CSC336 Assignment #3

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2016-03-10

Problem 1

$$f(x) \equiv xe^{-\frac{x}{2}} - \frac{e^{-1}}{2}$$

(a) Solution:
Exactly one root of $f(x)$ in $\left[0, 2\right]$:

- Every exponential function is continuous, x is a linear function, then the product of them is continuous, then subtracts a constant number, the result is still continous.
- $f(x)$ is continuous in $\left[0, 2\right]$, no jump discontinuities, no vertical asymptotes nor holes.
- $f(0) < 0, f(2) = \frac{3}{2}e^{-1} \approx 0.5519 > 0$, so $f(0) \cdot f(2) > 0$, Therefore, there exists a root of $f(x)$ between $\left[0, 2\right]$.
- $f(x)$ is differentiable in $\left(a, b\right)$ since $f'(x) = e^{\frac{-x}{2}} + x \cdot \frac{-1}{2}e^{-x/2} = (1 - \frac{x}{2})e^{-x/2}$ always exists in $(0, 2)$.
- $f'(x) \neq 0, \forall x \in (0, 2)$, so the root exists is unique.
- Hence there is exactly one root of $f(x)$ in $\left[0, 2\right]$.

Exactly one root of $f(x)$ in $\left(-\infty, 6\right]$:

- We know $f'(x) = (1 - \frac{x}{2})e^{-x/2} > 0$ for $x \in (-\infty, 0)$. So the function is monotonically increasing in this domain. We also know that $f(0) < 0$, so for any $x < 0, f(x) < f(0) < 0$, so there is no roots in $(-\infty, 0)$.
- We know that $f'(x) < 0$ for $x \in \left(2, 6\right]$. So the function is monotonically decreasing in this domain. We have $f(6) = 6e^{-3} - \frac{e^{-1}}{2} \approx 0.1148 > 0$. So for any $x \in \left(2, 6\right]$, $f(x) > 0$, so there is no roots in $\left(2, 6\right]$.
- But we do confirm that there is exactly one root in $\left[0, 2\right]$. And $\left(-\infty, 6\right] = (-\infty, 0) \cup \left[0, 2\right] \cup \left(2, 6\right]$, so there is exactly one root in $\left(-\infty, 6\right]$.

(b) Solution:
Newton's Method:

- Estimate $x^{(0)} = 0$
- Since $y = f(x^{(k)}) + f'(x^{(k)})(x - x^{(k)}) = 0, x^{(k+1)} = x^{(k)} - \frac{f(x^{(k)})}{f'(x^{(k)})}$

- Calculate $x^{(1)}$.

$$\begin{aligned} x^{(1)} &= x^{(0)} - \frac{f(x^{(0)})}{f'(x^{(0)})} \\ &= 0 - \frac{0 - e^{-1}/2}{1} \\ &= \frac{1}{2}\, e^{-1} \end{aligned}$$

(c) Solution:
Fixed-point iteration method:

- Estimate $x^{(0)} = 0$
- Since $f(x) = 0 \iff x = g(x)$
- Calculate $x^{(1)}$.

$$\begin{aligned} x^{(1)} &= g(x^{(0)}) \\ &= \frac{1}{2}\, e^{-1} e^{\frac{x^{(0)}}{2}} \\ &= \frac{1}{2}\, e^{-1} \cdot 1 \\ &= \frac{1}{2}\, e^{-1} \end{aligned}$$

(d) Solution:
The idea is to apply Theorem 4b in slides.

