MATH 3290 Mathematical Modeling

Chapter 11: Modeling with a Differential Equation

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Introduction

- We discuss modeling with a differential equation that relates a quantity of interest and its derivatives.
- 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

$$\frac{\mathrm{d}P}{\mathrm{d}t} = kP.$$

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

The model is

$$\frac{\mathrm{d}P}{\mathrm{d}t} = kP, \qquad P(t_0) = P_0.$$

To find P, we separate the variables

$$\frac{\mathrm{d}P}{P} = k\,\mathrm{d}t.$$

Integrate both sides

$$\int \frac{1}{P}\ \mathrm{d}P = \int k\ \mathrm{d}t \quad \Rightarrow \quad \ln P = kt + C.$$

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

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

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

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

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

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

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

Hence, the model becomes

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

Thus

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

When Δt is sufficiently small, we have

$$\frac{\mathrm{d}P}{\mathrm{d}t} = rP(M - P).$$

This is called the logistic model.

To find the solution, we separate the variables

$$\frac{\mathrm{d}P}{P(M-P)} = r\,\mathrm{d}t.$$

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

$$\frac{1}{P}\,\mathrm{d}P + \frac{1}{M-P}\,\mathrm{d}P = rM\,\mathrm{d}t.$$

Recall that

$$\frac{1}{P}\,\mathrm{d}P + \frac{1}{M-P}\,\mathrm{d}P = rM\,\mathrm{d}t.$$

Integrate both sides,

$$\int \frac{1}{P}\,\mathrm{d}P + \int \frac{1}{M-P}\,\mathrm{d}P = \int rM\,\mathrm{d}t.$$

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,

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

Recall that

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

Solving for P, we have

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

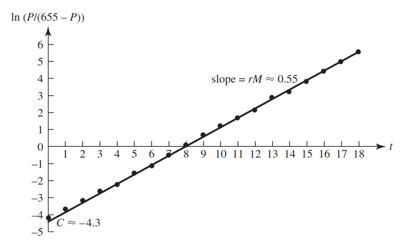
This gives a formula for finding P at any time t.

Remarks:

- We see that $P(t) \to M$ as $t \to \infty$.
- 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 $P(t) = \dfrac{MP_0}{P_0 + (M - P_0)\mathrm{e}^{-0.55(t-t_0)}}$.

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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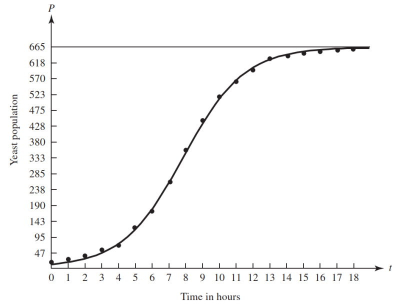


The model fits the data very well.

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.

Consider the equation

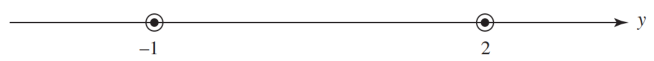
$$\frac{\mathrm{d}y}{\mathrm{d}x} = (y+1)(y-2).$$

Step $\boxed{1}$: locate the equilibrium points (EPs),

$$\frac{\mathrm{d}y}{\mathrm{d}x} = 0 \quad \to \quad (y+1)(y-2) = 0.$$

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

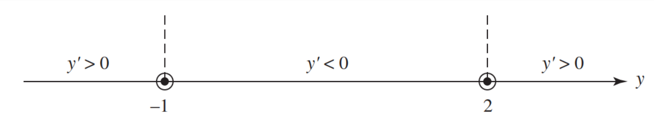
We indicate this in the phase line:



Recall the equation

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

Step 2: determine the sign of y'.



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

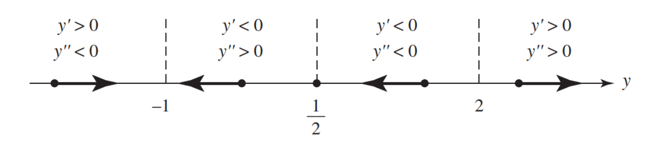
Recall the equation

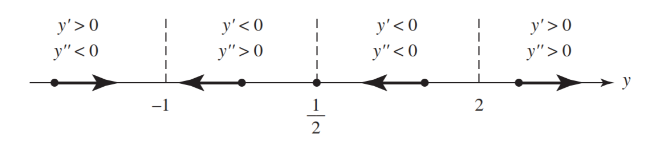
$$\frac{\mathrm{d}y}{\mathrm{d}x} = (y+1)(y-2).$$

Step 3: determine the sign of y''

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

Indicate the sign information in the phase line.



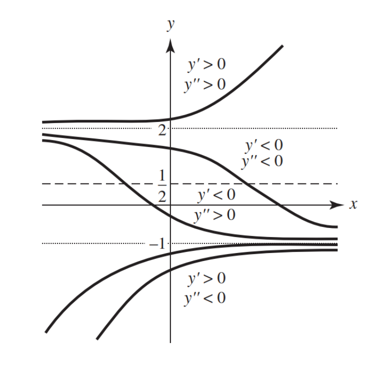


Step 4: sketch the solution using information from phase line.

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. You can download it from `https://www.cs.unm.edu/~joel/dfield/` (You need Java Runtime Environment to run it).

