**Department of Applied Mathematics and Statistics**
**COLORADO SCHOOL OF MINES**
MATH484: Capstone - Mathematical and Computational Modeling

**Assignment #1, Spring 2015**
**SOLUTIONS**

**1**. Friedman & Littman, p.14, Problem **1.8.1**
To show that the equation possesses at most two positive solutions, we first establish three facts, as mentioned in the problem. First, define the function

$$f(x) = \mu x^3 + c^* \exp(\Gamma/x)$$

and recall that all the constants are positive. Then, notice that

$$\lim_{x\to 0^+} f(x) = c^* \lim_{x\to 0^+} \exp(\Gamma/x) = \infty$$

and

$$\lim_{x\to\infty} f(x) = \mu \lim_{x\to\infty} x^3 = \infty.$$

Next, compute

$$f''(x) = 6\mu x + c^* \exp(\Gamma/x)\frac{\Gamma^2}{x^4} + 3c^* \exp(\Gamma/x)\frac{\Gamma}{x^3}$$

and notice that $f''(x) > 0$ for $x > 0$. Thus, $f(x)$ is convex and $f'(x)$ is increasing for $x > 0$. Additionally, because of the limits established above, the function $f(x)$ must change from decreasing (near $x = 0$) to increasing (as $x \to \infty$) at some point $x^* > 0$. Therefore, $f'(x^*) = 0$, $f''(x^*) > 0$, and $f$ attains a minimum at $x^*$. Additionally, $f'(x) < 0$ for $x < x^*$ and $f'(x) > 0$ for $x > x^*$ because $f'(x)$ is an increasing function.

Now, we consider the only three possible cases for values of $x^*$. First, if $f(x^*) > c_1$, then $f(x) > c_1$ for all $x > 0$ and the equation $f(x) = c_1$ has no solution. Next, if $f(x^*) = c_1$, then the equation has exactly one solution since the minimum can only be attained once. Finally, if $f(x^*) < c_1$, then by the continuity of $f(x)$ and the Intermediate Value Theorem there are values $z_1 \in (0, x^*)$ and $z_2 \in (x^*, \infty)$ such that $f(z_1) = f(z_2) = c_1$. However, because $f'(x) > 0$ for $x > x^*$ and $f'(x) < 0$ for $x < x^*$, we see that $f(x) > c_1$ for $x > z_2$ and $f(x) < c_1$ for $x < z_1$. Hence, in each case, there are at most two solutions.

**2**. Friedman & Littman, p.15, Problem **1.8.3**
(*Proof of Theorem* 1.8.3) To establish the first theorem, we let $x_\infty = \lim_{t\to\infty} x(t)$ and assume $x_\infty > \xi_2$. Then, because $x(0) > \xi_2$ and $x(t)$ is decreasing whenever $x(t) > \xi_2$, we see that $x(t)$ is decreasing for all $t > 0$. Let $z = \frac{1}{2}(x_\infty + \xi_2)$ so that for all $t > 0$, $G(x(t))$ (where $G$ is defined at the bottom of p. 6) satisfies $G(x(t)) \leq G(z) < 0$ for all $t > 0$. Since $x'(t) = G(x(t))$,

we see that $x'(t)$ is bounded above by a negative constant that is independent of $t$. Namely, $x'(t) \leq G(z)$ for every $t > 0$. Integrating both sides on $[0, t]$, we find

$$x(t) \leq x(0) + G(z)t$$

and since $G(z) < 0$, we see that the right side of the inequality tends to $-\infty$ as we let $t$ tend to $\infty$. Since the left side is less, it must also tend to $-\infty$ and this contradicts our original assumption that $x_\infty > \xi_2$. Therefore, we conclude that $x_\infty \leq \xi_2$.

For the next part, assume that $x_\infty < \xi_2$. Then, since $x'(t) > 0$ on this interval we again let $z = \frac{1}{2}(x_\infty + \xi_2)$ and notice that because $x(t)$ is tending to a number less than $\xi_2$ there exists $t_* > 0$ such that $G(x(t)) \geq G(z) > 0$ for $t \geq t_*$. Similar to the previous part, we can use the differential equation and integrate to find

$$x(t) \geq x(t_*) + G(z)t.$$

Since the right side tends to $\infty$ as $t$ grows large, the left side must as well, and this contradicts our assumption that $x_\infty < \xi_2$. Therefore, we have shown that $x_\infty \geq \xi_2$ and combining with the first part, we conclude $x_\infty = \xi_2$.

