3. Numerical analysis I

1. Root finding: Bisection method
2. Root finding: Newton-Raphson method
3. Interpolation
4. Curve fitting: Least square method
5. Curve fitting in MATLAB
6. Summary

Text

A. Gilat, *MATLAB: An Introduction with Applications*, 4th ed., Wiley

3.1. Root finding: Bisection method

- Formulation of the problem
- Idea of the bisection method
- MATLAB code of the bisection method
- Root finding with build-in MATLAB function fzero

Reading assignment

Gilat 7.9, 9.1

http://en.wikipedia.org/wiki/Bisection_method

3.1. Root finding: Bisection method

Problem statement

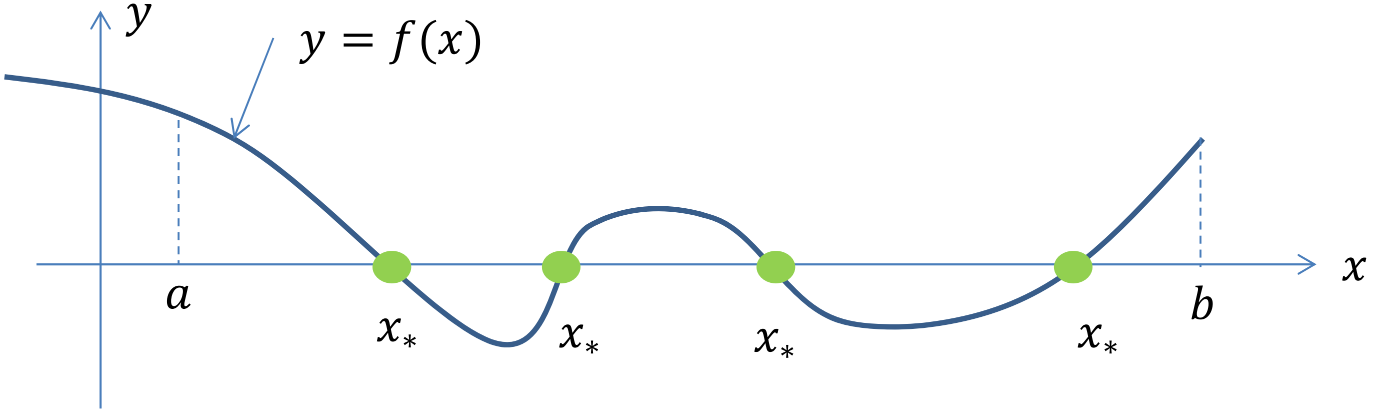
We need to find real **roots** x_*, of an equation

$$f(x_*) = 0 \tag{3.1.1}$$

in the interval $a < x < b$, where $f(x)$ is the **continuous** function.

Root of Eq. (3.1.1) is the (real) number that turns this equation into identity.

In general, a non-linear equation can have arbitrary number of roots in a fixed interval (a, b).



Examples:

- Linear equation

$$px_* = q, \qquad f(x) = px - q. \qquad \text{Only one root } x_* = q/p.$$

- Quadratic equation

$$px_*^2 + qx_* + r = 0, \qquad f(x) = px^2 + qx + r. \qquad \text{Can have 0, 1, or 2 real roots.}$$

- Transcendental equation

$$\sin x_* = a, \qquad f(x) = \sin x - a. \qquad \text{Multiple roots, Can not be solved algebraically.}$$

3.1. Root finding: Bisection method

Example: Roots finding in thermo-physical calculations

- The temperature dependence of the material properties is given by empirical equations. The specific heat C (J/kg/K) as a function of temperature T (K) of some material:

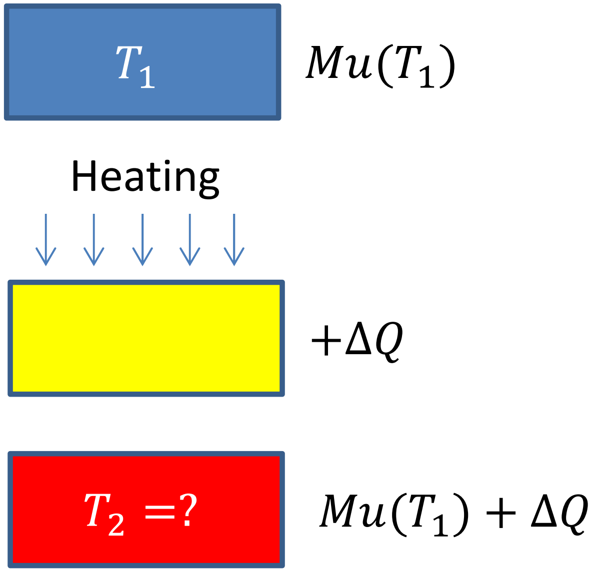
$$C(T) = C_0 + C_1 T + C_2 T^2 + C_3 T^3$$

Then the specific internal (thermal) energy u (J/kg) at temperature T is

$$u(T) = \int_0^T C(T) dT = C_0 T + \frac{C_1}{2} T^2 + \frac{C_2}{3} T^3 + \frac{C_3}{4} T^4$$

Let's assume that

1. We consider some body of that material of mass M (kg) with initial temperature T_1. Then the thermal energy of that body is equal to
$$U_1 = M\,u(T_1)$$
2. We heat the body by a laser and add energy ΔQ (J).
3. What is the body temperature T_2 after heating?
In order to answer this question we must find a root T_2 of the equation:
$$M\,u(T_2) = M\,u(T_1) + \Delta Q$$



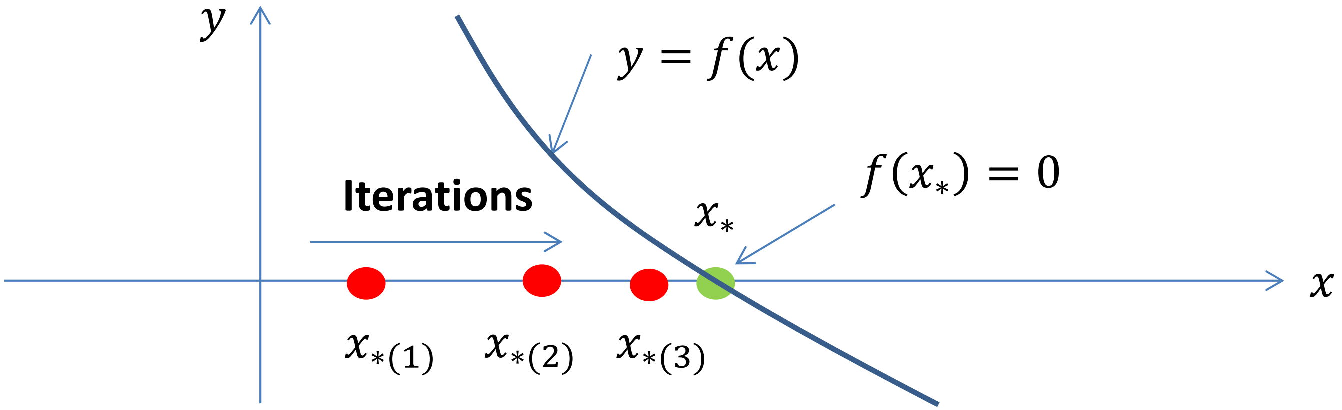
3.1. Root finding: Bisection method

Algebraic solution x_* is:

- An equation (formula) that defines the root of the equation $f(x_*) = 0$.
- An accurate solution.

Numerical solution $x_{*(num)}$:

- A **numerical** value which turns equation $f(x_*) = 0$ into identity.
- An approximate solution. It means that $f(x_{*(num)}) \neq 0$, but $|f(x_{*(num)})|$ is small.



The numerical methods for root finding of non-linear equations usually use **iterations** for successive approach to the root:

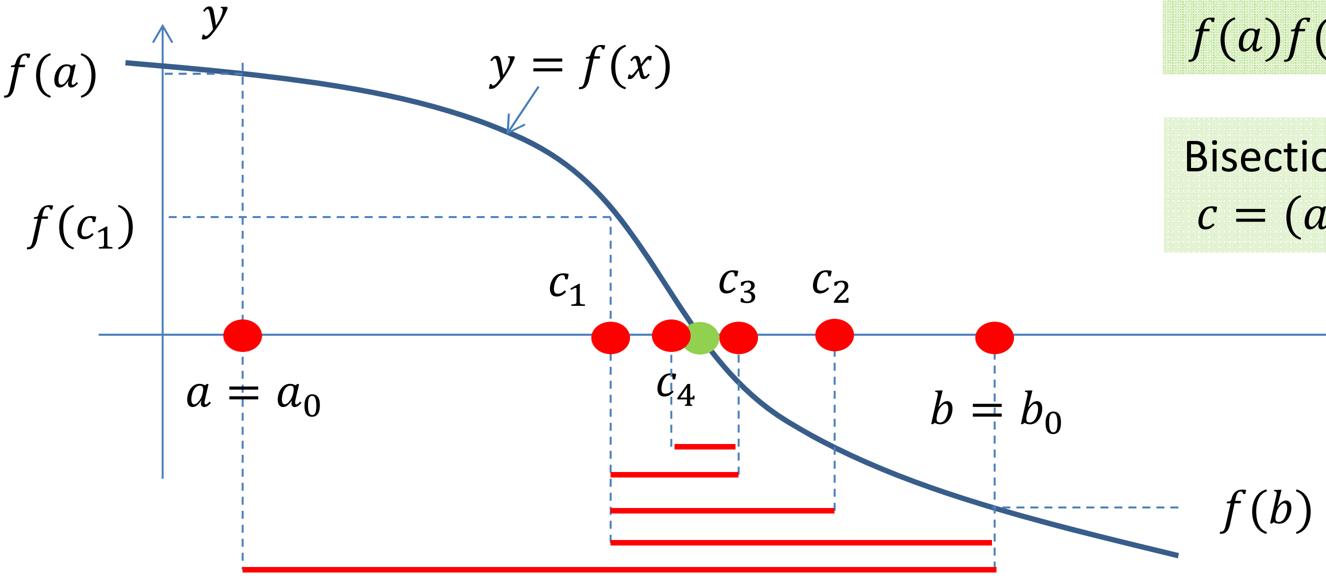
We find $x_{*(1)}, x_{*(2)}, x_{*(3)}, \dots$ such that $x_{*(i)} \to x_*$, i.e. $\varepsilon_i = |x_{*(i)} - x_*| \to 0$.

After finite number of iterations, we will be able to find the root with finite **numerical error** ε_i.

3.1. Root finding: Bisection method

Bisection method

- Let's assume that we **localize** a single root in an interval (a, b) and $f(x)$ changes sign in the root. If the interval (a, b) contains one root of the equation, then $f(a)f(b) < 0$.
- Let's iteratively shorten the interval by **bisections** until the root will be localized in the sufficiently short interval. For every bisection at the central point $c = (a + b)/2$, we replace either a or b by c providing $f(a)f(b) < 0$ after the replacement.



