Using EXCEL to solve a differential equation

Math 222

Department of Mathematics, UW - Madison

June 20, 2010

A chemical reaction

A chemical reactor contains two kinds of molecules, A and B.

A chemical reaction

A chemical reactor contains two kinds of molecules, A and B.

Whenever an A and B molecule bump into each other the B turns into an A:

$$\mathrm{A} + \mathrm{B} \longrightarrow 2\mathrm{A}$$

A chemical reaction

A chemical reactor contains two kinds of molecules, A and B.

Whenever an A and B molecule bump into each other the B turns into an A:

$$\mathrm{A} + \mathrm{B} \longrightarrow 2\mathrm{A}$$

As the reaction proceeds, all B gets converted to A. How long does this take?

Reaction rate for A+B$\longrightarrow$ 2A

The total number of molecules (A and B) stays constant.

Reaction rate for A+B$\longrightarrow$ 2A

The total number of molecules (A and B) stays constant.

Let $x(t)$ be the fraction of all molecules in the reactor which, at time t, are of type A.

Reaction rate for A+B$\longrightarrow$ 2A

The total number of molecules (A and B) stays constant.

Let $x(t)$ be the fraction of all molecules in the reactor which, at time t, are of type A.

Then $0 \le x(t) \le 1$, and the fraction of all molecules in the reactor which (at time t) are of type B is $1 - x(t)$.

Reaction rate for A+B$\longrightarrow$ 2A

The total number of molecules (A and B) stays constant.

Let $x(t)$ be the fraction of all molecules in the reactor which, at time t, are of type A.

Then $0 \leq x(t) \leq 1$, and the fraction of all molecules in the reactor which (at time t) are of type B is $1 - x(t)$.

Every time a reaction takes place, the ratio $x(t)$ increases, so

$$\frac{dx}{dt} \text{ is proportional to the reaction rate.}$$

Reaction rate for A+B$\longrightarrow$ 2A

"Chemistry" tells us that

$$\begin{aligned}\frac{dx}{dt} &= K \cdot \text{amount of A} \cdot \text{amount of B} \\ &= Kx(1-x).\end{aligned}$$

Reaction rate for A+B$\longrightarrow$ 2A

"Chemistry" tells us that

$$\frac{dx}{dt} = K \cdot \text{amount of A} \cdot \text{amount of B}$$
$$= Kx(1-x).$$

K is a proportionality constant, which depends on the particular kind of molecules A and B in this reaction. You would have to measure it to find its value.

Reaction rate for A+B$\longrightarrow$ 2A

"Chemistry" tells us that

$$\begin{aligned}\frac{dx}{dt} &= K \cdot \text{amount of A} \cdot \text{amount of B} \\ &= Kx(1-x).\end{aligned}$$

K is a proportionality constant, which depends on the particular kind of molecules A and B in this reaction. You would have to measure it to find its value.

This is a calculus class, so let's assume $K = 1$.

We have to solve the diffeq

$$\frac{dx}{dt} = x(1-x).$$

The solution will have an arbitrary constant ("C"). If we know what $x(0)$ is then we can compute C.

Solving $\frac{dx}{dt} = x(1-x)$

We have to solve the diffeq

$$\frac{dx}{dt} = x(1-x).$$

The solution will have an arbitrary constant ("C"). If we know what $x(0)$ is then we can compute C.

So (as an example) let's try to solve the following problem:

Solving $\frac{dx}{dt} = x(1-x)$

We have to solve the diffeq

$$\frac{dx}{dt} = x(1-x).$$

The solution will have an arbitrary constant ("C"). If we know what $x(0)$ is then we can compute C.

So (as an example) let's try to solve the following problem:

Suppose the tank initially holds 2% A and 98% B, We have to solve the diffeq

$$\frac{dx}{dt} = x(1-x).$$

The solution will have an arbitrary constant ("C"). If we know what $x(0)$ is then we can compute C.

So (as an example) let's try to solve the following problem:

Suppose the tank initially holds 2% A and 98% B, $x(0) = 0.02$

Solving $\frac{dx}{dt} = x(1-x)$

We have to solve the diffeq

$$\frac{dx}{dt} = x(1-x).$$

The solution will have an arbitrary constant ("C"). If we know what $x(0)$ is then we can compute C.

So (as an example) let's try to solve the following problem:

Suppose the tank initially holds 2% A and 98% B, $x(0) = 0.02$
Then what is the fraction of A molecules at time t?

Solving $\frac{dx}{dt} = x(1-x)$

We have to solve the diffeq

$$\frac{dx}{dt} = x(1-x).$$

The solution will have an arbitrary constant ("C"). If we know what $x(0)$ is then we can compute C.

