# MATH 227A: Mathematical Biology
# Homework 1

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## Problem 1

### Part (i)

Solve the ODE $y' = -\frac{1}{t}y + t$ using an appropriate integrating factor.

Given the ODE

$$\begin{aligned} y' &= -\frac{1}{t} \cdot y + t \\ y' + y \cdot \frac{1}{t} &= t \qquad (1) \end{aligned}$$

Comparing (1) with the standard linear ODE form, $y'(t) + y(t) \cdot p(t) = q(t)$, we have $p(t) = \frac{1}{t}$ and $q(t) = t$.

We now define an integrating factor $E(t)$

$$\begin{aligned} E(t) &= e^{\int_0^t p(z)\,dz} \\ &= e^{\int_0^t \frac{1}{z}\,dz} \\ &= e^{\ln t} \\ &= t \qquad (2) \end{aligned}$$

Using $(E(t) \cdot y(t))' = E(t) \cdot q(t)$ and integrating on both sides wrt $dt$

$$\begin{aligned}
E(t) \cdot y(t) &= \int E(t) \cdot q(t)\, dt \\
y(t) &= \frac{1}{E(t)} \int E(t) \cdot q(t)\, dt \\
&= \frac{1}{t} \int t^2\, dt \\
&= \frac{1}{t} \left( \frac{t^3}{3} + c_1 \right) \\
&= \frac{t^2}{3} + \frac{c_1}{t} \qquad (3)
\end{aligned}$$

### Part (ii)

Verify that you have found the right solution by plugging your solution into the ODE.

To verify, we ask if the given relation for $y'(t)$ in (1) can be obtained from the solution for $y(t)$ found in (3)

$$\begin{aligned}
-\frac{1}{t} \cdot y + t &= y'(t) \\
-\frac{1}{t} \cdot y + t &\stackrel{?}{=} \left( \frac{t^2}{3} + \frac{c_1}{t} \right)' \\
-\frac{1}{t} \cdot \left( \frac{t^2}{3} + \frac{c_1}{t} \right) + t &\stackrel{?}{=} \frac{2t}{3} - \frac{c_1}{t^2} \\
-\frac{t}{3} - \frac{c_1}{t^2} + t &\stackrel{?}{=} \frac{2t}{3} - \frac{c_1}{t^2} \\
\frac{2t}{3} - \frac{c_1}{t^2} &\stackrel{?}{=} \frac{2t}{3} - \frac{c_1}{t^2} \qquad (4)
\end{aligned}$$

QED $\square$

Since the relation in (4) holds true, the solution for $y(t)$ in (3) is verified.

## Problem 2

### Part (i)

Use separation of variables to find the general solution of the ODE $y' = b - ay$, where $b$ is a constant.

Given the ODE,

$$\begin{aligned} y' &= b - ay \\ y' &= (b - ay) \cdot 1 \end{aligned} \tag{5}$$

Comparing (5) with the standard separable ODE form, $y'(t) = g(y) \cdot h(t)$, we have $g(y) = b - ay$ and $h(t) = 1$.

Rewriting the separable ODE using Leibnitz's notation,

$$\begin{aligned} \frac{\mathrm{d}y}{\mathrm{d}t} &= g(y) \cdot h(t) \\ \frac{1}{g(y)} \cdot \frac{\mathrm{d}y}{\mathrm{d}t} &= h(t) \end{aligned}$$

Integrating both sides wrt $t$,

$$\begin{aligned} \int \frac{1}{g(y)} \frac{\mathrm{d}y}{\mathrm{d}t} \, dt &= \int h(t) \, dt \\ \int \frac{1}{b - ay} \, dy &= \int 1 \cdot dt \end{aligned}$$

Defining $m = b - ay$ and using that $\dfrac{\mathrm{d}m}{\mathrm{d}y} = -a$,

$$\begin{aligned} -\frac{1}{a} \int \frac{1}{m} \, dm &= t + c_1 \\ \ln|m| &= -a \cdot (t + c_2) && [\ \textit{absorbing integration consts into } c_2\ ] \\ \ln|b - ay| &= -a \cdot (t + c_2) && [\ \textit{since } m = b - ay\ ] \\ y &= \frac{b}{a} - \frac{1}{a} \cdot e^{-at} \cdot e^{ac_2} && [\ \textit{assuming } b - ay \geq 0\ ] \\ &= \frac{b}{a} - c_3 \cdot e^{-at} && [\ \textit{where } c_3 = c_2 \cdot e^{ac_2}\ ] \end{aligned} \tag{6}$$

**Part (ii)**

Find the solution for $y(0) = 3, a = 1, b = 2$.