$f(a)f(b) < 0$

Bisection point:
$c = (a + b)/2$

One **iteration** of the bisection method:

1. Assume the root is localized in the interval $a_i < x < b_i$.
2. Calculate middle point $c_i = (a_i + b_i)/2$. This is the i^{th} approximation to the root $x_{*(i+1)} = c_i$.
3. If $b_i - a_i < \varepsilon$, then stop iterations. The root is found with **tolerance** ε.
4. If $f(a_i)f(c) < 0$ then $a_{i+1} = a_i$, $b_{i+1} = c$ or $a_{i+1} = c$, $b_{i+1} = b_i$ otherwise.

3.1. Root finding: Bisection method

MATLAB code for the bisection method

Example: Solving equation $\sin x = 1/2$.

```
function [ x, N ] = Bisection ( a, b, Tol )
        N = 0 ;
        fa = Equation ( a )  ;
        while b – a > Tol
              c = 0.5 * ( a + b ) ;
              fc = Equation ( c  ) ;
              if fa * fc > 0
                      a = c;
              else
                      b = c ;
              end
              N = N + 1 ;
        end
        x = c ;
end

function f = Equation ( x )
       f = sin ( x ) – 0.5;
end
```

Notes:

1. Calculation of $f(x)$ is the most computationally "expensive" part of the algorithm. It is important to calculate $f(x)$ *only once* per pass of the loop.

2. **Advantage** of the bisection method: If we are able to localize *a single root*, the method allows us to find the root of an equation with *any continuous* $f(x)$ *that changes its sign in the root*. No any other restrictions applied.

3. **Disadvantage** of the bisection method: It is a slow method. Finding the root with small tolerance ε requires a large number N of bisections. Example: Let's assume $\Delta x = b - a = 1$, $\varepsilon = 10^{-8}$. Then the N can be found from equation $\varepsilon = \Delta x / 2^N$:

$$N = \frac{\log(\Delta x/\varepsilon)}{\log 2} = \frac{\log 10^8}{\log 2} \approx 27 .$$

3.1. Root finding: Bisection method

Summary on root finding with build-in MATLAB function fzero

The MATLAB build-in function **fzero** allows one to find a root of a nonlinear equation:

LHS of equation

```
x = fzero ( @fun, x0 )
```

Initial approximation

Example:

$$\sin(x) = \frac{1}{2} \quad \Longrightarrow \quad f(x) = \sin x - \frac{1}{2} = 0$$

```
function [ f ] = fun ( x )
        f = sin ( x ) – 0.5 ;
end

x = fzero ( @fun,  0.01 )
```

3.1. Root finding: Bisection method

- The MATLAB build-in function **fzero** allows one to find a root of a nonlinear equation:
  - ✓ x = **fzero** (@fun, x0).
  - ✓ fun is the (user-defined) function that calculates the LHS $f(x)$ of the equation.
  - ✓ x0 can be either a single real value or a vector of two values.
- If x0 is a single real number, then it is used as the initial approximation to the root. In this case the **fzero** function automatically finds another boundary of the interval x1 such that f(x1) * f(x0) < 0 and then iteratively shrinks that interval.
- If x0 is a vector of two numbers, then x0(1) and x0(1) are used as the boundaries of the interval, where the root is localized, such that f(x0(1)) * f (x0(2)) < 0.
- The function works only if $f(x)$ changes its sign in the root (not applicable for $f(x) = x^2$).
- The function utilizes a complex algorithm based on a combination of the **bisection**, **secant**, and **inverse quadratic interpolation** methods.
- **Example**: Roots of equation $\sin(x) = \frac{1}{2}$

```
function [ f ] = SinEq ( x )
        f = sin ( x ) – 0.5 ;
end

x = fzero ( @SinEq, [ 0, pi / 2 ] )
x = fzero ( @SinEq,  0.01 )
```

3.2. Root finding: Newton-Raphson method

- Idea of Newton-Raphson method: Linearization
- Graphical form of the root finding with Newton-Raphson method
- Examples: When Newton-Raphson method does not work
- MATLAB code for Newton-Raphson method
- MATLAB function function

Reading assignment

http://en.wikipedia.org/wiki/Newton's_method

Gilat 7.9, 9.1

3.2. Root finding: Newton-Raphson method

Problem statement

We need to find a real **root** x_* of a non-linear equation

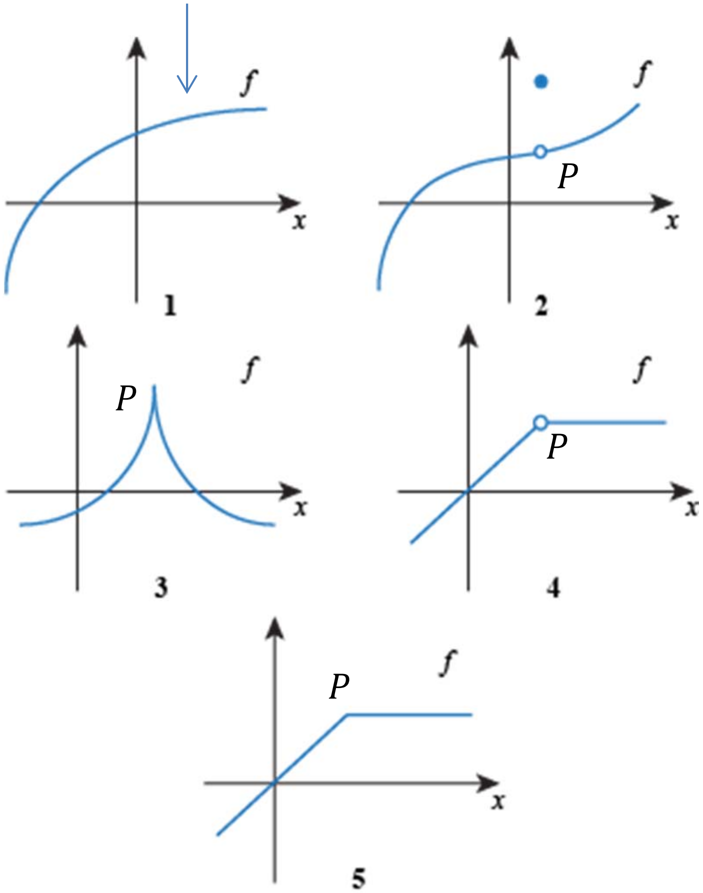
(3.2.1) $$f(x_*) = 0$$

in an $a < x < b$ interval, where $f(x)$ is the **differentiable** function with **continuous derivative** $f'(x)$.

Newton-Raphson method

- In the framework of Newton-Raphson (Newton's) method we start calculations from some **initial approximation** for the root, $x_{*(1)}$, and then **iteratively increase the accuracy of this approximation**, i.e. successively calculate $x_{*(2)}, x_{*(3)}, \dots$ such that $x_{*(i)} \to x_*$ and $\varepsilon_i = \left| x_{*(i)} - x_* \right| \to 0$.
- In order to find the next approximation to the root, $x_{*(i)}$, based on the previous approximation, $x_{*(i-1)}$, we use the idea of **linearization**: For one iteration, we replace non-linear Eq. (3.2.1) by a linear equation that is as close to Eq. (3.2.1) as possible.

Differentiable function



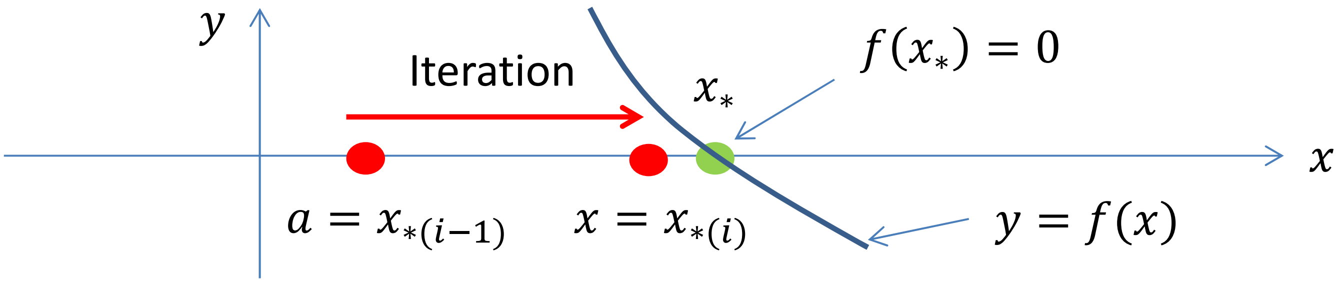
All other functions in this example are not differentiable if (a, b) includes point P

3.2. Root finding: Newton-Raphson method

- Linearization is based on the **Taylor series**. The Taylor series is the approximation of $f(x)$ in a vicinity of point $x = a$ by a polynomial:

$$f(x) = f(a) + f'(a)(x-a) + \frac{1}{2} f''(a)(x-a)^2 + \cdots$$

- Let's apply the Taylor series in order to find $x_{*(i)}$ based on $x_{*(i-1)}$, i.e. represent $f(x)$ in Eq. (3.2.1) in the form of the Taylor series at $x = x_{*(i)}$ and $a = x_{*(i-1)}$



Linearization (we retained only linear terms)

$$f\left(x_{*(i-1)}\right) + f'\left(x_{*(i-1)}\right)\left(x_{*(i)} - x_{*(i-1)}\right) + \xcancel{\frac{1}{2} f''\left(x_{*(i-1)}\right)\left(x_{*(i)} - x_{*(i-1)}\right)^2 + \cdots} = 0$$

- then drop all non-linear terms

$$f\left(x_{*(i-1)}\right) + f'\left(x_{*(i-1)}\right)\left(x_{*(i)} - x_{*(i-1)}\right) = 0 \qquad (3.2.2)$$

