

Lab Assignment 2

Bioaccumulation of Methyl Mercury

Written by

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Prepared for

Math 214: Discrete Math Modeling (Fall 2014)

Rhodes College

PreLab Assignment Due: **Thursday, 9/11/2014 before class begins**

Lab Assignment Due: **Tuesday, 9/16/2014 before class begins**

Material from the prelab is covered on the quiz on **9/11/2014**.

Scientists have known about the adverse affects of mercury on the health of humans for more than a century. The term “mad as a hatter” stems from the nineteenth-century use of mercuric nitrate in the making of felt hats. Human activities are responsible for most mercury emitted into the environment. For example, mercury, a by-product of coal, comes from the smokestack emissions of old, coal-fired power plants in the Midwest and South and is disseminated by acid rain. Particles containing mercury rise on the smokestack plumes and hitch a ride on prevailing winds, which often blow northeast. After colliding with mountains, the particles drop to earth. Once in the ecosystem, microorganisms in the soil and in reservoir/lake sediment break down the mercury and produce a very toxic chemical known as methyl mercury.

Methyl mercury undergoes a process known as bioaccumulation. This occurs when organisms take in contaminants more rapidly than their bodies can eliminate them. Therefore, the amount of methyl mercury in their bodies accumulates over time. Humans can eliminate the amount of methyl mercury in their system at a rate proportional to the amount remaining (i.e. the amount decays exponentially). Methyl mercury decays 50% every 65 to 75 days (known as the half-life of methyl mercury).

Officials in the town of Nowhere have collected and tested 2425 samples of largemouth bass from the reservoirs and found that all fish were contaminated. The mean concentration of methyl mercury in the fish samples was $0.43 \mu\text{g}$ (micrograms) per gram of fish mass. The average mass of the sampled largemouth bass was 0.817 kg.

Methyl mercury becomes lethal in humans when the concentration exceeds 30 mg/kg, but there can be detrimental effects to the fetuses of pregnant women if the concentration exceeds 0.02 mg/kg (referred to as fetal methyl mercury poisoning). Assuming the average adult person is 70 kg, what public health policy recommendation would you make to the people of Nowhere concerning the consumption of largemouth bass caught in local reservoirs?

The goals of this lab assignment are to:

- Construct a difference equation model of the amount of mercury in an average resident in the town of Nowhere who consumes fish.
- Utilize your model to make a public health policy recommendation for the residents of the town of Nowhere.

In this lab, we will be using MATLAB to help achieve these goals. Thus, as a part of this lab you will learn how to do the following in MATLAB:

- Create a cobweb diagram in MATLAB.

MATLAB Skills

After completing Lab 1 you have most of the skills necessary to complete to this lab project. In this lab you will generate cobweb plots of the models you construct to explore long-term behavior of your models. Here we examine a script m-file which will generate a cobweb diagram.

Generating Cobweb Diagrams

1. Open Matlab and navigate the current directory to the location where you will save your work.
2. Open a new script file (do you remember how to do this from Lab 1?) and save the file as L02Ex01.m.

