Project C No. 15

Final report

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Field of study : Computer Science

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1.1 Introduction.

The first task is to determine a polynomial function *y = f(x)* that fits the best, using least-square approximation, for the following data samples :

x_i	y_i
-5	-35.7986
-4	-19.4300
-3	-9.7370
-2	-3.1635
-1	-0.6503
0	1.5879
1	1.5176
2	2.1830
3	5.1024
4	11.0910
5	22.0003

The *approximation problem* can be defined in the following way : to find a function F^* belonging to set X_n closest to f in a certain sense, usually in the sense of a certain distance $\delta(f - F)$ defined by a norm $||\cdot||$. Thus, approximation of the function f means finding the coefficients $a_0,\dots,a_n$ of F such that the norm $||f - F||$ is minimized.

To perform least-square approximation, we must define A as a matrix Nxn, where N – number of samples, n – degree of polynomial, for every

$$A_{(i,j)} = {x_j}^{i-1}$$

$$i = 1, 2, 3, \dots, n;\ j = 1, 2, 3, \dots, N$$

Solving least-square task comes down to finding the vector *a* which contain coefficients of polynomial. In this case we will research two approaches :

Using and solving system of normal equations :

$$A^T A\, a = A^T y$$

Using and solving system resulting in QR factorization :

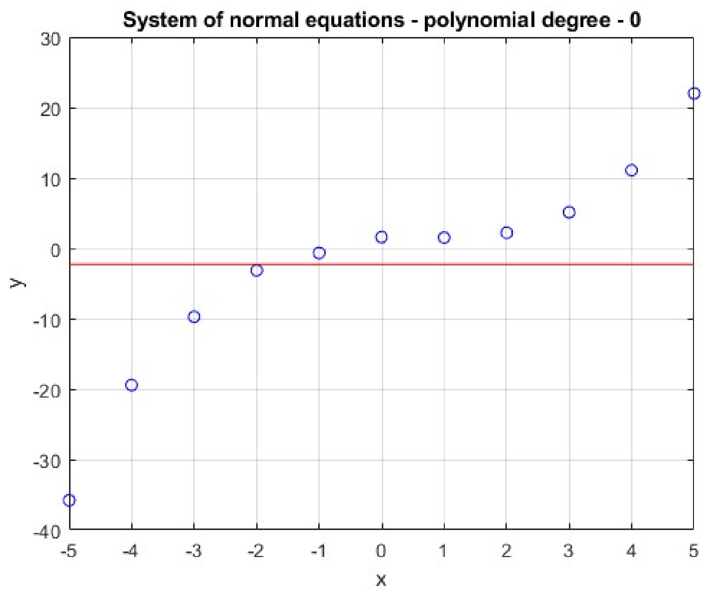
$$A = QR$$

$$Ra = Q^T y$$

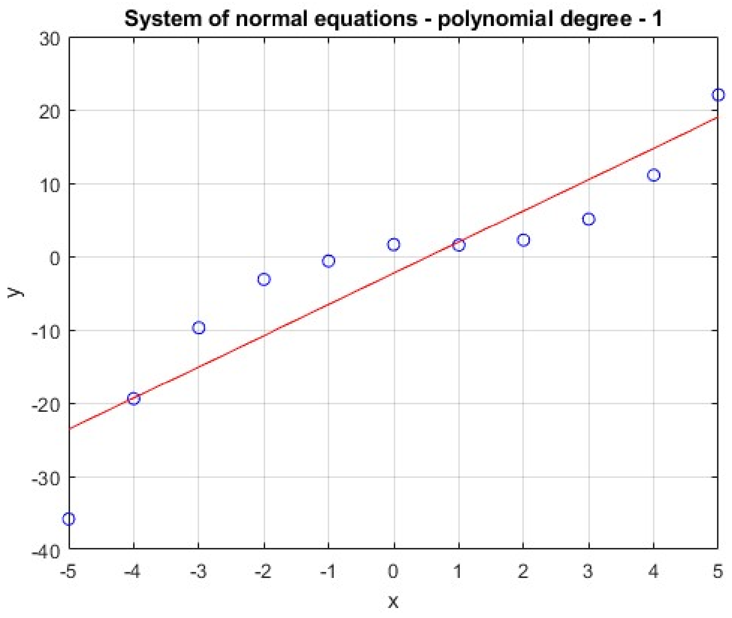
1.2 Approximation using system of normal equations – Results.

The following approximations of given function where obtain :