Setting $t = 0$, $y(0) = 3$, $a = 1$, and $b = 2$ in (6).

$$\begin{aligned} y(0) &= 2 - c_3 \cdot e^0 \\ 3 &= 2 - c_3 \\ c_3 &= -1 \end{aligned}$$

Thus, the specific solution under the given conditions becomes

$$y = e^{-t} + 2 \tag{7}$$

**Part (iii)**

Find the solution of the ODE $y' = \frac{t+y}{t-y}$.

Given the ODE

$$\begin{aligned} y' &= \frac{t+y}{t-y} \\ &= \frac{1 + \dfrac{y}{t}}{1 - \dfrac{y}{t}} && \text{[ \textit{dividing numer \& denom by } t \text{ ]}} \end{aligned} \tag{8}$$

We now have the form $y' = f\left(\frac{y}{t}\right)$. Defining $v = \frac{y}{t}$,

$$\begin{aligned} v &= \frac{y}{t} \\ y &= t \cdot v \\ y' &= v + t \cdot v' && \text{[ \textit{differentiating both sides wrt } t \text{ ]} } \\ f(v) &= v + t \cdot v' && (9) \end{aligned}$$

Rewriting (8) and using (9),

$$\begin{aligned} f(v) &= \frac{1+v}{1-v} \\ v + t \cdot v' &= \frac{1+v}{1-v} \\ t \cdot v' &= \frac{1 + v - v + v^2}{1-v} \\ t \cdot \frac{\mathrm{d}v}{\mathrm{d}t} &= \frac{1+v^2}{1-v} && \text{[ \textit{using Leibnitz's notation} ]} \\ \frac{1-v}{1+v^2}\, \frac{\mathrm{d}v}{\mathrm{d}t} &= \frac{1}{t} && (10) \end{aligned}$$

Integrating both sides wrt $t$,

$$\int \frac{1-v}{1+v^2}\,\frac{\mathrm{d}v}{\mathrm{d}t}\,dt = \int \frac{1}{t}\,dt$$
$$I_1 - I_2 = ln|t| + c_1 \tag{11}$$

$$\left[\text{ where } I_1 = \smallint \frac{1}{1+v^2}\,dv \text{ and } I_2 = \smallint \frac{v}{1+v^2}\,dv \;\right]$$

$$\begin{aligned} I_1 &= \int \frac{1}{1+v^2}\,dv \qquad & I_2 &= \int \frac{v}{1+v^2}\,dv \\ &= \arctan(v) + k_1 & &\text{Let } m = 1+v^2 \text{ and using } \frac{\mathrm{d}m}{\mathrm{d}v} = 2v, \\ & & I_2 &= \frac{1}{2}\int \frac{1}{m}\,dm \\ & & &= \frac{1}{2} ln|m| + k_2 \\ & & &= \frac{1}{2} ln(1+v^2) + k_2 \;[\; since\ 1+v^2 \geq 0 \;] \end{aligned}$$

Substituting $I_1$ and $I_2$ back in (11),

$$\arctan\left(\frac{y}{t}\right) - \frac{1}{2}\,ln\left(1+\frac{y^2}{t^2}\right) = ln|t| + c_2 \tag{12}$$

# Problem 4

Suppose that a patient is given an intravenous drug and that the hospital measures the patient's drug concentration at regular intervals. The concentration after 0, 3, 6, 9, 12 hours is 0, 400, 700, 900, and 750 uM (micro molar), respectively. The drug is being injected in such a way that the blood concentration influx is 100 uM per hour.

### Part (a)

Formulate a simple ODE model of intravenous drug delivery and explain the assumptions you're using. Plot a sample graph with arbitrary parameters.