So (as an example) let's try to solve the following problem:

Suppose the tank initially holds 2% A and 98% B, $x(0) = 0.02$
Then what is the fraction of A molecules at time t? $x(t) = ?$

Summary of the problem

We are going to solve an initial value problem:

Summary of the problem

We are going to solve an initial value problem:

Find $x(t)$ if you know

$$\underbrace{\frac{dx}{dt} = x(1-x)}_{\text{diffeq}} \quad \text{and} \quad \underbrace{x(0) = 0.02}_{\text{initial value}}$$

Summary of the problem

We are going to solve an initial value problem:

Find $x(t)$ if you know

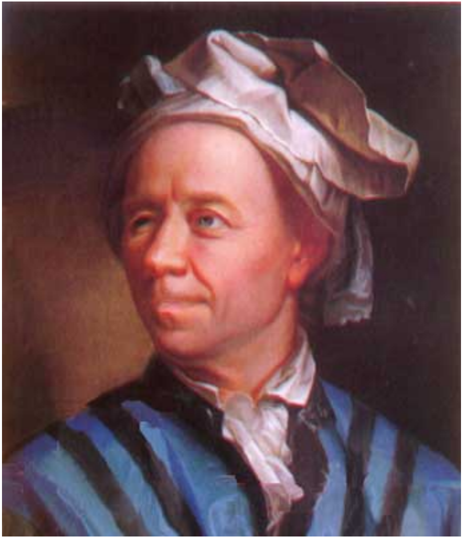
$$\underbrace{\frac{dx}{dt} = x(1-x)}_{\text{diffeq}} \quad \text{and} \quad \underbrace{x(0) = 0.02}_{\text{initial value}}$$

The solution is

$$x(t) = \frac{1}{1+49e^{-t}}.$$

(to be explained later this hour).

Leonhard "$e^{\pi i} + 1 = 0$" Euler (1707 - 1783)



Euler's idea:

Euler's idea:

I can't solve the equation because I don't know what $\frac{dx}{dt}$ is. So pick a small number $h > 0$ and say that

$$\frac{dx}{dt} \approx \frac{x(t+h) - x(t)}{h}.$$

Solving $\frac{dx}{dt} = x(1-x)$

Euler's idea:

I can't solve the equation because I don't know what $\frac{dx}{dt}$ is. So pick a small number $h > 0$ and say that

$$\frac{dx}{dt} \approx \frac{x(t+h) - x(t)}{h}.$$

The diffeq then becomes

$$\frac{x(t+h) - x(t)}{h} \approx x(t)(1 - x(t)).$$

Solving $\frac{dx}{dt} = x(1-x)$

Euler's idea:

I can't solve the equation because I don't know what $\frac{dx}{dt}$ is. So pick a small number $h > 0$ and say that

$$\frac{dx}{dt} \approx \frac{x(t+h) - x(t)}{h}.$$

The diffeq then becomes

$$\frac{x(t+h) - x(t)}{h} \approx x(t)(1 - x(t)).$$

If you know $x(t)$ and h then you can solve this equation for $x(t+h)$.

Solving $\frac{dx}{dt} = x(1-x)$

$$\frac{x(t+h) - x(t)}{h} \approx x(t)(1 - x(t)).$$

has as solution

$$x(t+h) \approx x(t) + h \cdot x(t)(1 - x(t)).$$

$$\frac{x(t+h) - x(t)}{h} \approx x(t)(1 - x(t)).$$

has as solution

$$x(t+h) \approx x(t) + h \cdot x(t)(1 - x(t)).$$

Example ($t = 0$): If we know $x(0)$, then this equation allows us to compute $x(0+h) = x(h)$.

Solving $\frac{dx}{dt} = x(1-x)$

$$\frac{x(t+h) - x(t)}{h} \approx x(t)(1-x(t)).$$

has as solution

$$x(t+h) \approx x(t) + h \cdot x(t)(1-x(t)).$$

Example ($t = 0$): If we know $x(0)$, then this equation allows us to compute $x(0+h) = x(h)$.

Example ($t = h$): Knowing $x(h)$ you can find $x(h+h) = x(2h)$

$$\frac{x(t+h) - x(t)}{h} \approx x(t)(1 - x(t)).$$

has as solution

$$x(t+h) \approx x(t) + h \cdot x(t)(1 - x(t)).$$

Example ($t = 0$): If we know $x(0)$, then this equation allows us to compute $x(0 + h) = x(h)$.

Example ($t = h$): Knowing $x(h)$ you can find $x(h + h) = x(2h)$,

And then $x(2h + h) = x(3h)$,

$$\frac{x(t+h) - x(t)}{h} \approx x(t)(1 - x(t)).$$

has as solution

$$x(t+h) \approx x(t) + h \cdot x(t)(1 - x(t)).$$

Example ($t = 0$): If we know $x(0)$, then this equation allows us to compute $x(0+h) = x(h)$.

Example ($t = h$): Knowing $x(h)$ you can find $x(h+h) = x(2h)$,

And then $x(2h+h) = x(3h)$, $x(3h+h) = x(4h)$, etc...