$$f(x) = -2.2997$$

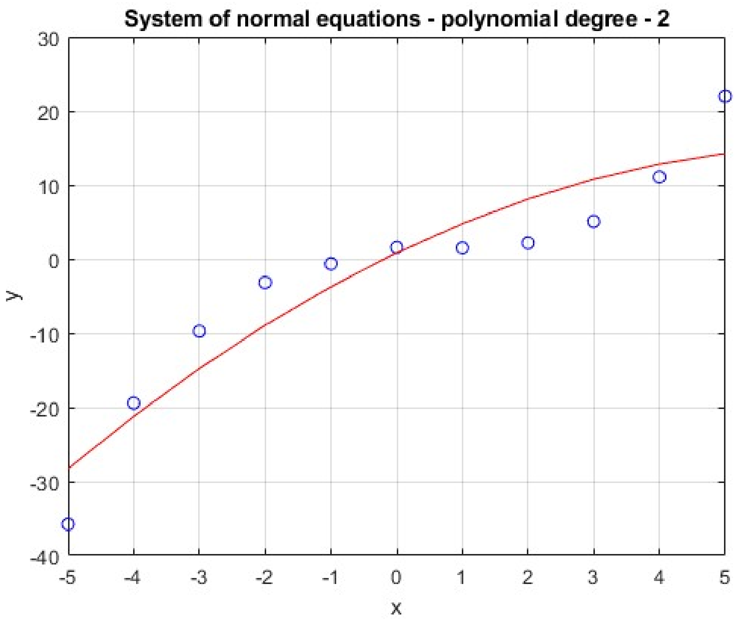


$$f(x) = 4.2587x - 2.2997$$

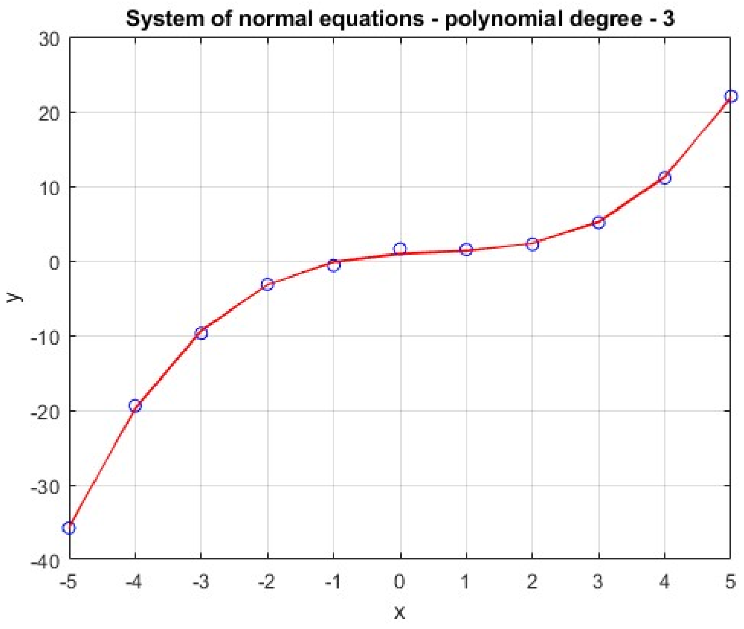


1.2 Approximation using system of normal equations – Results.

$$f(x) = -0.3149x^2 + 4.2587x + 0.8492$$

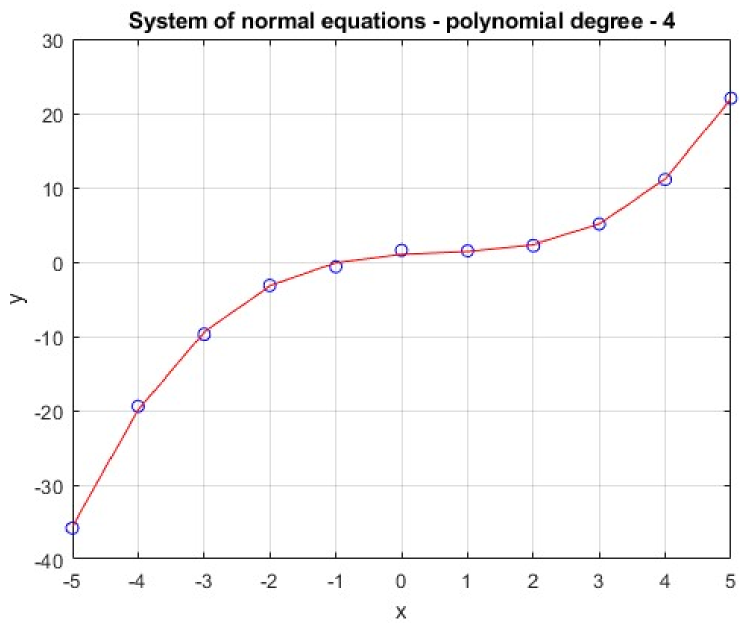


$$f(x) = 0.2081x^3 - 0.3149x^2 + 0.5553x + 0.8492$$

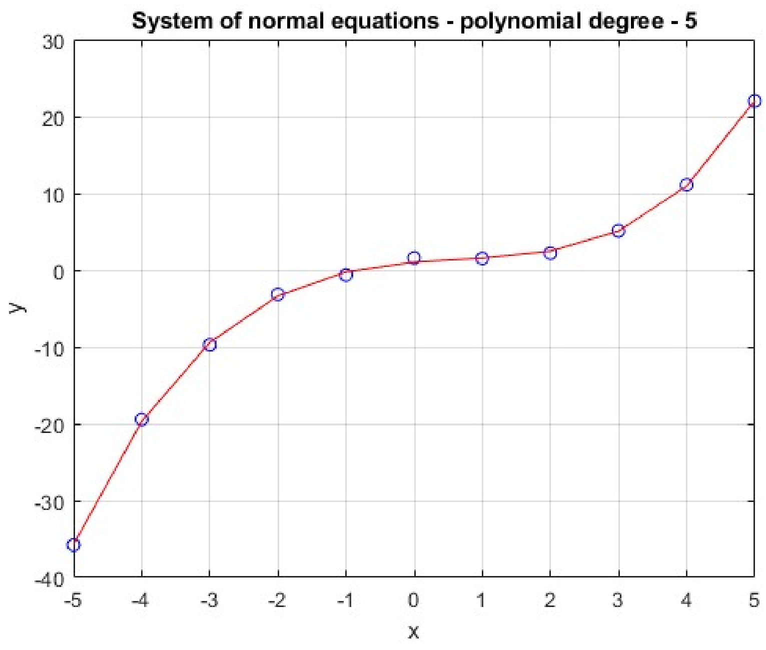


1.2 Approximation using system of normal equations – Results.

$$f(x) = 0.0026x^4 + 0.2081x^3 - 0.3807x^2 + 0.5554x + 1.0386$$



$$f(x) = 0.000879x^5 + 0.0026x^4 + 0.1801x^3 - 0.3807x^2 + 0.7230x + 1.0386$$



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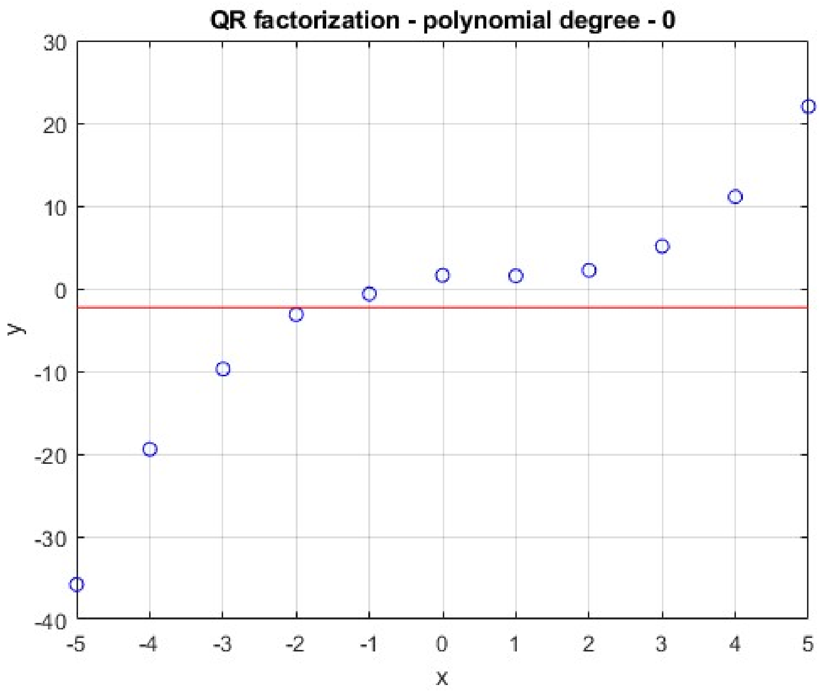

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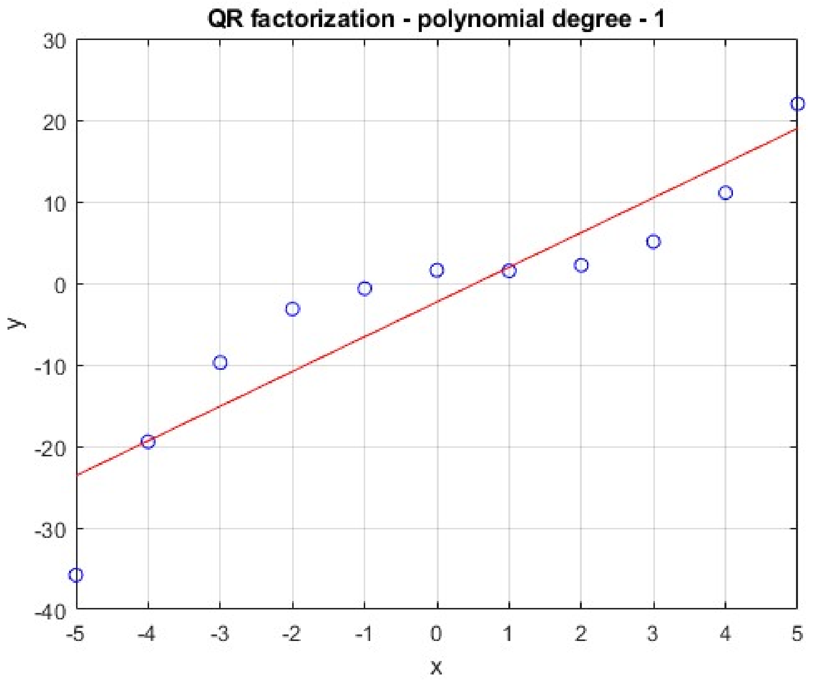

1.3 Approximation using QR distribution – Results.

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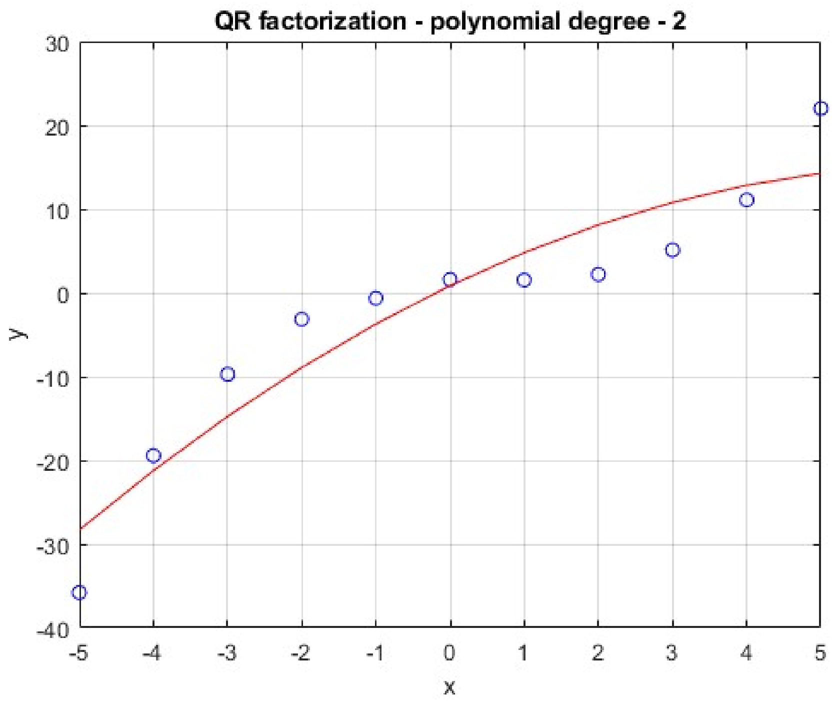

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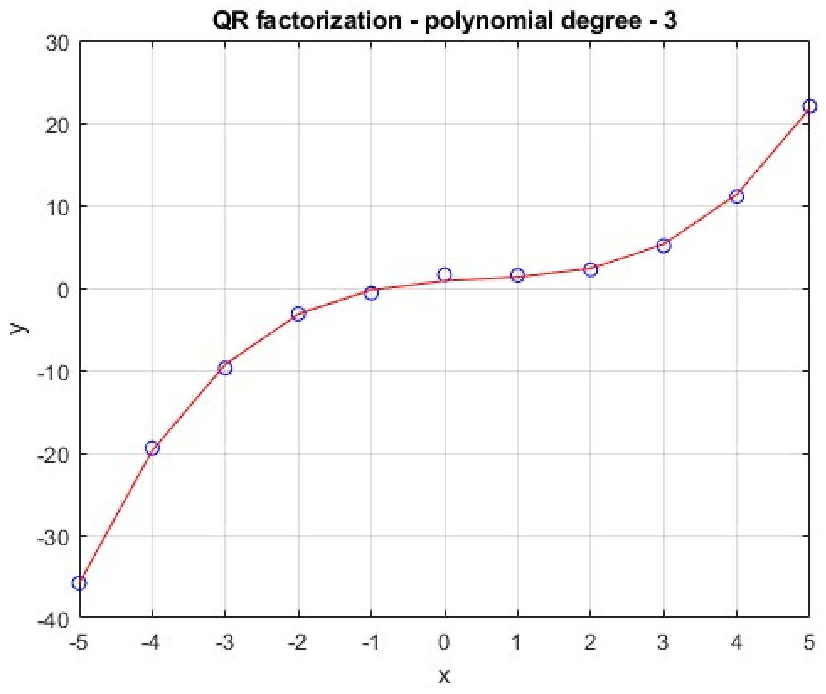

1.3 Approximation using QR distribution – Results.

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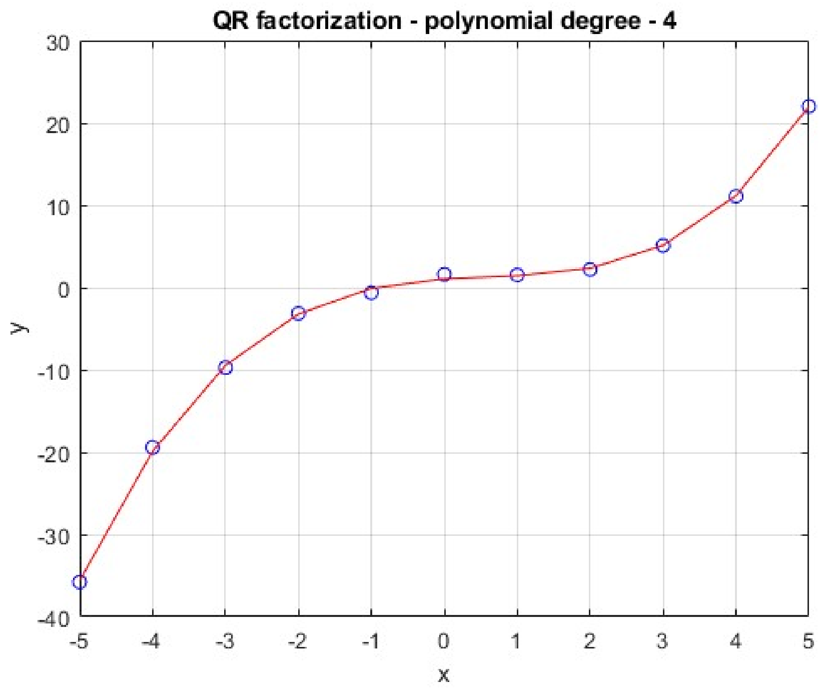

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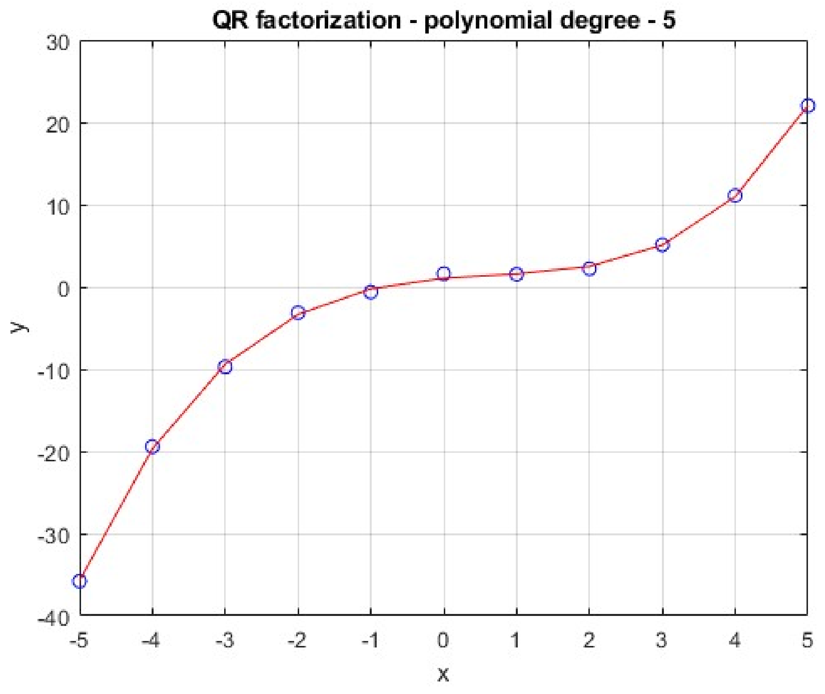


1.4 Comparison both method of finding least square approximation.

To compare both methods we will look at the residuum error obtain during computing approximate polynomial with a given degree. Table below shows the results of those calculations.