The ODE to describe the concentration $y$ over time can be expressed in terms of the influx rate $b$ and decay rate $a$ as shown in (13). Here, we assume that the influx rate ($b$) is independent of the current concentration and the decay rate ($a$) is linearly proportional to the current concentration.

$$y' = b - ay \tag{13}$$

Figure 1 shows the concentration as a function of concentration rate for an arbitrary parameter choice of $a = 1\mu M^{-1}$ and $b = 100\mu M$. Concentration ($y$) is expressed in $\mu M$. As expected, the plot is a straight line.

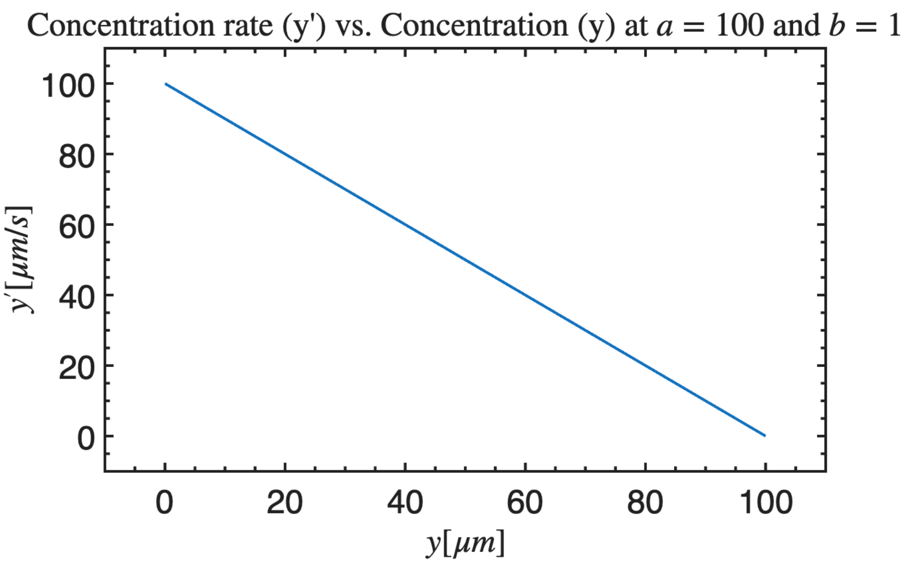


**Figure 1:** Concentration rate vs. concentration for arbitrary parameters.

### Part (b)

Using Matlab, for a given concentration function y(t) determine a formula for the error between the data and the concentration function y(t). (Note: There are multiple definitions of error, just stick to one)

For ODE formulated in (13),

$$\begin{aligned} y' &= b - ay \\ y' &= (b - ay) \cdot 1 \end{aligned} \tag{14}$$

Comparing (14) with the standard separable ODE form, $y'(t) = g(y) \cdot h(t)$, we have $g(y) = b - ay$ and $h(t) = 1$.

Rewriting the separable ODE using Leibnitz's notation,

$$\begin{aligned} \frac{\mathrm{d}y}{\mathrm{d}t} &= g(y) \cdot h(t) \\ \frac{1}{g(y)} \cdot \frac{\mathrm{d}y}{\mathrm{d}t} &= h(t) \end{aligned}$$

Integrating both sides wrt $t$,

$$\int \frac{1}{g(y)} \frac{\mathrm{d}y}{\mathrm{d}t} \, dt = \int h(t) \, dt$$
$$\int \frac{1}{b - ay} \, dy = \int 1 \cdot dt$$

Defining $m = b - ay$ and using that $\dfrac{\mathrm{d}m}{\mathrm{d}y} = -a$,

$$\begin{aligned}
-\frac{1}{a} \int \frac{1}{m} \, dm &= t + c_1 \\
\ln |m| &= -a \cdot (t + c_2) && [\ \textit{absorbing integration consts into } c_2\ ] \\
\ln |b - ay| &= -a \cdot (t + c_2) && [\ \textit{since } m = b - ay\ ] \\
y &= \frac{b}{a} - \frac{1}{a} \cdot e^{-at} \cdot e^{ac_2} && [\ \textit{assuming } b - ay \geq 0\ ] \\
&= \frac{b}{a} - c_3 \cdot e^{-at} && [\ \text{where } c_3 = c_2 \cdot e^{ac_2}\ ]
\end{aligned} \tag{15}$$