- First we need to confirm the function g is a contraction:
  - $g(x) = \frac{e^{-1}}{2}\, e^{\frac{x}{2}}$
  - $g'(x) = \frac{1}{2}\,\frac{e^{-1}}{2}\, e^{x/2} = \frac{1}{4}\, e^{-1} e^{x/2} > 0$. This is because, $e^{x/2}$ is a positive function, and $\frac{1}{4}\, e^{-1}$ is positive, so their product is positive.
  - $|g(a) - g(b)| \le |g(0) - g(2)| = \frac{1}{4} - \frac{1}{4}\, e^{-1} \le \lambda |a - b| \le \lambda |0 - 2| = 2\lambda, \forall a, b \in \ (0, 2)$.
  - $\therefore \lambda \ge \frac{1}{8} - \frac{1}{8}\, e^{-1} \approx 0.079 \in \ [0, 1)$
- Now we can safely apply Theorem 4b in slides, with g is a contraction in $I = \ [0, 2]$ with constant $\lambda = 0.079$.
- As we know $g'(x) > 0, \forall x \in \ [0, 2]$ indicating $g(x)$ is monotonically increasing, and we calculate:
  - $g(0) = \frac{e^{-1}}{2} \approx 0.1839 \in \ [0, 2]$
  - $g(2) = 1 \in \ [0, 2]$
  - therefore, for all $x \in I, g(x) \in \ [0, 2]$
- Then by Theorem 4b, $\exists$ a unique fixed point r of g of $[0, 2]$, $\forall x^{(0)} \in \ [0, 2]$, the iteration scheme $x^{(k+1)} = g(x^{(k)})$ converges to r no matter where we start in $[0, 2]$.

(e) Solution:

- Netwon's Method rate of convergence:
  - f is already differentiable with $f'(x) = (1 - \frac{x}{2})e^{-x/2}$, check for whether it is twice differentiable:

$$f''(x) = -\frac{1}{2}e^{-x/2} + (1 - \frac{x}{2}) \cdot (-\frac{1}{2})e^{-x/2} = (\frac{x}{4} - 1)e^{-x/2}$$

    $f''(x)$ always exists in $\left[0, 2\right]$, so it is twice differentiable.
  - As when Newton's method converges and started with close enough to r, it usually converges quadratically with rate 2.
  - Now we check if the rate is 2:

$$\begin{aligned}
g(x) &= x - \frac{f(x)}{f'(x)} \\
g'(x) &= 1 - \frac{f'(x) \cdot f'(x) - f(x) \cdot f''(x)}{f'(x) \cdot f'(x)} \\
&= 1 - \frac{(1-x)^2 e^{-x} - (xe^{-x/2} - \frac{e^{-1}}{2})(\frac{1}{2}x - \frac{3}{2})e^{-x/2}}{(1-x)^2 e^{-x}} \\
&= \frac{\frac{1}{2}x^2 e^{-x/2} - \frac{1}{4}e^{-1}x - \frac{3}{2}xe^{-x/2} + \frac{3}{4}e^{-1}}{(1-x)^2} \cdot e^{x/2} \\
&= \frac{\frac{1}{2}x^2 - \frac{1}{4}e^{x/2-1}x - \frac{3}{2}x + \frac{3}{4}e^{x/2-1}}{(1-x)^2}
\end{aligned}$$

Suppose we have root r such that $f(r) = 0 = re^{-r/2} - e^{-1}/2$, therefore,

$$e^{\frac{r}{2}-1} = 2r$$

Then we plug r back in g':

$$g'(r) = (\frac{1}{2}r^2 - \frac{1}{2}r^2 - \frac{3}{2}r + \frac{3}{4} \cdot 2r) \cdot \frac{1}{(1-r)^2} = 0$$

But for $g''(x)$, let
$Q(x) = \frac{1}{2}x^2 - \frac{1}{4}e^{x/2-1}x - \frac{3}{2}x + \frac{3}{4}e^{x/2-1}$, $Q'(x) = 2x - (\frac{1}{8}e^{x/2-1}x + \frac{1}{4}e^{x/2-1}) - \frac{3}{2} + (\frac{3}{8}e^{x/2-1})$

$$g''(x) = (Q'(x)(1-x)^2 - Q(x)2(x-1)) \cdot \frac{1}{(1-x)^4}$$

So:

$$
\begin{aligned}
g''(r) = & ((4r - (\frac{1}{4}r^2 + \frac{1}{2}r) - \frac{3}{2} + \frac{3}{4}r)(1-r)^2 \\
& - (\frac{1}{2}r^2 - \frac{1}{2}r^2 - 3r + \frac{3}{2}r)2(r-1)) \cdot \frac{1}{(1-r)^4} \\
& \neq 0
\end{aligned}
$$

