MATH3800-Mathematical Modeling and Computational Methods

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Contents

Introduction

Numerical methods: are mathematical methods that are used to approximate the solution of complicated problems. Numerical methods are very useful because they are suitable for the use with computers.

Finding roots: Solve $f(x) = 0$ for x, when an explicit analytical solution is impossible.

- Bisection Method.
- Fixed-point Iteration.
- Newton's Method.

Bisection Method: To solve $f(x) = 0$ for x, we want to construct a sequence x_0, x_1, x_2,..., which converges to the root.

1. Chose two initial values a and b such that $f(a)f(b) < 0$.
2. $x_0 = \dfrac{a+b}{2}$.
3. $x_1 = \frac{a+x_0}{2}$ if $f(a)f(x_0) < 0$, or $x_1 = \frac{x_0+b}{2}$ if $f(b)f(x_0) < 0$.
4. And so on.

Example 1 *Approximate the root of the equation $f(x) = x^3 - x + 1 = 0$ by bisection method.*

Solution: $f(-2) = -5$ and $f(0) = 1$.
$f(-2) = -5$ and $f(-1) = 1$.
$f(-1.5) = -0.875$ and $f(-1) = 1$.
$f(-1.25) = ...$

Fixed point method: If

$$g(a) = a,$$

then a is called a fixed point of the function $g(x)$. An fixed point a is called stable if the solutions that start near a stay near or approach a; if the solutions that start near a moves away from it, then a is unstable.

Theorem 1 *(Stability Theorem). Let a be a fixed point of $g(x)$.*

1. *If $|g'(a)| < 1$, then a is stable;*
2. *If $|g'(a)| > 1$, then a is unstable.*

To find zeros of $f(x) = x^5 + 5x - 5$, i.e.,

$$x^5 + 5x - 5 = 0, \quad x = \frac{5 - x^3}{5}.$$

Let

$$g(x) = \frac{5 - x^3}{5},$$

then any fixed point of $g(x)$, i.e., $x = g(x)$, will be a zero of $f(x)$.

Note that $f(0.5) < 0$, $f(1) > 0$, we start from $x_0 = 0.75$ to approximate the fixed point of $g(x)$. Since

$$g'(x) = -\frac{3}{5}x^2, \quad |g'(x)| < 1 \quad for \quad x \in (0.5, 1),$$

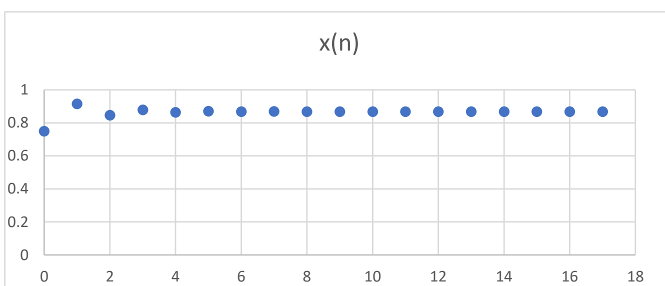
The recursive relation

$$x_{n+1} = g(x_n), \quad x_{n+1} = \frac{5 - x_n^3}{5}$$

will converge to the fixed point.

```
%% Matlab m-file for fixed point iteration to find the root of f(x)=x^3-5x-5 in (0,1)
%% Set initial guess
x(1)=0.75;
for n=1:17
          z(n+1)=(5-z(n)^3)/5;
          x(n)=z(n+1);
end
plot(x,"+r");
xlabel('Iteration n');
ylabel('x(n)');
```

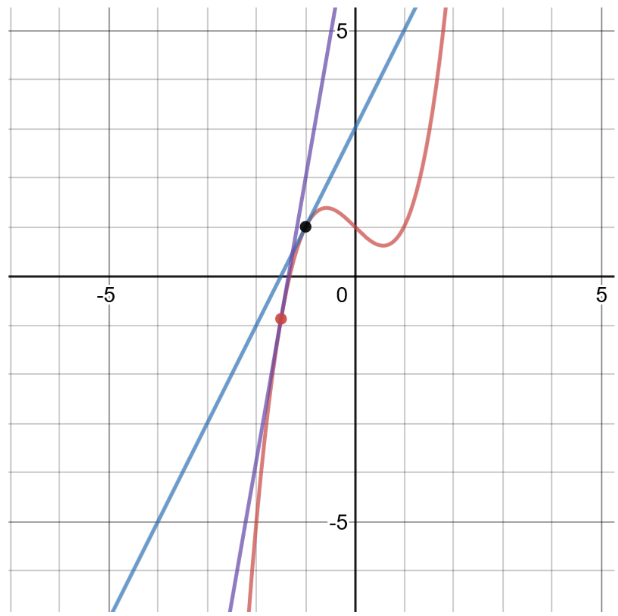
n	x(n)
0	0.75
1	0.915625
2	0.846473651
3	0.878697339
4	0.864309973
5	0.870866605
6	0.867905448
7	0.869248332
8	0.868640468
9	0.868915854
10	0.868791141
11	0.868847629
12	0.868822045
13	0.868833633
14	0.868828384
15	0.868830761
16	0.868829685
17	0.868830172



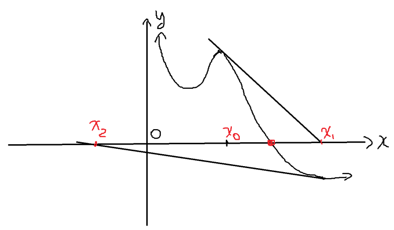
Newton's method: To approximate solutions of the equation $f(x) = 0$, start from x_0, we have approximate solutions

$$x_{n+1} = x_n - \frac{f(x_n)}{f'(x_n)}$$

provided we have started with a good value for x_0, this will produce approximate solutions to any degree of accuracy.



The following graph shows that with bad initial value, Newton's method fails: This is likely the case when $f'(x_0)$ is close to 0, we can see that x_2 is even outside the domain.



Example 2 *Find the roots $\sqrt[6]{2}$ by Newton's method, correct to 8 decimals.*

Solution: Let $f(x) = x^6 - 2$. Then $\sqrt[6]{2}$ is a solution of the equation $f(x) = 0$. Note that $f(2) = 62 > 0$ and $f(0) = -2 < 0$. This tells us that the root is between 0 and 2. So we chose $x_0 = 1$ for our initial guess.

$$x_{n+1} = x_n - \frac{x_n^6 - 2}{6x_n^5} = \frac{5x_n^6 + 2}{6x_n^5}.$$

With our initial guess of $x_0 = 1$, we can produce the following values:

x_0	1
x_1	1.16666667
x_2	1.12644368
x_3	1.12249707
x_4	1.12246205
x_5	1.12246205

Example 3 *Approximate the root of the polynomial $f(x) = x^3 - x + 1 = 0$ by Newton's method with $x_0 = -1$, correct to 6 decimals.*

Solution: Note that $f(-2) = -5$ and $f(0) = 1$. This tells us that the root is between -2 and 0. So we chose $x_0 = -1$ for our initial guess.

$$x_{n+1} = x_n - \frac{x_n^3 - x_n + 1}{3x_n^2 - 1} = \frac{2x_n^3 - 1}{3x_n^2 - 1}.$$

With our initial guess of $x_0 = -1$, we can produce the following values:

x_0	-1
x_1	-1.500000
x_2	-1.347826
x_3	-1.325200
x_4	-1.324718
x_5	-1.324717
x_6	-1.324717
x_7	-1.324717

Notice how the values for x_n become closer and closer to the same value. This means that we have found the approximate solution to six decimal places. In fact, this was obtained after only five relatively painless steps.

Mathematical Modelling

- Mathematical model: mathematical representations of the behavior of real devices or objects.
- By mathematical model, we can formulate and solve problems.
- How:

$$\begin{tikzcd}
\boxed{\textbf{Real world data}} \arrow[r, "Simplification"] & \boxed{\textbf{Model}} \arrow[d, "Analysis"'] \\
\boxed{\textbf{Predictions/explanations}} \arrow[u, "Verification"'] & \boxed{\textbf{Mathematical conclusions}} \arrow[l, "Interpretation"]
\end{tikzcd}$$

- Some check lists:
  - Identify the need for the model.
  - List the data we are seeking.
  - Identify the available relevant data.
  - Identify the circumstances.
  - How should we look at this model? Identify the governing principles.
  - Identify the equations that will be used, the calculations that will be made, and the answers that will result.
  - Validate the model: consistent with its principles and assumptions?
  - Verify the model: useful to initial problem?

1.1 Modeling Change with Difference Equation

Definition 1 *Two variables x and y are* **proportional** *if*

$$y = kx$$

for some nonzero constant k. We write $y \propto x$, y is proportional to x.

- Change = future value - present value.
- A sequence is a function, domain={all non-negative integers}, range={subset of real numbers}.
- A dynamical system (DTDS) is a relationship among terms in a sequence. A numerical solution is a table of values satisfying the dynamical system.
- Consider a sequence of numbers $A = \{a_0, a_1, a_2, ...\}$.

  $$\Delta a_0 = a_1 - a_0,\ \Delta a_1 = a_2 - a_1, ..., \Delta a_n = a_{n+1} - a_n, ...$$

  are called the first differences, and Δa_n is called the nth first difference.

Example 4 *You deposit \$ 100 into a bank account, that pays 1% interest annually. Model the balance after each year.*

Solution: Let a_n be the balance after n-th year. Then we have the following the sequence

$$A = \{100, 101, 102.01, 103.0301, ...\}.$$

The first differences are:

$$1, 1.01, 1.0201, ..., \Delta a_n = 0.01 a_n.$$

The general model is given by the following **difference equation**:

$$a_{n+1} = a_n + 0.01 a_n,\ i.e.,\ a_{n+1} = 1.01 a_n.$$

The solution of the difference equation is

$$a_n = 1.01^n a_0.$$

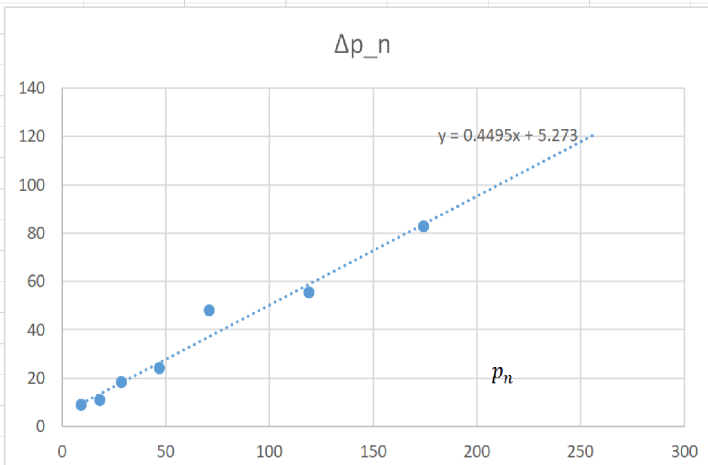
Remark. The balance a_n is proportional to 1.01^n, i.e., $a_n \propto 1.01^n$.