Degree of polynomial	Residuum error using system of normal equations	Residuum error using QR distribution
0	3.5527e-15	0
1	5.6954e-14	2.6645e-15
2	5.6954e-14	5.0242e-15
3	3.5527e-15	8.7023e-15
4	1.8189e-12	9.6710e-15
5	2.9104e-11	1.4947e-14
6	4.1319e-11	2.4027e-14
7	9.3178e-10	6.4035e-14
8	2.0827e-09	7.2071e-14
9	5.9815e-08	3.6645e-13
10	4.47089e-06	3.4017e-13

Conclusions : As you can see, the system of equations resulting from the QR distribution maintains a good conditioning longer in contrast to the system of normal equations, which quickly loses accuracy of result. Nevertheless, for the degrees of polynomials of a degree greater than or equal to 10, the approximate function in both cases begins to differ from the previous results. This is due to the fact that at some point we stop approximating the function and only measuring data. In both cases we can observe that approximation errors decrease with increasing polynomial degree.

2.1 Introduction.

The second task is to determine the trajectory of the motion of a point define by the equations:

$$x_1' = x_2 + x_1(0{,}5 - {x_1}^2 - {x_2}^2)$$

$$x_2' = -x_1 + x_2(0{,}5 - {x_1}^2 - {x_2}^2)$$

on the interval [0, 20]. The following initial conditions are given : $x_1(0) = 0, x_2(0) = 0.3$. We will evaluate the solution in two following ways :

a) Runge-Kutta method of 4th order (RK4) and Adams PC (P_5EC_5E) – each method a few times, with different constant step-sizes unital an „optimal" constant step size is found, i.e., when its decrese does not influence the solutions significantly but its increase does.
b) Runge-Kutta method of 4th order (RK4) with a variable step size automatically adjusted by the algorithm, making error estimation according to the step-doubling rule.

Runge-Kutta method 4th order(RK4, "classical") can be define using following formulas :

$$y_{n+1} = y_n + \frac{1}{6}\, h\,(k_1 + 2k_2 + 2k_3 + k_4)$$

$$k_1 = f(x_n, y_n)$$

$$k_2 = f(x_n + \frac{1}{2}h, y_n + \frac{1}{2}hk_1)$$

$$k_3 = f(x_n + \frac{1}{2}h, y_n + \frac{1}{2}hk_2)$$

$$k_4 = f(x_n + h, y_n + hk_3)$$

The coefficient k_1 represents the derivative at (x_n, y_n). The value k_2 is calculated as in the modifed Euler's method – as a derivative of the solution calculated by the standard Euler's method at the midpoint $(x_n + \frac{1}{2}h, y_n + \frac{1}{2}hk_1)$, the dashed tangent line correspond to this derivative. Next, the value k_3 is calculated similarly as it was for k_2, but this time at the point $(x_n + \frac{1}{2}h, y_n + \frac{1}{2}hk_2)$-i.e., with a tangent line corresponding to k_2.. Finally, we start with this line from the initial point until the endpoint $(x_n + h)$, i.e., the derivative k_4 of a solution at the point $(x_n + h, y_n + hk_3)$ over sthe one step intevral: one at the initial point, two at the midpoint and on at the endpoint. The final approximation of the solution derivative for the final full step of the method is calculated as a weighted mean value of these derivatives, with the weight 1 for the initial and end points and the weight 2 for the midpoint.

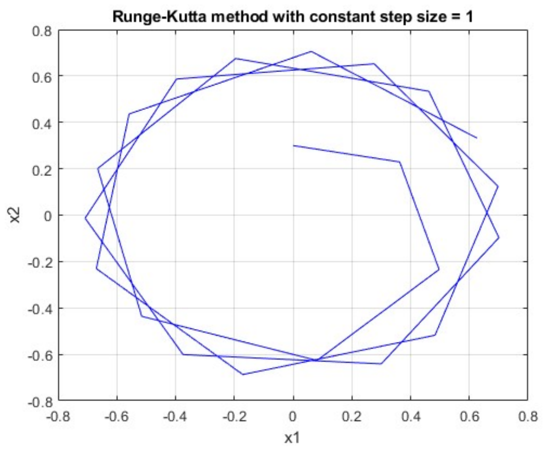
The step was decreased until the plot started to present sufficient accuracy. Error of single step can be calculated using formula :

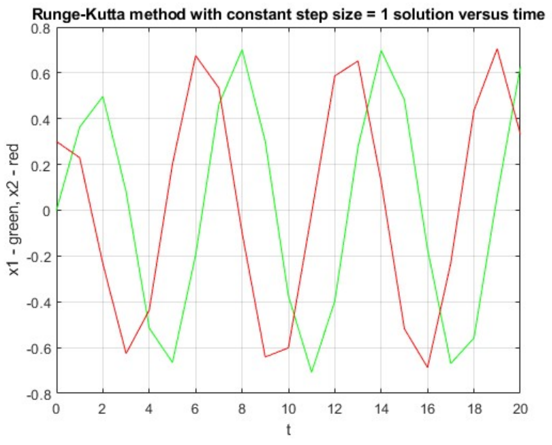
$$\delta_n(h) = \frac{2^p}{2^p - 1}({y_n}^{(2)} - {y_n}^{(1)})$$

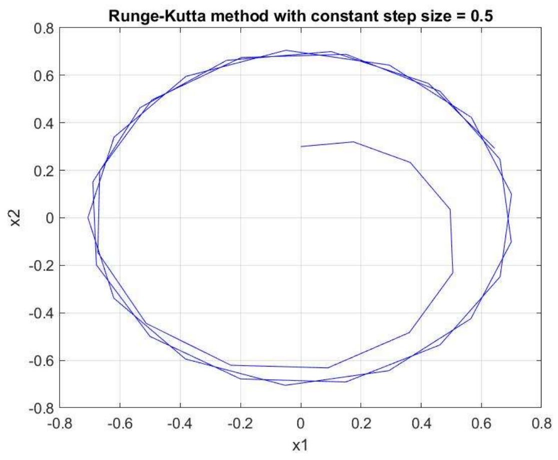
where, ${y_n}^{(1)}$ – new point obtained from the step of length h, ${y_n}^{(2)}$ – new point obtain from two additional steps of length $0.5h, p$ – order of method.

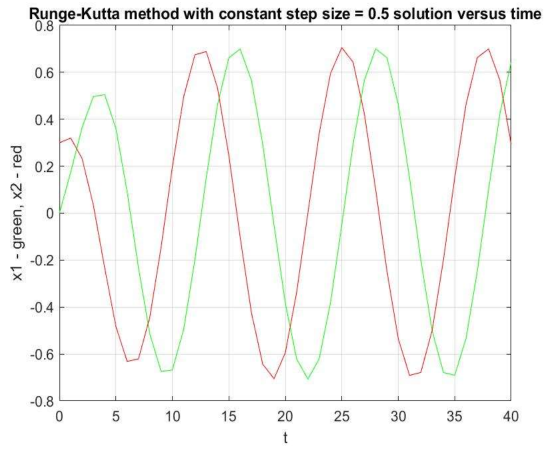
2.2 Runge-Kutta method of 4th order (RK4), a constant step size – Results.

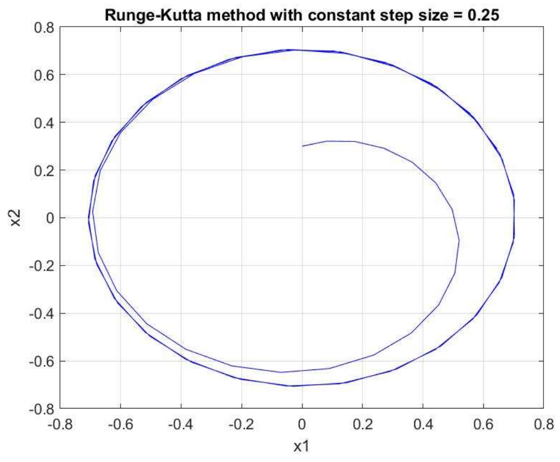
Results(for different step sizes) obtained using Runge-Kutta algorithm of 4th order presents as follow :