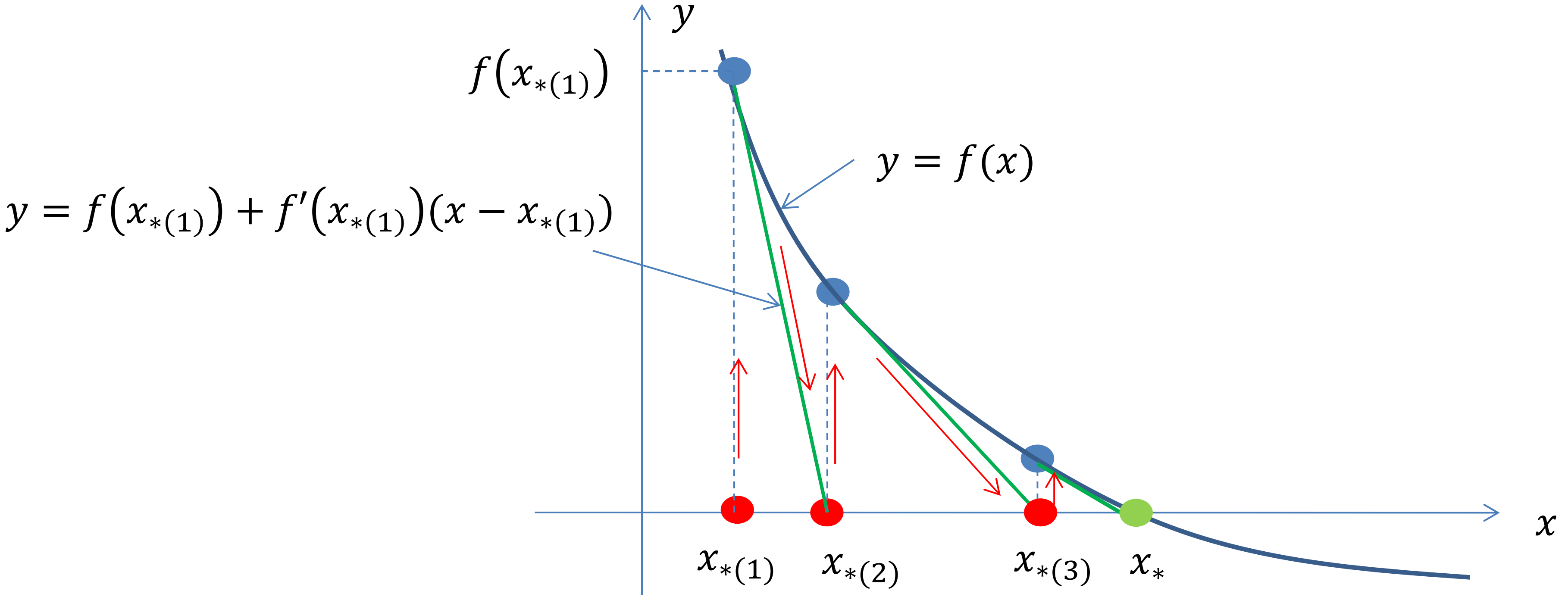
- and use this equation to find the next approximation to the root:

$$\boxed{x_{*(i)} = x_{*(i-1)} - \frac{f\left(x_{*(i-1)}\right)}{f'\left(x_{*(i-1)}\right)}} \qquad (3.2.3)$$

3.2. Root finding: Newton-Raphson method

Graphical representation of the Newton-Raphson method

- The plot of the function $y = f\left(x_{*(i-1)}\right) + f'\left(x_{*(i-1)}\right)\left(x - x_{*(i-1)}\right)$ is the straight line that is **tangent** to the plot of the function $f(x)$ in the point $x_{*(i-1)}$.
- When we find the root of Eq. (3.2.2), we find a point, where the tangent crosses the axis Ox.
- The iterative process of Newton-Raphson method can be graphically represented as follows:



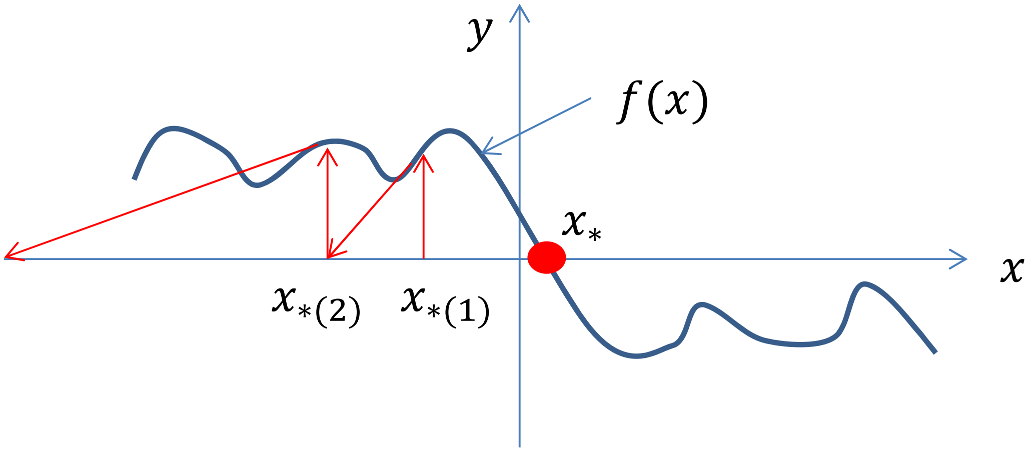
- **Advantages** of Newton-Raphson method:
  - It is the fast method. Usually only a few iterations are required to obtain the root.
  - It can be generalized for systems of non-linear equations.

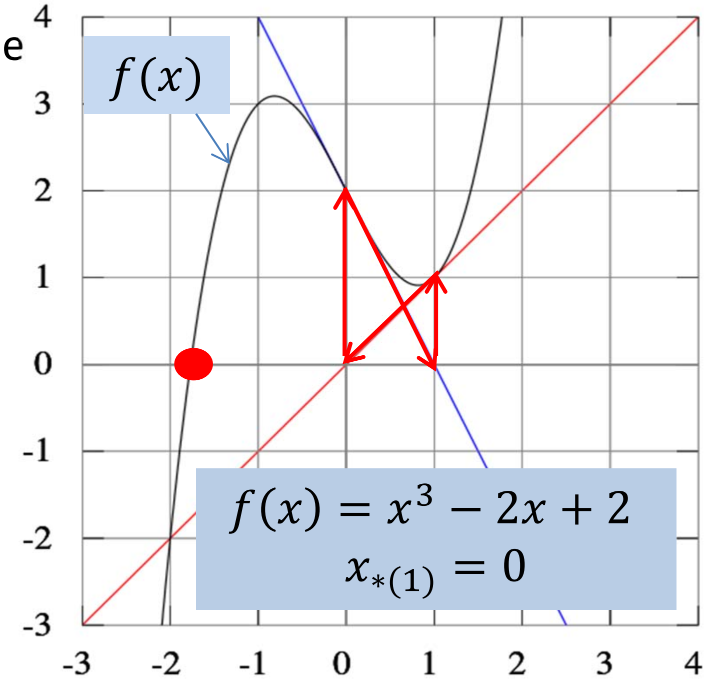
3.2. Root finding: Newton-Raphson method

- **Disadvantage** of the Newton-Raphson method: There are lot of situations, when the method does not work. Conditions that guarantee the **convergence** of $x_{*(1)}, x_{*(2)}, \ldots$ to x_*, i.e. $\left|x_{*(i)} - x_*\right| \to 0$, are complicated. Roughly, the Newton-Raphson method converges if
  - In some interval around the root x_*, $f(x)$ has the first and second derivatives (first derivative is continuous), $f'(x) \neq 0$, $f''(x)$ is finite.

    Example: $f(x) = \sqrt[3]{x}$ is the function that does not satisfy these properties and the root of equation $\sqrt[3]{x} = 0$ can not be find with the Newton-Raphson method.
  - Initial approximation, $x_{*(1)}$, is chosen to be "sufficiently close" to the root x_*.

Examples: Newton-Raphson method does not work when the initial point is too "far" from the root or enters a cycle





3.2. Root finding: Newton-Raphson method

MATLAB code for Newton-Raphson method

Example: Solving equation $\sin x = 1/2$.

```
function [ x, N ] = NewtonMethod ( a, Tol )
        N = 0 ;
        x  = a ;
        [ f, dfdx ] = Equation ( x ) ;
        while abs ( f ) > Tol
              x = x - f / dfdx ;
              [ f, dfdx ] = Equation ( x ) ;
              N = N + 1 ;
        end
end

function [ f, dfdx ] = Equation ( x )
       f = sin ( x ) – 0.5 ;
       dfdx = cos ( x ) ;
end
```

Notes:

1. Calculation of $f(x)$ and $f'(x)$ is the most computationally "expensive" part of the algorithm. It is important to calculate $f(x)$ and $f'(x)$ *only once* per pass of the loop.

2. Disadvantage of the current version of the code: For solving *different* equations we need to prepare different versions of the NewtonMethod function. They will be different only by the name of the function (Equation) that calculates $f(x)$ and $f'(x)$. We can make NewtonMethod universal (capable of solving different equations) by programming the MATLAB **function function**.

- Only 3 iterations is necessary to get the root with tolerance $\varepsilon = 10^{-8}$.

3.2. Root finding: Newton-Raphson method

MATLAB function function

- **Function function** is a function that accepts the name of another function as an input argument.
- Definition of the function function:

  function [...] = Function1 (Fun, ...) : Here Fun the name of input function argument
- Use of the function function :

  [...] = Function1 (@Fun1, ...) : Here Fun1 is the name of a MATLAB function

MATLAB code for the Newton-Raphson method based on function function

File NewtonMethodFF.m

```
function [ x, N ] = NewtonMethodFF ( Eq, a, Tol )
        N = 0 ;
        x  = a ;
        [ f, dfdx ] = Eq ( x ) ;
        while abs ( f ) > Tol
                x = x - f / dfdx ;
                [ f, dfdx ] = Eq ( x ) ;
                N = N + 1 ;
        end
end
```

File SinEq.m

```
function [ f, dfdx ] = SinEq ( x )
        f = sin ( x ) – 0.5 ;
        dfdx = cos ( x ) ;
end
```

In the MATLAB command window:

```
[ x, N ] = NewtonMethodFF ( @SinEq, 0.01, 1e-08 )
```

3.3. Interpolation

- Interpolation problem
- Reduction of the interpolation problem to the solution of a SLE
- Polynomial interpolation
- Example: Interpolations of smooth and non-smooth data

Reading assignment

3.3. Interpolation

Interpolation problem

Let's assume that a functional dependence between two variables x and y is given in the **tabulated form**: We know values of the function, $y_i = y(x_i)$, for some discrete values of the argument x_i, $i = 1, \dots, N$.

Arg.	x_1	x_2	…	x_{i-1}	x_i	x_{i+1}	…	x_{N-1}	x_N
Fun.	y_1	y_2	…	y_{i-1}	y_i	y_{i+1}	…	y_{N-1}	y_N

(3.3.1)

Such tabulated data can be produced in experiments. **Example**: $x = t$ is time and $y = T$ is temperature, in the experiment we measure the temperature T_i at a discrete times t_i.

We are interested in the question : How can we predict the values of the function $y(x)$ (and its derivatives $y'(x)$, etc.) at arbitrary x which does not coincide with any of x_i?