1.2 Approximating Change with Difference Equation

- Discrete-time Dynamical System (DTDS): The depositing of interest into a bank account.
- Continuous Dynamical System: Change of temperature of a cup of coffee.

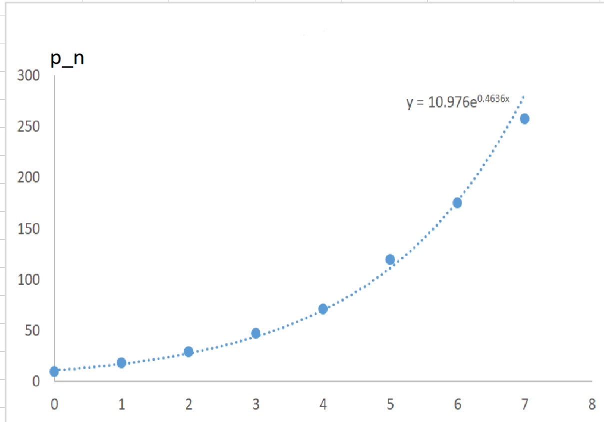
Example 5 (Yeast culture 1): *Here we have data for yeast culture. From dot plot, we can approximate the change in population as linear relation to population size. Find the model.*

p_n	Δp_n
9.6	8.7
18.3	10.7
29	18.2
47.2	23.9
71.1	48
119.1	55.5
174.6	82.7
257.3	



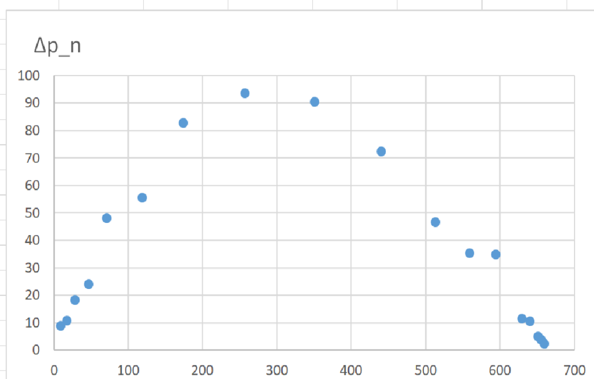
The solution p_n can be modeled by exponential function.

n	p_n	Δp_n
0	9.6	8.7
1	18.3	10.7
2	29	18.2
3	47.2	23.9
4	71.1	48
5	119.1	55.5
6	174.6	82.7
7	257.3	



Example 6 (Yeast culture 2): *With more data, the model may be changed.*

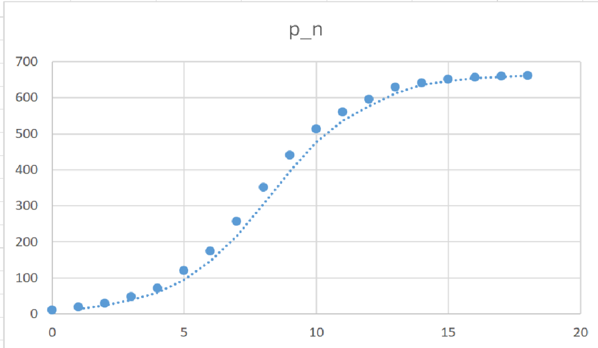
n	p_n	Δp_n
0	9.6	8.7
1	18.3	10.7
2	29	18.2
3	47.2	23.9
4	71.1	48
5	119.1	55.5
6	174.6	82.7
7	257.3	93.4
8	350.7	90.3
9	441	72.3
10	513.3	46.4
11	559.7	35.1
12	594.8	34.6
13	629.4	11.4
14	640.8	10.3
15	651.1	4.8
16	655.9	3.7
17	659.6	2.2
18	661.8	



The solution p_n:

$$\Delta p_n = -0.0008 p_n^2 + 0.5161 p_n + 6.4112,$$
$$p_{n+1} = p_n - 0.0008 p_n^2 + 0.5161 p_n + 6.4112,$$
$$p_{n+1} = -0.0008 p_n^2 + 1.5161 p_n + 6.4112.$$

n	p_n	Δp_n
0	9.6	8.7
1	18.3	10.7
2	29	18.2
3	47.2	23.9
4	71.1	48
5	119.1	55.5
6	174.6	82.7
7	257.3	93.4
8	350.7	90.3
9	441	72.3
10	513.3	46.4
11	559.7	35.1
12	594.8	34.6
13	629.4	11.4
14	640.8	10.3
15	651.1	4.8
16	655.9	3.7
17	659.6	2.2
18	661.8	



Numerical solutions from the model:

n	p_n	p_n from the mo
0	9.6	9.6
1	18.3	14.892032
2	29	22.81159162
3	47.2	34.57955909
4	71.1	51.88067281
5	119.1	76.91420467
6	174.6	112.2881898
7	257.3	160.5644145
8	350.7	223.2181639
9	441	298.9711793
10	513.3	382.1743921
11	559.7	462.9799831
12	594.8	530.8547806
13	629.4	579.7946944
14	640.8	610.508426
15	651.1	627.8265941
16	655.9	636.9261135
17	659.6	641.5149814
18	661.8	643.7788862

Another method is given by the text book, page 12.

1.3 Solutions to Dynamical Systems

The Method of Conjecture

1. Observe a pattern.
2. Conjecture the solution of the dynamical system.
3. Test the conjecture by substitution.
4. Conclusion.

Example 7 *Consider the dynamical system*

$$a_{n+1} = 1.03a_n,$$

which can model account balance with annual interest rate 3%*. Predict the solution.*

Solution: If the initial is \$100, then the dynamical system is:

$$100, 1.03(100), 1.03 * 1.03(100), ...$$

Conjecture: $a_n = 1.03^n a_0$.
Test: $a_{n+1} = 1.03^{n+1}a_0 = 1.03 * 1.03^n a_0 = 1.03a_n$, same as the dynamical system.
Conclusion: $a_n = 1.03^n a_0$.

Example 8 *Find the general solution of the basic exponential discrete-time dynamical system: $b_{n+1} = rb_n$.*

Solution:

$$b_n = r^n b_0.$$

Equilibrium (or fixed point):

Definition 2 *A point a is called an equilibrium (or fixed point) of the discrete-time dynamical system*

$$a_{n+1} = f(a_n)$$

if

$$f(a) = a,$$

where $f(x)$ is called the updating function of the DTDS.

Remark. At any equilibrium, $f(x)$ neither increases nor decreases, remains the same.

Graphic approach: The intersections of the updating function and the line $y = x$.

Stability of equilibrium: Consider the DTDS

$$a_{n+1} = f(a_n)$$

with an equilibrium a.

1. If $|f'(a)| < 1$, then a is stable;
2. If $|f'(a)| > 1$, then a is unstable;
3. If $|f'(a)| = 1$, then use Cobwebbing method to classify.

Example 9 $a_{n+1} = 4a_n^3$. *Find and classify all equilibria.*

Solution: Note that $f(x) = 4x^3$.
Step 1: Construct the equation $a = 4(a)^3$;
Step 2: Solve the equation, we obtain $0, 1/2, -1/2$.

Step 3: $f(x) = 4x^3$. $f'(x) = 12x^2$. Thus $f'(0) = 0$, $|f'(\pm\frac{1}{2})| = 3 > 1$.
By Stability Thm, it is stable at 0, unstable at $1/2, -1/2$.

Linear dynamical systems

Theorem 2 *Consider the dynamical system of the form*

$$a_{n+1} = ra_n + b,$$

where r and b are constants.

- *If $r = 1$: the solution is*

$$a_n = a_0 + nb.$$

- *If $r \neq 1$: the solution is*

$$a_n = r^n (a_0 - a) + a, \quad a = \frac{b}{1-r},$$

  where a is the equilibrium.

  - *If $|r| > 1$: a is unstable.*
  - *If $|r| < 1$: a is stable.*

Solution:
$a_1 = ra_0 + b,$
$a_2 = ra_1 + b = r(ra_0 + b) + b = r^2 a_0 + (r+1)b,$
$a_3 = r^3 a_0 + (r^2 + r + 1)b,$
$a_n = r^n a_0 + (r^{n-1} + \cdots + r^2 + r + 1)b = r^n a_0 + \dfrac{(1-r^n)b}{1-r} = r^n a_0 + (1-r^n)a = r^n(a_0 - a) + a.$
Note that $f(x) = rx + b$. Set

$$a = f(a), \quad a = ra + b, \quad a = \frac{b}{1-r}.$$

Since $f'(a) = r$,

- if $|r| > 1$: $|f'(a)| > 1$, a is unstable.
- If $|r| < 1$: $|f'(a)| < 1$, a is stable.

Example 10 *By c_t we denote the amount (in mg) of caffeine at time t (in hours). On average, our body eliminates 13% per hour. Assume that at the end of the same time interval we consume 94.8 extra mg of caffeine.*

- *Construct the model.*
- *Solve the model.*

- *What is the long-term behaviour?*

Solution:

1. The model will be:

$$c_{t+1} = 0.87c_t + 94.8.$$

2. The solution is

$$c_t = 0.87^t c_0 + \frac{(1-0.87^n)94.8}{0.13}.$$

3. The equilibrium is

$$a = \frac{b}{1-r} = \frac{94.8}{0.13} \doteq 729.$$

Since $|r| = 0.87 < 1$, a is stable, which is long-term behaviour.

1.4 Systems of Difference Equations

Example 11 *MATH3800 Tutoring Ottawa has two branches in Ottawa: Andrew Park, and Billings Bridge, with market portion a_0 and b_0 respectively. According to market statistics, due to variety of tutors, after each year, 40% of AP's customers will switch to BB's, while 30% of BB's customers will switch to AP's.*

(a) Construct the dynamical system model.

(b) Find the equilibrium values.

(c) Analyse the data. Predict the long term market share of the two branches.