Stable and unstable equilibrium

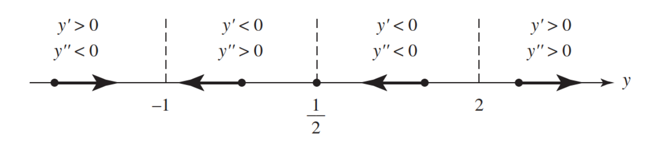
Let y^* be an equilibrium point (EP).

- 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

$$\frac{\mathrm{d}y}{\mathrm{d}x} = (y+1)(y-2).$$

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

$$\frac{\mathrm{d}P}{\mathrm{d}t} = rP(M - P), \qquad r, M > 0.$$

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

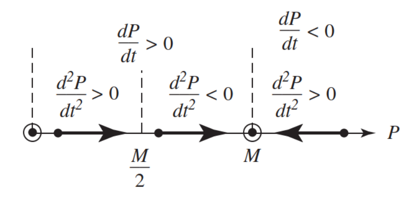
Moreover, we have

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

We see that

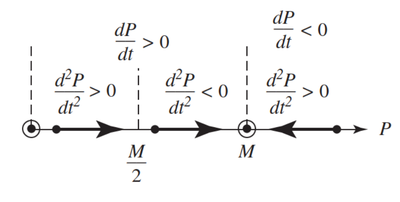
- $P' > 0$ when $0 < P < M$, and $P' < 0$ when $P > M$;
- $P'' > 0$ when $M - 2P$ and P' have the same sign, and $P'' < 0$ otherwise.

We have the following phase line.

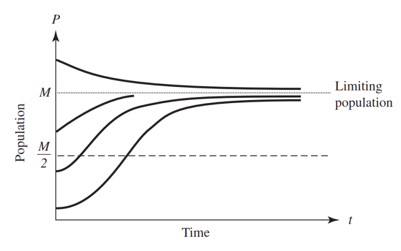


From the phase line, we see that

- $P = 0$ 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

$$\frac{\mathrm{d}y}{\mathrm{d}x} = g(x, y).$$

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

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

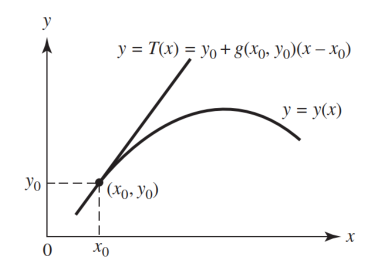
Main idea

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

$$T(x) = y_0 + \frac{\mathrm{d}y}{\mathrm{d}x}(x_0)(x - x_0).$$

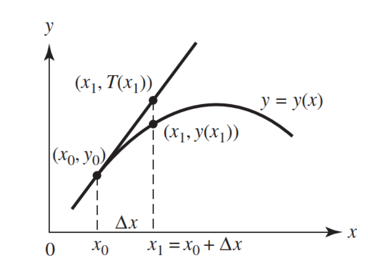
Using the differential equation

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



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.

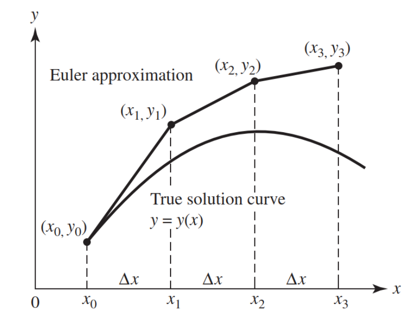
$$y_2 = y_1 + g(x_1, y_1)\Delta x.$$

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

$$\frac{\mathrm{d}S}{\mathrm{d}t} = r(S)S.$$

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

$$\frac{\mathrm{d}S}{\mathrm{d}t} = r(S)S = S\,\frac{1+2S}{100+100S}, \quad S(0) = 10.$$

- Let $S_0 = 10$. then

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

- Next, we have

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

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

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

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

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

$$\frac{\mathrm{d}P}{\mathrm{d}t} = rP(M-P).$$

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

$$\frac{\mathrm{d}C}{\mathrm{d}t} = -kC.$$

Determine unknown parameters a and b in the model

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

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

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

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

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

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

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

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

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

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

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

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

$$\frac{\mathrm{d}y_i}{\mathrm{d}x} = af(x,y_i) + bg(x,y_i),$$
$$y_i(0) = \alpha_i.$$

Taking derivative with respect to a, we have

$$\frac{\mathrm{d}A_i}{\mathrm{d}x} = f(x,y_i) + af_y(x,y_i)A_i + bg_y(x,y_i)A_i,$$
$$A_i(0) = 0.$$

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

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

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

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

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

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

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

Let a_k and b_k be known.

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

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

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

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

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

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

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

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

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

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

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

$$\frac{\mathrm{d}y}{\mathrm{d}x} = ay.$$

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

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

$$\frac{\mathrm{d}y_i}{\mathrm{d}x} = a_k y_i,$$
$$y_i(0) = \alpha_i.$$

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

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

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

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

$$\frac{\mathrm{d}A_i}{\mathrm{d}x} = R(x) + Q(x)A_i.$$

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

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

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

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

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

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

Consider some data

α_i	1	2	3
β_i	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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