There are two major of approaches to introduce $y(x)$ based on tabulated data in the form (3.3.1). We will consider two major methods:

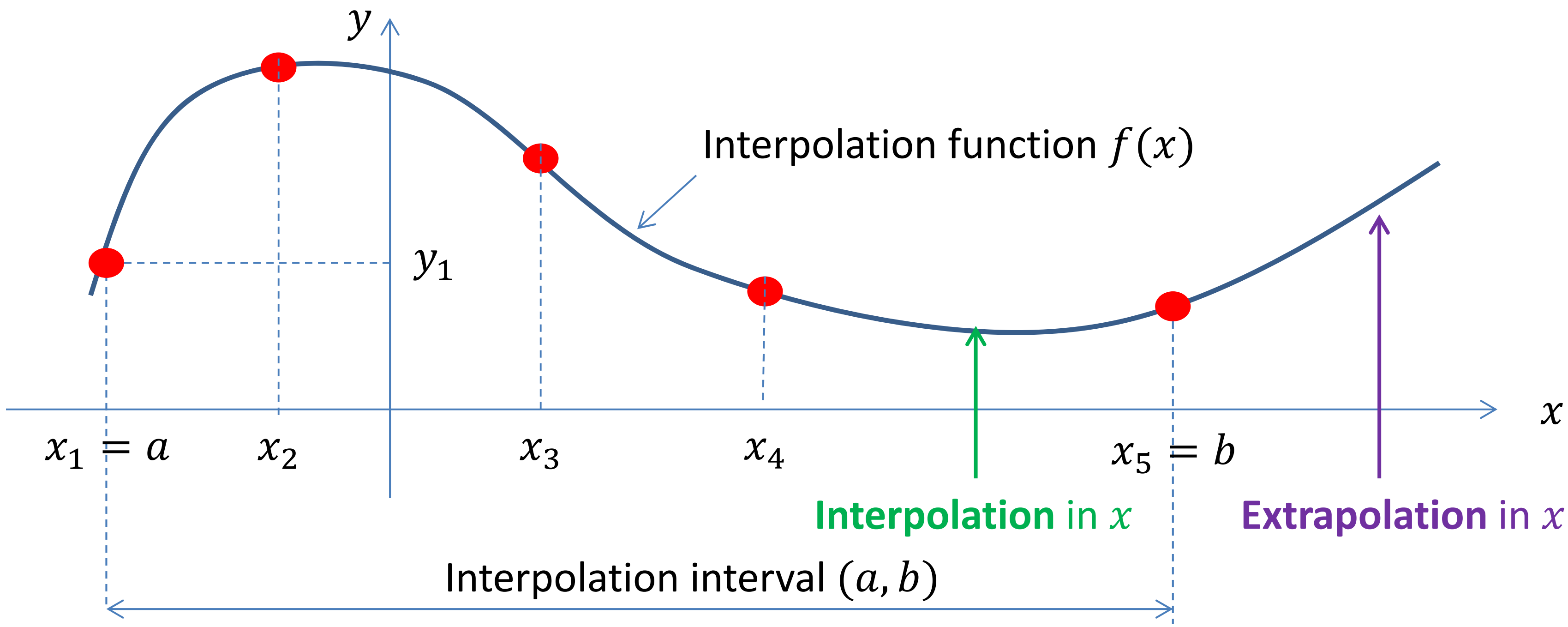
1. **Interpolation**.
2. **Fitting** (will be considered later).

Interpolation implies that we introduce a continuous **interpolation function** $f(x)$ such that

$$f(x_i) = y_i, \qquad i = 1, \dots, N. \tag{3.3.2}$$

This means that the interpolation function goes through every point (x_i, y_i) on the plane (x, y).

3.3. Interpolation



- We assume that all x_i are given in ascending order: $x_{i-1} < x_i$
- **Interpolation** is the process of constructing of new data points within the observation interval:

  $x_1 \leq x \leq x_N$: $y = f(x)$ is the **interpolated value** of the function
- **Extrapolation** is the process of constructing of new data points beyond the observation interval:

  $x < x_1$ or $x > x_N$: $y = f(x)$ is the **extrapolated value** of the function
- Both interpolation and extrapolation can be performed only approximately, but extrapolation is subject to greater uncertainty and higher risk of producing meaningless results.

3.3. Interpolation

Solution of the interpolation problem

- Let's introduce a system of N known functions

$$f_1(x),\quad f_2(x),\quad f_3(x),\quad f_4(x),\quad .....$$

Usually these functions are assumed to be smooth(have continuous derivatives of any order).

- Now, let's look for the interpolation function in the following form:

$$f(x) = C_1 f_1(x) + C_2 f_2(x) + \cdots + C_N f_N(x) = \sum_{i=1}^{N} C_i f_i(x) \tag{3.3.3}$$

where C_i are unknown coefficients. In order to be an interpolation function, $f(x)$ should satisfy conditions (3.3.2), i.e.

$$\begin{gathered} C_1 f_1(x_1) + C_2 f_2(x_1) + \cdots + C_N f_N(x_1) = y_1 \\ C_1 f_1(x_2) + C_2 f_2(x_2) + \cdots + C_N f_N(x_2) = y_2 \\ \ldots \\ C_1 f_1(x_N) + C_2 f_2(x_N) + \cdots + C_N f_N(x_N) = y_N \end{gathered} \tag{3.3.4}$$

- Eqs. (3.3.4) is the linear system of N equations with respect to N coefficients C_i . It can be rewritten in the matrix form as follows:

$$\begin{bmatrix} f_1(x_1) & \cdots & f_N(x_1) \\ \vdots & \ddots & \vdots \\ f_1(x_N) & \cdots & f_N(x_N) \end{bmatrix} \begin{bmatrix} C_1 \\ \vdots \\ C_N \end{bmatrix} = \begin{bmatrix} y_1 \\ \vdots \\ y_N \end{bmatrix} \tag{3.3.5}$$

Thus solution of the interpolation problem reduces to solution of a SLE.

3.3. Interpolation

The interpolation function in the form

$$f(x) = C_1 x^{N-1} + \cdots + C_{N-2} x^2 + C_{N-1} x + C_N \qquad (3.3.6)$$

is called the **interpolation polynomial**.

- In order to find the interpolation polynomial one needs to solve the SLE given by Eqs. (3.3.5):

$$f_1(x) = x^{N-1}, \qquad f_2(x) = x^{N-2}, \qquad \ldots, \qquad f_{N-1}(x) = x, \qquad f_N(x) = 1. \qquad (3.3.7)$$

$$\text{Eq. (3.3.5)} \quad \Longrightarrow \quad \begin{bmatrix} x_1^{N-1} & \cdots & 1 \\ \vdots & \ddots & \vdots \\ x_N^{N-1} & \cdots & 1 \end{bmatrix} \begin{bmatrix} C_1 \\ \vdots \\ C_N \end{bmatrix} = \begin{bmatrix} y_1 \\ \vdots \\ y_N \end{bmatrix}. \qquad (3.3.8)$$

Elements of the matrix of coefficients $\mathbf{A}$ are equal to $a_{ij} = x_i^{N-j}$

- If the interpolation data includes N points (x_i, y_i) , then we can find the interpolation polynomial of degree $N - 1$.

- The chosen order of functions in Eqs. (3.3.7) and (3.3.8) (C_1 is the coefficient at the highest degree of x) allows us to use the MATLAB **polyval** function in order to calculate value of the interpolation polynomial.

3.3. Interpolation: General approach

Problem 3.3.1: Interpolation of various functions

File InterpolationProblem.m

```
function [ C ] = InterpolationProblem ( x_i, y_i )
    N = length ( x_i );
    A = zeros ( N, N );
    for i = 1 : N % i is the row index
        for j = 1 : N % j is the column index
            A(i,j) = x_i(i)^(N-j);
        end
    end
    C = inv ( A ) * y_i';
end
```

$$\mathbf{A} = \begin{bmatrix} x_1^{N-1} & \cdots & 1 \\ \vdots & \ddots & \vdots \\ x_N^{N-1} & \cdots & 1 \end{bmatrix}$$

File Interpolation.m

```
function [ C ] = Interpolation ( Fun, a, b, N, NN )
    % Preparation of tabulated data
    x_i = linspace ( a, b, N );
    y_i = arrayfun ( Fun, x_i );
    % Solving the interpolation problem
    C = InterpolationProblem ( x_i, y_i );
    % Now we plot the function, interpolation polynomial, and data points
    x = linspace ( a, b, NN );
    f = polyval ( C, x ); % Interpolation polynomial
    y = arrayfun ( Fun, x ); % Original function
    plot ( x, y, 'r', x_i, y_i, 'bx', x, f, 'g' )
end
```

File Problem_3_3_1

```
C = Interpolation ( @TriangleFun, -1, 3, 5, 101 )
```

These functions can be used to generate data points:

File PolyFun.m

```
function [ y ] = PolyFun ( x )
        Coeff = [ 1 2 3 ];
        y = polyval ( Coeff, x ) ;
end
```

File SinFun.m

```
function [ y ] = SinFun ( x )
        y = sin ( pi * x / 2 ) ;
end
```

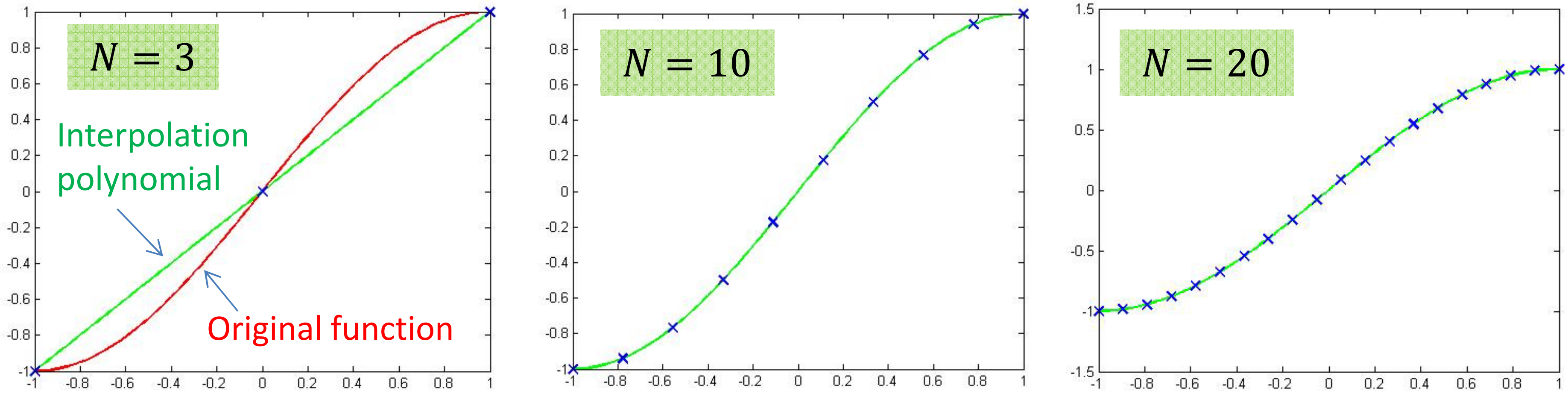
File TriangleFun.m

```
function [ y ] = TriangleFun ( x )
    if x < 0
            y = 0 ;
    elseif x < 1
            y = x ;
    elseif x < 2
            y = 2 - x;
    else
            y = 0;
    end
end
```