Solution:

(a) Let a_n and b_n be the number of customers at the branch Andrew Park and the branch Billings Bridge respectively, at the end of year n. Then

$$\begin{aligned} a_{n+1} &= 0.6a_n + 0.3b_n \\ b_{n+1} &= 0.4a_n + 0.7b_n \end{aligned}$$

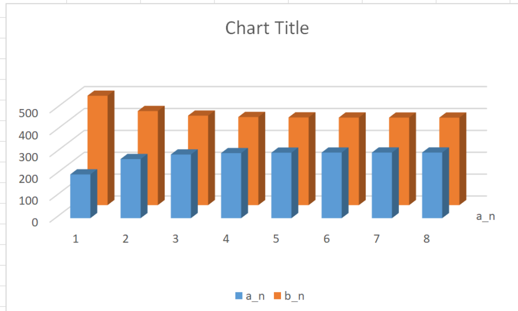
(b) Set up system:

$$\begin{aligned} a &= 0.6a + 0.3b \\ b &= 0.4a + 0.7b \end{aligned}$$

$a = b = 0$, and $a = 3000$, $b = 4000$.

(c) We will show that the equilibrium values $a = 3000$, $b = 4000$ are stable later. The system is insensitive to initial values. We predict that 3/7 customers will end up in Andre Park, 4/7 in BB.

a_n	b_n
200	500
270	430
291	409
297.3	402.7
299.19	400.81
299.757	400.243
299.9271	400.0729
299.9781	400.0219



Dynamics in a Discrete Competition System. Consider fish population oscillations in Ontario Rideau Lake. Let a_n be the population of pike fish at the end of year n, and Let b_n be the population of bass fish at the end of year n. The model is based on the following assumptions:

1. In the absence of other species, each individual species will grow unconstrained, and the population change is proportional to the population size.

2. The effect of the presence of the second species is to diminish the growth of the other species. The decrease is proportional to the product of both populations.

The Model:

$$\begin{aligned} a_{n+1} - a_n &= k_1 a_n - k_3 a_n b_n \\ b_{n+1} - b_n &= k_2 b_n - k_4 a_n b_n, \end{aligned}$$

or

$$\begin{aligned} a_{n+1} &= (1+k_1)a_n - k_3 a_n b_n \\ b_{n+1} &= (1+k_2)b_n - k_4 a_n b_n, \end{aligned}$$

where k_1, k_2 , k_3, k_4 are positive constants.

- $(1+k_1)$ is pike population growth rate if no bass fish.

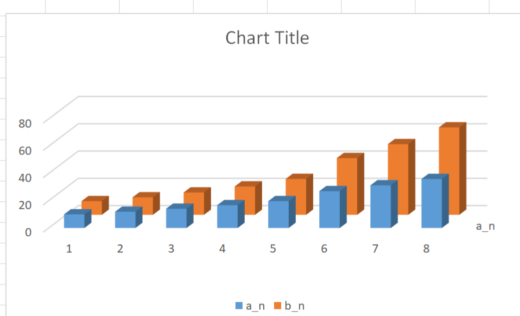
- $(1 + k_2)$ is bass population growth rate if no pike fish.
- k_3: the pike population decrease rate by the presence of bass fish.
- k_4: the bass population decrease rate by the presence of pike fish.

Example 12 *Consider the case where* $k_1 = 0.2$, $k_2 = 0.3$, $k_3 = 0.001$, $k_4 = 0.002$. *Find the equilibrium values and analyse sensitivity to initial values.*

Solution:

$(a, b) = (0, 0)$, or $(150, 200)$.

a_n	b_n
10	10
11.9	12.8
14.12768	16.33536
16.72244	20.77441
19.71952	26.31193
27.00583	41.58282
31.28402	51.81171
35.91994	64.11347
40.80098	78.7416



Dynamics of a discrete-time predator-prey system

predator

prey

$$\begin{cases} x_{n+1} = ax_n - bx_n y_n, \\ y_{n+1} = cy_n + dx_n y_n, \end{cases}$$

where x_n represents prey population densities at time n, and y_n represents predator population densities at time n, and a, b, c, d are positive parameters.

- Here $a > 1$ represents the natural growth rate of the prey in the absence of predators.
- b represents the consumption rate of the predators (where bx_n is the average number of prey eaten per predator in time n), i.e., the decrease rate of the prey by the presence of predator.
- $0 < c < 1$ is the survival rate of the predator (decrease rate) in the absence of its prey source.
- $d > 0$ is the growth rate of the predator population due to the consumption of prey.

The amount of prey consumed by the predator at each time step depends on not only on the numbers of predators present, but also the numbers of prey present. When the prey density is higher, it is easier for the predators to find prey and thus more prey will be consumed. Likewise, the growth rate the predators depends not only on the number of predators present (more predators should produce more offspring overall), but also on the number of prey present (a large food source often correlates with higher reproductive rates and/or larger litter or clutch sizes).

The system has two fixed point $(0, 0)$, and $(\frac{1-c}{d}, \frac{a-1}{b})$.

2.2 Modelling Using Proportionality

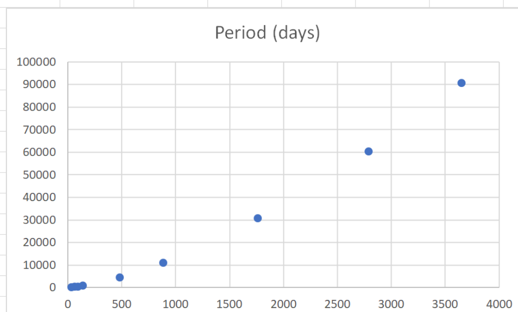
Kepler's third law - shows the relationship between the period (days) of a planet and mean distance to the sun (can be used for anything naturally orbiting around any other thing). Formula:

$$T^2 = kR^3,\ or,\ T = cR^{3/2},$$

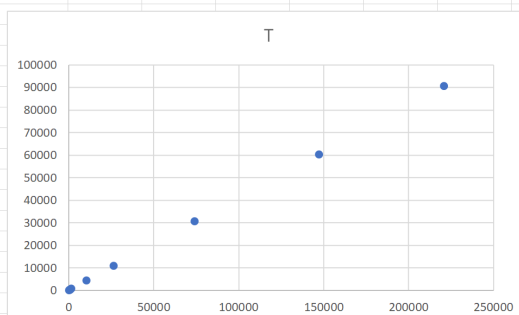
where:

T = period of the orbit, measured in days.
R = average distance of the object, measured in units of distance.
k, c = constants.

Planet	Mean distance (millions miles)	Period (days)
Mercury	36	88
Venus	67.25	224.7
Earth	93	365.3
Mars	141.75	687
Jupital	483.8	4331.8
Saturn	887.97	10760
Uranus	1764.5	30684
Neptune	2791.05	60188.3
Pluto	3653.9	90466.8



R^(3/2)	T
216	88
551.4910046	224.7
896.8595208	365.3
1687.658618	687
10641.40068	4331.8
26460.46306	10760
74119.50223	30684
147452.2572	60188.3
220869.1125	90466.8



Example 13 *$T \propto R^{3/2}$, i.e., $T = cR^{3/2}$. Estimate c value.*

Solution:

$$c \doteq \frac{90466.8 - 0}{220869.1115 - 0} = 0.41.$$

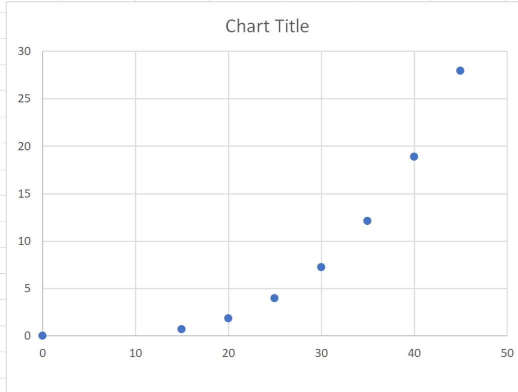
Example 14 *The following is the data for Ontario muskie fish:*

Length (in)	Weight (lp)
0	0
15	0.724258237
20	1.885014704
25	3.958590112
30	7.258020301
35	12.11759
40	18.89032709
45	27.94612614

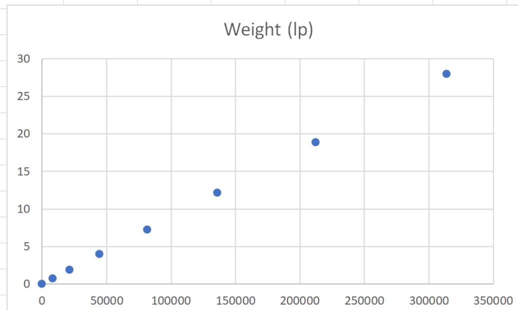
(a) Is weight $\propto$ *length?*

(b) Is weight $\propto$ *length*$^{3.325}$ *?*

Length (in)	Weight (lp)
0	0
15	0.724258237
20	1.885014704
25	3.958590112
30	7.258020301
35	12.11759
40	18.89032709
45	27.94612614



Length (in)	L^(3.325)	Weight (lp)
0	0	0
15	8137.732997	0.7242582
20	21179.94049	1.8850147
25	44478.54058	3.9585901
30	81550.7899	7.2580203
35	136152.6967	12.11759
40	212250.8661	18.890327
45	314001.4173	27.946126



(a) No.

(b) Yes. $W = 0.000089L^{3.325}$.

3.1 Fitting Models to Data Graphically

When we analyse data,

- Fitting a selected model type to the data.

- Chose the most appropriate model.

- Making predictions from data.

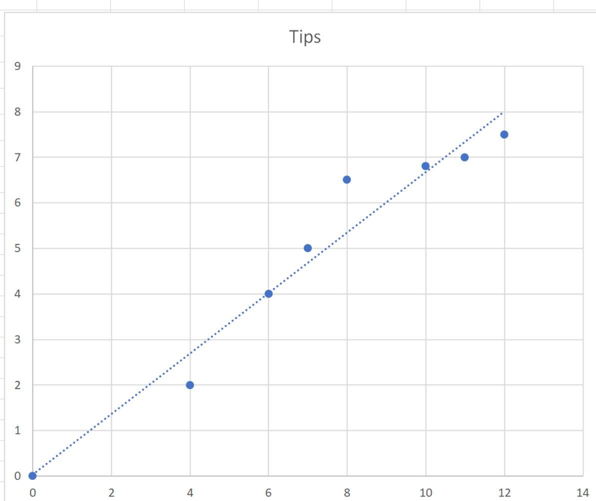
1. Visual model fitting with the original data

Example 15 *(The best-fitting line) A waiter at a restaurant received tips according to his working hours. The data are:*

Hours	0	4	6	7	8	10	11	12
Tips	0	2	4	5	6.5	6.8	7	7.5

Model the data with the best-fitting line such that **the sum of absolute deviations is minimum**.