Euler's (approximate) solution

Pick a small number $h > 0$, and compute

$$x(h) = x(0) + h \cdot x(0)[1 - x(0)]$$

$$\searrow$$

Euler's (approximate) solution

Pick a small number $h > 0$, and compute

$$
\begin{aligned}
x(h) &= x(0) + h \cdot x(0)[1 - x(0)] \\
&\searrow \\
x(2h) &= x(h) + h \cdot x(h)[1 - x(h)] \\
&\searrow
\end{aligned}
$$

Euler's (approximate) solution

Pick a small number $h > 0$, and compute

$$
\begin{array}{rcl}
x(h) & = & x(0) + h \cdot x(0)[1 - x(0)] \\
 & \searrow & \\
x(2h) & = & x(h) + h \cdot x(h)[1 - x(h)] \\
 & \searrow & \\
x(3h) & = & x(2h) + h \cdot x(2h)[1 - x(2h)] \\
 & \searrow &
\end{array}
$$

Euler's (approximate) solution

Pick a small number $h > 0$, and compute

$$\begin{aligned} x(h) &= x(0) + h \cdot x(0)[1 - x(0)] \\ &\searrow \\ x(2h) &= x(h) + h \cdot x(h)[1 - x(h)] \\ &\searrow \\ x(3h) &= x(2h) + h \cdot x(2h)[1 - x(2h)] \\ &\searrow \\ x(4h) &= x(3h) + h \cdot x(3h)[1 - x(3h)] \\ &\vdots \end{aligned}$$

Euler's (approximate) solution

Pick a small number $h > 0$, and compute

$$\begin{array}{rcl} x(h) & = & x(0) + h \cdot x(0)[1 - x(0)] \\ & \searrow & \\ x(2h) & = & x(h) + h \cdot x(h)[1 - x(h)] \\ & \searrow & \\ x(3h) & = & x(2h) + h \cdot x(2h)[1 - x(2h)] \\ & \searrow & \\ x(4h) & = & x(3h) + h \cdot x(3h)[1 - x(3h)] \\ & \vdots & \end{array}$$

Now let's choose $h = 0.2$ and $x(0) = 0.02$, and compute $x(0.2)$, $x(0.4)$, $x(0.6)$, $x(0.8)$, $x(1.0)$, ...

Doing the calculations

Doing all these calculations is a drag of course. How did Euler do this? By hand!! (and with a lot of patience).

Doing the calculations

Doing all these calculations is a drag of course. How did Euler do this? By hand!! (and with a lot of patience).

How do we do this in the 21st century? With a computer.

Doing the calculations

Doing all these calculations is a drag of course. How did Euler do this? By hand!! (and with a lot of patience).

How do we do this in the 21st century? With a computer.

For more complicated diffeqs one should learn to program a computer, but for the example we've been looking at you can get Excel (or some other spreadsheet program like Open Office) to compute and plot the solutions.

What the spreadsheet computed

Here are the numbers, and graphs. The exact solution is $x(t) = 1/(1 + 49e^{-t})$.

h	t	x(t)	x'(t)	exact solution
0.2	0	0.020000	0.019600	0.020000
0.2	0.2	0.023920	0.023348	0.024320
0.2	0.4	0.028590	0.027772	0.029546
0.2	0.6	0.034144	0.032978	0.035853
0.2	0.8	0.040740	0.039080	0.043446
0.2	1	0.048556	0.046198	0.052559
0.2	1.2	0.057795	0.054455	0.063458
0.2	1.4	0.068686	0.063968	0.076434
0.2	1.6	0.081480	0.074841	0.091803
0.2	1.8	0.096448	0.087146	0.109894
0.2	2	0.113877	0.100909	0.131037
0.2	2.2	0.134059	0.116087	0.155537
0.2	2.4	0.157277	0.132541	0.183649
0.2	2.6	0.183785	0.150008	0.215545
0.2	2.8	0.213786	0.168082	0.251276
0.2	3	0.247403	0.186195	0.290734
0.2	3.2	0.284642	0.203621	0.333628
0.2	3.4	0.325366	0.219503	0.379465
0.2	3.6	0.369266	0.232909	0.427558
0.2	3.8	0.415848	0.242918	0.477061
0.2	4	0.464432	0.248735	0.527019
0.2	4.2	0.514179	0.249799	0.576441
0.2	4.4	0.564138	0.245886	0.624380
0.2	4.6	0.613316	0.237160	0.669999
0.2	4.8	0.660748	0.224160	0.712628
0.2	5	0.705580	0.207737	0.751790
0.2	5.2	0.747127	0.188928	0.787208
0.2	5.4	0.784913	0.168825	0.818791
0.2	5.6	0.818678	0.148445	0.846600
0.2	5.8	0.848367	0.128641	0.870815
0.2	6	0.874095	0.110053	0.891696
0.2	6.2	0.896105	0.093101	0.909552
0.2	6.4	0.914725	0.078003	0.924713
0.2	6.6	0.930326	0.064820	0.937508
0.2	6.8	0.943290	0.053494	0.948249
0.2	7	0.953989	0.043894	0.957229
0.2	7.2	0.962768	0.035846	0.964708
0.2	7.4	0.969937	0.029159	0.970920
0.2	7.6	0.975769	0.023644