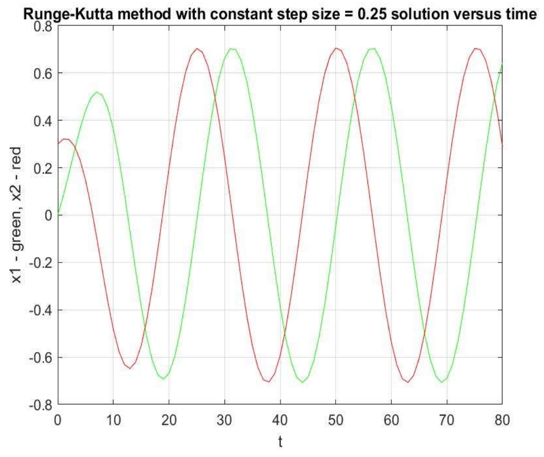












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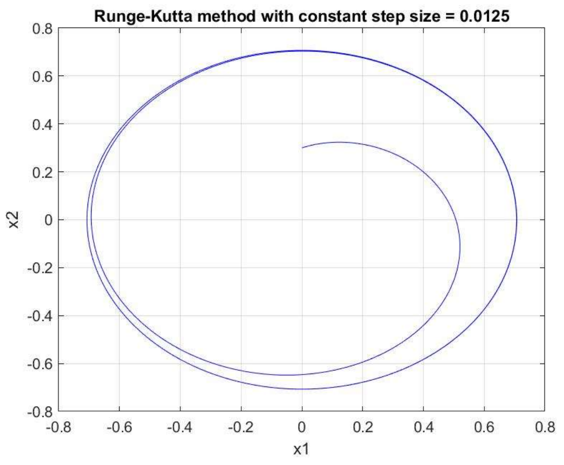
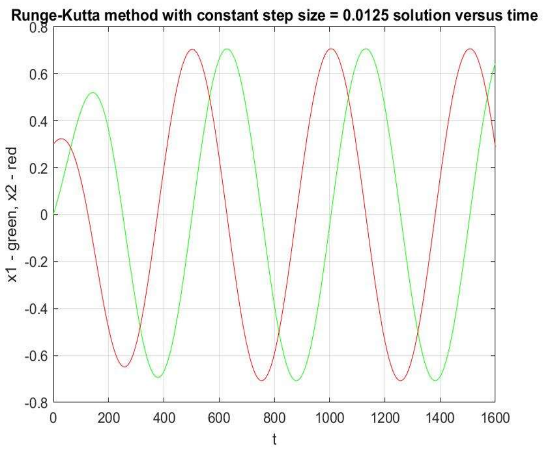
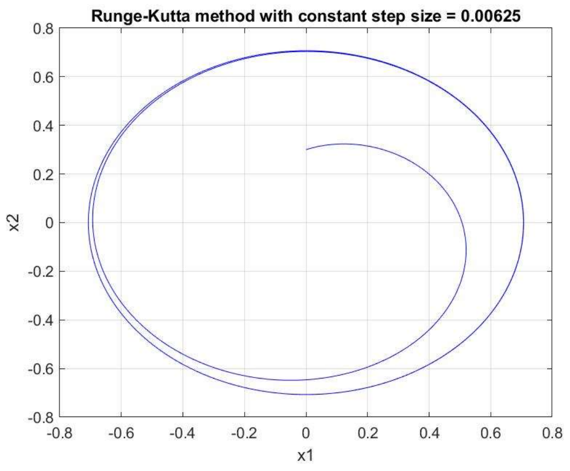
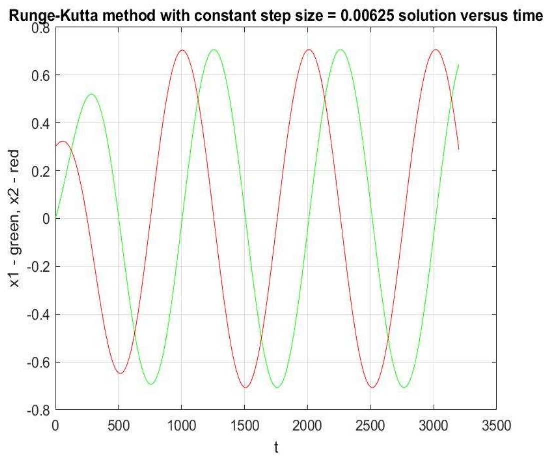
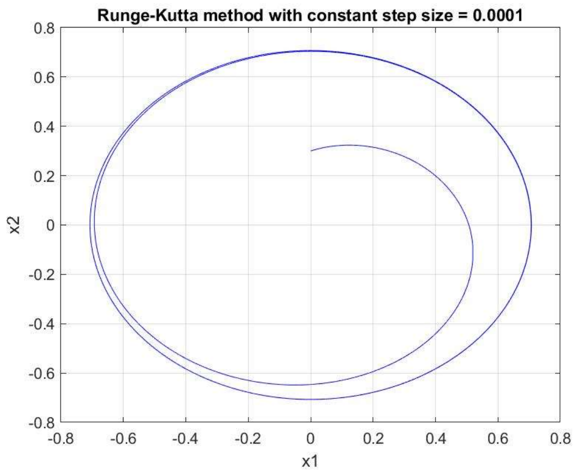
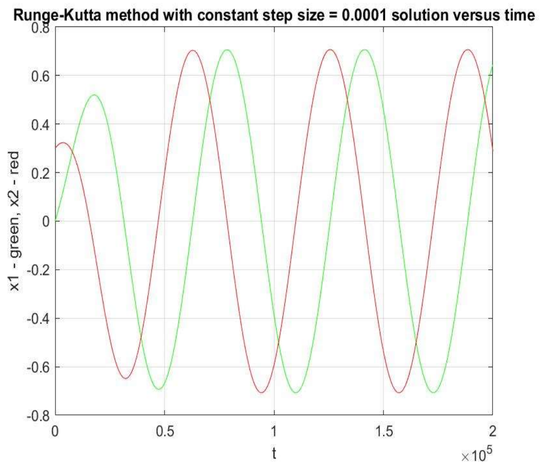








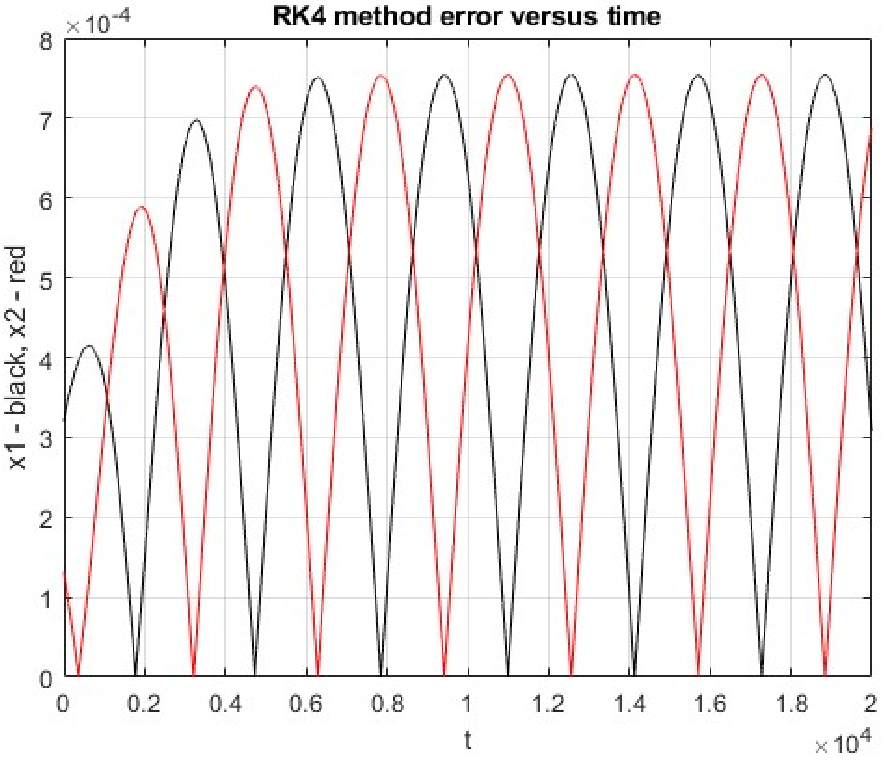




2.2 Runge-Kutta method of 4th order (RK4), a constant step size – Results.

Conclusion : We can see that starting from *h = 0.0125* obtained trajectory does not change a lot(probably if we zoom and compare plots we would see some differences). For that matter, we can conclude that it presents a proper function.

Errors versus time for such chosen step presents as follow :



2.3 Adams PC (P_5EC_5E) – Results.

The second method that will be researched is so called Adams PC (P_5EC_5E) method.

An initial differential equation problem :

$$y'(x) = f\big(x, y(x)\big),$$

$$y(a) = \ y_a, x \in [a, b]$$

can be equivalently formulated in the form of an integral equation:

$$y(x) = y(a) + \int_a^x f(t, y(t)dt$$

Consider this integral on the interval [xn-1, xn]:

$$(x_n) = y(x_{n-1}) + \int_{x_{n-1}}^{x_n} f(t, y(t)dt$$

leads to Adams methods.

There can be two forms of Adams method distinguished – explicit and implicit.

Explicit Adams methods :

The function *f* (*x* , *y* (*x*)) is replaced by an interpolation polynomial *W(x)* of order *k-1*, calculated at the points *xn*−1 , ... , *xn*−*k* . Using the Lagrange interpolation formula we have:

$$f\big(x, y(x)\big) \approx W(x) = \sum_{j=1}^{k} f\big(x_{n-j}, y_{n-j}\big)\, L_j(x)$$

$$y_n = y_{n-1} + \sum_{j=1}^{k} f\big(x_{n-j}, y_{n-j}\big) \ \int_{x_{n-1}}^{x_n} L_j(t)dt$$

where *Lj* (*x*) are the Lagrange polynomials:

$$L_j(x) = \prod_{m=1, m\neq j}^{k} \frac{x - \ x_{n-m}}{x_{n-j} - \ x_{n-m}}$$

Assuming that the points are equally spaced *xn*− *j* = *xn* − *jh* , *j* = 1, 2, ... , *k* , the integration process yields:

$$y_n = y_{n-1} + h \sum_{j=1}^{k} \beta_j f\big(x_{n-j}, y_{n-j}\big)$$

where values of the coefficients β *j* are given.

2.3 Adams PC (P_5EC_5E) – Results.

Implicit Adams methods:

The function *f* (*x* , *y* (*x*)) is now replaced by an interpolation polynomial *W*(x)* of order *k*, calculated at the points x_n , ... , x_{n-k} with the corresponding solution values $y\ (x_{n-1}) \approx y_{n-j}$. Reasoning in the same way as it was done in the case of the explicit methods, we finally get:

$$y_n = y_{n-1} + h\sum_{j=0}^{k} \beta_j^* f\left(x_{n-j}, y_{n-j}\right) = y_{n-1} + \beta_0^* f(x_n, y_n) + h\sum_{j=1}^{k} \beta_j^* f\left(x_{n-j}, y_{n-j}\right)$$

where values of the parameters β_j^*, for *k* = 1, ... , 7, are given.

The predictor-corrector method P_kEC_kE:

For the Adams methods the P_kEC_kE algorithm has the following form:

P: $y_n{}^{[0]} = y_{n-1} + h\ \sum_{j=1}^{k} \beta_j f_{n-j}$

E: $f_n{}^{[0]} = f(x_n, y_n{}^{[0]})$

K: $y_n = y_{n-1} + h\ \sum_{j=1}^{k-1} \beta_j^* f_{n-j} + h\,\beta_0^*\, f_n{}^{[0]}$

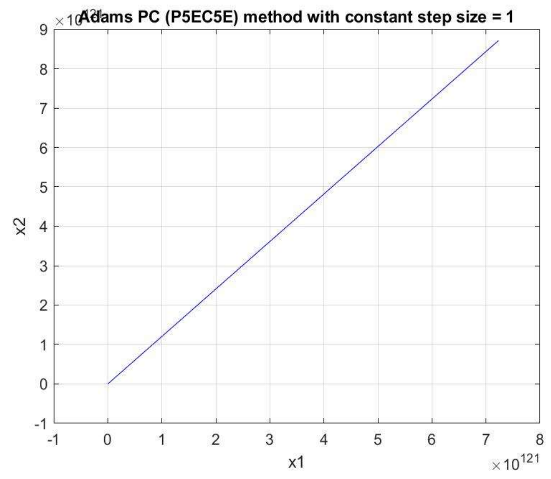
E: $f_n = f(x_n, y_n)$

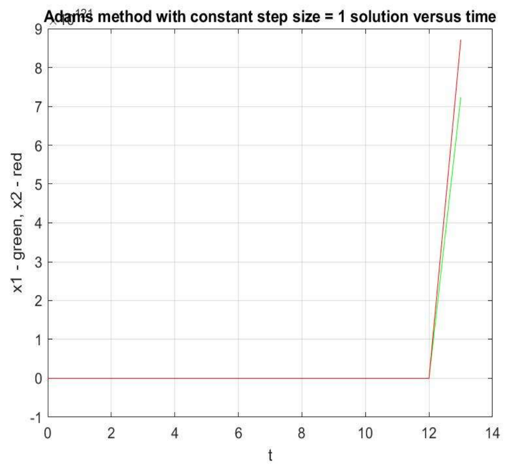
The error approximation is calculated by the formula:

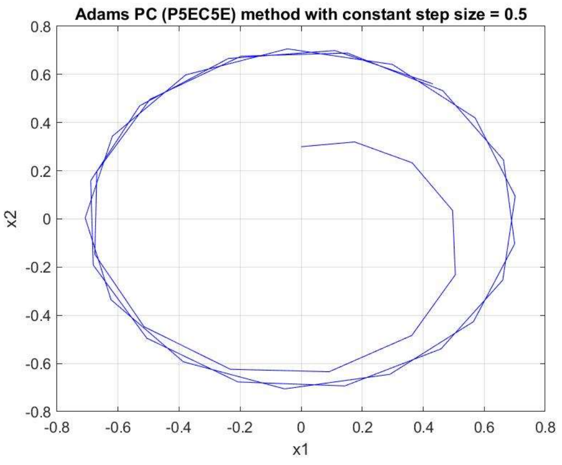
$$\delta_n(h_{n-1}) = -0.0452(y_n{}^{[0]} - y_n)$$

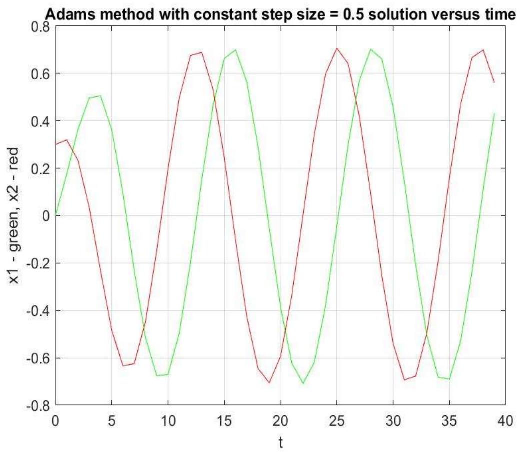
2.3 Adams PC (P_5EC_5E) – Results.