(*Proof of Theorem* 1.8.4) To establish the second theorem, we notice that since $x(0) < \xi_1$, the function $G(x(t)) < 0$ as long as $x(t)$ remains in the interval $[0, \xi_1]$. Since $x'(t) = G(x(t))$, this implies that $x'(t) < 0$ and $x(t)$ is decreasing. Moreover, because $G'(x) > 0$, we see that $x'(t) = G(x(t)) \leq G(x(0)) < 0$ and integrating over $[0, t]$ as before yields

$$x(t) \leq x(0) + G(x(0))t.$$

We then define $t_* = -x(0)/G(x(0))$ and notice that letting let $t = t_*$ forces $x(t_*) \leq 0$. Finally, by the Intermediate Value Theorem since $x(0) > 0$ and $x(t_*) \leq 0$, there is a time $t_0 \in (0, t_*]$ such that $x(t_0) = 0$.

(*Proof of Theorem* 1.8.5) The last theorem is proved exactly as the first with the exception that $x'(t)$ has a different sign in each of the respective contradiction proofs.

**3**. Friedman & Littman, p.17, Problem **1.10.2**
For Problems $3 - 5$, the code and pictures are included below. The corresponding values of $\xi_1$ and $\xi_2$ are provided in the text.

```
% Ostwald Ripening - Problem 1.10.2
clc;clear;
format long g;

% Parameter Initialization
G = 4e-3;
mu = 1e-3;
cs = 7.52e-7;
```

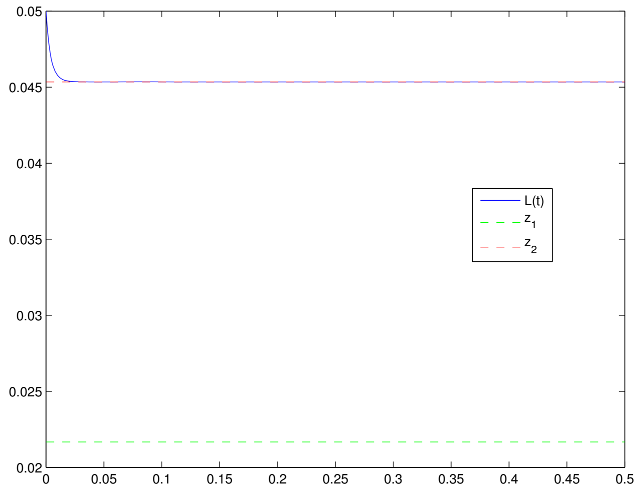


Figure 1: Graph for Problem 3

```
c0 = 1.05*cs;
k = 5e7;

% Initial condition
x0 = 0.05;

% c1
c1 = c0 + mu*x0^3;

% Find the Roots
g = @(x) mu*x.^3 + cs*exp(G./x) - c1;

% Plot function
y = 0.02:0.001:0.06;
plot(y,g(y))

format long e
xi1 = fzero(g, 0.025)
xi2 = fzero(g, 0.045)

% Right side of ODE
f = @(t,x) k*(c1 - mu*x^3 - cs*exp(G/x));

% Time span
tSpan = [0 0.5];

% Differential Equation
[tOut xOut] = ode15s(f, tSpan, x0);
```

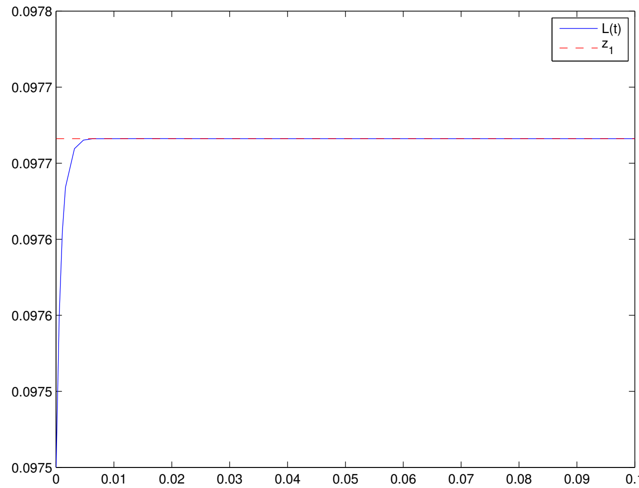


Figure 2: Graph for Problem 4

```
figure;
plot(tOut, xOut)
hold on
plot([0,tOut(end)], [xi1,xi1], '--g')
plot([0,tOut(end)], [xi2,xi2], '--r')
legend('L(t)', 'z_1', 'z_2')
```