3. In the m-file editor, type the following exactly (or download the file from Moodle):

[L02Ex01.m](#)

```

1  % Lab 2 L02Ex01 by Prof Bodine
2  % This script will generate a cobweb diagram for a first order linear
3  % difference equation:  $x(t+1) = ax(t) + b$ 
4
5  % Clear all variables stored in the workspace
6  clear all;
7
8  %% User Defined Parameters
9  a = 1.5;          % Exponential growth coefficient
10 b = -6114;        % Constant growth coefficient
11 x0 = 12230;       % Initial value
12 N=25;            % Number of time steps
13
14 %% Generate Plot of Sequence  $x(0), \dots, x(N)$ 
15 x(1) = x0;
16 for t = 1:N
17     x(t+1) = a*x(t) + b;
18 end
19 subplot(2,1,1); plot([0:N],x,'r.-');
20 xlabel('Time Step'); ylabel('x(t)');
21
22 %% Generate Cobweb Diagram
23 % Get limits of the y-axis from previous plot
24 yrange = get(gca,'ylim');
25
26 % Generate the curve of the difference equation over yrange
27 r = yrange(1):0.01:yrange(2);
28 y = a.*r + b;
29
30 % Plot curve of diff eqn (black) and ' $x(t+1)=x(t)$ ' line (cyan)
31 subplot(2,1,2); plot(r,y,'c-'); hold on; plot(r,r,'k-')
32 xlabel('x(t)'); ylabel('x(t+1)')
33
34 % Generate cobweb
35 plot(x0,0,'r. '); % note starting point with a dot
36 plot([x0 x0],[0 x(1)],'r-'); % first vert line up to curve
37 for t = 1:N-1
38     plot([x(t) x(t+1)], [x(t+1) x(t+1)], 'r-'); % horz line to  $x(t+1)=x(t)$  line
39     plot([x(t+1) x(t+1)], [x(t+1) x(t+2)], 'r-'); % vert line up to curve
40 end

```

41

```
hold off;
```

Make sure to save the file after you have written it, and make note of where you saved the file. If you save the file in a location other than the current folder, make sure you change the current folder to the location where `L02Ex01.m` is saved.

Now, let us take a moment to understand everything contained within this script. Several new elements were used in this script.

- (a) The `clear` command in MATLAB will erase from the workspace the value of any variable or parameter listed after the command. If `all` is given after the `clear` command, then all existing parameters in the workspace are erased. When writing scripts where the size of an array could change each time you run the script (depending on different parameter values you use), it is a good idea to place a `clear all` command at the top of script to avoid accidentally retaining information from a previous run that you do not want.

For example, suppose you have a script that the first time you run it should generate the array

$$\mathbf{x} = 18 \ 21 \ 36 \ 42 \ 58 \ 69$$

Notice that the array \mathbf{x} has 6 elements. The second time you run your script you have changed some parameters and now the array \mathbf{x} should only have 4 elements: 1 2 3 4. If you do not clear the variable \mathbf{x} before the second run, your second run will produce the array

$$\mathbf{x} = 1 \ 2 \ 3 \ 4 \ 58 \ 69$$

Notice the array still has six elements, and the last two are left over from the previous run.

- (b) You should notice that in Matlab, use of the double percent sign, `%%` causes a gray horizontal bar to appear above the line containing the `%%`. This can be useful for visually breaking up longer scripts.
- (c) Examine lines 9–12 in the code. From your work in Lab 1, you should understand these lines. Note, in this script the comments are placed on the same lines, to the right of, executable code. If you do not understand these lines of code, review Lab 1.
- (d) In lines 15–18 we create an array called \mathbf{x} whose first element is x_0 and whose subsequent elements are defined by the first order linear difference equation through the for-loop. Note, the array \mathbf{x} contains a total of $N + 1$ elements. If you do not understand why the array \mathbf{x} contains $N + 1$ elements, now is the time to stop and ask your instructor.

In lines 19–20 we plot the elements of the sequence $x_{t+1} = ax_t + b$, however notice the use of the MATLAB command `subplot`. The `subplot` command allows you to place multiple graphs in one figure window. The command takes in three arguments (separated by commas); the first argument defines the number of rows of graphs within the figure, the second argument defines the number of columns of graphs within the figure, and the third argument indicates where the next graph will be placed (by counting across then down). In this script we generate two plots: one of the sequence values and one showing the cobweb diagram. Thus, we create 2 rows and 1 column of subplots within the figure window.