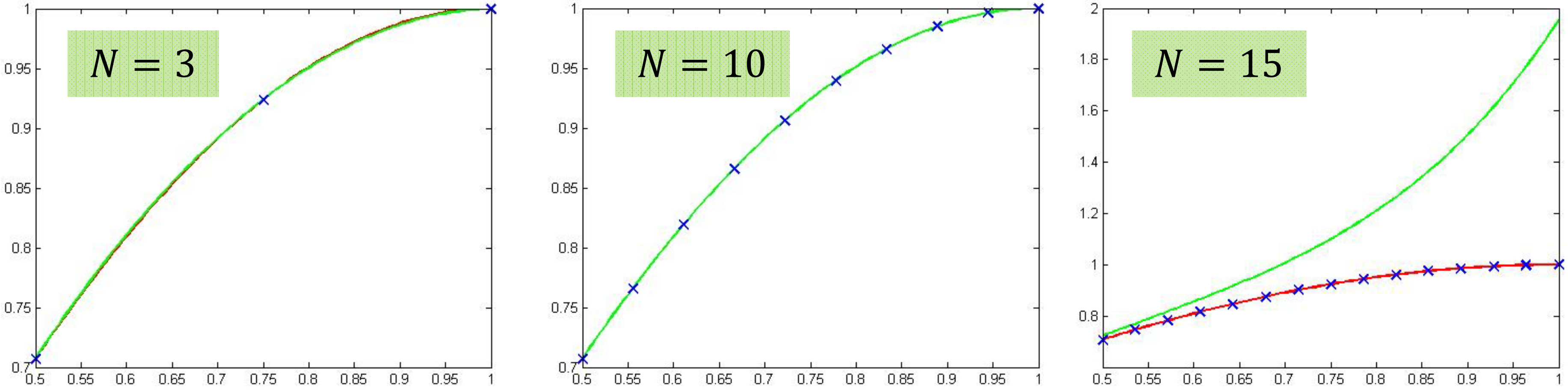
3.3. Interpolation

Example 1: Smooth data $y = \sin(\pi x/2)$, N is the number of interpolation points

A. Symmetric interpolation interval (-1,1)



B. Non-symmetric interpolation interval (0.5, 1)

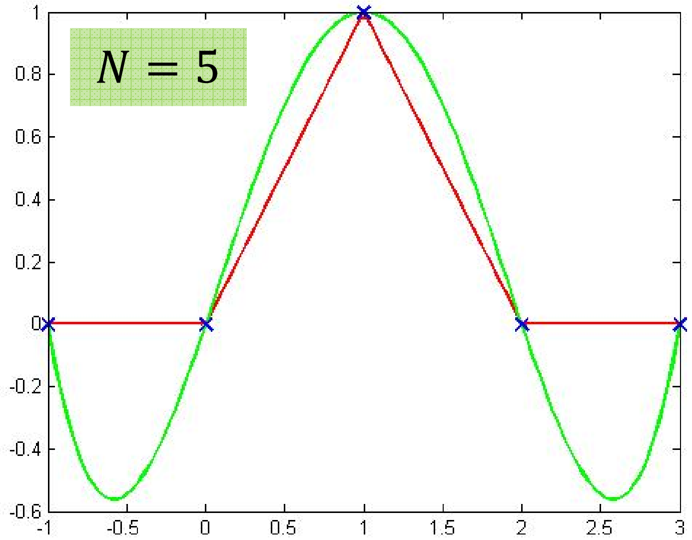


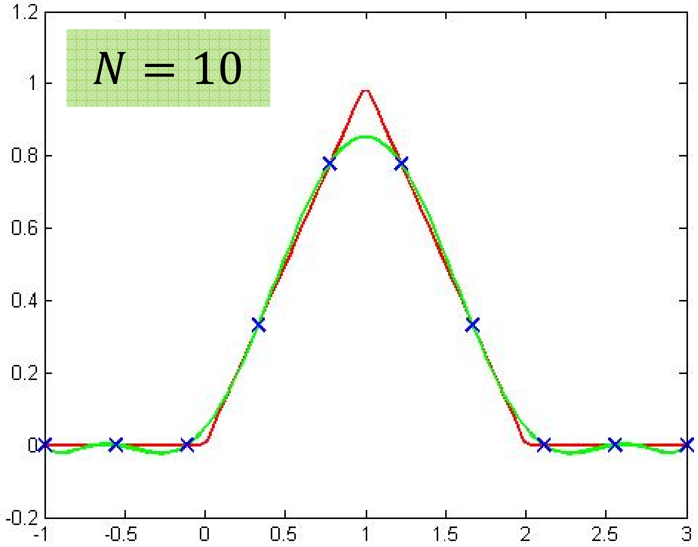
- ➢ In general, it is difficult to build and calculate interpolation polynomials at large N (>10-20) due to strong enhancement of **round-off errors. We are limited by small N!**

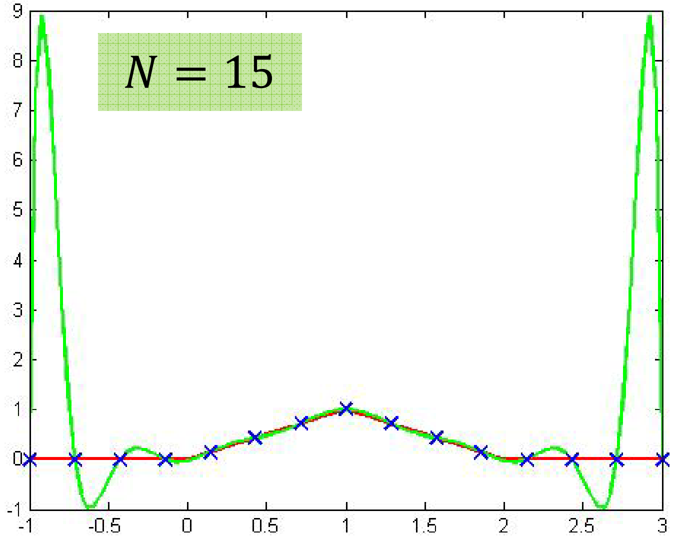
3.3. Interpolation

Example 2: Non-smooth data in the form of a triangle pulse

Symmetric interpolation interval (-1,3)







- For non-smooth data, an increase in the number of data points N (and degree of the polynomial) can deteriorate the accuracy.
- The values of the interpolation polynomial for non-smooth data are subject to "oscillations."

3.4. Curve fitting: Least square method

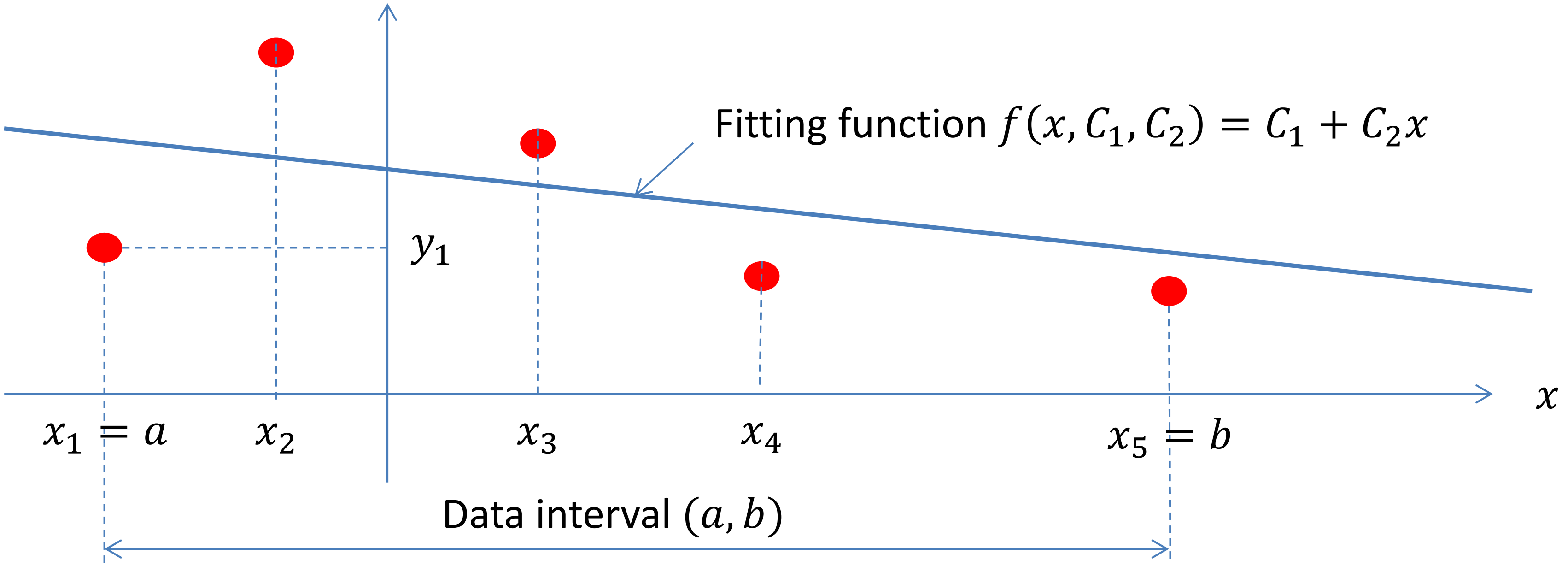
- Fitting problem
- When is interpolation not a viable approach?
- Least square method: General approach
- Least square method: Polynomial fitting

Reading assignment

Gilat 8.2, 8.4, 8.5

3.4. Curve fitting: Least square method

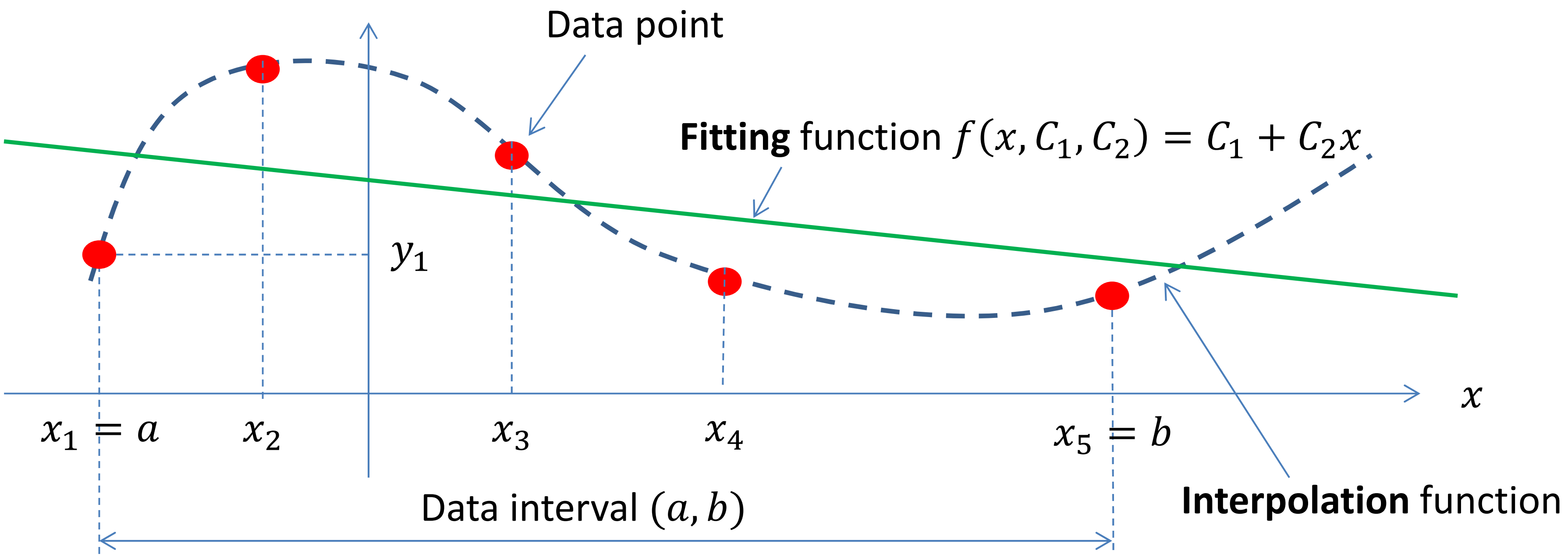
Curve fitting is the process of constructing a curve, or mathematical function, that has the best fit to a series of discrete data points.



