



MATH 3290 Mathematical Modeling

Chapter 11: Modeling with a Differential Equation

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<https://www.math.cuhk.edu.hk/course/2324/math3290>



Midterm report

- There are 31 answer sheets collected with 2 students absent.
- Nine achieved the full score 35, with the average score 30.58.
- Solutions will be released later.
- Keep up the great work!

Future arrangements

- The second assignment has been released. Due: 5pm, **April 2nd**.
- The final assignment will be released **next week**, possibly due by **April 16th**.

Introduction

- We discuss modeling with a differential equation.
- A differential equation is an equation relating a quantity of interest and its derivatives.
- Derivatives represent instantaneous rates of change of a quantity.
- Differential equations model quantities that change continuously in time, e.g., populations, concentration of chemicals.
- In contrast, difference equations model quantities that change in discrete time intervals.

Population growth

Suppose that the population at time $t = t_0$ is known, P_0 .

We want to predict the **future** population $P(t)$, $t \geq t_0$.

Let k be the **percentage** growth per **unit time** and **assume** k is a constant.

Then, from time t to $t + \Delta t$,

$$\frac{P(t + \Delta t) - P(t)}{P(t)} = k\Delta t.$$

Thus,

$$\frac{P(t + \Delta t) - P(t)}{\Delta t} = kP(t).$$

If Δt is very **small**, we have

$$\frac{dP}{dt} = kP.$$

Moreover, we have $P(t_0) = P_0$.

The model is

$$\frac{dP}{dt} = kP, \quad P(t_0) = P_0.$$

To find P , we **separate** the variables

$$\frac{dP}{P} = k dt.$$

Integrate both sides

$$\int \frac{1}{P} dP = \int k dt \Rightarrow \ln P = kt + C.$$

Use the condition $P(t_0) = P_0$ to **determine C** ,

$$\ln P_0 = kt_0 + C \Rightarrow C = \ln P_0 - kt_0.$$

Finally, we have $\ln P = kt + C = kt + \ln P_0 - kt_0$,

$$P(t) = P_0 e^{k(t-t_0)}, \quad \text{exponential growth.}$$

The percentage growth rate per unit time k should **not** be a constant.

One choice of k (due to a mathematician P. F. Verhulst) is

$$k(t) = r(M - P(t)), \quad r > 0.$$

This suggests that the growth rate should be small when the population reaches the **maximum population** M .

Hence, the model becomes

$$\frac{P(t + \Delta t) - P(t)}{P(t)} = r(M - P)\Delta t.$$

Thus

$$\frac{P(t + \Delta t) - P(t)}{\Delta t} = rP(M - P).$$

When Δt is sufficiently small, we have

$$\frac{dP}{dt} = rP(M - P).$$

This is called the **logistic model**.

To find the solution, we **separate** the variables

$$\frac{dP}{P(M - P)} = r dt.$$

Using **partial fractions**, we have

$$\frac{1}{P(M - P)} = \frac{1}{M} \left(\frac{1}{P} + \frac{1}{M - P} \right).$$

The differential equations become

$$\frac{1}{P} dP + \frac{1}{M - P} dP = rM dt.$$

Recall that

$$\frac{1}{P} dP + \frac{1}{M - P} dP = rM dt.$$

Integrate both sides,

$$\int \frac{1}{P} dP + \int \frac{1}{M - P} dP = \int rM dt.$$

Assuming $P > 0$ and $P < M$, we have

$$\ln P - \ln(M - P) = rMt + C.$$

Using the initial condition $P(t_0) = P_0$ to determine C ,

$$\ln P_0 - \ln(M - P_0) = rMt_0 + C.$$

Consequently,

$$\ln P - \ln(M - P) = rMt + (\ln P_0 - \ln(M - P_0) - rMt_0).$$

Recall that

$$\ln P - \ln(M - P) = rMt + (\ln P_0 - \ln(M - P_0) - rMt_0).$$

Solving for P , we have

$$P(t) = \frac{MP_0}{P_0 + (M - P_0)e^{-rM(t-t_0)}}.$$

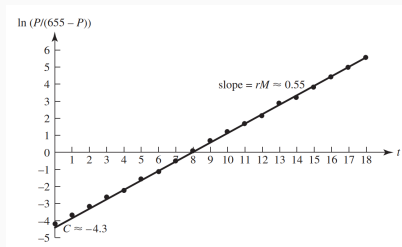
This gives a formula for finding P at any time t .