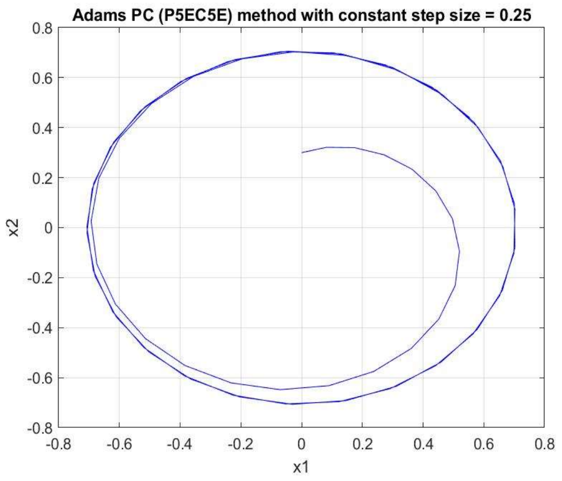
Results(for different step sizes) obtained using Adams PC (P_5EC_5E) algorithm presents as follow :

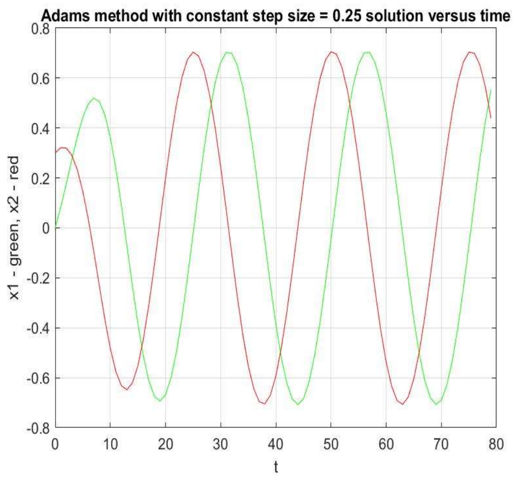




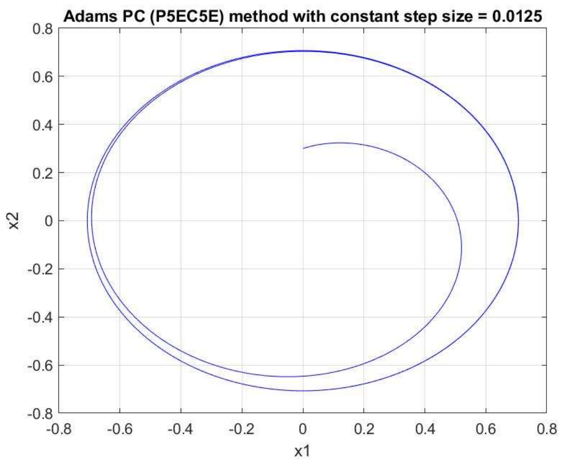


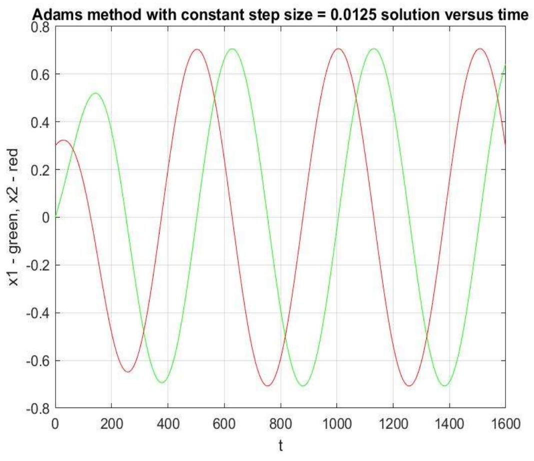


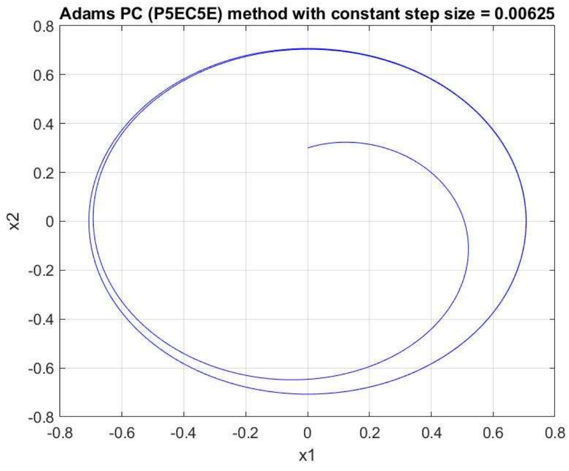


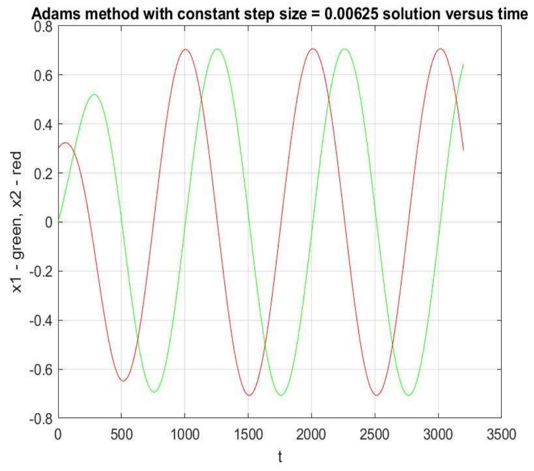


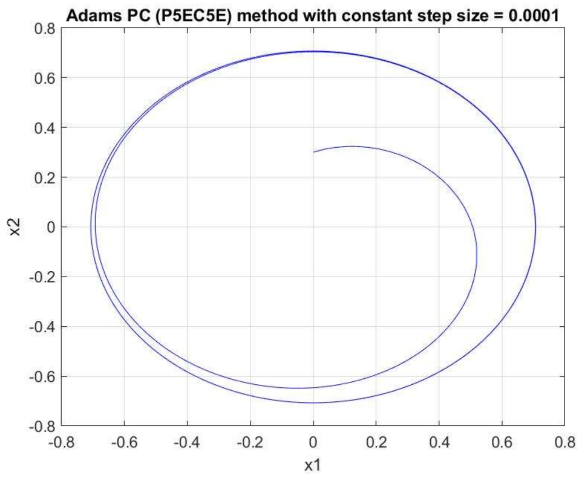
2.3 Adams PC (P_5EC_5E) – Results.

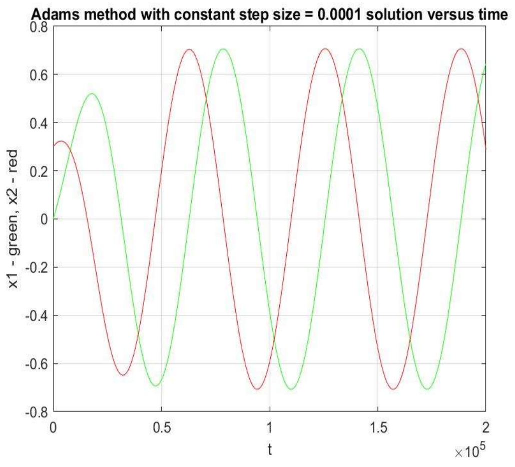








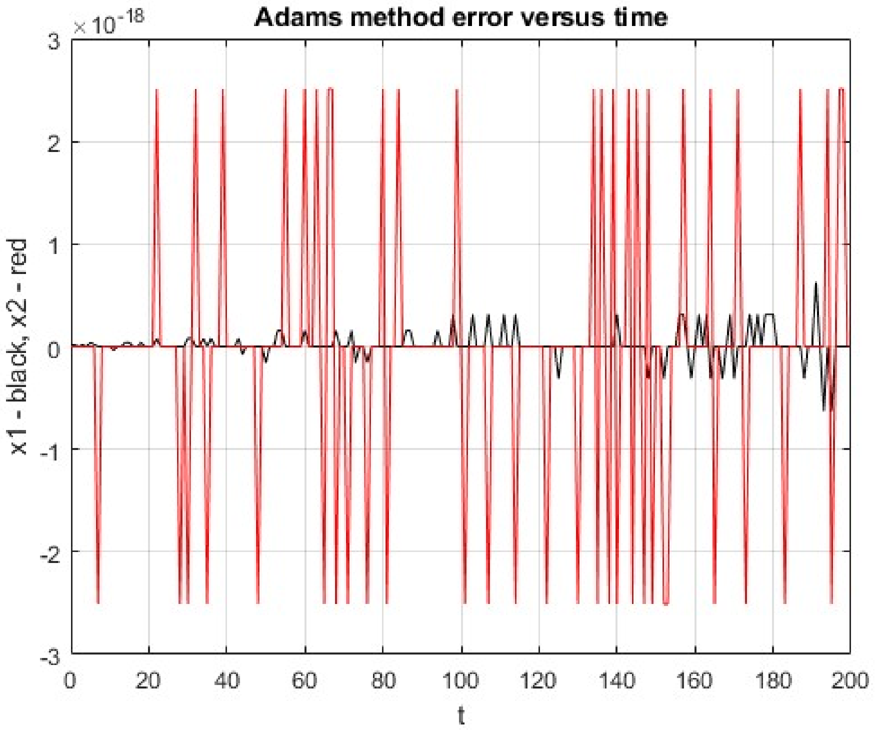




2.3 Adams PC (P_5EC_5E) – Results.

Conclusion : We can see that starting from *h = 0.0125* obtained trajectory does not change a lot(probably if we zoom and compare plots we would see some differences). For that matter, we can conclude that it presents a proper function.