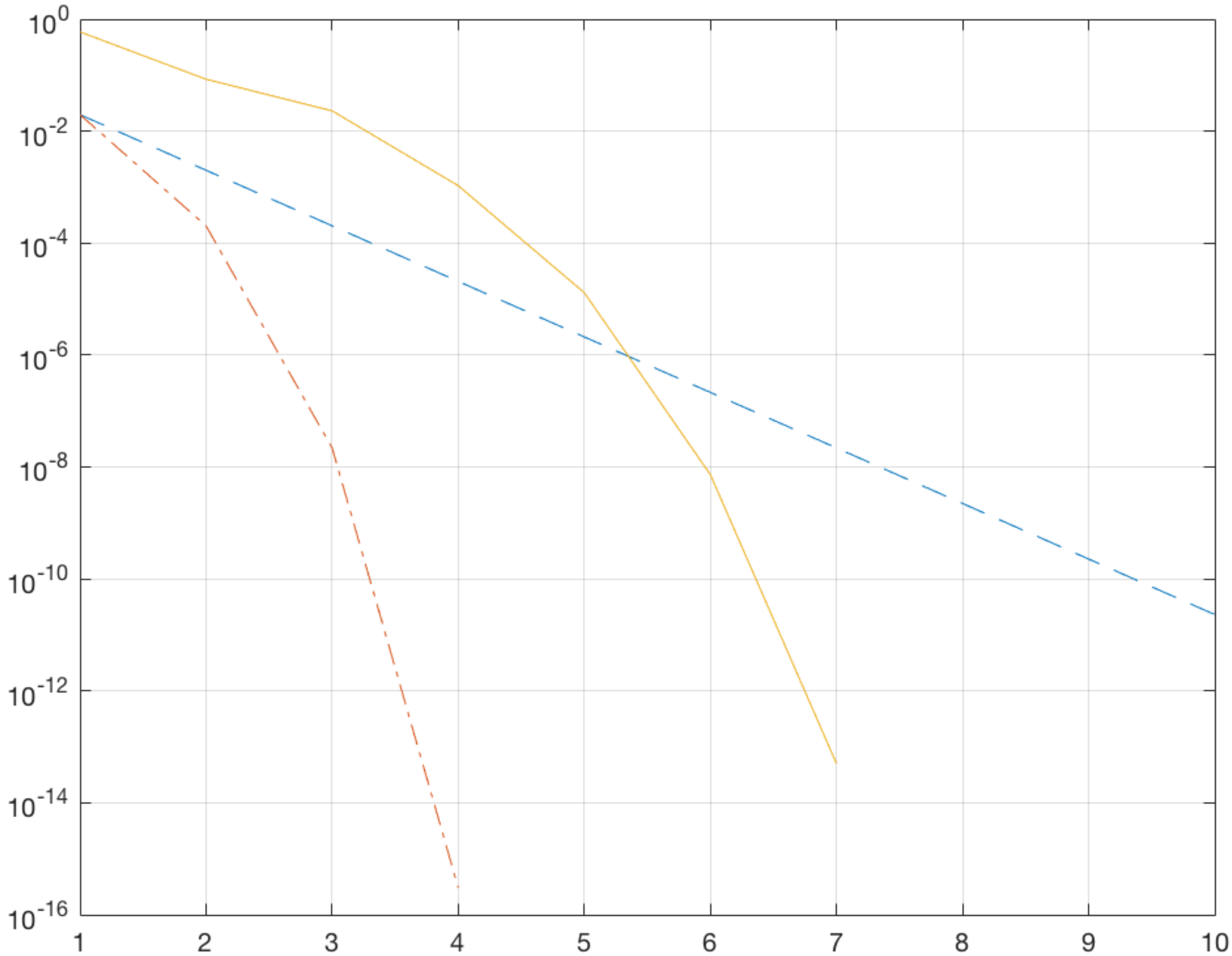
- Hence the rate of convergence of Newton's method here is 2.
- Fixed-point iteration:
  - By Theorem 6, $g'(r) = \frac{1}{4}e^{-1}e^{r/2} \neq 0$, so $\beta = 1$, i.e., the rate of convergence is 1.