Remarks:

- We see that $P(t) \rightarrow M$ as $t \rightarrow \infty$.
- Usually we **assume** M is given.
- To find the model parameter $r > 0$, we plot $\ln \frac{P}{M-P}$ against t , and **the slope** of the line is rM .

Consider the following data. We take $M = 665$.

Time (hr)	Observed yeast biomass	Biomass calculated from logistic equation (11.13)	Percent error
0	9.6	8.9	-7.3
1	18.3	15.3	-16.4
2	29.0	26.0	-10.3
3	47.2	43.8	-7.2
4	71.1	72.5	2.0
5	119.1	116.3	-2.4
6	174.6	178.7	2.3
7	257.3	258.7	0.5
8	350.7	348.9	-0.5
9	441.0	436.7	-1.0
10	513.3	510.9	-4.7
11	559.7	566.4	1.2
12	594.8	604.3	1.6
13	629.4	628.6	-0.1
14	640.8	643.5	0.4
15	651.1	652.4	0.2
16	655.9	657.7	0.3
17	659.6	660.8	0.2
18	661.8	662.5	0.1



We plot $\ln \frac{P}{665-P}$ against t , the slope is rM .

The value of rM can be obtained by the least squares method. We have $r = 8.27 \times 10^{-4}$.

How to determine P_0 ?

- Use the **original** data point, that is $P_0 = 9.6$ from the **table**.
- Recall that

$$\ln\left(\frac{P}{M-P}\right) = rMt + \ln\left(\frac{P_0}{M-P_0}\right) - rMt_0.$$

From the least squares method, we could obtain a linear model

$$\ln\left(\frac{P}{M-P}\right) \approx kt + C,$$

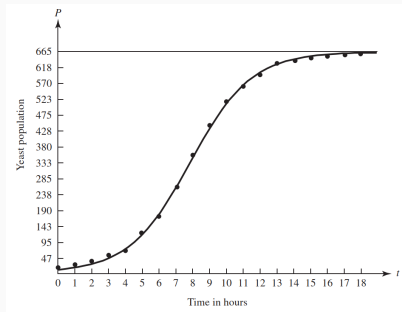
and we can hence **solve** P_0 by

$$C = \ln\left(\frac{P_0}{M-P_0}\right) - rMt_0.$$

Those two options should produce **similar** results.

Hence, the model is $P(t) = \frac{MP_0}{P_0 + (M - P_0)e^{-0.55(t-t_0)}}$.

Time (hr)	Observed yeast biomass	Biomass calculated from logistic equation (11.13)	Percent error
0	9.6	8.9	-7.3
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The model fits the data very well.

Example: Drug dosage

We combine differential and difference equations in a model.

Q: How can the **doses** and the **time** between doses be adjusted to maintain a safe but effective concentration of drug?

Assumption 1: decay of drug.

Let $C(t)$ be the concentration of the drug. Then we assume

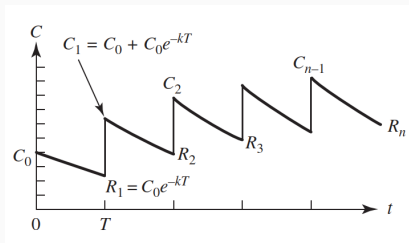
$$\frac{dC}{dt} = -kC,$$

where $k > 0$ is the decay rate. We will obtain a **differential equation** model.

Assumption 2: constant dosage.

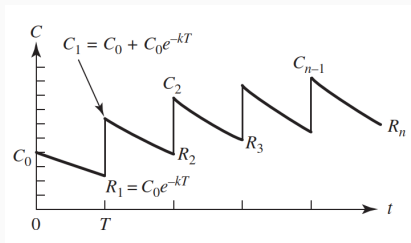
A dose of C_0 is added at fixed time intervals of length T . We will obtain a **difference equation** model

An illustration of C as a function of time t :



Some notations:

- R_n is the residual after n doses, **before** the next dose,
- C_n is the residual **after** $n + 1$ doses.



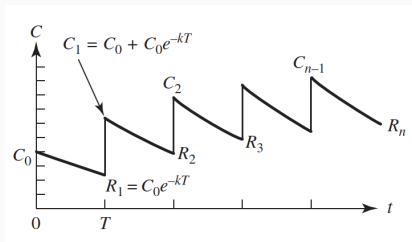
From Assumption 1, we have

$$C(t) = C(t_0)e^{-k(t-t_0)}$$

We see that $R_1 = C_0 e^{-kT}$.