Given that at $t = 0$, $y = 0$ and the influx rate $b = 100\mu M$,

$$\begin{aligned}
0 &= \frac{100}{a} - c_3 \cdot e^0 \\
c_3 &= \frac{100}{a}
\end{aligned}$$

So, the specific solution at the given initial conditions becomes,

$$y = \frac{100}{a} \left(1 - e^{-at}\right) \tag{16}$$

In this formulation, we define the square root of the sum of mean squared error (MSE) over all data points as the measure of error between data and prediction; this is shown in (17) and is called the L2-norm.

$$e_{L2} = \sqrt{\sum_{i=1}^{N} \left(\hat{y}_i - y_i\right)^2} \tag{17}$$

The Matlab code to compute the error between observed data and model prediction using the ODE solution found in (16) and the error formulation in (17) is shown in Listing 1.

```
% define the ODE as an anonymous function.
yprime_function = @(y, a, b) b - a*y;

% part (a): plot the ODE with arbitrary parameters.
b = 100;    % influx.
```

```
a = 1;       % decay.
y_vals = linspace(0, 100, 200);
disp(yprime_function(y_vals, a, b));
figure();
plot(y_vals, yprime_function(y_vals, a, b));
title( concentration rate (y') vs. concentration (y) at $a=100$ and $b=1$ , 'Interpreter', 'latex');
xlabel( $y [\mu m]$ , 'Interpreter', 'latex');
ylabel( $y^\prime [\mu m/s]$ , 'Interpreter', 'latex');

% part (b): define an error function.
function err = compute_error(y_fun, y_true, t_true, a, b, k)
    %y(x)=\frac{a}{b}-ke^{-bt}
    y_pred = y_fun(t_true, a, b, k);
    err = norm(y_pred - y_true);
end
```

**Listing 1:** Matlab script for 4(a) and 4(b).

### Part (c)

Plot the error E as a function of the degradation parameter a, and from this graph find the value that minimizes the error.

The plot of error as a function of degradation parameter, $a$, is shown in Figure 2 with the least error point marked in red. This occurs at $a = 0.0470$. The solution function in (16) now becomes,

$$y = \frac{100}{0.0470}\left(1 - e^{-(0.0470)t}\right) \tag{18}$$

The code to generate the plot is shown in Listing 2.

```
% part (c): plot error as a function of parameter a (decay rate).
% encode real data points.
y_true = [1e-4 400 700 900 750];
t_true = [1e-4 3 6 9 12];
b = 100;     % given influx rate.

% anonoymous function to compute y.
y_function = @(t_vals, a, b, k) b/a - (k .* exp(-a .* t_vals));

% sample values of a between 0 and 0.5.
n_points = 1000;
a_vals = linspace(0, 0.5, n_points);
k_vals = b ./ a_vals;        % k=b/a based on initial conditions.
error_vals = zeros(1, n_points);
for idx=1:length(a_vals)
    error = compute_error(y_function, y_true, t_true, a_vals(idx), b, k_vals(idx));
    error_vals(idx) = error;
```

