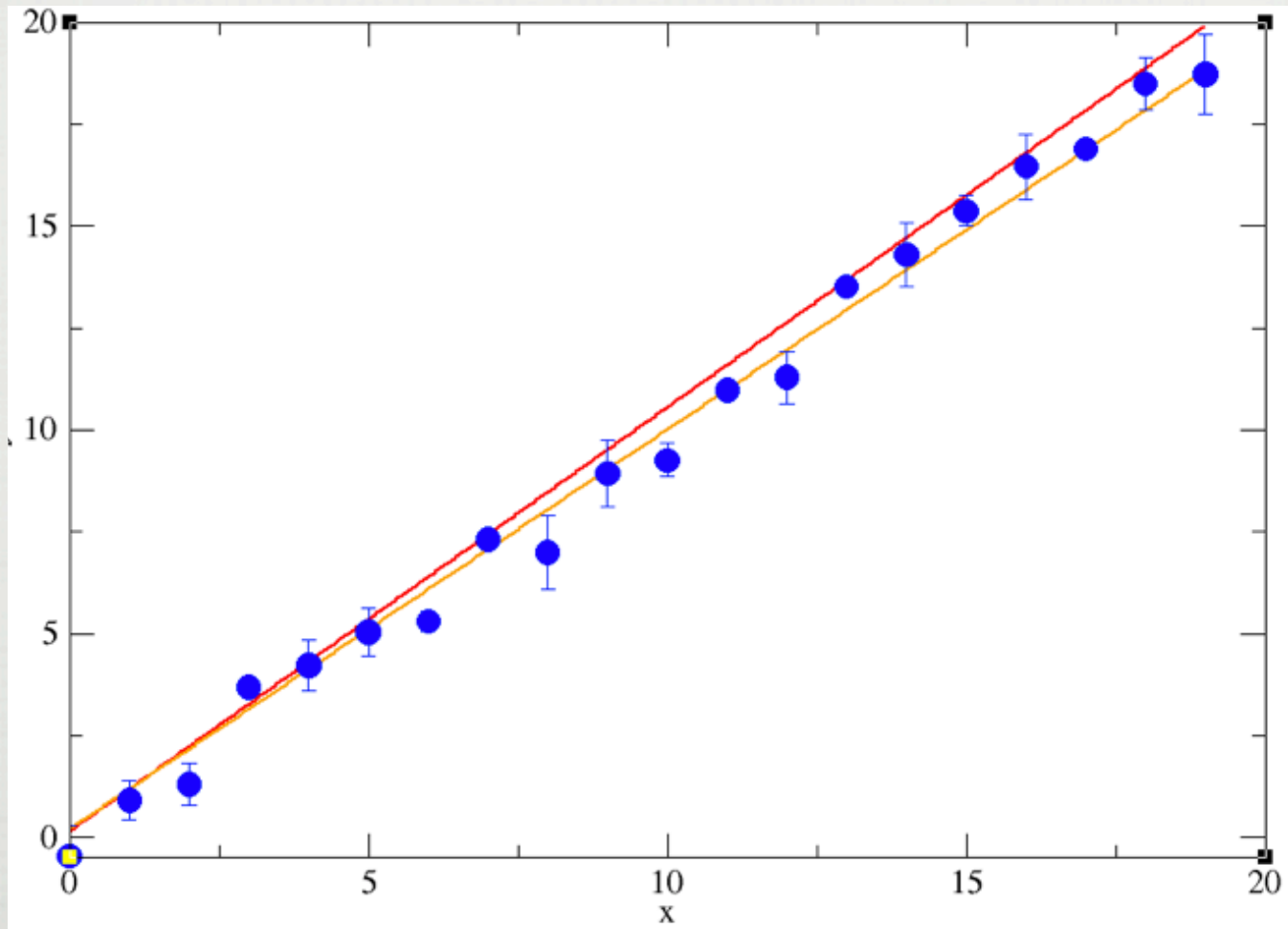
REGRESSION



REGRESSION WITH ERRORS



COMPARISON



SUMMARY

- ☐ **Polynomial fits**

- ☐ Lagrange formula and Neville's algorithm

- ☐ Can fit polynomial of order $N-1$ passing exactly through N points

- ☐ **Spline fits**

- ☐ More pleasing for the eye

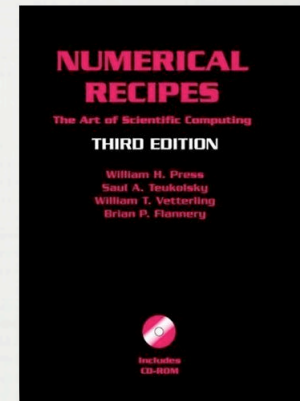
- ☐ 3rd order polynomial with continuity of slope and curvature

- ☐ **Least $\sum x_i^2$ fits**

- ☐ best fit does not necessarily goes though all the points

- ☐ very powerful when we know the analytical form of the solution

IN PRACTICE



- ☐ We use “numerical recipes”
- ☐ Today: we will work on computing splines using numrec.
- ☐ See LMS


```

#include <iostream>
#include "nr3.h"
#include "interp_1d.h"
using namespace std;
int main () {
    int i,k;
    int kmax=50;
    double xx=0, gxx=0;
    double xxmin, xxmax;
    //
    int npoints;

    //GET INPUT
    cin >> npoints;
    //allocate memory
    VecDoub x(npoints), g(npoints);
    //read in data points
    for (i=0;i<npoints;i++){
        cin >> x[i] >> g[i];
    }
    //CREATE SPLINE OBJECT
    Spline_interp myspline (x,g);

    //CREATE INTERPOLATION
    xxmin=x[0];
    xxmax=x[npoints-1];
    //
    for(k=0;k<kmax;k++){
        xx=xxmin+(double)k*(xxmax-xxmin)/((double)kmax-1);
        gxx= myspline.interp(xx);
        cout << xx << " " << gxx << endl;
    }
}

```

SPLINE WITH NUMREC