**4**. Friedman & Littman, p.17, Problem **1.10.3**

```
% Ostwald Ripening - Problem 1.10.3
clc;clear;
format long g;

% Parameter Initialization
G = 4e-3;
mu = 1e-3;
cs = 7.52e-7;
c0 = 1.05*cs;
k = 5e7;

% Initial condition
x0 = 0.0975;

% c1
c1 = c0 + mu*x0^3;

% Find the Roots
```

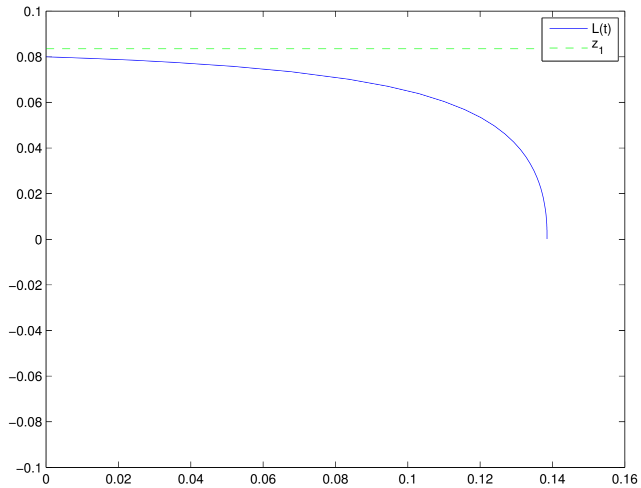


Figure 3: Graph for Problem 5

```
g = @(x) mu*x.^3 + cs*exp(G./x) - c1;

% Plot function
y = 0.003:0.001:0.1;
plot(y,g(y))

format long e
xi1 = fzero(g, 0.005)
xi2 = fzero(g, 0.1)

% Right side of ODE
f = @(t,x) k*(c1 - mu*x^3 - cs*exp(G/x));

% Time span
tSpan = [0 0.1];

% Differential Equation
[tOut xOut] = ode15s(f, tSpan, x0);

figure;
plot(tOut, xOut)
hold on
plot([0,tOut(end)], [xi2,xi2], '--r')
legend('L(t)', 'z_1')
```

**5**. Friedman & Littman, pp.17-18, Problem **1.10.4**

```
% Ostwald Ripening - Problem 1.10.4
```

```
clc;clear;
format long g;

% Parameter Initialization
G = 4e-3;
cs = 7.52e-7;
c0 = 1.05*cs;
k = 5e7;
mu = 5e2/k;

% Initial condition
x0 = 0.08;

% c1
c1 = c0 + mu*x0^3;

% Find the Roots
g = @(x) mu*x.^3 + cs*exp(G./x) - c1;

% Plot function
%y = 0:0.001:0.11;
y = 0.06:0.001:0.12;
plot(y,g(y))

format long e
xi1 = fzero(g, 7e-2)
xi2 = fzero(g, 2e-1)

% Right side of ODE
f = @(t,x) k*(c1 - mu*x^3 - cs*exp(G/x));

% Time span
tSpan = [0 0.16];

% Differential Equation
[tOut xOut] = ode15s(f, tSpan, x0);

figure;
plot(tOut, xOut)
hold on
plot([0,tOut(end)], [xi1,xi1], '--g')
axis([0, 0.16, -0.1, 0.1])
legend('L(t)', 'z_1')
```

**6**. Friedman & Littman, p.24, Problem **1.13.1**

For this problem use $N = 2$ and investigate each of the three different cases in 1.10.2, 1.10.3, and 1.10.4. For the initial lengths use $x_1(0) = \frac{1}{2}x^*$, $x_2(0) = x^*$, and for the $\mu$-values use $\mu_1 = \mu_2 = \mu$, where $x^*$ and $\mu$ are given in each problem.

**7**. Friedman & Littman, p.24, Problem **1.13.2**
For this problem use $N = 2$ and investigate each of the three different cases in 1.10.2, 1.10.3, and 1.10.4. Since there are two crystals, use the initial lengths and $\mu$-values from Problem 6. Don't perform any simulations - you can calculate these limits analytically given the necessary constants and the results of the previous problems. Note that when the first crystal dissolves at time $\tau_1$, the problem reduces to the single-crystal case and the "initial length" in this situation can be determined by the remaining crystal length at time $\tau_1$.

Problems 6 and 7 are also grouped together. The code and output values are included below.