Then a dosage of C_0 is **added**, we have

$$C_1 = C_0 + R_1 = C_0 + C_0 e^{-kT}.$$



Then at time $2T$, the residual is

$$R_2 = C_1 e^{-kT} = C_0(e^{-kT} + e^{-2kT}).$$

Then a dosage of C_0 is added

$$C_2 = C_0 + R_2 = C_0(1 + e^{-kT} + e^{-2kT}).$$

Continuing the above process, at time nT ,

$$R_n = C_0 e^{-kT} (1 + e^{-kT} + \dots + e^{-(n-1)kT}).$$

That is

$$R_n = C_0 e^{-kT} \frac{1 - e^{-nkT}}{1 - e^{-kT}}.$$

We see that, in the long run ($n \rightarrow \infty$):

$$R = \lim_{n \rightarrow \infty} C_0 e^{-kT} \frac{1 - e^{-nkT}}{1 - e^{-kT}} = \frac{C_0}{e^{kT} - 1}.$$

Recall:

- C_0 is the **constant dosage** level;
- T is the **time interval**;
- R is the concentration of drug in the **long run**.

Assume the drug is ineffective if the concentration is below L , and harmful if above H .

We set $R = L$ (in the long run, the concentration is L), and $C_0 = H - L$. Then

$$R = \frac{C_0}{e^{kT} - 1}$$

becomes

$$L = \frac{H - L}{e^{kT} - 1}.$$

Solving, we have

$$T = \frac{1}{k} \ln \frac{H}{L},$$

which gives guidance of how much ($C_0 = H - L$) and when ($T = \frac{1}{k} \ln \frac{H}{L}$) one should take the drug.

Graphical methods

Most differential equations cannot be solved easily.

Graphical method gives a sketch of the solution.

The following information could be derived from the sketch:

1. equilibrium points (EPs) (points at which the derivative is **zero**),
2. signs of the first order derivative (**increase/decrease**),
3. signs of the second order derivative (**convex/concave**).

To obtain the above information, a **phase line** is helpful.

Drawing a phase line

Consider the equation

$$\frac{dy}{dx} = (y + 1)(y - 2).$$

Step 1: locate the equilibrium points (EPs),

$$\frac{dy}{dx} = 0 \quad \rightarrow \quad (y + 1)(y - 2) = 0.$$

Hence, the equilibrium points (EPs) are $y = -1$ and $y = 2$.

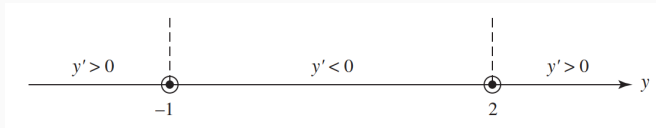
We indicate this in the phase line:



Recall the equation

$$\frac{dy}{dx} = (y + 1)(y - 2).$$

Step 2: determine the sign of y' .



We also put arrows (left \rightarrow decrease, right \rightarrow increase) to indicate how the value of y change.



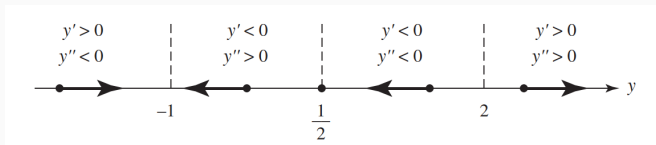
Recall the equation

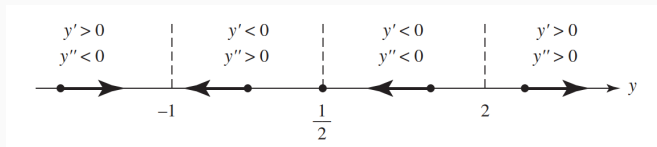
$$\frac{dy}{dx} = (y + 1)(y - 2).$$

Step 3: determine the sign of y''

$$\frac{d^2y}{dx^2} = (y + 1) \frac{dy}{dx} + (y - 2) \frac{dy}{dx} = (2y - 1)(y + 1)(y - 2).$$

Indicate the sign information in the phase line.