- (e) Lines 22–45 generate the second plot showing the cobweb diagram. Recall that to generate a cobweb diagram, you are plotting the curve $x_{t+1} = f(x_t)$ and the line $x_{t+1} = x_t$. To ensure that we plot these two curves over an appropriate range of x_t values, we obtain the range of the vertical axis from the first

subplot (see line 24). Note `gca` refers to the axes of the most recent plot, and `ylim` refers to the limits of the vertical axis of a plot. As you might now guess, the command `get(gca,'ylim')` “gets” the limits of the vertical axis of the most recent plot which happens to be the plot of the x_t sequence. The command returns an array with two elements: (1) the lower limit of the vertical axis and (2) the upper limit of the vertical axis. To plot the curve $x_{t+1} = f(x_t)$ and the line $x_{t+1} = x_t$, we generate an array of many values (spaced 0.01 units apart) between the lower and upper limit of vertical axis (see line 27), generate the corresponding values of the curve $x_{t+1} = f(x_t) = ax_t + b$ (see line 28), and then plot both on the same graph (see lines 31–32). The curve $x_{t+1} = ax_t + b$ is plotted in cyan, and the line $x_{t+1} = x_t$ is plotted in black.

Note that in line 28, the variable `r` is an array, and the parameters `a` and `b` are real numbers. The expression `y=a*r+b`, first multiplies every element in `r` by the value of `a`, then adds the value of `b` to every element in the array, and lastly saves the transformed array as the variable `y`.

As of line 33, we have still not drawn the cobwebbing on the graph (the second subplot). Lines 35–41 add the cobwebbing to the plot of the curve $x_{t+1} = f(x_t)$ and the line $x_{t+1} = x_t$ drawn on the graph in lines 32–33. Recall that to create a cobweb diagram we start at $(x_0, 0)$. Thus, in `L02Ex01`, we start by placing a dot at the starting point $(x_0, 0)$ (see line 37). To plot a point you list the x coordinate, the y coordinate, and then the color and marker style. Next, in line 36 we draw the cobweb (a red line) from $(x_0, 0)$ up to the curve $x_{t+1} = ax_t + b$ (cyan curve). In Matlab, if you wish to draw a green line from (a, b) to (c, d) , you would use the following command

```
plot([a c],[b d], 'g-')
```

Recall from Lab 1 that the first two arguments in MATLAB's `plot` function are arrays of values which give the horizontal and vertical coordinates, respectively, of points on the graph. In this case we have only two points, so each array has only two values. Note the third argument, `'g-'` indicates that we want a green line (`g` for green, `-` for solid line).

To draw the rest of the cobweb we use the for-loop on lines 37–40. Each iteration (one pass) through the for-loop draws one horizontal line from the cyan curve over to the black line, and then one vertical from the black line up to the cyan curve.

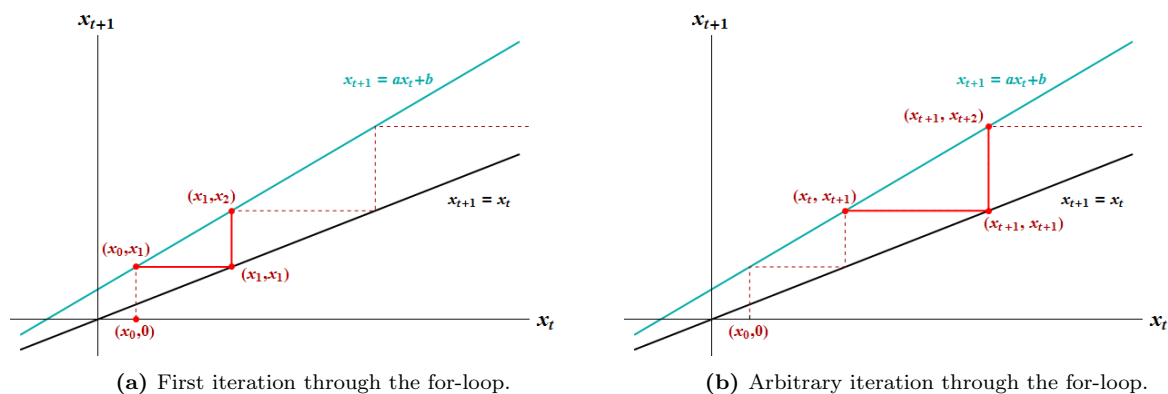


Figure 1: The thick red lines show the portion of the cobweb drawn in one iteration of the for-loop on lines 37–40 of `L02Ex01.m`.