Hours	Tips
0	0
4	2
6	4
7	5
8	6.5
10	6.8
11	7
12	7.5

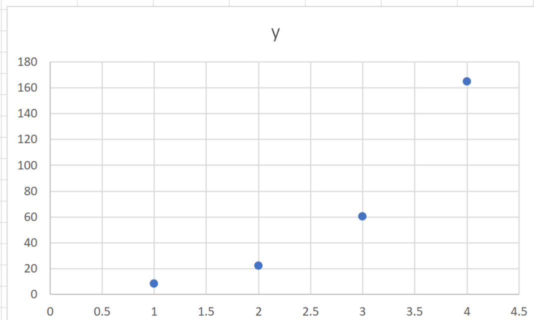


2. Transforming the data

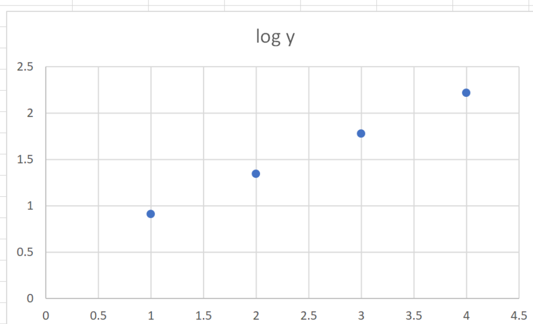
Sometimes we may not be easy to predict model visually. In this case, we can try to transform data. Such as

- Apply log function to data.
- Apply exponential function to data.
- Apply power function to data, e.g., muskie fish length to weight.

x	1	2	3	4
y	8.1	22.1	60.1	165



x	1	2	3	4
log y	0.908485	1.344392	1.778874	2.217484



3.2 Analytic Methods of Model Fitting

LEAST SQUARES CRITERION: Fitting the data set

$$\{(x_1, y_1), ..., (x_m, y_m)\}$$

by the function $y = f(x)$ such that

$$S = \sum_{i=1}^{m} [y_i - f(x_i)]^2$$

is minimum.

"Predictions from models are not always correct, the least squares criterion proves minimized predictions based on this assumption."

3.3 Applying the Least-Squares Criterion

Here we apply the LS Criterion to estimate the parameters for several types of curves.

1. Fitting a Straight Line

Theorem 3 *Fitting the data set*

$$\{(x_1, y_1), ..., (x_m, y_m)\}$$

by the function

$$y = f(x) = ax + b$$

such that

$$S = \sum_{i=1}^{m} [y_i - f(x_i)]^2$$

is minimum. Then

$$a = \frac{m \sum_{i=1}^{m} x_i y_i - (\sum_{i=1}^{m} x_i)(\sum_{i=1}^{m} y_i)}{m \sum_{i=1}^{m} x_i^2 - (\sum_{i=1}^{m} x_i)^2},$$

$$b = \frac{(\sum_{i=1}^{m} x_i^2)(\sum_{i=1} y_i) - (\sum_{i=1}^{m} x_i y_i)(\sum_{i=1}^{m} x_i)}{m \sum_{i=1}^{m} x_i^2 - (\sum_{i=1}^{m} x_i)^2},$$

where a is called the slope, b is the intercept.

Remark. If we define

$$\bar{x} = \frac{\sum_{i=1}^{m} x_i}{m}, \quad \bar{y} = \frac{\sum_{i=1}^{m} y_i}{m}, \quad \overline{x^2} = \frac{\sum_{i=1}^{m} x_i^2}{m}, \quad \overline{xy} = \frac{\sum_{i=1}^{m} x_i y_i}{m},$$

then

$$a = \frac{\overline{xy} - \bar{x}\bar{y}}{\overline{x^2} - \bar{x}^2},$$

$$b = \frac{\overline{x^2}\bar{y} - \overline{xy}\bar{x}}{\overline{x^2} - \bar{x}^2}, \quad or \quad b = \bar{y} - a\bar{x}.$$

Solution:

$$S = \sum_{i=1}^{m} [y_i - ax_i - b]^2.$$

To have optimality,

$$\frac{\partial S}{\partial a} = 0, \quad \frac{\partial S}{\partial b} = 0.$$

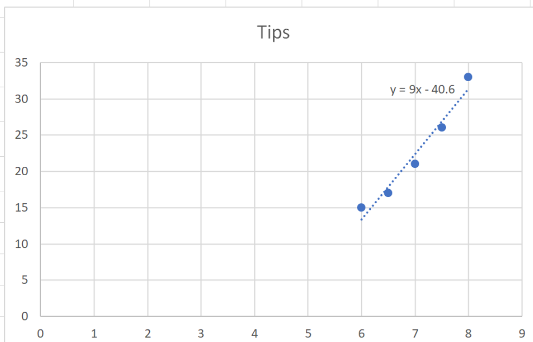
We derive the system

$$\begin{aligned} \sum_{i=1}^{m} y_i &= a \sum_{i=1}^{m} x_i + mb \\ \sum_{i=1}^{m} x_i y_i &= a \sum_{i=1}^{m} x_i^2 + b \sum_{i=1}^{m} x_i. \end{aligned}$$

By solving the system we get a and b.

Example 16

Hours	Tips
6	15
6.5	17
7	21
7.5	26
8	33



Solution: Here is the calculation according to the formula:

	Hours	Tips	xy	x^2		a-num	a-den	a	b-num	b
	6	15	90	36		112.5	12.5	9	-507.5	-40.6
	6.5	17	111	42.3						
	7	21	147	49						
	7.5	26	195	56.3						
	8	33	264	64						
Sum	35	112	807	248						

2. Fitting a Power Curve

Theorem 4 *Fitting the data set*

$$\{(x_1, y_1), ..., (x_m, y_m)\}$$

by the power function

$$y = f(x) = ax^n$$

such that

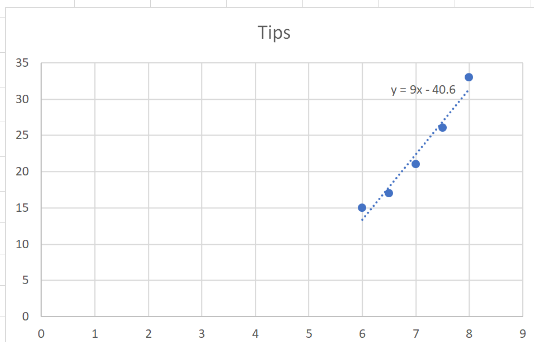
$$S = \sum_{i=1}^{m} [y_i - f(x_i)]^2$$

is minimum, where a is the parameter to be determined, n is a constant. Then

$$a = \frac{\sum_{i=1}^{m} x_i^n y_i}{\sum_{i=1}^{m} x_i^{2n}}.$$

Example 17 *Consider the data:*

Hours	Tips
6	15
6.5	17
7	21
7.5	26
8	33



We are going to fit the set with power function $y = ax^2$. Find a.

Solution: Here is the calculation according to the formula: $y = 0.46003x^2$.

	Hours	Tips	xy	x^2	x^2y	x^4	a
	6	15	90	36	540	1296	0.46003
	6.5	17	110.5	42.25	718.25	1785.1	
	7	21	147	49	1029	2401	
	7.5	26	195	56.25	1462.5	3164.1	
	8	33	264	64	2112	4096	
Sum	35	112	806.5	247.5	5861.8	12742	

3. Transformed Least-Squares Fit

Theorem 5 *Fitting the data set*

$$\{(x_1, y_1), ..., (x_m, y_m)\}$$

by the general power function

$$y = f(x) = ax^n$$

such that

$$S = \sum_{i=1}^{m} [y_i - f(x_i)]^2$$

is minimum, where both a and n are parameters. Then

$$n = \frac{m \sum_{i=1}^{m} \ln x_i \ln y_i - (\sum_{i=1}^{m} \ln x_i)(\sum_{i=1}^{m} \ln y_i)}{m \sum_{i=1}^{m} \ln x_i^2 - (\sum_{i=1}^{m} \ln x_i)^2},$$

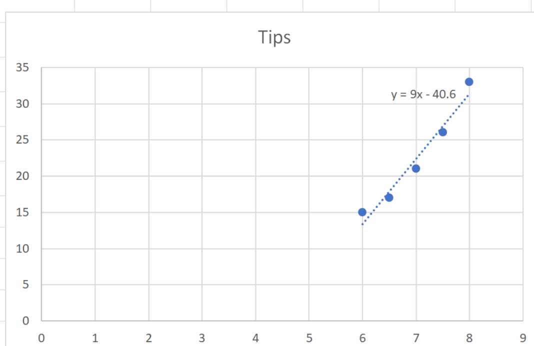
$$\ln a = \frac{(\sum_{i=1}^{m} \ln x_i^2)(\sum_{i=1} \ln y_i) - (\sum_{i=1}^{m} \ln x_i \ln y_i)(\sum_{i=1}^{m} \ln x_i)}{m \sum_{i=1}^{m} \ln x_i^2 - (\sum_{i=1}^{m} \ln x_i)^2}.$$

Proof.

$$\ln y = n \ln x + \ln a.$$

Example 18 *Consider the data:*

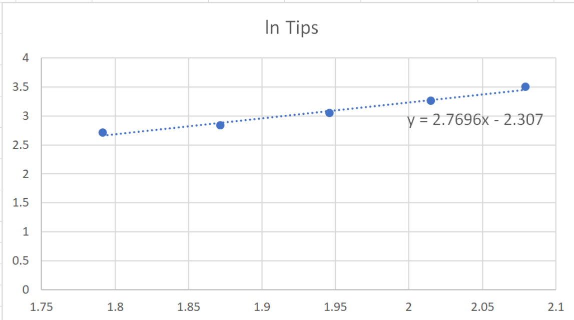
Hours	Tips
6	15
6.5	17
7	21
7.5	26
8	33



We are going to fit the set with power function $y = ax^n$. Find a and n.

Solution: Here is the calculation according to the formula: $y = 0.09956x^{2.7696}$.