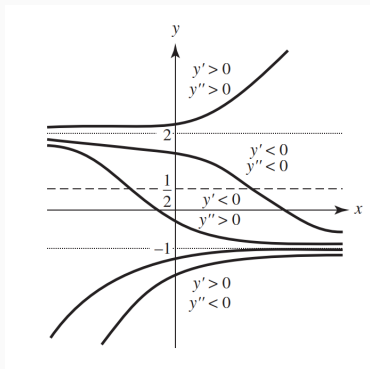


Step 4: sketch the solution using information from phase line.

we observe

- for $y < -1$, the function is **increasing**, slope is **decreasing**;
- for $-1 < y < 1/2$, the function is **decreasing**, slope is **increasing**;
- for $1/2 < y < 2$, the function is **decreasing**, slope is **decreasing**;
- for $y > 2$, the function is **increasing**, slope is **increasing**.

Then we get the following sketch:



A useful program for phase plots: [dfield](https://www.cs.unm.edu/~joel/dfield/). You can download it from <https://www.cs.unm.edu/~joel/dfield/> (You need Java Runtime Environment to run it).

Stable and unstable equilibrium

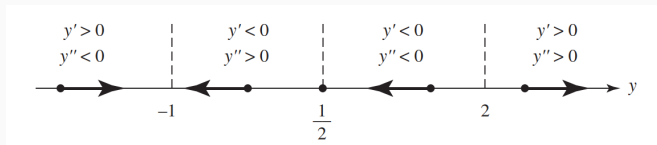
Let y^* be an equilibrium point (EP).

- It is a **stable** equilibrium point (EP) if the solution starts at a point **close** to y^* , then the solution for all future time remains **close** to y^* (e.g., pendulum).
- It is an **asymptotic stable** equilibrium point (EP) if the solution starts at a point **close** to y^* , then the solution **converges** to y^* .
- It is an **unstable** equilibrium point (EP) if the solution starts at a point **close** to y^* , then the solution **moves away** from y^* .

Example: for the differential equation

$$\frac{dy}{dx} = (y + 1)(y - 2).$$

Recall that the phase line is



We see that

- $y = -1$ is an **asymptotic stable** equilibrium point (EP),
- $y = 2$ is an **unstable** equilibrium point (EP).

Another example: consider the logistic equation

$$\frac{dP}{dt} = rP(M - P), \quad r, M > 0.$$

Equilibrium points are $P = 0$ and $P = M$.

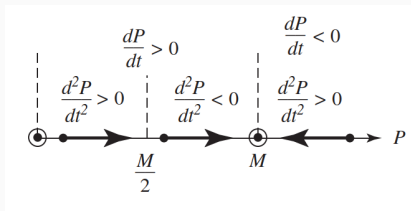
Moreover, we have

$$\frac{d^2P}{dt^2} = r(M - 2P) \frac{dP}{dt}.$$

We see that

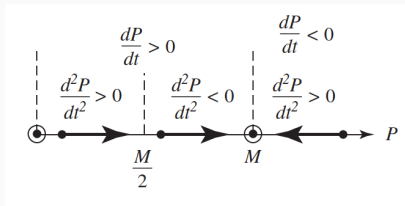
- $P' > 0$ when $0 < P < M$, and $P' < 0$ when $P > M$;
- $P'' > 0$ when $M - 2P$ and P' have the same sign, and $P'' < 0$ otherwise.

We have the following phase line.

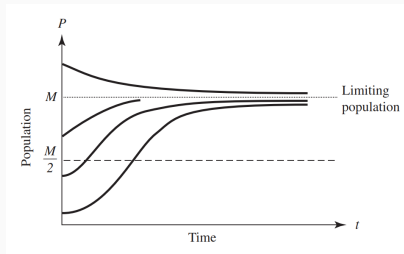


From the phase line, we see that

- $P = 0$ is an **unstable** equilibrium point (EP),
- $P = M$ is an **asymptotic stable** equilibrium point (EP).



Phase line



Sketch

Finding approximate solutions

Note, graphical method does not give the **values** of solutions.

We present a simple method, called the **Euler's method**, to find approximate values of solutions.

Specifically, we consider the differential equation

$$\frac{dy}{dx} = g(x, y).$$

Assume that a starting value is given: $y(x_0) = y_0$.

We will approximate values of $y(x)$ for future values of x ($x \geq x_0$).