(f) Solution:
We already know $g'(x)$ is monotonically increasing from part (d).
Then we only need to consider the interval keeps $|g'(r)| < 1$,
so try to solve:

- $g'(x_{max}) = \frac{1}{4}e^{-1}e^{x_{max}/2} < 1$ so $x_{max} < 2 + 4\log(2)$
- $g'(x_{min}) = \frac{1}{4}e^{-1}e^{x_{min}/2} > -1$ so x_{min} could be any because $g'(x) > 0$

Hence the largest interval is $\left(-\infty, 2 + 4\log(2)\right)$

(g) Solution:



- Starting from y-axis, the curves from up to down are: secant, fixed-point and Newton.
- As we can observe from plot, Newton has the fastest rate of convergence, then secant method is at the second place, and fixed-point method converges linearly.
- Also, we observe the error of Newton's method, it seems that the number of correct digits doubles after each iteration.

Output:

```
>> script
fixed-point:
  1  0.183939720586   1.77e-02
  2  0.201658961000   1.79e-03
  3  0.203453520626   1.83e-04
  4  0.203636157289   1.86e-05
  5  0.203654753852   1.89e-06
  6  0.203656647500   1.93e-07
  7  0.203656840327   1.96e-08
  8  0.203656859962   2.00e-09
  9  0.203656861962   2.04e-10
 10  0.203656862165   2.07e-11
Newton:
```

```
  1  0.183939720586  -1.97e-02
  2  0.203453654804  -2.03e-04
  3  0.203656840374  -2.18e-08
  4  0.203656862188  -3.05e-16
secant:
  1 -0.389803526129  -5.93e-01
  2  0.288179216834   8.45e-02
  3  0.226709585970   2.31e-02
  4  0.202596233016  -1.06e-03
  5  0.203669858498   1.30e-05
  6  0.203656869469   7.28e-09
  7  0.203656862188  -5.00e-14
```

- Function for fixed-point iteration:

```
function res = fp(x)
format long
g = exp(-1)/2*exp(1)^(x/2);
index = 0;
diff = abs(g-x);
res = zeros(1,3);

while diff > 10^(-10)
    index = index + 1;
    x = g;
    g = exp(-1)/2*exp(1)^(x/2);
    diff = abs(g-x);
    fprintf('%3d %15.12f %10.2e\n', index, x, diff);
    res(index,1) = index;
    res(index,2) = x;
    res(index,3) = diff;
end
end
```

- Function for Newton's Method:

```
function res = newton(x)
format long
f = x*exp(1)^(-x/2)-exp(-1)/2;
fprime = (1-x/2)*exp(1)^(-x/2);
index = 0;
r1 = 0.203656862188284;
res = zeros(1,3);

while abs(f) > 10^(-10)
    index = index + 1;
    x = x-f/fprime;
    f = x*exp(1)^(-x/2)-exp(-1)/2;
    fprime = (1-x/2)*exp(1)^(-x/2);
    residual = x - r1;
    fprintf('%3d %15.12f %10.2e\n', index, x, residual);
    res(index,1) = index;
    res(index,2) = x;
```

```
    res(index,3) = residual;
end
end
```