Errors versus time for such chosen step presents as follow :

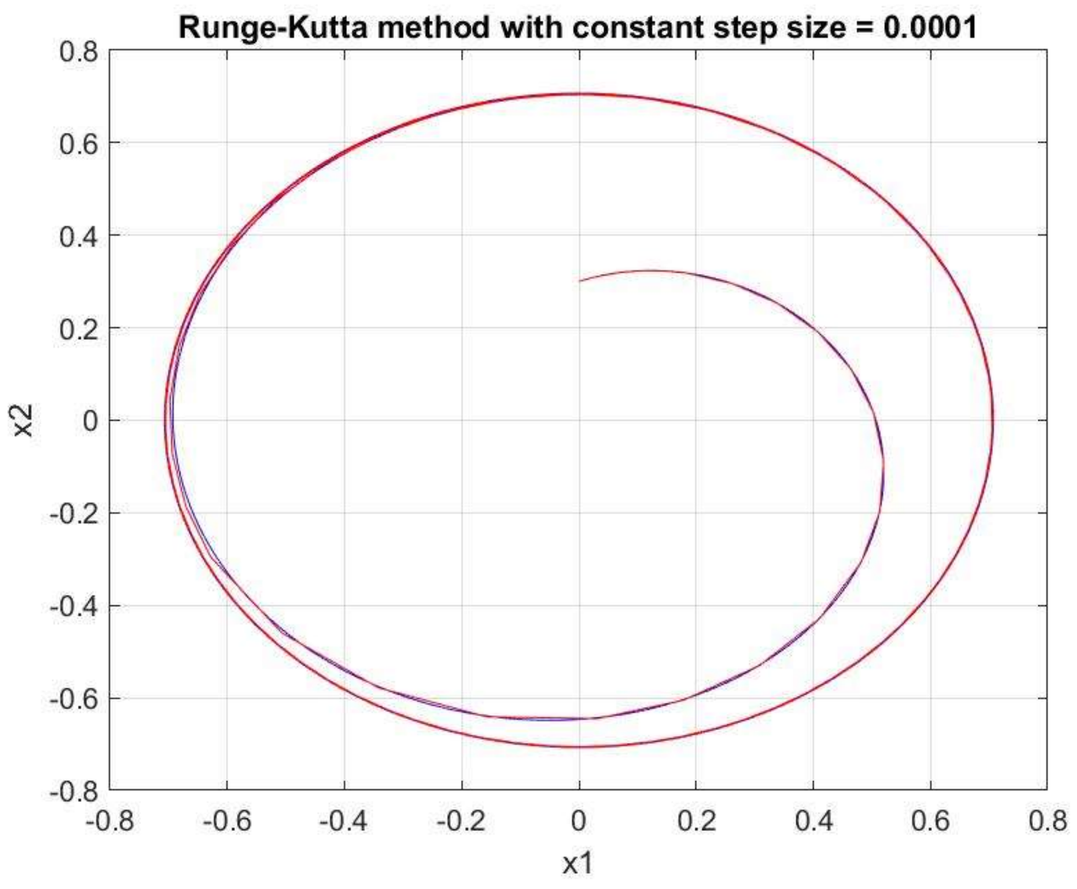


2.4 Testing and comparing both method from subpoint a.

To test my implementations of algorithms I used ***ode45*** build-in Matlab function. Next I plot two functions, one obtained from my algorithm and the second one from *ode45* function, and see whether they differ or not. The step size that I choose for my algorithm is equal 0.0001.

Runga-Kutta method of order 4th, my implementation – color BLUE

ode45, build-in Matlab function – color *RED*

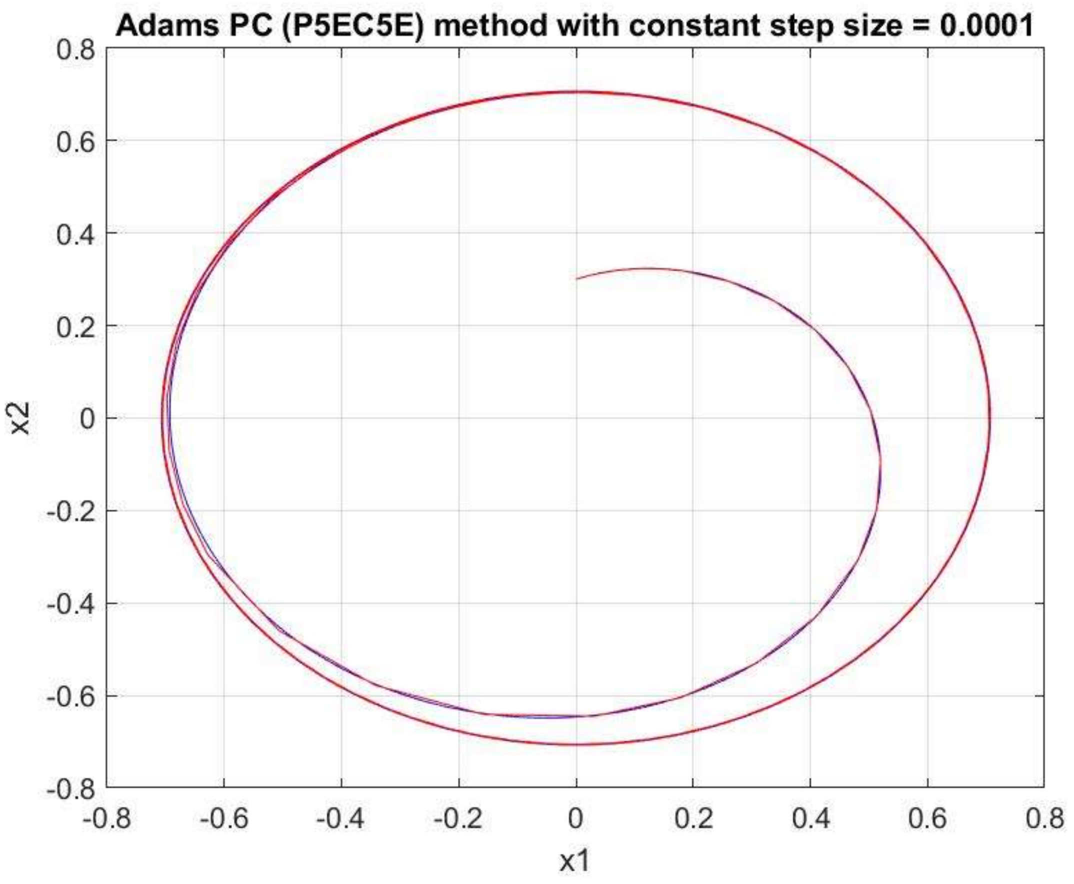


Conclusion : We can assume that our algorithm works fine even though there are some small differences which may be erased if we choose smaller step size.

2.4 Testing and comparing both method from subpoint a.

Adams PC (P_5EC_5E), my implementation – color BLUE

ode45, build-in Matlab function – color *RED*



Conclusion : We can assume that our algorithm works fine even though there are some small differences which may be erased if we choose smaller step size.

As we can see, in each case the methods gave results similar to the results obtained with the command *ode45*. However, in all cases the predictor-corrector method found the result faster. Moreover, each time it generated smaller errors: in the case of the first two at the very beginning they are larger, but remember that the first four points in the Adams PC (P_5EC_5E) method are calculated using the RK4 method, then the errors stabilize quickly and reach very small values. However, the Adams PC (P_5EC_5E) method requires more calculation than RK4 due to the double evaluation of the function value. It can be reduced by examining the variability of functions and introducing a variable step (larger for less variable intervals and smaller for intervals of high variability).

2.5 Runge-Kutta method of 4th order with a variable step size.

We can modify Runge-Kutta method and make algorithm to choose the best fitting next step size.

Choosing the length of the step size

The basic issue in the practical implementation of methods for solving differential equations is the question of choosing the step length h_n. When determining the step length, there are two opposing cases :

- If the step h_n decreases, the method error decreases, for the convergent method the error decreases to zero with h going toward zero
- If the step h_n decreases, the number of iterations needed to determine the solution on the given distance [a, b] increases, hence the number of calculations and related numerical errors also increases.

From the above points it appears that there should be an optimal step, for which both method and numerical errors will not be too great.

Estimating the error value according to the step-doubling rule

In order to estimate the error, in addition to the step of length h, we additionally carry out two additional steps of $\frac{1}{2}h$ each in parallel and exactly the same method.

Starting from the formula :

$$y(x_n + h) = y_n^{(1)} + \frac{r_n^{(p+1)}(0)}{(p+1)!} * h^{p+1} + O(h^{p+2}) \text{ – for single step}$$

$$y(x_n + h) \approx y_n^{(2)} + 2 * \frac{r_n^{(p+1)}(0)}{(p+1)!} * (\frac{h}{2})^{p+1} + O(h^{p+2}) \text{ – for double step}$$

After some transformations we receiving the following error's formulas :

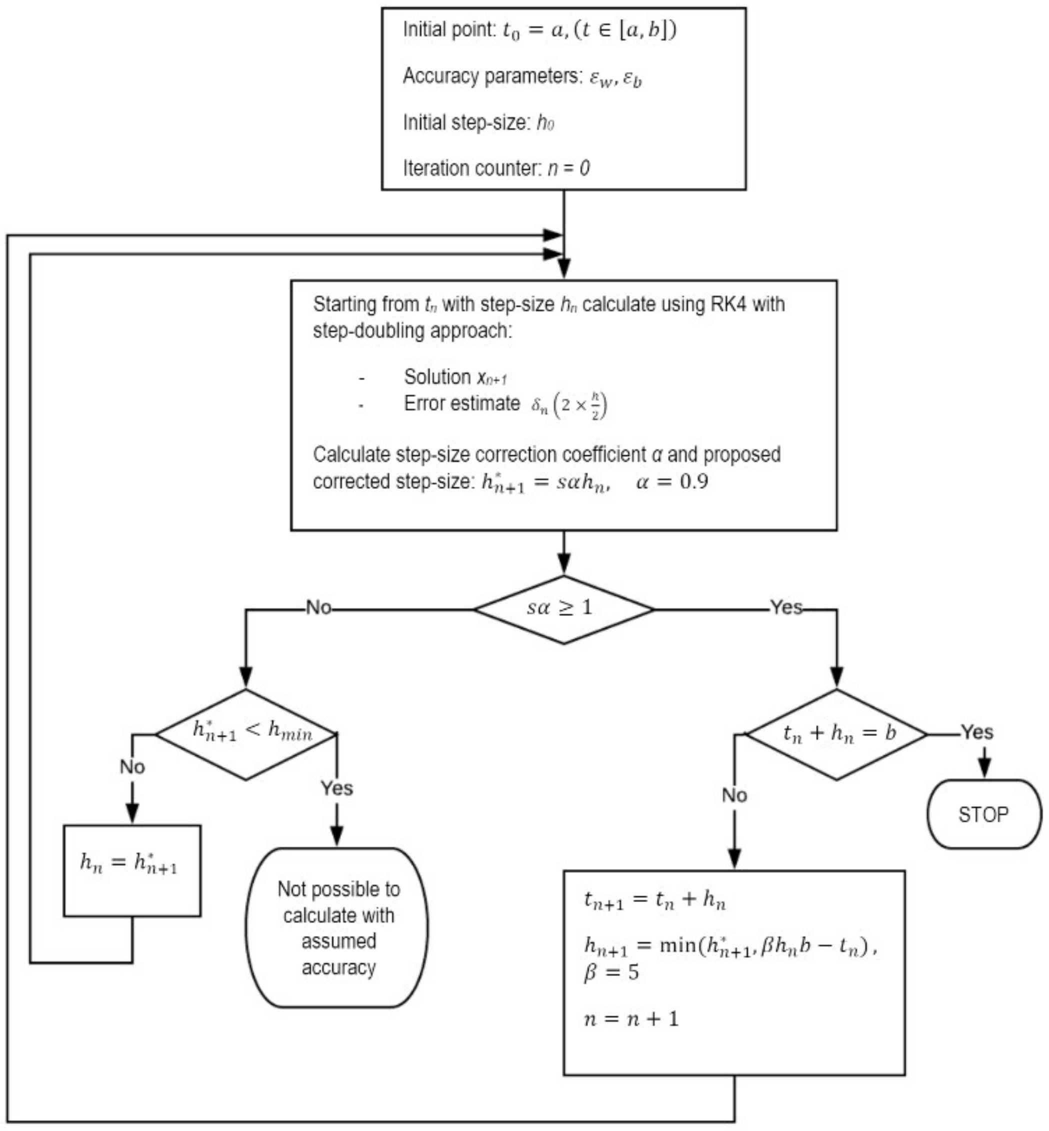
$$\sigma_n(h) = \frac{2^p}{2^p - 1}(y_n^{(2)} - y_n^{(1)}) \xrightarrow{p=4} \frac{16}{15}(y_n^{(2)} - y_n^{(1)}) \text{ – estimating error after single step}$$