Hours	Tips	ln Hours	ln Tips		y=ax^n
6	15	1.791761	2.708		n=2.7696
6.5	17	1.871803	2.833		ln a=-2.307
7	21	1.945911	3.045		a=0.09956
7.5	26	2.014904	3.258		
8	33	2.079443	3.497		



6.3 Linear Regression

Least Squares criteria is only for a single observation. For multiple observations, we use linear regression. Our objectives are

- Illustrate basic linear regression model
- Define and interpret R^2
- Examine and interpret the residual plots

The Linear Regression Model: Given paired data $(x_1, y_1), \cdots, (x_m, y_m)$, the basic linear regression model is

$$y_i = ax_i + b, \quad i = 1, ..., m.$$

Solve the system

$$\begin{aligned} \sum_{i=1}^m y_i &= a\sum_{i=1}^m x_i + mb \\ \sum_{i=1}^m x_i y_i &= a\sum_{i=1}^m x_i^2 + b\sum_{i=1}^m x_i. \end{aligned}$$

We have

$$a = \frac{m\sum_{i=1}^m x_i y_i - (\sum_{i=1}^m x_i)(\sum_{i=1}^m y_i)}{m\sum_{i=1}^m x_i^2 - (\sum_{i=1}^m x_i)^2}, \quad b = \frac{(\sum_{i=1}^m x_i^2)(\sum_{i=1}^m y_i) - (\sum_{i=1}^m x_i y_i)(\sum_{i=1}^m x_i)}{m\sum_{i=1}^m x_i^2 - (\sum_{i=1}^m x_i)^2}.$$

For convenience, we define

$$\bar{x} = \sum_{i=1}^m x_i/m, \quad \bar{y} = \sum_{i=1}^m y_i/m, \quad \overline{x^2} = \sum_{i=1}^m x_i^2/m, \quad \overline{xy} = \sum_{i=1}^m x_i y_i/m.$$

Then

$$a = \frac{\overline{xy} - \bar{x}\bar{y}}{\overline{x^2} - (\bar{x})^2}, \quad b = \overline{y} - a\overline{x}.$$

The **error sum of squares (SSE)**, which reflects variation about the regression line, is given by

$$SSE = \sum_{i=1}^m [y_i - (ax_i + b)]^2.$$

The **total sum of squares (SST)** measures the total amount of variation in observed y values, and is defined as

$$SST = \sum_{i=1}^{m} (y_i - \bar{y})^2.$$

Regression sum of squares (SSR) given by

$$SSR = SST - SSE.$$

SSR reflects the amount of variation in the y values explained by the linear regression line $y = ax + b$ when compared with the variation in the y values about the line $y = \bar{y}$.
Coefficient of determination measures the proportion of the total variations in y that can be explained by the linear model and it is defined as

$$R^2 = 1 - \frac{SSE}{SST}$$

1. R is called the *sample correlation coefficient.*
2. $R^2 \leq 1$.
3. The value of R^2 does not depend on which of the two variables is labeled x and which is labeled y.
4. The value of R^2 is independent of the unit of x and y.

Residuals: The residuals are the errors between the actual and predicted values

$$r_i = y_i - (ax_i + b).$$

1. One way to evaluate the reasonableness of the fit of the model is to look at the plot of residuals versus the independent variable.
2. The residuals should be randomly distributed and contained in a reasonable small band that corresponds with the accuracy of the data.
3. An extremely large residual should indicate that we need to take a further look at the associated data point to discover the cause of the large residual.
4. A pattern or trend in the residuals indicates that some effect or aspect on the data has not been captured in the model. The nature of the pattern can provide hints as to how to refine our model.

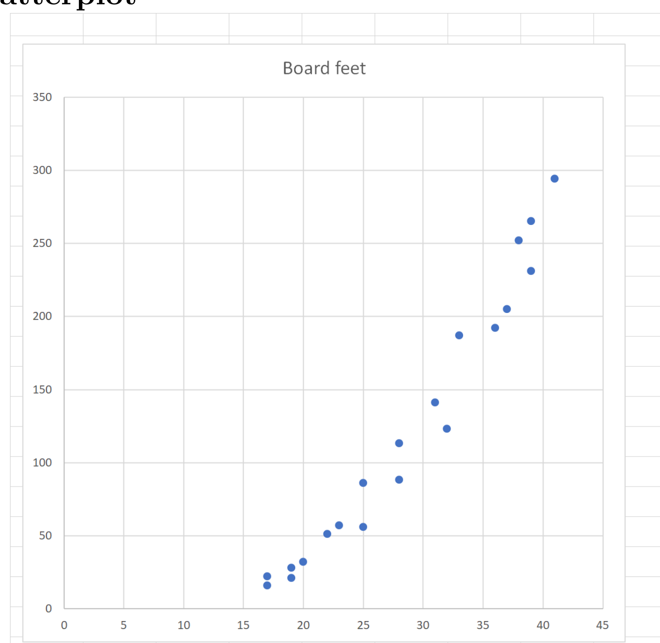
Example 19 *Ponderosa pines: Diameter versus volume.*

Data

Diameter	Volume
36	192
28	113
28	88
41	294
19	28
32	123
22	51
38	252
25	56
17	16
31	141
20	32
25	86
19	21
39	231
33	187
17	22
37	205
23	57
39	265

Problem Identification: Predict the volume as a function of the diameter.

Scatterplot



The plot is concave up and increasing, which suggests a power function model or exponential model.

Model Formulation: If we may assume that the height is proportional to the diameter. Then

$$V \propto a(d^3) + b.$$

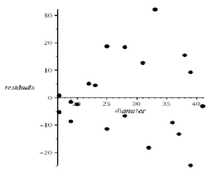
If we assume that the pines have constant height. Then

$$V \propto a(d^2) + b.$$

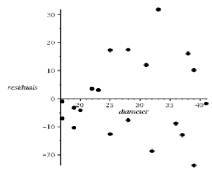
Model Solutions:

Model	SSE	SSR	SST	R^2
$V = 0.00431d^2$	3742	458 536	462 278	0.9919
$V = 0.00426d^3 + 2.08$	3712	155986	159 698	0.977
$V = 0.152d^2$	12 895	449 383	462 278	0.9721
$V = 0.194d^2 - 45.7$	3910	155 788	159 698	0.976

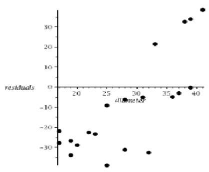
Residuals Plot:



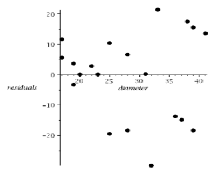
$V = 0.00431d^3$



$V = 0.00426d^3 + 2.08$



$V = 0.152d^2$



$V = 0.194d^2 - 45.7$

Remark:

- R^2 values are close to 1, which indicates a strong linear relationship.
- For the model $V = 0.152d^2$, SSE is much bigger than other models, residuals plot shows an apparent trend, we would probably reject the model.

4.1 One-Term Models

When we construct empirical model, we always begin with DATA analysis:

1. Any existence of a trend? If yes, find a function that transform data into **a straight line**. Most often transformations are:

$$y = a(x^b), \quad y = a(b^x).$$

2. Are there data points lie obviously outside the trend? If yes, we may need to discard them.

Sometimes it is hard to construct a good model. We may think about the following transformations:

Ladder of powers
$\vdots$
z^2
z
$\sqrt{z}$
$\log z$
$\frac{1}{\sqrt{z}}$
$\frac{1}{z}$
$\frac{1}{z^2}$

How to use the ladder?

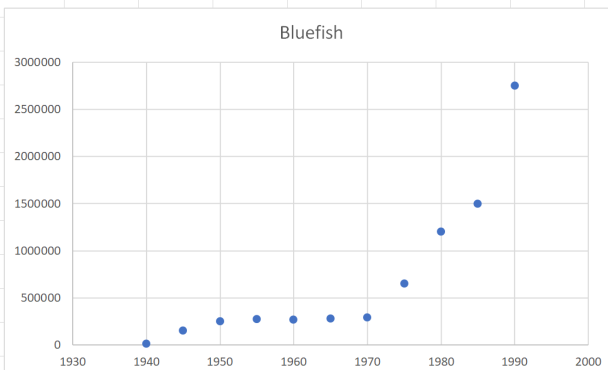
- If the data concave up, then go down the ladder (below z).
- If the data concave down, then go up the ladder (above z).

Example 20 *Consider the following data set, Harvesting of bluefish and blue crabs versus time:*

Year	Bluefish (lb)	Blue crabs (lb)
1940	15,000	100,000
1945	150,000	850,000
1950	250,000	1,330,000
1955	275,000	2,500,000
1960	270,000	3,000,000
1965	280,000	3,700,000
1970	290,000	4,400,000
1975	650,000	4,660,000
1980	1,200,000	4,800,000
1985	1,500,000	4,420,000
1990	2,750,000	5,000,000

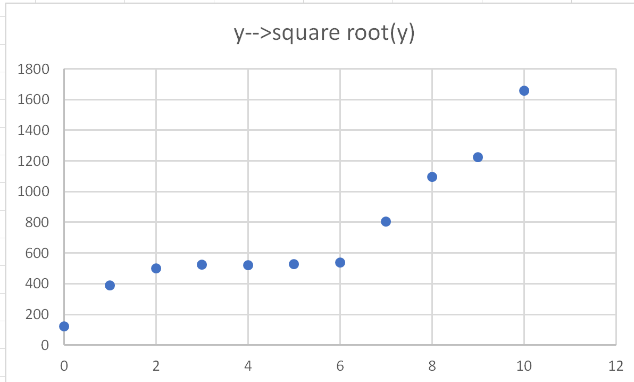
By plotting Bluefish data,

Year	Bluefish
1940	15000
1945	150000
1950	250000
1955	275000
1960	270000
1965	280000
1970	290000
1975	650000
1980	1200000
1985	1500000
1990	2750000



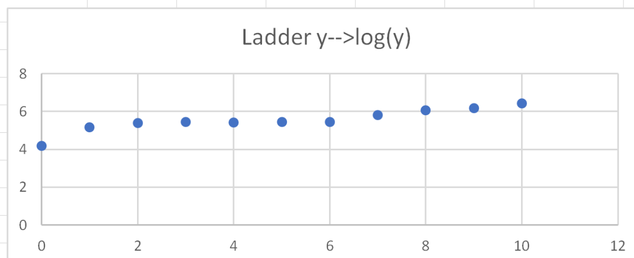
Now we try Ladder of powers: $y \to \sqrt{y}$

x (Ye	y(Bluefish	y-->square root(y)
0	15000	122.4744871
1	150000	387.2983346
2	250000	500
3	275000	524.4044241
4	270000	519.6152423
5	280000	529.1502622
6	290000	538.5164807
7	650000	806.2257748
8	1200000	1095.445115
9	1500000	1224.744871
10	2750000	1658.312395