Curve fitting implies that

1. We choose a form of the fitting function (e.g. linear fitting function $f(x, C_1, C_2) = C_1 + C_2 x$) with some number of unknown coefficients (C_1, C_2). In general, the choice of the fitting function is *arbitrary* and the number of unknown coefficients is *much smaller* than the number N of data points.
2. We introduce a *measure of difference*, R, between the data points (x_i, y_i) and the fitting function $f(x)$.
3. We find such unknown coefficients (C_1, C_2) that allow us to *minimize* the value of R.

3.4. Curve fitting: Least square method



Curve fitting is an *alternative to interpolation*.

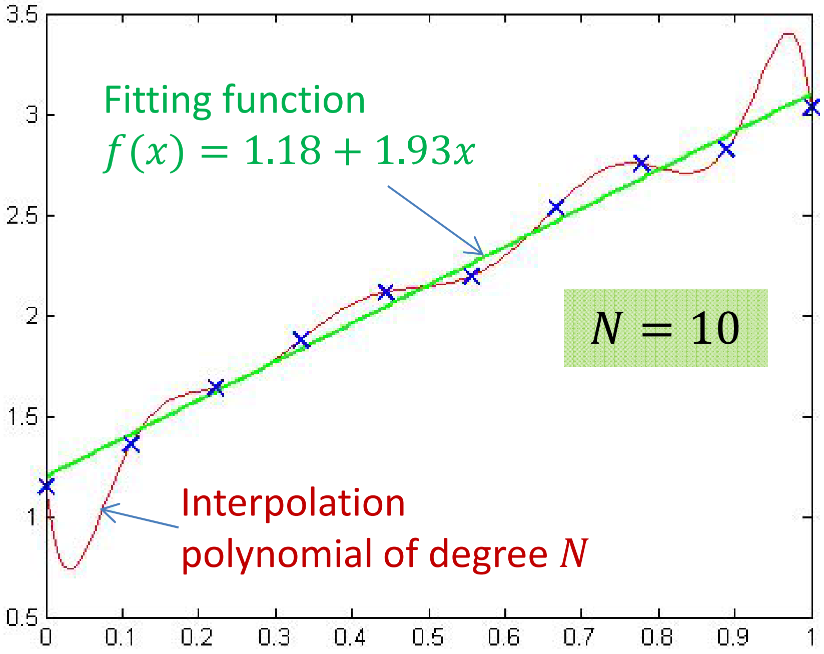
Difference between interpolation and fitting functions:

- Interpolation function passes precisely through every data point.
  Fitting function goes closely to data points and follows the general trend in data behavior.
- Interpolation function has N coefficients, where N is the number of data points.
  Fitting function has M coefficients, usually $M \ll N$.

3.4. Curve fitting: Least square method

- Curve fitting can (and must!) be used instead of interpolation if
  - ✓ There are *too many data points* in order to build an interpolating function ($N > \sim 10$).
  - ✓ Input data are *noisy*.
  - ✓ We are interested in revealing general trends in the data behavior (Curve fitting can be used as a tool for *data analysis)*.

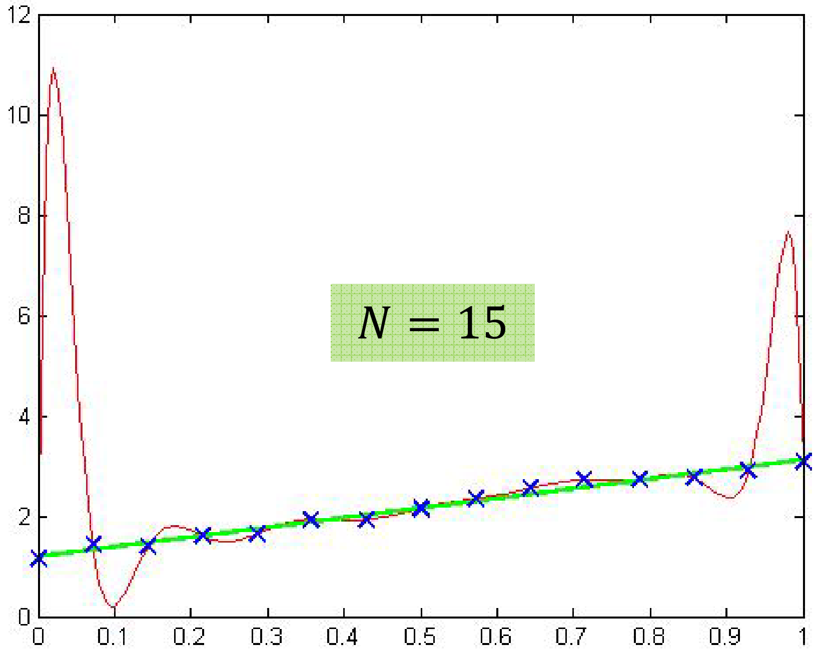
Example: Fitting vs. interpolation of noisy data (see solution in **FittingVsInterpolation.m**)
Data points are given by the law $y(x) = 1 + 2x$ + *random noise*



Fitting function
$f(x) = 1.18 + 1.93x$

Interpolation
polynomial of degree N

$N = 10$



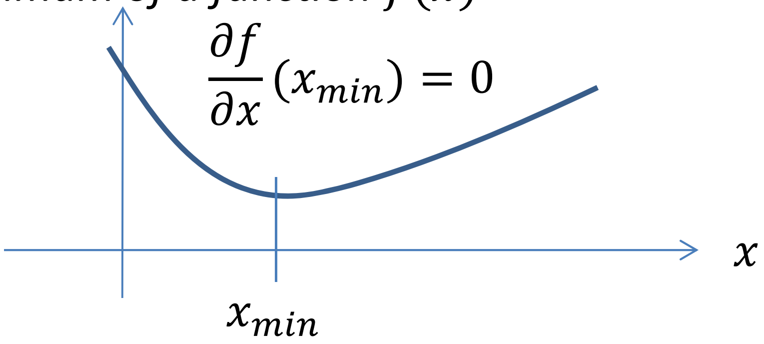
$N = 15$

3.4. Curve fitting: Least square method

Least square method: General idea

Least square method for finding coefficients of fitting functions is based on the general conditions that allow one to find a minimum of a function

Minimum of a function $f(x)$



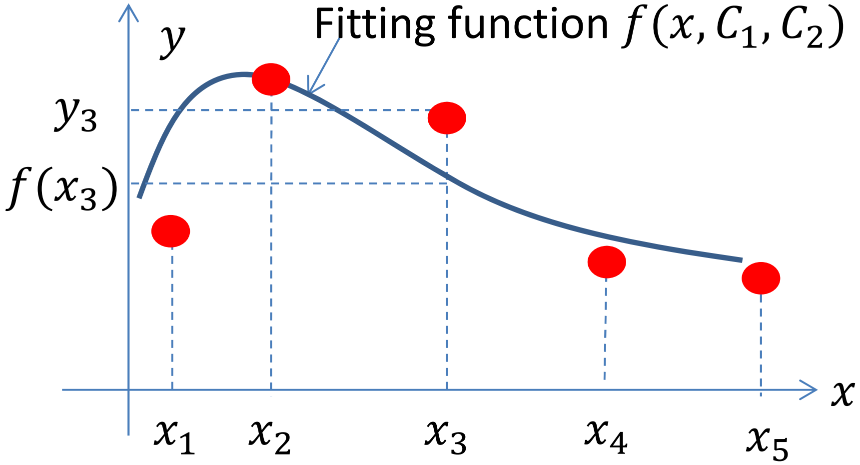
$$\frac{\partial f}{\partial x}(x_{min}) = 0$$

Minimum of a function $f(x, y)$

$$\frac{\partial f}{\partial x}(x_{min}, y_{min}) = 0$$

$$\frac{\partial f}{\partial y}(x_{min}, y_{min}) = 0$$

In the least square method, the same *conditions of a minimum* are applied to the **mean-square difference** R between the fitting function and tabulated data.