$$\sigma_n\left(2\ x\ \frac{h}{2}\right) = \frac{y_n^{(2)} - y_n^{(1)}}{2^p - 1} \xrightarrow{p=4} \frac{y_n^{(2)} - y_n^{(1)}}{15} \text{ – estimating error after double step}$$

where $y_n^{(1)}$ is a new point received after step of length h, $y_n^{(2)}$ is a new point received after double step of length h.

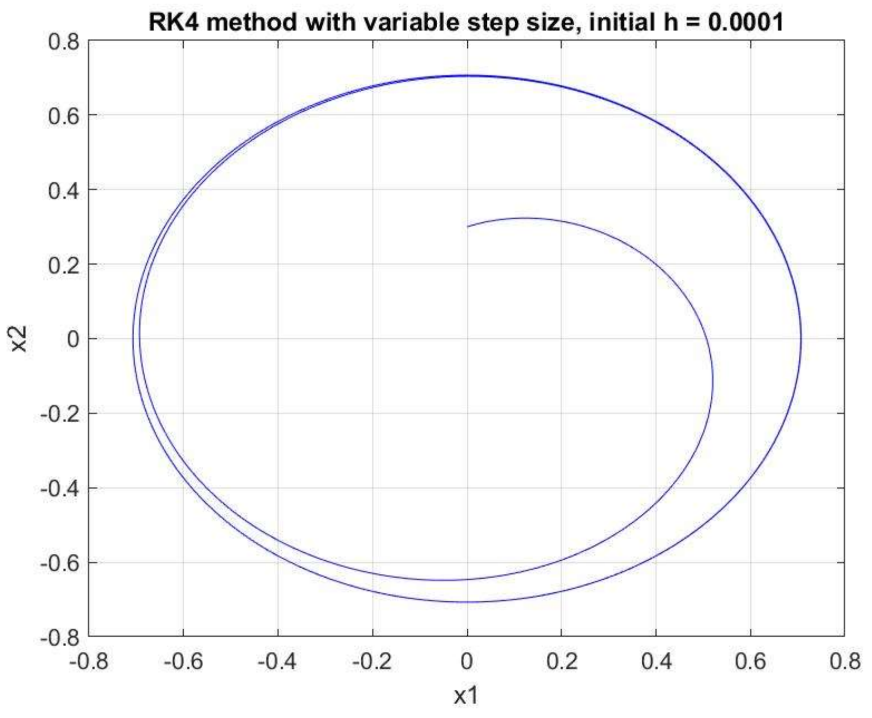
2.5 Runge-Kutta method of 4th order with a variable step size.

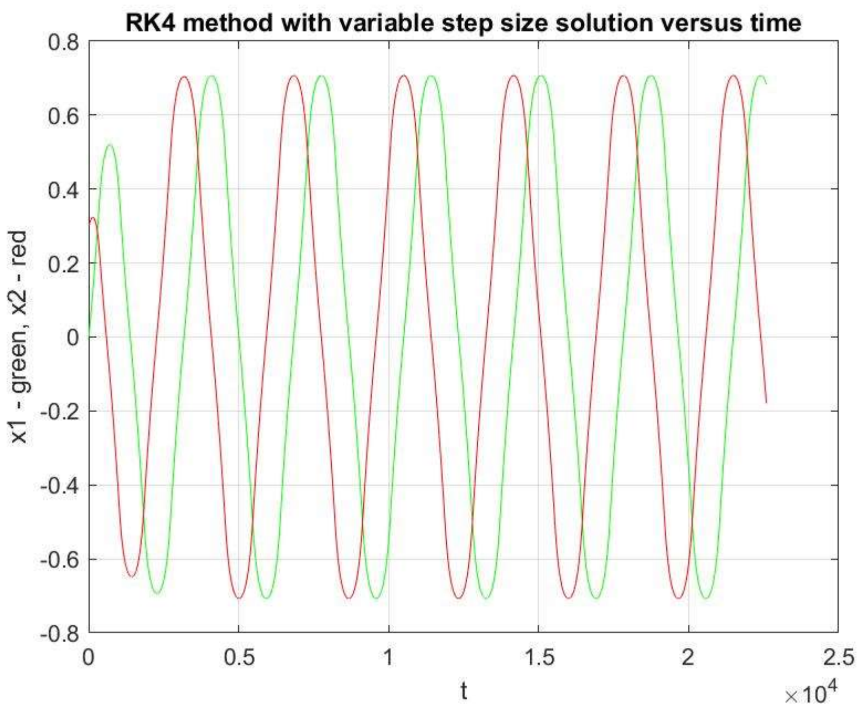
Flowchart of an algorithm :


Initial point: $t_0 = a, (t \in [a, b])$
Accuracy parameters: $\varepsilon_w, \varepsilon_b$
Initial step-size: h_0
Iteration counter: $n = 0$
Starting from t_n with step-size h_n calculate using RK4 with step-doubling approach:
- Solution x_{n+1}
- Error estimate $\delta_n\left(2 \times \frac{h}{2}\right)$
Calculate step-size correction coefficient α and proposed corrected step-size: $h^*_{n+1} = s\alpha h_n, \quad \alpha = 0.9$
$s\alpha \geq 1$
No
Yes
$h^*_{n+1} < h_{min}$
No
Yes
$h_n = h^*_{n+1}$
Not possible to calculate with assumed accuracy
$t_n + h_n = b$
Yes
No
STOP
$t_{n+1} = t_n + h_n$
$h_{n+1} = \min(h^*_{n+1}, \beta h_n b - t_n)$, $\beta = 5$
$n = n + 1$

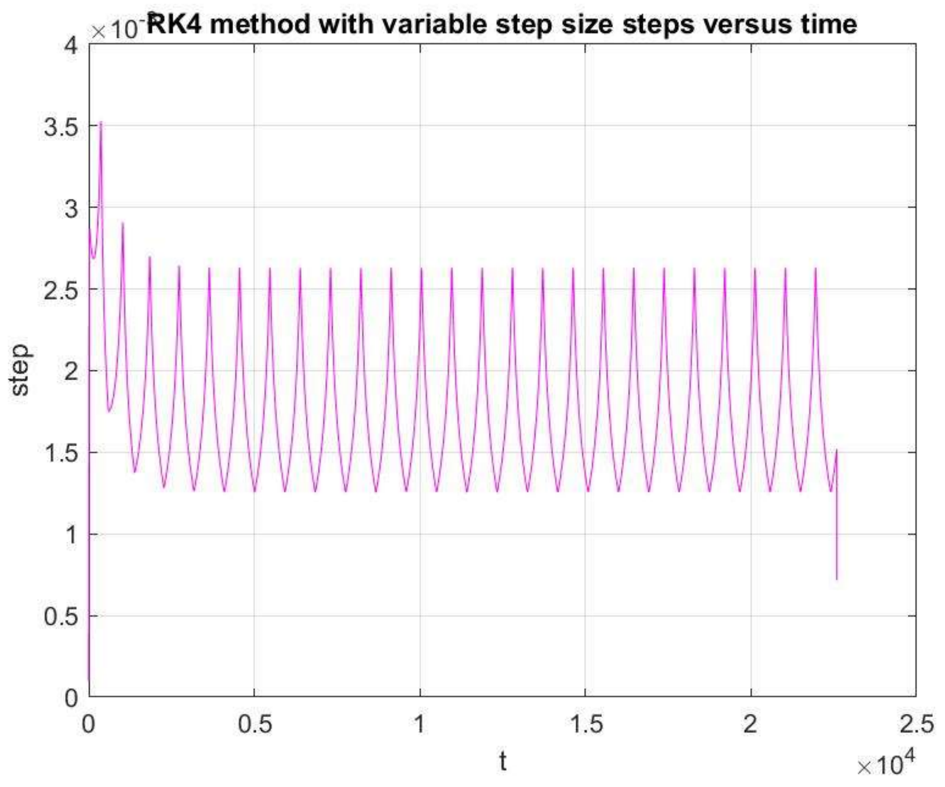
2.5 Runge-Kutta method of 4th order with a variable step size.