Next we try Ladder of powers: $y \to \log(y)$

x (Year)	y(Bluefish)	Ladder y-->log(y)
0	15000	4.176091259
1	150000	5.176091259
2	250000	5.397940009
3	275000	5.439332694
4	270000	5.431363764
5	280000	5.447158031
6	290000	5.462397998
7	650000	5.812913357
8	1200000	6.079181246
9	1500000	6.176091259
10	2750000	6.439332694



The line of best fit is:

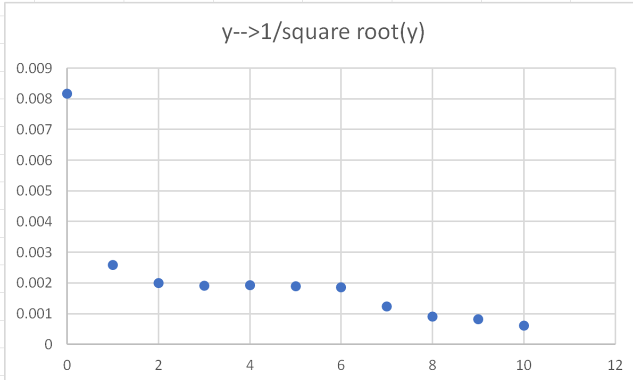
$$\log y = (0.1654)x + 0.7231.$$

Thus

$$y = 10^{0.7231} 10^{0.1654x} = 5.2857(1.4635)^x.$$

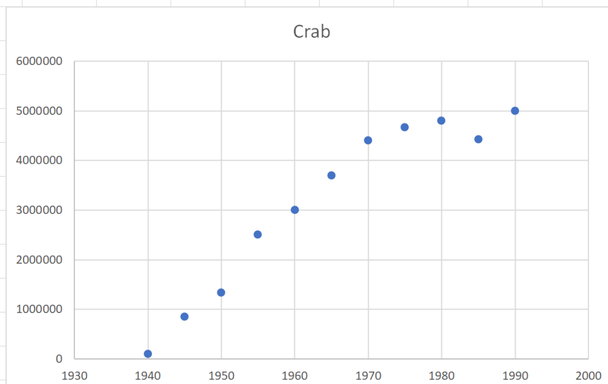
Next we try Ladder of powers: $y \to \frac{1}{\sqrt{y}}$

x (Ye	y(Bluefish	y-->1/square root(y)
0	15000	0.008164966
1	150000	0.002581989
2	250000	0.002
3	275000	0.001906925
4	270000	0.001924501
5	280000	0.001889822
6	290000	0.001856953
7	650000	0.001240347
8	1200000	0.000912871
9	1500000	0.000816497
10	2750000	0.000603023

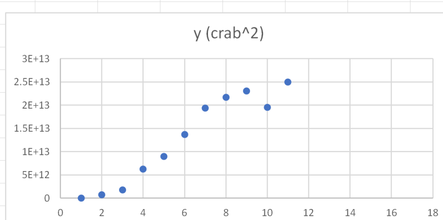


Similarly, by plotting crab data,

Year	Crab
1940	100000
1945	850000
1950	1330000
1955	2500000
1960	3000000
1965	3700000
1970	4400000
1975	4660000
1980	4800000
1985	4420000
1990	5000000



Year	Crab	x	y (crab^2)
1940	100000	0	10000000000
1945	850000	1	7.225E+11
1950	1330000	2	1.7689E+12
1955	2500000	3	6.25E+12
1960	3000000	4	9E+12
1965	3700000	5	1.369E+13
1970	4400000	6	1.936E+13
1975	4660000	7	2.17156E+13
1980	4800000	8	2.304E+13
1985	4420000	9	1.95364E+13
1990	5000000	10	2.5E+13



We imply that

$$y = 158.34\sqrt{x}.$$

4.3 Smoothing: Low-Order Polynomial Models

Interpolation

We try to a polynomial

$$p_n(x) = a_0 + a_1 x + ...a_n x^n$$

fitting data $(x_1, y_1), ..., (x_n, y_n), (x_{n+1}, y_{n+1})$, i.e.,

$$p_n(x_j) = y_j, \quad j = 1, ..., n+1.$$

The method is called **Lagrange polynomial interpolation**:

$$p_n(x) = \sum_{j=1}^{n+1} L_j(x) y_j,$$

where

$$L_j(x) = \Pi_{i=1, i \neq j}^{n+1} (x - x_i) / \Pi_{i=1, i \neq j}^{n+1} (x_j - x_i).$$

Example 21 *Given three points* $(1.3, 3.2)$, $(1.7, 4.4)$, $(2.1, 5.2)$. *Then*

$$L_1(x) = \frac{(x - x_2)(x - x_3)}{(x_1 - x_2)(x_1 - x_3)} = \frac{(x - 1.7)(x - 2.1)}{(1.3 - 1.7)(1.3 - 2.1)} = 3.125x^2 - 11.875x + 11.15625,$$

$$L_2(x) = \frac{(x - x_1)(x - x_3)}{(x_2 - x_1)(x_2 - x_3)} = \frac{(x - 1.3)(x - 2.1)}{(1.7 - 1.3)(1.7 - 2.1)} = -6.25x^2 + 21.25x - 17.0025,$$

$$L_3(x) = \frac{(x - x_1)(x - x_2)}{(x_3 - x_1)(x_3 - x_2)} = \frac{(x - 1.3)(x - 1.7)}{(2.1 - 1.3)(2.1 - 1.7)} = 3.125x^2 - 9.375x + 6.90625.$$

Then

$$\begin{aligned} P_2(x) &= L_1(x)(3.2) + L_2(x)(4.4) + L_3(x)(5.2) \\ &= -1.25x^2 + 6.75x - 3.4625. \end{aligned}$$

Example 22 *Given four points* $(0,1)$, $(1,-1)$, $(2,-3)$, $(3,1)$. *Then*

$$L_1(x) = \frac{(x-x_2)(x-x_3)(x-x_4)}{(x_1-x_2)(x_1-x_3)(x_1-x_4)} = \frac{(x-1)(x-2)(x-3)}{(0-1)(0-2)(0-3)} = -\frac{1}{6}x^3 + x^2 - 2x + 1,$$

$$L_2(x) = \frac{(x-0)(x-2)(x-3)}{(1-0)(1-2)(1-3)} = \frac{1}{2}x^3 - \frac{5}{2}x^2 + 3x,$$

$$L_3(x) = \frac{(x-0)(x-1)(x-3)}{(2-0)(2-1)(2-3)} = -\frac{1}{2}x^3 + 2x^2 - \frac{3}{2}x,$$

$$L_4(x) = \frac{(x-0)(x-1)(x-2)}{(3-0)(3-1)(3-2)} = \frac{1}{6}x^3 - \frac{1}{3}x^2 + \frac{1}{3}x.$$

Then

$$\begin{aligned} P_3(x) &= L_1(x)(1) + L_2(x)(-1) + L_3(x)(-3) + L_4(x)(1) \\ &= x^3 - 3x^2 + 1. \end{aligned}$$

Divided Differences

Consider the model

$$P(x) = a + bx + cx^2 + \cdots .$$

We have

$P'(x) = b + 2cx + ...$

$P''(x) = 2c + ...$

Recall the definition of the derivative

$$f'(x) = \lim_{h \to 0} \frac{f(x+h) - f(x)}{x+h-x} = \lim_{h \to 0} \frac{\Delta y}{\Delta x}.$$

Thus

$$P' \approx \frac{\Delta P}{\Delta x}, \quad P'' \approx \frac{\Delta P'}{\Delta x}, ...$$

Definition 3 *Given the data set* $\{(x_1, y_1), ..., (x_m, y_m)\}$.

The first differences are

$\Delta = y_{i+1} - y_i, \quad i = 1..., m-1.$

The second differences are

$\Delta^2 = (y_{i+2} - y_{i+1}) - (y_{i+1} - y_i), \quad i = 1..., m-2.$

The kth differences Δ^k are computed by finding the difference between successive $k-1$th differences.

The first divided differences (1DD) are

$$f[x_i, x_{i+1}] = \frac{y_{i+1} - y_i}{x_{i+1} - x_i}, \quad i = 1..., m-1.$$

The second divided differences (2DD) are

$$f[x_i, x_{i+1}, x_{i+2}] = \frac{f[x_{i+1}, x_{i+2}] - f[x_i, x_{i+1}]}{x_{i+2} - x_i}, \quad i = 1..., m-2.$$

The kth divided differences (kDD) are

$$f[x_i, x_{i+1}, ..., x_{i+k}] = \frac{f[x_{i+1}, ..., x_{i+k}] - f[x_i, x_{i+1}, ..., x_{i+k-1}]}{x_{i+k} - x_i}, \quad i = 1..., m-k.$$

Theorem 6 *Given the data set $\{(x_1, y_1), ..., (x_m, y_m)\}$.*

The kth degree polynomial model is given by

$$P(x) = f(x_0) + f[x_0, x_1](x - x_0) + f[x_0, x_1, x_2](x - x_0)(x - x_1)$$

$$+ ... + f[x_0, x_1, ..., x_k](x - x_0)(x - x_1)...(x - x_{k-1}).$$

Example 23 *Consider the following data:*

x_i	y_i	1DD	2DD	3DD	4DD	
0	1					
		2				
1	3		7			
		23		3		
3	49		19			
		80		3		
4	129		37			
		228				
7	813					

$$P(x) = 1 + 2x + 7x(x-1) + 3x(x-1)(x-3) = 3x^3 - 5x^2 + 4x + 1.$$

Error Estimates

If we use a polynomial $p_n(x)$ to approximate $f(x)$ such that

$$p_n(x_j) = f(x_j), j = 1, ..., n+1,$$

then the error

$$e_n(x) = |f(x) - p_n(x)| = |(x-x_1)...(x-x_{n+1})\ \frac{f^{(n+1)}(c)}{(n+1)!}|,$$

where c is some (unknown) point in the interval $[a,b]$ containing all x_j.