- Function for Secant method:

```
function res = secant(x0,x1)
format long
f0 = x0*exp(1)^(-x0/2)-exp(-1)/2;
f1 = x1*exp(1)^(-x1/2)-exp(-1)/2;
x = x1 - f1 * (x1 - x0) / (f1 - f0);
f = x*exp(1)^(-x/2)-exp(-1)/2;
index = 0;
r1 = 0.203656862188284;
res = zeros(1,3);

while abs(f) > 10^(-10)
    index = index + 1;
    x0 = x1;
    x1 = x;
    f0 = x0*exp(1)^(-x0/2)-exp(-1)/2;
    f1 = x1*exp(1)^(-x1/2)-exp(-1)/2;
    x = x1 - f1 * (x1 - x0) / (f1 - f0);
    f = x*exp(1)^(-x/2)-exp(-1)/2;
    residual = x - r1;
    fprintf('%3d %15.12f %10.2e\n', index, x, residual);
    res(index,1) = index;
    res(index,2) = x;
    res(index,3) = residual;
end
end
```

- Script:

```
disp('fixed-point:');
res1 = fp(0);
disp('Newton:');
res2 = newton(0);
disp('secant:');
res3 = secant(0,2);
r1 = 0.203656862188284;

figure
semilogy(res1(:,1),abs(res1(:,2)-r1),'--');
hold on
semilogy(res2(:,1),abs(res2(:,3)),'-.');
hold on
semilogy(res3(:,1),abs(res3(:,3)),'-');
grid;
```

A3Q2

Problem 2

(a) Solution:

$$
\begin{aligned}
f_1 &= 4x^2 + y^2 - 25 = 0 \\
f_2 &= xye^{-(x+y)/4} - 0.2 = 0 \\
J &= \begin{pmatrix} \dfrac{df_1}{dx} & \dfrac{df_1}{dy} \\ \dfrac{df_2}{dx} & \dfrac{df_2}{dy} \end{pmatrix} \\
&= \begin{pmatrix} 8x & 2y \\ y(1 - \dfrac{x}{4})e^{-(x+y)/4} & x(1 - \dfrac{y}{4})e^{-(x+y)/4} \end{pmatrix}
\end{aligned}
$$

(b) Solution:

The condition that Newton's method is applicable is that Jacobian matrix J is non-singular, i.e. $\det(J) \neq 0$.

$$
\begin{aligned}
\det(J) &= 8x \cdot x(1 - \frac{y}{4})e^{-(x+y)/4} - 2y \cdot y(1 - \frac{x}{4})e^{-(x+y)/4} \\
&= e^{-(x+y)/4}\left(8x^2 - 2x^2y - 2y^2 + \frac{1}{2}xy^2\right) \\
&\neq 0
\end{aligned}
$$

Since $e^{-(x+y)/4} \neq 0$, we only need to make sure that:

$$8x^2 - 2x^2y - 2y^2 + \frac{1}{2}xy^2 \neq 0$$

Plug in initial guess $\left[1, 1\right]^T$, we have the condition:

$$8 - 2 - 2 + \frac{1}{2} = 4.5 \neq 0$$

So this initial guess is applicable for Newton's Method.

(c) Solution:

We know

$$\bar{x}^{(k+1)} = \bar{x}^{(k)} - J^{-1}(\bar{x}^{(k)})\bar{f}(\bar{x}^{(k)})$$

We have

$$\bar{x}^{(0)} = \begin{pmatrix} 1 \\ 0 \end{pmatrix},$$
$$\bar{f}(\bar{x}^{(0)}) = \begin{pmatrix} -21 \\ -0.2 \end{pmatrix},$$
$$J(\bar{x}^{(0)}) = \begin{pmatrix} 8 & 0 \\ 0 & e^{-0.25} \end{pmatrix}.$$