Example: Fitting function with *two coefficients*:

$$R(C_1, C_2) = \frac{1}{N} \sum_{i=1}^{N} \left(f(x_i, C_1, C_2) - y_i\right)^2$$

Conditions of minimum of $R(C_1, C_2)$:

$$\frac{\partial R}{\partial C_1} = 0, \qquad \frac{\partial R}{\partial C_2} = 0$$

These are *two equations* with respect to C_1 and C_2

3.4. Curve fitting: Least square method

Least square method: Polynomial fitting

- Assume that we have N data points (x_k, y_k) , $k = 1, .., N$.
- Consider the fitting function in the form of a polynomial of degree M $(M \ll N)$

$$f(x) = f(x, C_1, C_2, .., C_M) = C_1 x^{M-1} \ldots + C_{M-2} x^2 + C_{M-1} x + C_M = \sum_{j=1}^{M} C_j x^{M-j} \quad (3.4.1)$$

- Introduce the **mean square difference** R

$$R(C_1, C_2, .., C_M) = \frac{1}{N} \sum_{k=1}^{N} \left(f(x_k) - y_k\right)^2$$

- Apply **conditions of a minimum** of $R(C_1, C_2, .., C_M)$:

$$\frac{\partial R}{\partial C_i} = 0 \qquad \Longrightarrow \qquad \frac{2}{N} \sum_{k=1}^{N} \left(f(x_k) - y_k\right) \frac{\partial f}{\partial C_i}(x_k) = 0, \qquad i = 1, .., M$$

Eq. (3.4.1) $\Longrightarrow \dfrac{\partial f}{\partial C_i}(x_k) = x_k^{M-i} \Rightarrow \displaystyle\sum_{k=1}^{N} x_k^{M-i} f(x_k) = \sum_{k=1}^{N} y_k x_k^{M-i}$, (3.4.2)

$$\sum_{k=1}^{N} x_k^{M-i} \sum_{j=1}^{M} C_j x_k^{M-j} = \sum_{k=1}^{N} y_k x_k^{M-i} ,$$

3.5. Curve fitting: Least square method

$$\sum_{j=1}^{M}\left(\sum_{k=1}^{N} x_k^{M-j} x_k^{M-i}\right) C_j = \sum_{k=1}^{N} y_k x_k^{M-i}$$

$$\boxed{\sum_{j=1}^{M} a_{ij} C_j = b_i, \qquad i = 1,..,M} \quad \Longrightarrow \quad \begin{bmatrix} a_{11} & \cdots & a_{1M} \\ \vdots & \ddots & \vdots \\ a_{M1} & \cdots & a_{MM} \end{bmatrix} \begin{bmatrix} C_1 \\ \vdots \\ C_M \end{bmatrix} = \begin{bmatrix} b_1 \\ \vdots \\ b_M \end{bmatrix} \qquad (3.4.3)$$

Eq. (3.4.3) is the SLE with respect to coefficients $C_1, C_2, .., C_M$, where the matrix of coefficients and the RHS are

$$a_{ij} = \sum_{k=1}^{N} x_k^{2M-(i+j)} \quad , \qquad b_i = \sum_{k=1}^{N} y_k x_k^{M-i} . \qquad (3.4.4)$$

Solution of the polynomial fitting problem reduces to a SLE given by Eq. (3.4.3) with respect to unknown coefficients C_i ($i = 1,..,M$) of the fitting polynomial.

Once coefficients are found, values of the fitting polynomial can be calculated with the MATLAB **polyval** function.

3.5. Curve fitting in MATLAB

- Polynomial curve fitting with the MATLAB build-in functions
- Other fitting functions
- Data analysis based on the curve fitting
- MATLAB basic fitting interface

Reading assignment

Gilat 8.2, 8.4, 8.5

3.5. Curve fitting in MATLAB

Least square method: Polynomial fitting in the MATLAB

- Assume that we have N data points (x_k, y_k) , $k = 1, .., N$.
- Consider the fitting polynomial of degree $K = M - 1$ $(M \ll N)$

$$f(x) = f(x, C_1, C_2, .., C_M) = C_1 x^{M-1} \ldots + C_{M-2} x^2 + C_{M-1} x + C_M$$

- In the MATLAB, coefficients of the fitting polynomial, $C_1, C_2, .., C_M$, can be calculated with the build-in **polyfit** function.
- This function implements the solution of the SLE given by Eq. (3.4.3).
- Syntax:

C = **polyfit** (x_i, y_i, K)

x_i (= [1 : N]) is a 1D array of x-coordinates of the data points

y_i (= [1 : N]) is a 1D array of y-coordinates of the data points

K= M-1 is the degree of the fitting polynomial

C = [C[1], C[2], ..., C[M]] is an array of M coefficients of the fitting polynomial

f = **polyval** (C, x) can be used in order to calculate the value of the fitting polynomial

3.5. Curve fitting in MATLAB

Problem 3.5.1: Fitting of polynomial data. Initial data points are obtained with the polynomial $y(x) = (x - 0.1)(x - 0.4)(x - 0.75)(x - 0.8)(x - 0.9)$ in the interval $[0,1]$ at $N = 10$.

File Fitting.m

```
function [ C ] = Fitting ( Fun, a, b, N, K, NN )
   % Preparation of tabulated data
   x_i = linspace ( a, b, N );
   y_i = arrayfun ( Fun, x_i );
   % Solving the fitting problem
   C = polyfit ( x_i, y_i, K );
   % Now we plot the function, fitting polynomial, and data points
   x = linspace ( a, b, NN );
   f = polyval ( C, x ); % Fitting polynomial
   y = arrayfun ( Fun, x ); % Original function
   plot ( x, y, 'r', x_i, y_i, 'bx', x, f, 'g' )
end
```

File PolyFun.m

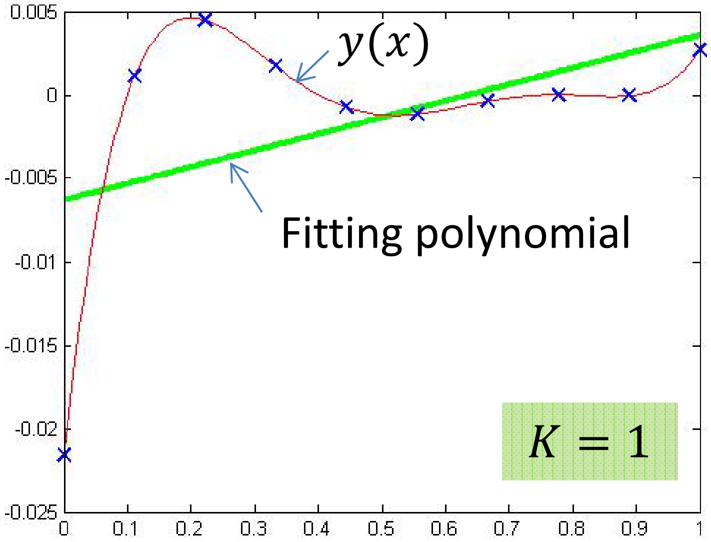
```
function [ y ] = PolyFun ( x )
   y = ( x - 0.1 ) * ( x - 0.4 ) * ( x - 0.75 ) * ( x - 0.8 ) * ( x - 0.9 );
end
```

File Problem_3_5_1.m

```
C = Fitting ( @PolyFun, 0.0, 1.0, 10, 3, 101 )
```

3.5. Curve fitting in MATLAB

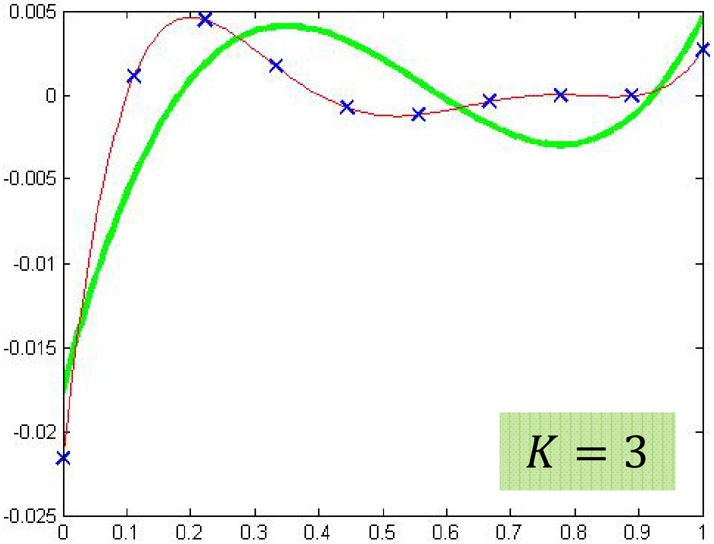
Solution of problem 3.5.1:



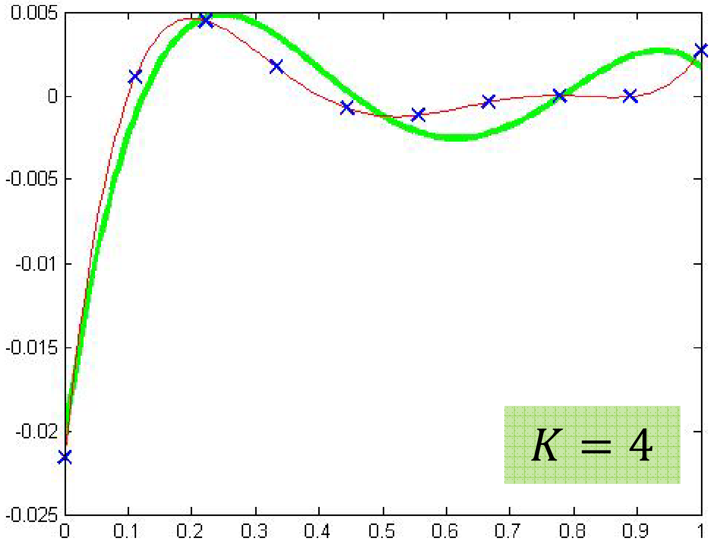
$y(x)$

Fitting polynomial

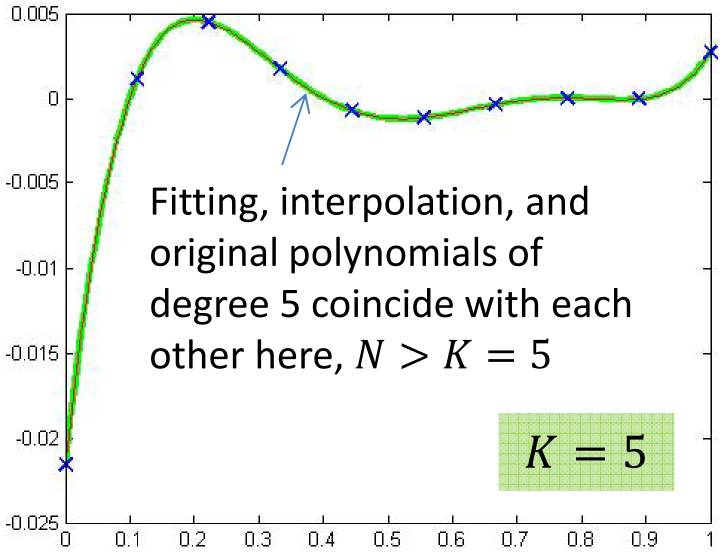
$K = 1$



$K = 3$



$K = 4$



Fitting, interpolation, and original polynomials of degree 5 coincide with each other here, $N > K = 5$

$K = 5$

3.5. Curve fitting in MATLAB

Curve fitting with functions other than polynomials

- Theoretically, any function can be used to model data within some *short range* of x.
- For a given problem, some particular function provide a better fit than others (better fit in a *broader range* of x).
- The choice of the fitting function for the experimental data points is often based on preliminary theoretical consideration of scaling laws governing the dependence $y = y(x)$.
- Curve fitting with power, exponential, logarithmic, and reciprocal functions are of particular importance since these functions often occur in science and engineering

$f = bx^m$: **Power function**

$f = be^{mx}$: **Exponential function**

$f = b + m \log x$: **Logarithmic function**

$f = 1/(b + mx)$: **Reciprocal function**

Any such function has only two fitting parameters ("coefficients"): b and m

- **Fitting with these functions can be reduced to fitting with a polynomial of the first degree and, thus, can be performed with the polyfit function.**

3.5. Curve fitting in MATLAB

- For this purpose, one needs to *rewrite* any of such functions in a form that can be fitted with a linear polynomial:

$\log f = \log b + m \log x$	: Power function	: Linear relation between $\ln x$ and $\ln f$
$\log f = \ln b + mx$	: Exponential function	: Linear relation between x and $\ln f$
$f = b + m \log x$	: Logarithmic function	: Linear relation between $\ln x$ and f
$1/f = b + mx$	: Reciprocal function	: Linear relation between x and $1/f$

Then the fitting problem can be solved in three steps:

1. Transform tabulated data (x_i, y_i) to (t_i, z_i) such that for the chosen fitting function relationship between t and z is linear.