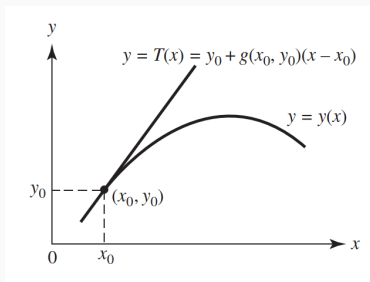
Main idea

The **tangent line** at the point (x_0, y_0) can be written as

$$T(x) = y_0 + \frac{dy}{dx}(x_0)(x - x_0).$$

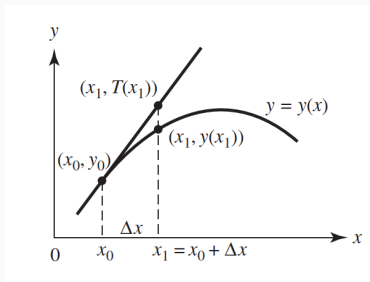
Using the differential equation

$$T(x) = y_0 + g(x_0, y_0)(x - x_0).$$



Let $x_1 = x_0 + \Delta x$ be a point near x_0 .

Then we can use the value $y_1 = T(x_1)$ of the **tangent line** to approximate the value of the exact solution $y(x_1)$.



We have

$$y_1 = y_0 + g(x_0, y_0)\Delta x.$$

Similarly, the tangent line of $y(x)$ at $(x_1, y(x_1))$ is

$$T(x) = y(x_1) + g(x_1, y(x_1))(x - x_1).$$

Let $x_2 = x_1 + \Delta x$ be a point near x_1 .

Then we can use the value $T(x_2)$ to approximate the value of the exact solution $y(x_2)$ by replacing $y(x_1)$ with y_1 .

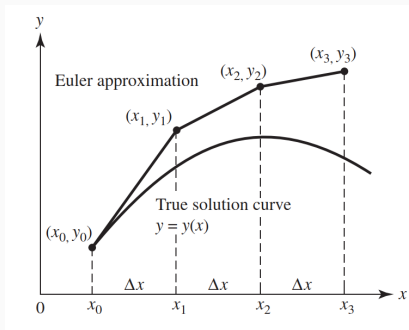
$$y_2 = y_1 + g(x_1, y_1)\Delta x.$$

In general, we can use the formula

$$y_{n+1} = y_n + g(x_n, y_n)\Delta x.$$

Euler's method

$$y_{n+1} = y_n + g(x_n, y_n)\Delta x.$$



Example: consider a saving account with variable interest rate.

We assume the interest rate r depends on the amount of saving S ,

$$S(t + \Delta t) = S(t) + r(S)S(t)\Delta t.$$

We obtain the model

$$\frac{dS}{dt} = r(S)S.$$

We take:

- the initial deposit is \$10, that is, $S(0) = 10$;
- the **variable** interest rate

$$r(S) = \frac{1 + 2S}{100 + 100S}$$

(it is increasing from 1% to 2%);

- $\Delta t = 1$.

Recall

$$\frac{dS}{dt} = r(S)S = S \frac{1 + 2S}{100 + 100S}, \quad S(0) = 10.$$

- Let $S_0 = 10$. then

$$S_1 = S_0 + \Delta t \left(S_0 \frac{1 + 2S_0}{100 + 100S_0} \right) = 10.1909.$$

- Next, we have

$$S_2 = S_1 + \Delta t \left(S_1 \frac{1 + 2S_1}{100 + 100S_1} \right) = 10.3856.$$

So, the deposit in the second day is $S(2) \approx \$10.3856$.

Application: Parameter identification

The aim is to determine **unknown parameters** a and b in the model

$$\frac{dy}{dx} = af(x, y) + bg(x, y),$$
$$y(0) = \alpha.$$

Motivation: parameters are needed in order to solve the model.

- In population model, we need to determine $r > 0$

$$\frac{dP}{dt} = rP(M - P).$$

- In drug concentration model, we need to determine $k > 0$

$$\frac{dC}{dt} = -kC.$$

Determine unknown parameters a and b in the model

$$\frac{dy}{dx} = af(x, y) + bg(x, y),$$
$$y(0) = \alpha.$$

Idea: perform experiments and collect data.

- Given the **initial condition** $y(0) = \alpha$, we measure $y(T) = \beta$, that is, the **response** at time T .
- Repeat the experiment with **different initial conditions**.