Let $\bar{a} = J^{-1}(\bar{x}^{(0)})\bar{f}(\bar{x}^{(0)})$,

$$\bar{f}(\bar{x}^{(0)}) = J(\bar{x}^{(0)})\bar{a}$$
$$\begin{pmatrix} -21 \\ -0.2 \end{pmatrix} = \begin{pmatrix} 8 & 0 \\ 0 & e^{-0.25} \end{pmatrix} \cdot \begin{pmatrix} a_1 \\ a_2 \end{pmatrix}$$

And this is equal to solve:

$$8a_1 = -21$$
$$e^{-0.25} a_2 = -0.2$$

Hence, $\begin{pmatrix} a_1 \\ a_2 \end{pmatrix} = \begin{pmatrix} -2.625 \\ -0.2568 \end{pmatrix}$.

And

$$\bar{x}^{(1)} = \bar{x}^{(0)} - \begin{pmatrix} -2.625 \\ -0.2568 \end{pmatrix} = \begin{pmatrix} 3.625 \\ 0.2568 \end{pmatrix}.$$

A3Q3

Problem 3

(a) Solution:
NDD table:

x	y		
-1	e^{-1}		
		1-e^{-1}	
0	1		(e+e^{-1}-2)/2
		e-1	
1	e		

with

$$\frac{1-e^{-1}}{0-(-1)} = 1 - e^{-1}$$
$$\frac{e-1}{1-0} = e - 1$$
$$\frac{(e-1)-(1-e^{-1}}{1-(-1)} = \frac{e+e^{-1}-2}{2}$$

So

$$\begin{aligned} p_2(x) &= e^{-1} + (1-e^{-1})(x+1) + \frac{e+e^{-1}-2}{2}(x+1)x \\ &= 1 + \frac{e-e^{-1}}{2}x + \frac{e+e^{-1}-2}{2}x^2 \end{aligned}$$

(b) Solution:
By Theorem (error in polynomial interpolation), f has 3 continuous derivatives and $p_2(x)$ is the polynomial of degree at most 2 interpolating f at distinct points x_0, x_1, x_2, then for any x

$$
\begin{aligned}
f(x) - p_2(x) &= e^x - 1 - \frac{e - e^{-1}}{2} x - \left(\frac{e + e^{-1}}{2} - 1 \right) x^2 \\
&= \frac{f^{(3)}(\xi)}{3!} (x - x_0)(x - x_1)(x - x_2) \\
&= \frac{e^\xi}{6} (x^3 - x)
\end{aligned}
$$

where ξ is an unknown point in the open spread of $\{x_0, x_1, x_2, x\}$, which is $\xi \in opsr\,(-1, 0, 1, x)$.

(c) Solution:

The error contains two parts:

- Since $e^\xi/6$ is always monotonically increasing, so it is maximized when ξ is maximal.
- Let $W = (x - x_0)(x - x_1)(x - x_2) = x^3 - x$whose derivative W' is quadratic. Then it is easy to find the roots r_1, r_2 of $W'(x)$. In fact, $W'(x) = 3x^2 - 1 = 0, r_1 = \frac{\sqrt{3}}{3}, r_2 = -\frac{\sqrt{3}}{3}$. Then

$$
\max_{a \le x \le b} |W(x)| = \max\{|W(x)| x = a, x = b, x = r_1, x = r_2\}
$$

So

- The upper bound of $|e^{1.5} - p_2(1.5)|, \xi_{max} = 1.5$:

$$
\begin{aligned}
|e^{1.5} - p_2(1.5)| &= |\frac{e^\xi}{6} (1.5^3 - 1.5)| \\
&= \frac{e^\xi}{6} (1.5^3 - 1.5) \\
&\le \frac{e^{1.5}}{6} (1.5^3 - 1.5) \\
&= 1.4005
\end{aligned}
$$