In the first iteration through the loop (see Figure 1a), in line 38 we draw the cobweb line from (x_0, x_1) on the $x_{t+1} = ax_t + b$ curve to (x_1, x_1) on the line $x_{t+1} = x_t$. Then, in line 39 we draw the cobweb line from

(x_1, x_1) to (x_1, x_2) back on the cyan curve. In an arbitrary iteration through the loop, in line 38 we draw the cobweb line from (x_t, x_{t+1}) on the $x_{t+1} = ax_t + b$ curve to (x_{t+1}, x_{t+1}) on the line $x_{t+1} = x_t$. Then, in line 39 we draw the cobweb line from (x_{t+1}, x_{t+1}) to (x_{t+1}, x_{t+2}) back on the cyan curve. Notice that the for-loop will only work for $t = 1, 2, \dots, N - 1$, because the array \mathbf{x} only has $N + 1$ elements. In the $t = (N - 1)^{th}$ iteration through the for-loop, the code $\mathbf{x}(\mathbf{t}+2)$ in line 39 will access the

$$t + 2 = (N - 1) + 2 = N + 1$$

element of \mathbf{x} (which is the last element of the \mathbf{x} array).

- (f) Take another moment to review L02Ex01.m. **Do you understand what each line of code is doing now?** If not, now is the time to stop and ask.
4. Run the script file. Do you remember how to do this from Lab 1? A window containing the graph should appear and should look like Figure 2.

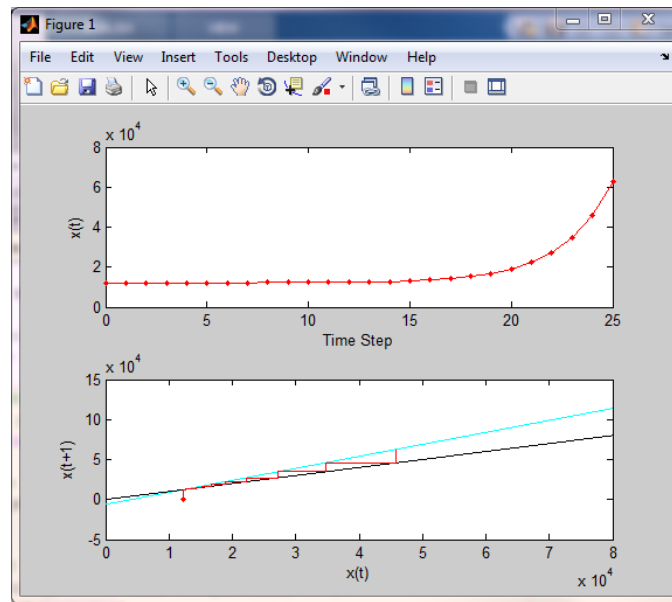


Figure 2: Plot produced from L02Ex01.m script.

PreLab Assignment

Suppose a patient with heart disease is being treated with digoxin (see Exercise 3 and Example 5 in reference readings). The patient takes a 0.1 mg dose every day, and the half-life of the drug is 1.868 days.

1. Construct a difference equation of the form $x_{t+1} = e^{-k\tau}x_t + b$, where x_t is the amount of digoxin in the patient's body at day t , k is the elimination rate of digoxin in the patient, τ is the number of days between doses, and b is the size of the dose. *Hint: Use the half-life of digoxin to find the value of k .*
2. Modify the m-file L02Ex01.m to draw a cobweb diagram for the model you constructed in part (1). *Hint: Remember, for pharmacokinetics models, $a = e^{-k\tau}$. You may assume that time step $t = 0$ occurs at the time*

the patient takes the initial dose. Save your modified file as `PLab02_YourLastName.m`. Run the file and save the figure as `PLab02_YourLastName.jpg`.