Determine unknown parameters a and b in the model

$$\begin{aligned}\frac{dy}{dx} &= af(x, y) + bg(x, y), \\ y(0) &= \alpha.\end{aligned}$$

The solution is denoted by $y(x; a, b)$.

Given a set of initial values $\alpha_1, \alpha_2, \dots, \alpha_N$, we measure the corresponding responses $\beta_1, \beta_2, \dots, \beta_N$ at time T .

We find the parameters a and b so that $S(a, b)$ is **minimized**:

$$S(a, b) = \sum_{i=1}^N \left(\beta_i - y_i(T; a, b) \right)^2,$$

where $y_i(T; a, b)$ is the response at time T with parameters a and b , and initial condition α_i .

We will minimize

$$S(a, b) = \sum_{i=1}^N \left(\beta_i - y_i(T; a, b) \right)^2.$$

We can use the **gradient method**. Given initial guess a_0 and b_0 , we generate a sequence (a_k, b_k) by the following

$$a_{k+1} = a_k - \lambda_k \frac{\partial S}{\partial a}(a_k, b_k),$$
$$b_{k+1} = b_k - \lambda_k \frac{\partial S}{\partial b}(a_k, b_k),$$

where

$$\frac{\partial S}{\partial a} = -2 \sum_{i=1}^N \left(\beta_i - y_i(T; a, b) \right) \frac{\partial y_i}{\partial a}(T; a, b),$$
$$\frac{\partial S}{\partial b} = -2 \sum_{i=1}^N \left(\beta_i - y_i(T; a, b) \right) \frac{\partial y_i}{\partial b}(T; a, b).$$

Next, we discuss how to compute

$$A_i(x; a, b) = \frac{\partial y_i}{\partial a}(x; a, b) \quad \text{and} \quad B_i(x; a, b) = \frac{\partial y_i}{\partial b}(x; a, b).$$

Recall that $y_i(x; a, b)$ satisfies

$$\begin{aligned} \frac{dy_i}{dx} &= af(x, y_i) + bg(x, y_i), \\ y_i(0) &= \alpha_i. \end{aligned}$$

Taking derivative with respect to a , we have

$$\begin{aligned} \frac{dA_i}{dx} &= f(x, y_i) + af_y(x, y_i)A_i + bg_y(x, y_i)A_i, \\ A_i(0) &= 0. \end{aligned}$$

From the above calculations, we see that to compute

$$A_i(T; a, b) = \frac{\partial y_i}{\partial a}(T; a, b).$$

We need the following steps:

Step 1: solve the following

$$\begin{aligned}\frac{dA_i}{dx} &= f(x, y_i) + af_y(x, y_i)A_i + bg_y(x, y_i)A_i, \\ A_i(0) &= 0,\end{aligned}$$

to get $A_i(x; a, b)$.

Step 2: evaluate A_i at $x = T$.

Similarly, to compute

$$B_i(T; a, b) = \frac{\partial y_i}{\partial b}(T; a, b),$$

we need the following steps:

Step 1: solve the following

$$\begin{aligned}\frac{dB_i}{dx} &= af_y(x, y_i)B_i + g(x, y_i) + bg_y(x, y_i)B_i, \\ B_i(0) &= 0,\end{aligned}$$

to get $B_i(x; a, b)$.

Step 2: evaluate B_i at $x = T$.

Summary of steps

Aim: determine unknown parameters a and b in the model

$$\frac{dy}{dx} = af(x, y) + bg(x, y),$$
$$y(0) = \alpha.$$

Assume that an initial guess a_0 and b_0 have been chosen.

Let a_k and b_k be known.

Step 1: find $y_i(x; a_k, b_k)$, $i = 1, 2, \dots, N$, by solving

$$\frac{dy_i}{dx} = a_k f(x, y_i) + b_k g(x, y_i),$$
$$y_i(0) = \alpha_i.$$

Then evaluate $y_i(T; a_k, b_k)$.

Step 2: find $A_i(x; a_k, b_k)$, $i = 1, 2, \dots, N$, by solving

$$\begin{aligned}\frac{dA_i}{dx} &= f(x, y_i) + a_k f_y(x, y_i) A_i + b_k g_y(x, y_i) A_i, \\ A_i(0) &= 0,\end{aligned}$$

where y_i need to be determined from Step **1**. Then evaluate $A_i(T; a_k, b_k)$.