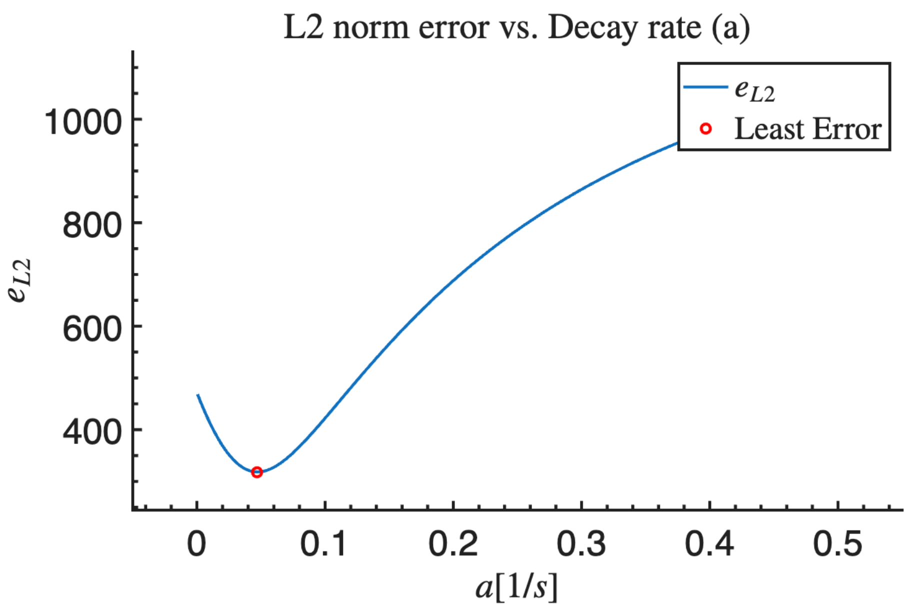


**Figure 2:** Error as a function of decay rate parameter choice.

```
end

figure(); hold on;
plot(a_vals, error_vals);
title( L2 norm error vs. decay rate (a) , 'Interpreter', 'latex');
xlabel( $a[1/s]$ , 'Interpreter', 'latex');
ylabel( $e_{L2}$ , 'Interpreter', 'latex');

% least error param fit.
[min_error, min_idx] = min(error_vals);
best_a = a_vals(min_idx);
plot(best_a, min_error,  ro );
hold off;
legend( $e_{L2}$ ,  Least Error , 'Interpreter', 'latex');
```

**Listing 2:** Matlab script to plot error as a function of decay rate.

### Part (d)

Using that value of the degradation parameter a, plot the best fitting graph y (t) together with the experimental data.

The best fit plot based on the value of decay rate, $a = 0.0470$, chosen at least $e_{L2}$ is shown in Figure 3. Specifically, (18) was used to predict concentrations at the same time points for which they were measured experimentally. The predictions are in agreement with data with reasonable variation. Notably, all data measurements are in the exponential growth region of the function;

consequently, it is difficult to comment on how the predictions will hold up close to saturation values. The Matlab code used to generate the plot is included as Listing 3.

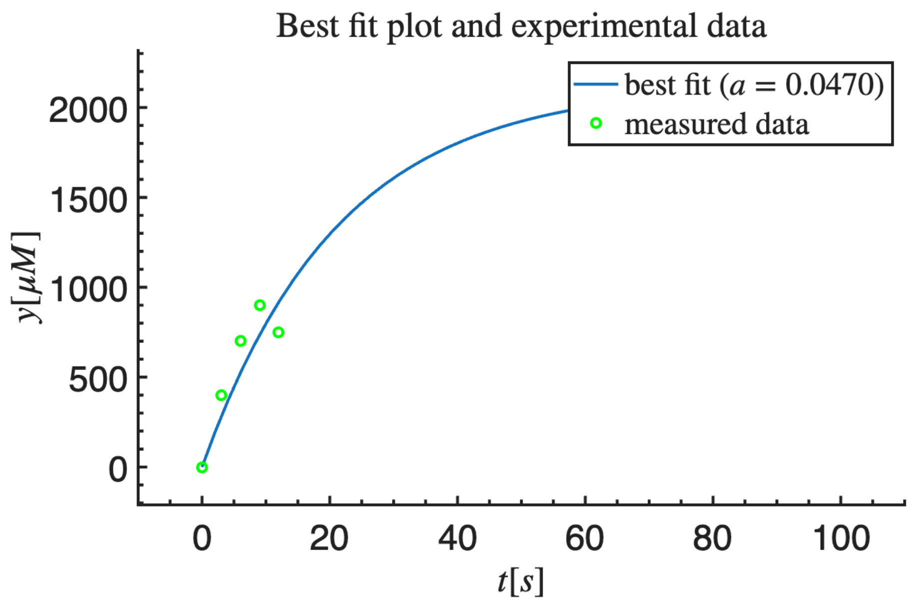


**Figure 3:** Best fit predictions overlayed on data points.

```
% part (d): plot y(t) for best b found along with data pts.
best_a = a_vals(min_idx);
figure(); hold on;
k = b/best_a;
% sample t to show (pseudo)-continuous prediction.
t_trend = linspace(0, 100, 50);
y_trend = y_function(t_trend, best_a, b, k);
plot(t_trend, y_trend);
plot(t_true, y_true, 'bo');
title( Best fit plot and experimental data , 'Interpreter', 'latex'
    );
xlabel( $t [s]$ , 'Interpreter', 'latex');
ylabel( $y [\mu M]$ , 'Interpreter', 'latex');
hold off; PrettyFig;
```

**Listing 3:** Matlab script to plot the best fit along with experimental data points.

### Part (e)

Predict for the same patient how the drug concentration would decrease if there was no influx of drug and initial drug concentration was $1000\mu M$ (say, after a single pill dose).