   Example: For the power fit, $t_i = \log x_i$, $z_i = \log y_i$.

2. Apply **C = polyfit (t, z, 1)** to (t_i, z_i) and obtain the coefficients C_2 and C_1 in the linear fitting function for transformed data

$$z = C_1 t + C_2$$
$$\log y = m \log x + \log b$$

3. Obtain coefficients m and b in the original fitting function

   Example: For the power fit, $m = C_1, b = \exp C_2$.

3.5. Curve fitting in MATLAB

Problem 3.5.2: Fitting data with the power function: Data points are given by the equation $y = (1 + 2\sqrt{x})x^2$ in the interval $[0.1, 10]$ at $N = 10$.

The part of the code that prepares coefficients of the fitting functions:

File PowerFitting.m

```
function [ m1, b1 ] = PowerFitting ( Fun, a, b, N, NN )
   % Preparation of tabulated data
   x_i = linspace ( a, b, N );
   y_i = arrayfun ( Fun, x_i );
   % Solving the fitting problem
   C = polyfit ( log ( x_i ), log ( y_i ), 1 );
   % Coefficients of the power fitting function
   m1 = C(1);
   b1 = exp ( C(2) );
   % Now we plot the function, power fitting function, and
   x = linspace ( a, b, NN );
   f = b1 * x.^m1; % Power fitting function
   y = arrayfun ( Fun, x ); % Original function
   loglog ( x, y, 'r', x_i, y_i, 'bx', x, f, 'g' )
end
```

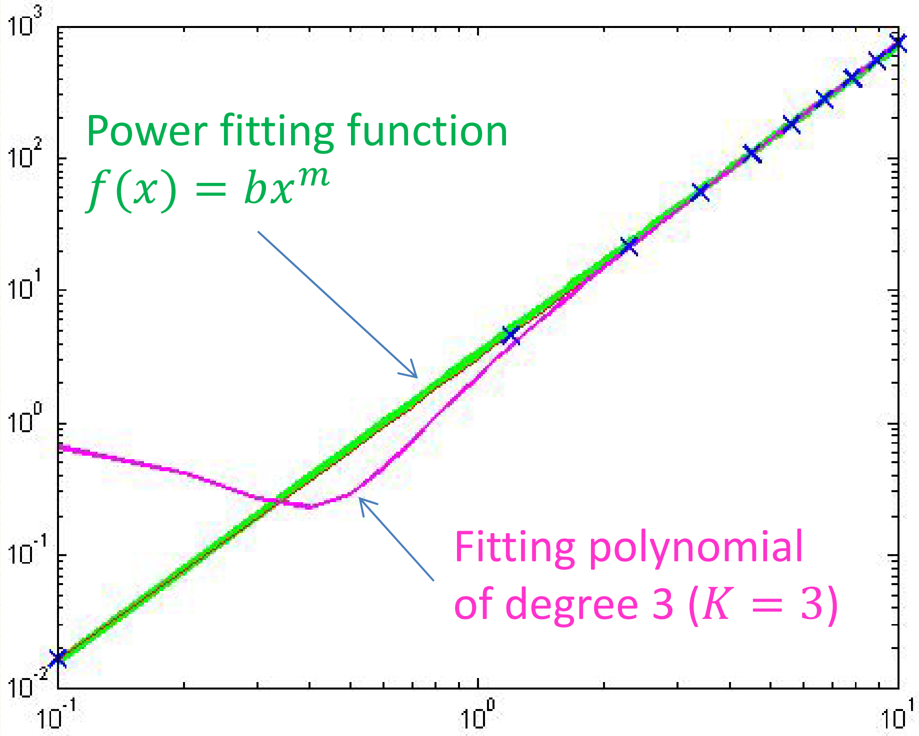
File QuasiPowerFun.m

```
function [ y ] = QuasiPowerFun ( x )
   y = ( 1 + 2.0 * sqrt ( x ) ) * x^2;
end
```

File Problem_3_5_2.m

```
[ m1, b1 ] = PowerFitting ( @QuasiPowerFun, 0.1, 10.0, 10, 101 )
```

Results in the double logarithmic scale



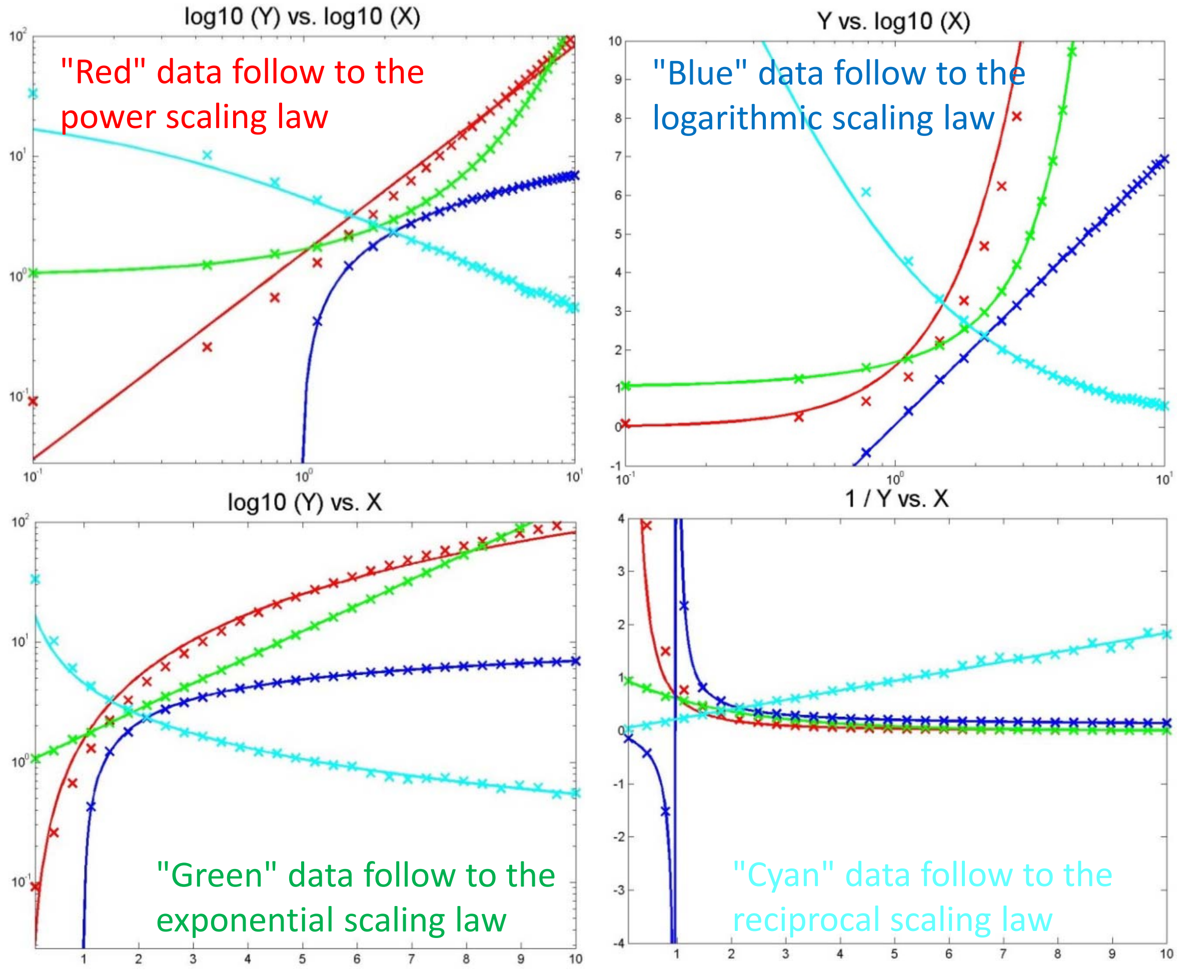
Power fitting function $f(x) = bx^m$

Fitting polynomial of degree 3 $(K = 3)$

3.5. Curve fitting in MATLAB

Data analysis based on the curve fitting

- "Basic" fitting functions (linear, power, exponential, logarithmic, and reciprocal) are specific for many engineering problems since many fundamental physical laws are described in terms of these functions.
- We can visually judge about the best shape of the fitting function by plotting data in different scales (normal, semi logarithmic, double logarithmic) or by plotting reciprocal ($1/y$) data points.



log10 (Y) vs. log10 (X)

"Red" data follow to the power scaling law

Y vs. log10 (X)

"Blue" data follow to the logarithmic scaling law

log10 (Y) vs. X

"Green" data follow to the exponential scaling law

1 / Y vs. X

"Cyan" data follow to the reciprocal scaling law

- If the data points follow to one of the "basic" functions (or **scaling laws**), there will be a scale type when the data points fall on a line plot.
- Four data sets are plotted using different plot scales.

$$f = bx^m$$
$$f = be^{mx}$$
$$f = b + m\ln x$$
$$f = 1/(b + mx)$$

$$\ln f = \ln b + m\ln x$$
$$\ln f = \ln b + mx$$
$$f = b + m\ln x$$
$$1/f = b + mx$$

- See **DataAnalysis.m**

3.5. Curve fitting in MATLAB

Basic fitting tool of the MATLAB figure window

- Fitting functions can be added to the MATLAB figure window by using the **Basic fitting tool**.
- For this purpose we need to do only two steps:
  - ✓ Plot data points using **plot**, **semilogx**, **semilogy**, or **loglog** commands.
  - ✓ In the opened figure window, go to menu Tools->Basic Fitting
- The Basic fitting panel allows us to
  - ✓ Add fitting functions to the figure window.
  - ✓ See coefficients of fitting functions.
  - ✓ Plot residuals.
- Similar interactive fitting tools are build in MS Excel and other data processing software.

3.6. Summary

For the exam we must know how

- To implement and use the bisection method for finding roots of a non-linear equation.
- To implement and use the Newton-Raphson method for finding roots of a non-linear equation.
- To use the build-in **fzero** function for finding roots of an individual non-linear equation.
- To find coefficients of an interpolation polynomial by solving a SLE.
- To understand the basic idea of the least square method and how to reduce the fitting problem to the solution of a SLE.
- To use **polyfit** function in order to find coefficients of the fitting polynomial.
- To use **polyfit** function to fit data to power, exponential, logarithmic, and reciprocal functions.
- To chose the best shape of the fitting function by changing plot scales.