Low-order polynomial is a technique to model data points. For example, if we decided to use quadratic, it is not possible to force a quadratic to pass through all data points. Thus it must be decided which quadratic best ts the data. This process is called **smoothing**. This smoothing process requires two decisions:

1. The order of the polynomial.
2. The coefficients of the polynomial.

Theorem 7 *If*

$$P_2(x) = a + bx + cx^2$$

is the model of best-fit to the data set

$$\{(x_1, y_1), \cdots,\ (x_m, y_m)\},$$

$$\begin{aligned}
ma + \left(\sum_{i=1}^{m} x_i\right) b + \left(\sum_{i=1}^{m} x_i^2\right) c &= \sum_{i=1}^{m} y_i \\
\left(\sum_{i=1}^{m} x_i\right) a + \left(\sum_{i=1}^{m} x_i^2\right) b + \left(\sum_{i=1}^{m} x_i^3\right) c &= \sum_{i=1}^{m} x_i y_i \\
\left(\sum_{i=1}^{m} x_i^2\right) a + \left(\sum_{i=1}^{m} x_i^3\right) b + \left(\sum_{i=1}^{m} x_i^4\right) c &= \sum_{i=1}^{m} x_i^2 y_i
\end{aligned}$$

Equivalently,

$$\begin{aligned}
a + \overline{x}b + \overline{x^2}c &= \overline{y} \\
\overline{x}a + \overline{x^2}b + \overline{x^3}c &= \overline{xy} \\
\overline{x^2}a + \overline{x^3}b + \overline{x^4}c &= \overline{x^2y}
\end{aligned}$$

By Cramer's Rule, we have

$$a = \frac{\begin{vmatrix} \overline{y} & \overline{x} & \overline{x^2} \\ \overline{xy} & \overline{x^2} & \overline{x^3} \\ \overline{x^2y} & \overline{x^3} & \overline{x^4} \end{vmatrix}}{\begin{vmatrix} 1 & \overline{x} & \overline{x^2} \\ \overline{x} & \overline{x^2} & \overline{x^3} \\ \overline{x^2} & \overline{x^3} & \overline{x^4} \end{vmatrix}}, \quad b = \frac{\begin{vmatrix} 1 & \overline{y} & \overline{x^2} \\ \overline{x} & \overline{xy} & \overline{x^3} \\ \overline{x^2} & \overline{x^2y} & \overline{x^4} \end{vmatrix}}{\begin{vmatrix} 1 & \overline{x} & \overline{x^2} \\ \overline{x} & \overline{x^2} & \overline{x^3} \\ \overline{x^2} & \overline{x^3} & \overline{x^4} \end{vmatrix}}, \quad c = \frac{\begin{vmatrix} 1 & \overline{x} & \overline{y} \\ \overline{x} & \overline{x^2} & \overline{xy} \\ \overline{x^2} & \overline{x^3} & \overline{x^2y} \end{vmatrix}}{\begin{vmatrix} 1 & \overline{x} & \overline{x^2} \\ \overline{x} & \overline{x^2} & \overline{x^3} \\ \overline{x^2} & \overline{x^3} & \overline{x^4} \end{vmatrix}}$$

Proof. To minimize

$$S = \sum_{i=1}^{m} \left[y_i - (a + bx_i + cx_i^2)\right]^2,$$

$$\frac{\partial S}{\partial a} = \frac{\partial S}{\partial b} = \frac{\partial S}{\partial c} = 0.$$

Example 24 *Consider the data collected for the tape recorder problem*

c_i	100	200	300	400	500	600	700	800
t_i	205	430	677	945	1233	1542	1872	2224

where c_i are the counter reading, $P_2(c)$ are the elapsed time. Then

$$P_2(c) = 0.14286 + 1.94226c + 0.00105c^2.$$

Solution:

$$\begin{aligned}
8a + 3600b + 2040000c &= 9128 \\
3600a + 2040000b + 1296000000c &= 5318900 \\
2040000a + 1296000000b + 8.772 \times 10^{11}c &= 3435390000
\end{aligned}$$

Solving this we get the solution.

Testing of the model: The deviations

c_i	100	200	300	400	500	600	700	800
t_i	205	430	677	945	1233	1542	1872	2224
$t_i - P_2(c_i)$	0.167	-0.45	0	0.524	0.119	-0.21	-0.48	0.333

A divided difference table for the tape recorder data

c	t	1DD	2DD	3DD
100	205			
		2.25		
200	430		0.0011	
		2.47		-2E-07
300	677		0.00105	
		2.68		-2E-07
400	945		0.001	
		2.88		2E-07
500	1233		0.00105	
		3.09		0
600	1542		0.00105	
		3.3		2E-07
700	1872		0.0011	
		3.52		
800	2224			

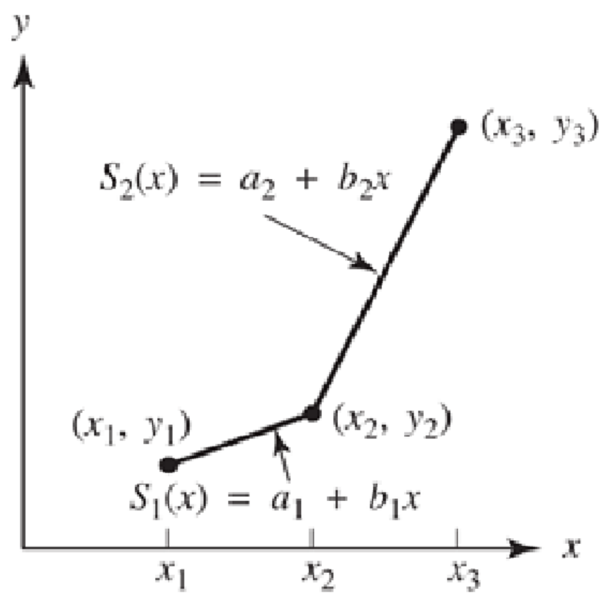
Example 25 *Consider the following data, which degree of polynomial will be good model?*

x	1		2		3		4		5		6		7
y	-5		-24		-27		64		375		1080		2401
1DD		-19		-3		91		311		705		1321	
2DD			8		47		110		197		308		
3DD				13		21		29		37			
4DD					2		2		2				
5DD						0		0					

4.4 Cubic Spline Models

Consider the data set $\{(x_1, y_1),\ (x_2, y_2),\ (x_3, y_3)\}$.
Linear Splines: Using piecewise linear functions model the data as follows:

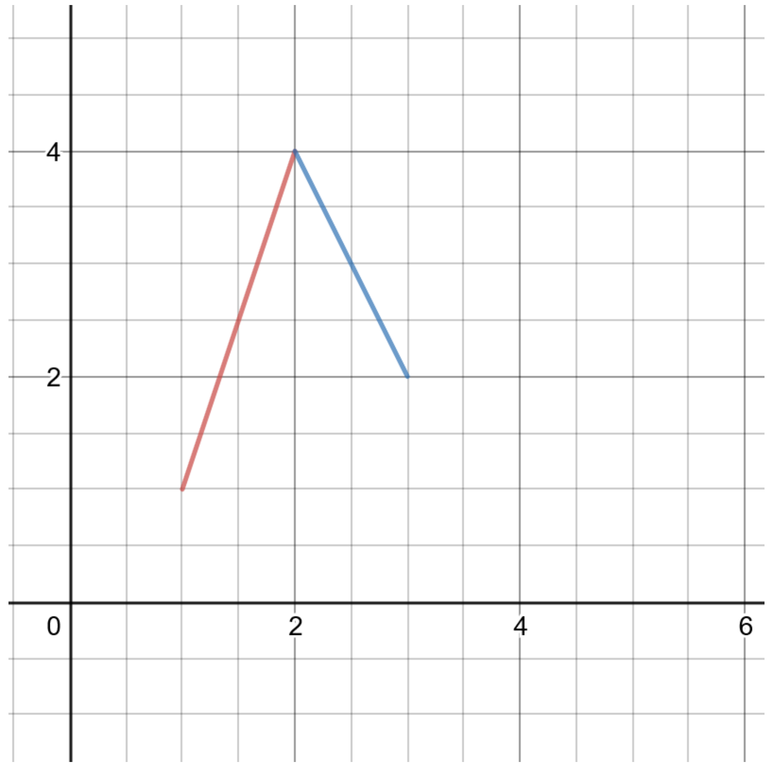
$$\begin{cases} S_1(x) = a_1 + b_1 x, & for \quad x \in [x_1, x_2) \\ S_2(x) = a_2 + b_2 x, & for \quad x \in [x_2, x_3] \end{cases}$$



- Unfortunately the function is not smooth at $x = x_2$.
- Usually it fails to capture the trend of data.

Example 26 *Given the data set* $(x_i, y(x_i)) = (1, 1),\ (2, 4),\ (3, 2)$*. The spline model is:*

$$\begin{cases} S_1(x) = -2 + 3x, & for \quad x \in [1, 2) \\ S_2(x) = 8 - 2x, & for \quad x \in [2, 3] \end{cases}$$



Cubic Splines (**Natural Spline**): Consider the data set $\{(x_1, y_1),\ (x_2, y_2),\ (x_3, y_3)\}$ (3 points can be extended to N points). The Cubic Spline Model constructs 2 third-order piecewise continuous cubic polynomials (cubic splines) that connect 3 data points:

$$\begin{cases} S_1(x) = a_1 + b_1 x + c_1 x^2 + d_1 x^3, & for \quad x \in [x_1, x_2) \\ S_2(x) = a_2 + b_2 x + c_2 x^2 + d_2 x^3, & for \quad x \in [x_2, x_3] \end{cases}$$

Polynomial coefficients are chosen such that the resulting curve and its first derivative are smooth at the points.

$$\begin{aligned} y_1 = S_1(x_1) \quad &: \quad y_1 = a_1 + b_1 x_1 + c_1 x_1^2 + d_1 x_1^3 \\ y_2 = S_1(x_2) \quad &: \quad y_2 = a_1 + b_1 x_2 + c_1 x_2^2 + d_1 x_2^3 \\ y_2 = S_2(x_2) \quad &: \quad y_2 = a_2 + b_2 x_2 + c_2 x_2^2 + d_2 x_2^3 \\ y_3 = S_2(x_3) \quad &: \quad y_3 = a_2 + b_2 x_3 + c_2 x_3^2 + d_2 x_3^3 \\ S_1'(x_2) = S_2'(x_2) \quad &: \quad b_1 + 2c_1 x_2 + 3d_1 x_2^2 = b_2 + 2c_2 x_2 + 3d_2 x_2^2 \\ S_1''(x_2) = S_2''(x_2) \quad &: \quad 2c_1 + 6d_1 x_2 = 2c_2 + 6d_2 x_2 \\ S_1''(x_1) = 0 \quad &: \quad 2c_1 + 6d_1 x_1 = 0 \\ S_2''(x_3) = 0 \quad &: \quad 2c_2 + 6d_2 x_3 = 0. \end{aligned}$$

Remark. If we replace the last two equations by $S_1'(x_1) = f'(x_1)$, $S_2'(x_3) = f'(x_3)$, then the cubic spline is called **clamped spline**.