- The upper bound of $\max_{-1 \le x \le 1} |e^x - p_2(x)|, \xi_{max} = 1$:
  - Calculate $W(x) = x^3 - x$ for $x = -1, 1, \frac{\sqrt{3}}{3}, -\frac{\sqrt{3}}{3}$.
  - $|W(-1)| = |W(1)| = 0$
  - $|W(\frac{\sqrt{3}}{3})| = |W(-\frac{\sqrt{3}}{3})| = \frac{2}{9}\sqrt{3}$

$$
\begin{aligned}
\max_{-1 \le x \le 1} |e^x - p_2(x)| &\le \frac{e^\xi}{6} \cdot \frac{2}{9} \sqrt{3} \\
&= \frac{e}{27} \sqrt{3} \\
&= 0.1744
\end{aligned}
$$

- The upper bound of $\max_{-1 \le x \le 2} |e^x - p_2(x)|, \xi_{max} = 2$:

- Calculate $W(x) = x^3 - x$ for $x = -1, 2, \frac{\sqrt{3}}{3}, -\frac{\sqrt{3}}{3}$.
- $|W(-1)| = 0$
- $|W(2)| = 8 - 2 = 6$
- $|W(\frac{\sqrt{3}}{3})| = |W(-\frac{\sqrt{3}}{3})| = \frac{2}{9}\sqrt{3}$

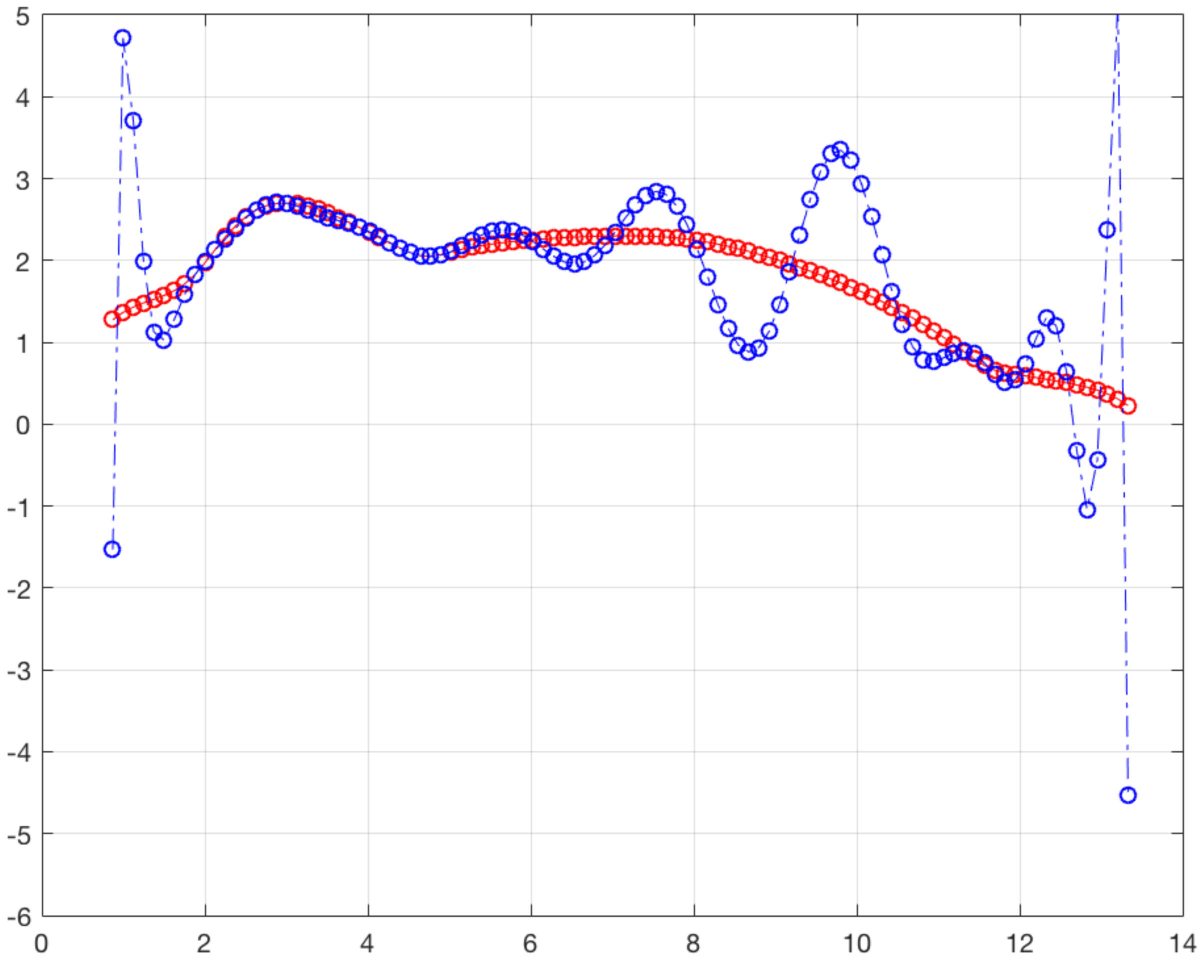
$$\begin{aligned}\max_{-1 \le x \le 2} |e^x - p_2(x)| &\le \frac{e^{\xi}}{6} \cdot 6 \\ &= e^2 \\ &= 7.3891\end{aligned}$$