If the patient had no influx of drug, the influx rate would be zero, i.e., $b = 0$. In addition, there is a change in initial condition: at time $t = 0$, $y = 1000\mu M$. Solving (15) again with these new conditions,

$$
\begin{aligned}
y(0) &= \frac{0}{a} - c_3 \cdot e^0 \\
1000 &= -c_3 \\
c_3 &= -1000
\end{aligned}
$$

So, the specific solution at these conditions becomes,

$$y = 1000 \cdot 1 - e^{-at} \tag{19}$$

Using the same best fit parameter value $a = 0.0470$ as before, we have,

$$y = 1000 \cdot e^{-(0.0470)t} \tag{20}$$

The solution for $y$ obtained in (19) is used to predict concentration as a function of time, and the obtained plot is shown in Figure 4. The code used to make predictions and generate the plot is shown in Listing 4.

```
% part (e): solve if influx is 0, init is (0, 1000).
k_noinflux = -1000;
b_noinflux = 0;
a_noinflux = best_a;
figure(); hold on;
t_trend = linspace(0, 20, 50);
y_trend = y_function(t_trend, a_noinflux, b_noinflux, k_noinflux);
title( Concentration evolution when $a=0$ and $y(0)=1000\mu M$ , '
    Interpreter', 'latex');
xlabel( $t [s]$ , 'Interpreter', 'latex');
ylabel( $y [\mu M]$ , 'Interpreter', 'latex');
plot(t_trend, y_trend);
hold off; PrettyFig;
```

**Listing 4:** Matlab script to predict concentration evolution over time when there is no drug influx and the patient starts off with an initial drug level in the blood.

The complete Matlab script is included as a submission file on Canvas.

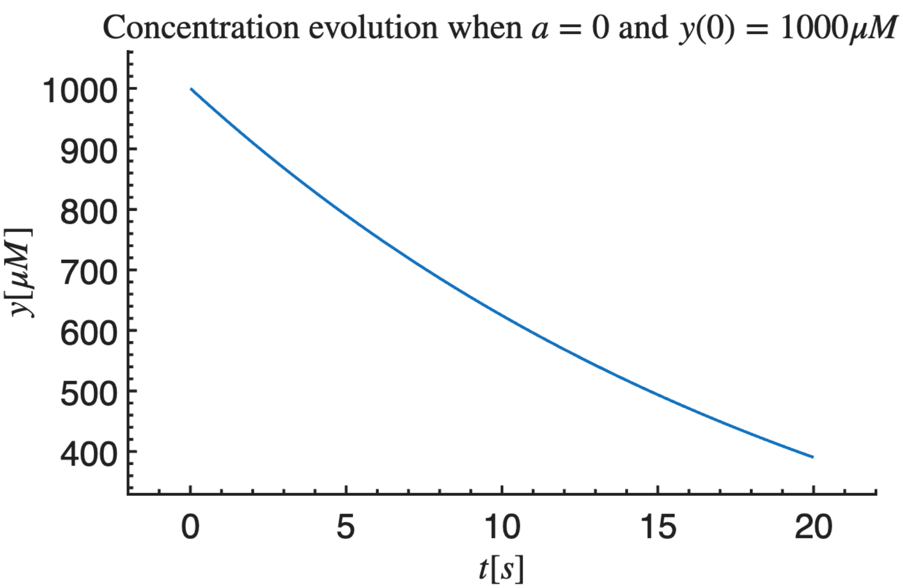


**Figure 4:** Concentration evolution over time when there is no drug influx and the patient starts off with an initial drug level in the blood.