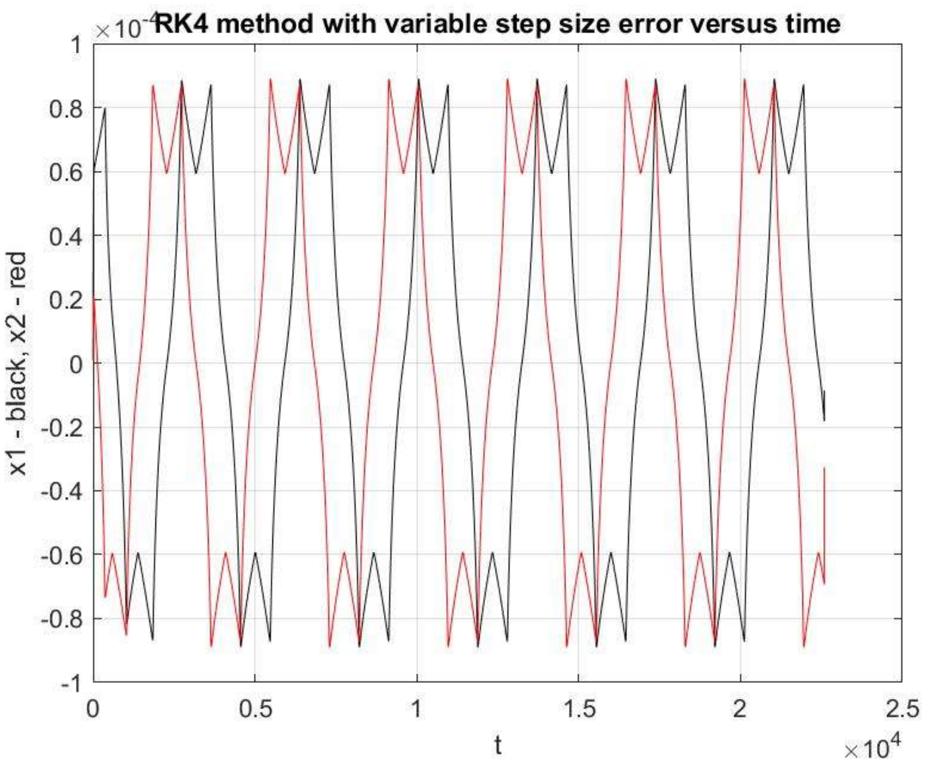
Result obtained using Runge-Kutta method of 4th order with variable step size algorithm presents as follow :





2.5 Runge-Kutta method of 4th order with a variable step size.





2.5 Runge-Kutta method of 4th order with a variable step size.

The parameters h_{min}, absolute and relative tolerance where chosen using trial and error method. It occurs that it is the best for our problem to assign them as follow :

$h_{min} = 10^{-10}$, because if we choose smaller the time performance will not be sufficient.

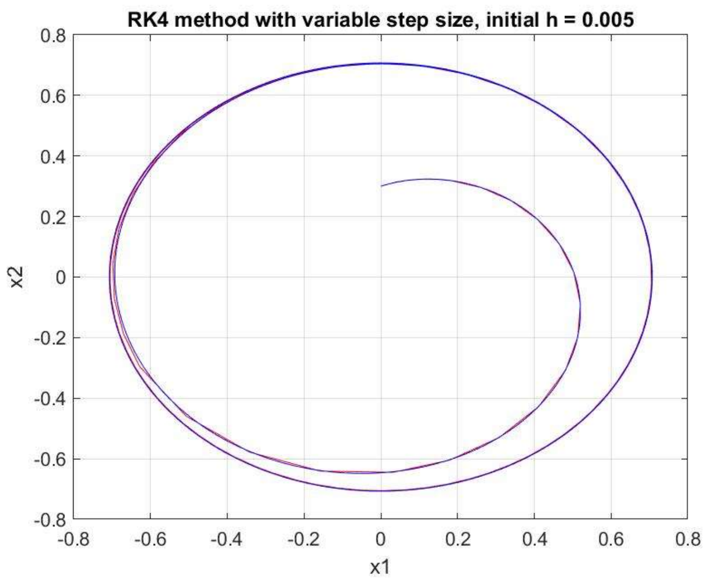
$\text{eps\_absolute} = 10^{-4}$

$\text{eps\_relative} = 10^{-4}$, those configuration allows to get very precise solution as shown above within the sufficient time, because if we decrease both parameters to 10^{-5} the solution does not differ very much but the period of computation is significantly longer.

To test my implementations of algorithms I used ***ode45*** build-in Matlab function. Next I plot two functions, one obtained from my algorithm and the second one from *ode45* function, and see whether they differ or not. The initial step size that I choose for my algorithm is equal 0.005.

Runga-Kutta method of order 4th variable step size – color BLUE

ode45, build-in Matlab function – color *RED*



Final conclusions : This method significantly reduces the number of iterations performed in relation to the method unmodified (the step grows - the number of iterations decreases and, consequently, the number related calculations and numeric errors). However, more iterations are done in each iteration, often repeatedly the step on the corresponding accuracy is changed. The advantage of this method is the fact that automatic step selection depending on the direction of the trajectory, the program itself adapts to the conditions of the function, e.g. in the moments of bending the function increases its accuracy to better approximate it. This method also relieves the user from obligation to determine the optimal step by trial and error, which saves a huge amount of time.

3.1 Approximation using system of normal equations.

```
function [a, residuum] = approxUsingSysNormEq(x, y, n)
% approxUsingSysNormEq is a function which computes       approximation
% of a function based on
% x - xs of function
% y - values of f(x)
% n - degree of an approximate polynomial

N = size(x, 1);
A = zeros(N, n + 1);

for i = 1:N
    for j = 1:n + 1
        A(i, j) = x(i, 1) ^ (j - 1);
    end
end

a = (A' * A) \ (A' * y);
residuum = norm((A' * y) - (A' * A) * a);

end
```

3.2 Approximation using QR factorization.

```
function [a, residuum] = approxUsingQRdistr(x, y, n)
% approxUsingSysNormEq is a function which computes approximation
% of a function based on
% x - xs of function
% y - values of f(x)
% n - degree of an approximate polynomial

N = size(x, 1);
A = zeros(N, n + 1);

for i = 1:N
    for j = 1:n + 1
        A(i, j) = x(i, 1) ^ (j - 1);
    end
end

[Q, R] = qrmgs(A);
a = R \ Q' * y;
residuum = norm(R * a - Q' * y);

end
```

3.3 Runge-Kutta method of 4th order with a constant step.

```
function [x1, x2, errX1, errX2] = RK4(fun1, fun2, h, initX1, initX2)

x1(1) = initX1;
x2(1) = initX2;

for i = 1:1:(20 / h)

    [k1, k2] = computeKs(fun1, fun2, x1(i), x2(i), h);

    x1(i + 1) = x1(i) + h * (k1(1) + 2 * k1(2) + 2 * k1(3) + k1(4)) / 6;
    x2(i + 1) = x2(i) + h * (k2(1) + 2 * k2(2) + 2 * k2(3) + k2(4)) / 6;

    errX1(i) = (16 / 15) * abs(x1(i + 1) - x1(i));
    errX2(i) = (16 / 15) * abs(x2(i + 1) - x2(i));

end
```

```
function [k1, k2] = computeKs(fun1, fun2, x, y, h)

%first ks
k1(1) = fun1(x, y);
k2(1) = fun2(x, y);
%second ks
k1(2) = fun1(x + 0.5 * h * k1(1), y + 0.5 * h * k2(1));
k2(2) = fun2(x + 0.5 * h * k1(1), y + 0.5 * h * k2(1));
%third ks
k1(3) = fun1(x + 0.5 * h * k1(2), y + 0.5 * h * k2(2));
k2(3) = fun2(x + 0.5 * h * k1(2), y + 0.5 * h * k2(2));
%fourth ks
k1(4) = fun1(x + h * k1(3), y + h * k2(3));
k2(4) = fun2(x + h * k1(3), y + h * k2(3));

end
```

3.4 Adams PC (P_5EC_5E).

```
function [x1, x2, errX1, errX2] = adams5(fun1, fun2, h, initX1, initX2)

err_fac = (863/60480) / ((-95/288) + (863 / 60480));

x1(1) = initX1;
x2(1) = initX2;

betaE = [1901, -2774, 2616, -1274, 251];
betaE = betaE / 720;

betaI = [475, 1427, -798, 482, -173, 27];
betaI = betaI / 1440;

for i = 1:4
    [k1, k2] = computeKs(fun1, fun2, x1(i), x2(i), h);
    x1(i + 1) = x1(i) + h * (k1(1) + 2 * k1(2) + 2 * k1(3) + k1(4)) / 6;
    x2(i + 1) = x2(i) + h * (k2(1) + 2 * k2(2) + 2 * k2(3) + k2(4)) / 6;
end

for i = 6:ceil(20 / h)
    sumX1 = 0;
    sumX2 = 0;
    for j = 1:5
        sumX1 = sumX1 + betaE(j) * fun1(x1(i - j), x2(i - j));
        sumX2 = sumX2 + betaE(j) * fun2(x1(i - j), x2(i - j));
    end

    tempX1 = x1(i - 1) + h * sumX1;
    tempX2 = x2(i - 1) + h * sumX2;

    sumX1 = 0;
    sumX2 = 0;
    for j = 1:5
        sumX1 = sumX1 + betaI(j + 1) * fun1(x1(i - j), x2(i - j));
        sumX2 = sumX2 + betaI(j + 1) * fun2(x1(i - j), x2(i - j));
    end

    x1(i) = x1(i - 1) + h * sumX1 + h * betaI(1) * fun1(tempX1, tempX2);
    x2(i) = x2(i - 1) + h * sumX2 + h * betaI(1) * fun2(tempX1, tempX2);

    errX1 = err_fac * (tempX1 - x1(i));
    errX2 = err_fac * (tempX2 - x2(i));
end

end
```

3.5 Runge-Kutta method of 4th order with a variable step size

```
function [x1values, x2values, errors, steps] = RK4variable(fun1, fun2, x1, x2, h, epsr, epsa)
% x1 - first value of x1
% x2 - first value of x2
% h - step
% epsr - relative epsilon
% epsa - absolute epsilon
i = 1;
a = 0;

x1values(1) = x1;
x2values(1) = x2;
steps(i) = h;

while (a < 20)
    %next points
    [k1, k2] = computeKs(fun1, fun2, x1, x2, h);

    x1 = x1 + h * (k1(1) + 2 * k1(2) + 2 * k1(3) + k1(4)) / 6;
    x2 = x2 + h * (k2(1) + 2 * k2(2) + 2 * k2(3) + k2(4)) / 6;

    x1values(i + 1) = x1;
    x2values(i + 1) = x2;

    %first half-step
    h = 0.5 * h;

    [k1, k2] = computeKs(fun1, fun2, x1, x2, h);

    tmp1 = x1 + h * (k1(1) + 2 * k1(2) + 2 * k1(3) + k1(4)) / 6;
    tmp2 = x2 + h * (k2(1) + 2 * k2(2) + 2 * k2(3) + k2(4)) / 6;

    %second half-step
    [k1, k2] = computeKs(fun1, fun2, tmp1, tmp2, h);

    tmp1 = tmp1 + h * (k1(1) + 2 * k1(2) + 2 * k1(3) + k1(4)) / 6;
    tmp2 = tmp2 + h * (k2(1) + 2 * k2(2) + 2 * k2(3) + k2(4)) / 6;

    h = 2 * h;

    errors(i, 1) = (tmp1 - x1) / 15;
    errors(i, 2) = (tmp2 - x2) / 15;

    eps1 = abs(tmp1) * epsr + epsa;
    eps2 = abs(tmp2) * epsr + epsa;

    alpha1 = (eps1 / abs(errors(i, 1)))^(1/5);
    alpha2 = (eps2 / abs(errors(i, 2)))^(1/5);

    alpha = min(alpha1, alpha2);

    hnew = 0.9 * alpha * h;

    if (0.9 * alpha >= 1)
        if (a + h >= 20)
            break;
        else
            a = a + h;
            h = min([hnew, 5 * h, 20 - a]);
            i = i + 1;
            steps(i) = h;
            continue;
        end
    else
        if (hnew < 10^-10)
            error('Cant solve with this epsilon');
        else
            h = hnew;
        end
    end

    i = i + 1;
    steps(i) = h;
end
```