3. Submit the files `PLab02_YourLastName.m` and `PLab02_YourLastName.jpg` on Moodle, and in the textbox report the values of k , τ , b , and x_0 .

Lab Assignment

You may complete this lab assignment with a partner.

1. Calculate the amount of methyl mercury in an average size largemouth bass.
2. Given the half-life of methyl mercury in humans, calculate the decay rate of methyl mercury in humans. That is, find the value of k in the equation $x(t) = x(0)e^{-kt}$, where $x(t)$ is the amount of methyl mercury in a human at time t (measured in days), and k is the decay rate.
3. Assume the average adult citizen of Nowhere consumes one largemouth bass per day (they must really like to eat fish!). Construct a difference equation which models the amount of methyl mercury in an average adult over time, where the time step is one day.
4. Using the model you constructed in part (3), determine the maximum amount of methyl mercury that will accumulate in an adult citizen of Nowhere over their lifetime. *Hint: How are the equilibrium value and maximum drug amount in pharmacokinetics problems related?* For an average adult citizen of Nowhere with a mass of 70 kg, what is the concentration of methyl mercury (in mg/kg) in their body?
5. Modify the m-file `L02Ex01.m` to draw a cobweb diagram for the model you constructed in part (3). You may assume that time step $t = 0$ occurs at the time the citizen eats their first largemouth bass (i.e. $x_0 = b$). Save your modified file as `Lab02_YourLastName.m`. Run the file with `N=500` on line 12 and save the figure as `Lab02a_YourLastName.jpg`.
6. Examining your results from parts (4) and (5), is the average adult citizen of Nowhere likely to accumulate a lethal dose of methyl mercury by eating one fish a day?
7. Using your m-file `Lab02_YourLastName.m`, determine how many fish an individual would have to eat each day such that the accumulated amount of methyl mercury in their body would exceed 30 mg/kg. Do this by considering multiples of the dose size b . For example, if one average largemouth bass has 0.1 mg of methyl mercury, you would have modified line 10 of `L02Ex01.m` to be `b = 0.1;`. If you wanted to model an average adult citizen of Nowhere eating 2 largemouth bass each day, you could change line 10 to `b = 0.1 * 2;`. Is this amount of fish reasonable for one person to consume every day? When you find the number of largemouth bass consumed per day which would lead to an accumulated lethal amount of methyl mercury, save the figure as `Lab02b_YourLastName.jpg`.
8. Examining your results from parts (4) and (5), is a pregnant women in the town of mercury likely to have fetal methyl mercury poisoning by eating one largemouth bass a day? You may assume the average mass of pregnant woman in Nowhere is also 70 kg.
9. Using your m-file `Lab02_YourLastName.m`, determine how often a pregnant woman in Nowhere should eat one largemouth bass such that the accumulated amount of methyl mercury in her body would not exceed 0.02

mg/kg. Do this by changing the value of τ . For example, if a pregnant woman eats one largemouth bass a day, then $\tau = 1$, but if she eats one largemouth bass every 3 days then $\tau = 3$. Note, that when $\tau = 1$, the one time step represents 1 day, but when $\tau = 3$ one time step represents 3 days. Thus, at $t = 2$, 6 days would have passed. When you find how often a pregnant woman in Nowhere should eat largemouth bass so that she does not run the risk of fetal methyl mercury poisoning, save the figure as `Lab02c_YourLastName.jpg`.

10. Submit:

- 1 script file (`Lab02_YourLastName.m`)
- 3 image files (`Lab02a_YourLastName.jpg`, `Lab02b_YourLastName.jpg`, `Lab02c_YourLastName.jpg`)
- Answers to parts (1) - (9) above. Additional, write 1-2 sentences giving your official recommendation on eating largemouth bass to the citizen of Nowhere.