- The upper bound of $\max_{-2 \le x \le 1} |e^x - p_2(x)|, \xi_{max} = 1$:
  - Calculate $W(x) = x^3 - x$ for $x = -2, 1, \frac{\sqrt{3}}{3}, -\frac{\sqrt{3}}{3}$.
  - $|W(1)| = 0$
  - $|W(-2)| = |-8 + 2| = 6$
  - $|W(\frac{\sqrt{3}}{3})| = |W(-\frac{\sqrt{3}}{3})| = \frac{2}{9}\sqrt{3}$

$$\begin{aligned}\max_{-2 \le x \le 1} |e^x - p_2(x)| &\le \frac{e^{\xi}}{6} \cdot 6 \\ &= e \\ &= 2.7183\end{aligned}$$

Problem 4

Solution:




```
x = [ 0.9  1.3  1.9  2.1  2.6  3.0  3.9  4.4  4.7  5.0  6.0  7.0  8.0  9.2 ...
     10.5 11.3 11.6 12.0 12.6 13.0 13.3];
y = [ 1.3  1.5  1.85 2.1  2.6  2.7  2.4  2.15 2.05 2.1  2.25 2.3  2.25 1.95...
      1.4  0.9  0.7  0.6  0.5  0.4  0.25];
xv = linspace(0.87, 13.33, 100);
yvs = spline(x,y,xv);

p = polyfit(x,y,20);
yvs2 = polyval(p,xv);

figure
plot(xv,yvs,'red-o',xv,yvs2,'blue-.o')
axis([0 14 -6 5])
```

```
grid;
```

Comments: We got the following warning along with the plot:

> Warning: Polynomial is badly conditioned. Add points with distinct X values, reduce the degree of the polynomial, or try centering and scaling as described in HELP POLYFIT.

- As we can see, the blue curve indicating polynomial interpolation has lots of "up-and-downs", however, the red curve indicating cubic spline is rather smooth.
- In other words, when we try to interpolate values using a polynomial, we get unexpected oscillations (Runge's phenomenon) in the interpolation. Moreover, if we use higher degree polynomials, the oscillations could be more extreme. And this is why in the warning message, it suggests us to reduce the degree of polynomial.
- Using cubic spine to interpolate has one advantage, which is the ability to control the curve locally, i.e. if we change a data point then only the area around such point is affected, the general trend of our red curve still remains. But if we do the same to polynomial interpolation, it might dramatically change the blue curve. That's why we have so many oscillations.