Step 3: find $B_i(x; a_k, b_k)$, $i = 1, 2, \dots, N$, by solving

$$\begin{aligned}\frac{dB_i}{dx} &= a_k f_y(x, y_i) B_i + g(x, y_i) + b_k g_y(x, y_i) B_i, \\ B_i(0) &= 0,\end{aligned}$$

where y_i need to be determined from Step **1**. Then evaluate $B_i(T; a_k, b_k)$.

Step 4: update

$$a_{k+1} = a_k - \lambda_k \frac{\partial S}{\partial a}(a_k, b_k),$$

$$b_{k+1} = b_k - \lambda_k \frac{\partial S}{\partial b}(a_k, b_k),$$

where

$$\frac{\partial S}{\partial a}(a_k, b_k) = -2 \sum_{i=1}^N (\beta_i - y_i(T; a_k, b_k)) A_i(T; a_k, b_k),$$

$$\frac{\partial S}{\partial b}(a_k, b_k) = -2 \sum_{i=1}^N (\beta_i - y_i(T; a_k, b_k)) B_i(T; a_k, b_k).$$

Step 5: stop when

$$\frac{\partial S}{\partial a}(a_k, b_k) \quad \text{and} \quad \frac{\partial S}{\partial b}(a_k, b_k)$$

are small.

A simple example

Consider finding the model parameter a for

$$\frac{dy}{dx} = ay.$$

We follow the above procedure and set $T = 1$.

Step 1: Assume a_k is already **known**, find $y_i(x; a_k)$, $i = 1, 2, \dots, N$, by solving

$$\begin{aligned}\frac{dy_i}{dx} &= a_k y_i, \\ y_i(0) &= \alpha_i.\end{aligned}$$

Hence, we have $y_i(x; a_k) = \alpha_i e^{a_k x}$. So, $y_i(T; a_k) = \alpha_i e^{a_k}$.

Step 2: find $A_i(x; a_k)$, $i = 1, 2, \dots, N$, by solving

$$\begin{aligned}\frac{dA_i}{dx} &= y_i + a_k A_i = \alpha_i e^{a_k x} + a_k A_i, \\ A_i(0) &= 0,\end{aligned}$$

and then evaluate $A_i(T; a_k)$. In general, for equations in the form

$$\frac{dA_i}{dx} = R(x) + Q(x)A_i.$$

We multiply the equation by $e^{-\int_0^x Q(z) dz}$ (integrating factor method), then

$$\frac{d}{dx} \left(A_i e^{-\int_0^x Q(z) dz} \right) = R(x) e^{-\int_0^x Q(z) dz}.$$

Integrate from $x = 0$ to $x = T$ and recall that $A_i(0; a_k) = 0$,

$$A_i(T; a_k) e^{-\int_0^T Q(z) dz} = \int_0^T R(x) e^{-\int_0^x Q(z) dz} dx.$$

Letting $Q(x) = a_k$ and $R(x) = \alpha_i e^{a_k x}$, we have (recall $T = 1$)

$$A_i(T; a_k) e^{-a_k} = \int_0^1 \alpha_i e^{a_k x} e^{-a_k x} dx.$$

Thus,

$$A_i(T; a_k) = \alpha_i e^{a_k}.$$

Step 4: update

$$a_{k+1} = a_k - \lambda_k \frac{\partial S}{\partial a}(a_k),$$

where

$$\begin{aligned} \frac{\partial S}{\partial a}(a_k) &= -2 \sum_{i=1}^N (\beta_i - y_i(T; a_k)) A_i(T; a_k) \\ &= -2 \sum_{i=1}^N (\beta_i - \alpha_i e^{a_k}) \alpha_i e^{a_k}. \end{aligned}$$

Consider some data

α_j	1	2	3
β_j	3.5	6.9	10.5

Let $a_0 = 1.1$ and $\lambda_k = 0.005$.

Iteration	a	$\frac{\partial S}{\partial a}(a)$	$S(a)$
0	1.100	-40.506	3.254
1	1.303	19.867	0.528
2	1.203	-14.452	0.343
3	1.275	9.487	0.133
4	1.228	-6.810	0.078
\vdots	\vdots	\vdots	\vdots
48	1.249	-0.000	0.007
49	1.249	0.000	0.007

Hence, we have $a = 1.249$.

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