**<u>MATLAB Code - 1.10.2 Values</u>**

```
% Ostwald Ripening
clc;clear;
format long g;

% Parameter Initialization - from 1.10.2
G = 4e-3;
mu = [1e-3, 1e-3];
cs = 7.52e-7;
c0 = 1.05*cs;
k = 5e7;

% Initial condition
x0 = [0.025; 0.05];

% constants of concentration
c1 = c0 + mu*x0.^3;

% Right side of ODE
f = @(t,x)  [k*(c1 - mu*x.^3 - cs*exp(G/x(1)));
    k*(c1 - mu*x.^3 - cs*exp(G/x(2)))];

% Time span
tSpan = [0 5e-3];

% Differential Equation
[tOut xOut] = ode15s(f, tSpan, x0);
plot(tOut, xOut)

format long e
```

```
ind = find(xOut(:,1) > 0);
tau1 = tOut(ind(end))
L1 = xOut(ind(end),2)

%Steady states
newc1 = c0 + mu(2)*L1^3;
g = @(x) mu(2)*x.^3 + cs*exp(G./x) - newc1;

xi1 = fzero(g, 0.025)
xi2 = fzero(g, 0.045)

if L1 > xi1
    c_infty1 = c1 - mu(2)*L1^3;
else
    c_infty1 = c1;
end
c_infty1
```

**Output**

```
tau1 = 2.374607042668533e-03

L1 = 4.873212256868187e-02

xi1 = 2.333276679247936e-02

xi2 = 4.313542908246693e-02

c_infty1 = 8.144949918874417e-07
```

**MATLAB Code - 1.10.3 Values**

```
clc;clear;
format long g;

% Parameter Initialization - from 1.10.3
G = 4e-3;
mu = [1e-3, 1e-3];
cs = 7.52e-7;
c0 = 1.05*cs;
k = 5e7;

% Initial condition
x0 = [0.0975/2; 0.0975];
```

```
% constants of concentration
c1 = c0 + mu*x0.^3;

% Right side of ODE
f = @(t,x)  [k*(c1 - mu*x.^3 - cs*exp(G/x(1)));
    k*(c1 - mu*x.^3 - cs*exp(G/x(2)))];

% Time span
tSpan = [0 1];

% Differential Equation
[tOut xOut] = ode15s(f, tSpan, x0); %ode15s
plot(tOut, xOut)

format long e
ind = find(xOut(:,1) > 0);
tau2 = tOut(ind(end))
L2 = xOut(ind(end),2)

%Steady states
newc1 = c0 + mu(2)*L2^3;
g = @(x) mu(2)*x.^3 + cs*exp(G./x) - newc1;

xi1 = fzero(g, 0.005)
xi2 = fzero(g, 1)

if L2 > xi1
    c_infty2 = c1 - mu(2)*L2^3;
else
    c_infty2 = c1;
end
c_infty2
```

**Output**

```
tau2 = 1.233902480658632e-02

L2 = 1.015165180519177e-01

xi1 =  4.482072658595226e-03

xi2 = 1.017569390893384e-01

c_infty2 = 7.861278194877671e-07
```

## MATLAB Code - 1.10.4 Values

```
clc;clear;
format long g;

% Parameter Initialization- from 1.10.4
G = 4e-3;
mu = [1e-3, 1e-3];
cs = 7.52e-7;
c0 = 1.05*cs;
k = 5e2/mu(1);

% Initial condition
x0 = [0.04; 0.08];

% constants of concentration
c1 = c0 + mu*x0.^3;

% Right side of ODE
f = @(t,x)  [k*(c1 - mu*x.^3 - cs*exp(G/x(1)));
    k*(c1 - mu*x.^3 - cs*exp(G/x(2)))];

% Time span
tSpan = [0 2];

% Differential Equation
[tOut xOut] = ode15s(f, tSpan, x0); %ode15s
plot(tOut, xOut)

format long e
ind = find(xOut(:,1) > 0);
tau3 = tOut(ind(end))
L3 = xOut(ind(end),2)

%Steady states
newc1 = c0 + mu(2)*L3^3;
g = @(x) mu(2)*x.^3 + cs*exp(G./x) - newc1;

y = 0.005:0.001:0.12;
plot(y,g(y))

xi1 = fzero(g, 2e-2)
xi2 = fzero(g, 8e-2)

if L3 > xi1
```

```
    c_infty3 = c1 - mu(2)*L3^3;
else
    c_infty3 = c1;
end
c_infty3
```

**Output**

```
tau3 =  7.950464354836737e-01

L3 =  8.292122718125193e-02

xi1 = 6.755606435295322e-03

xi2 = 8.294281080431155e-02

c_infty3 =  7.954394532497777e-07
```