Example 27 *Given the data set* $(x_i, y(x_i)) = (1,5),\ (2,8),\ (3,25)$.

(1) Construct the natural spline model, i.e.,

$$\begin{cases} S_1(x) = a_1 + b_1 x + c_1 x^2 + d_1 x^3, & for \quad x \in [1,2) \\ S_2(x) = a_2 + b_2 x + c_2 x^2 + d_2 x^3, & for \quad x \in [2,3] \end{cases}$$

(2) Use (1) to estimate $y(1.5)$, $y(2.5)$.

Solution: (1)

$$\begin{aligned}
y_1 = S_1(x_1) \quad &: \quad 5 = a_1 + b_1 + c_1 + d_1 && (1)\\
y_2 = S_1(x_2) \quad &: \quad 8 = a_1 + 2b_1 + 4c_1 + 8d_1 && (2)\\
y_2 = S_2(x_2) \quad &: \quad 8 = a_2 + 2b_2 + 4c_2 + 8d_2 && (3)\\
y_3 = S_2(x_3) \quad &: \quad 25 = a_2 + 3b_2 + 9c_2 + 27d_2 && (4)\\
S_1'(x_2) = S_2'(x_2) \quad &: \quad b_1 + 4c_1 + 12d_1 = b_2 + 4c_2 + 12d_2 && (5)\\
S_1''(x_2) = S_2''(x_2) \quad &: \quad 2c_1 + 12d_1 = 2c_2 + 12d_2 && (6)\\
S_1''(x_1) = 0 \quad &: \quad 2c_1 + 6d_1 = 0 && (7)\\
S_2''(x_3) = 0 \quad &: \quad 2c_2 + 18d_2 = 0. && (8)
\end{aligned}$$

$$\begin{cases} S_1(x) = 2 + 10x - 10.5x^2 + 3.5x^3, \\ S_2(x) = 58 - 74x + 31.5x^2 - 3.5x^3. \end{cases}$$

(2) $S_1(1.5) = 5.188$, $S_2(2.5) = 15.188$.

Summary.

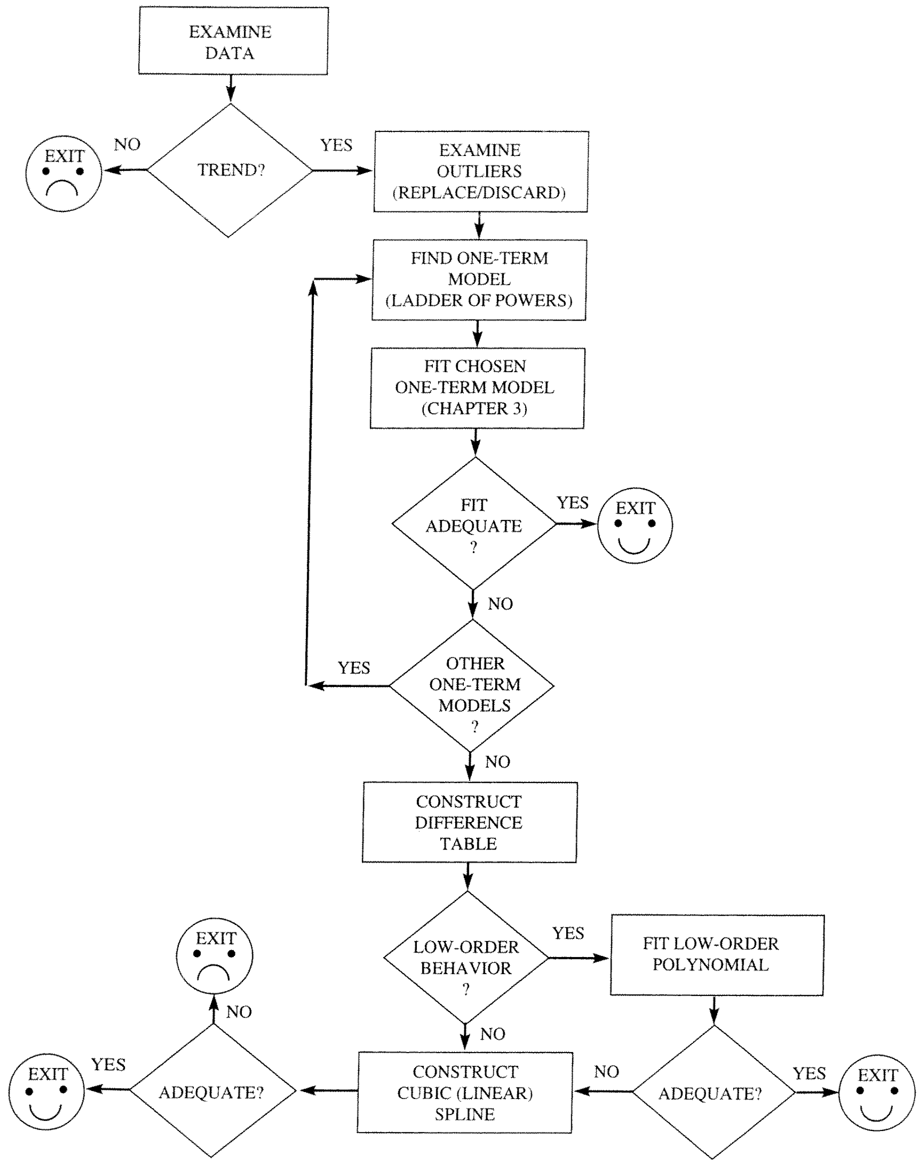


Figure 4.28
A flowchart for empirical model building

Numerical Differentiation and Integration

Numerical differentiation

First Order Derivatives

We start from Taylor series:

$$f(x) = f(x_i) + f'(x_i)h + \frac{f''(x_i)}{2!}h^2 + \frac{f'''(x_i)}{3!}h^3 + ... + \frac{f^{(n)}(x_i)}{n!}h^n + ... \quad h = x - x_i.$$

- The first forward finite divided difference: Let $x = x_{i+1}$,

$$f(x_{i+1}) = f(x_i) + f'(x_i)h + \frac{f''(x_i)}{2!}h^2 + \frac{f'''(x_i)}{3!}h^3 + ... + \frac{f^{(n)}(x_i)}{n!}h^n + ... \quad h = x_{i+1} - x_i$$

Then

$$f'(x_i) \approx \frac{f(x_{i+1}) - f(x_i)}{h}, \quad error = O(h).$$

- The first backward finite divided difference: Let $x = x_{i-1}$,

$$f(x_{i-1}) = f(x_i) - f'(x_i)h + \frac{f''(x_i)}{2!}h^2 - \frac{f'''(x_i)}{3!}h^3 + ... + \frac{f^{(n)}(x_i)}{n!}h^n + ... \quad h = x_i - x_{i-1}$$

Then

$$f'(x_i) \approx \frac{f(x_i) - f(x_{i-1})}{h}, \quad error = O(h).$$

- The first centred finite divided difference:

$$f(x_{i+1}) - f(x_{i-1}) = 2f'(x_i)h + O(h^3) \quad 2h = x_{i+1} - x_{i-1}$$

Then

$$f'(x_i) \approx \frac{f(x_{i+1}) - f(x_{i-1})}{2h}, \quad error = O(h^2).$$

Example 28 *Estimate the first derivative of*

$$f(x) = -0.1x^4 - 0.15x^3 - 0.5x^2 - 0.25x + 1.2$$

at $x_i = 0.5$ *with* $h = 0.25$.

Solution: The exact value is:

$$f'(x) = -0.4x^3 - 0.45x^2 - x - 0.25, \quad f'(0.5) = -0.9125.$$

When $h = 0.25$, $x_i = 0.5$, $x_{i+1} = 0.75$, $x_{i-1} = 0.25$,

$$f(x_i) = 0.925, \quad f(x_{i+1}) = 0.6363, \quad f(x_{i-1}) = 1.1035.$$

- The first forward finite divided difference:

$$f'(x_i) \approx -1.155.$$

- The first backward finite divided difference:

$$f'(x_i) \approx -0.714.$$

- The first centred finite divided difference:

$$f'(x_i) \approx -0.934.$$

Lower approximation error comes from centered finite divided difference.

Second Order Derivatives

- The second forward finite divided difference: We start from Taylor series:

$$f(x_{i+1}) = f(x_i) + f'(x_i)h + \frac{f''(x_i)}{2!}h^2 + \frac{f'''(x_i)}{3!}h^3 + ... + \frac{f^{(n)}(x_i)}{n!}h^n + ... \quad h = x_{i+1} - x_i$$

$$f(x_{i+2}) = f(x_i) + f'(x_i)(2h) + \frac{f''(x_i)}{2!}(2h)^2 + \frac{f'''(x_i)}{3!}(2h)^3 + ... + \frac{f^{(n)}(x_i)}{n!}(2h)^n + ... \quad 2h = x_{i+2} - x_i$$

Then

$$f''(x_i) \approx \frac{f(x_{i+2}) - 2f(x_{i+1}) + f(x_i)}{h^2}, \quad error = O(h).$$

- The second backward finite divided difference: Similarly,

$$f''(x_i) \approx \frac{f(x_i) - 2f(x_{i-1}) + f(x_{i-2})}{h^2}, \quad error = O(h).$$

- The second centred finite divided difference: Similarly,

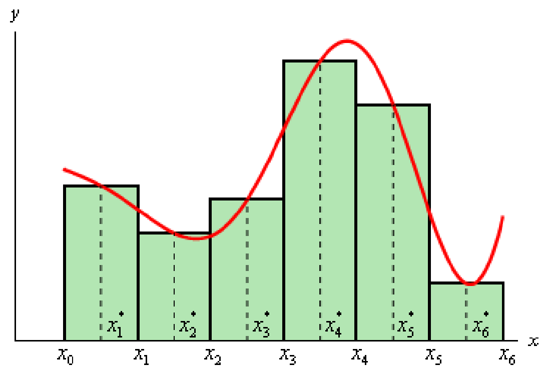
$$f''(x_i) \approx \frac{f(x_{i+1}) - 2f(x_i) + f(x_{i-1})}{h^2}, \quad error = O(h^2).$$

Numerical integration

Methods approximating definite integrals $\int_a^b f(t)dt$: Let $h = \frac{b-a}{n}$, $t_i = a + ih$, $i = 0, 1, ..., n$.

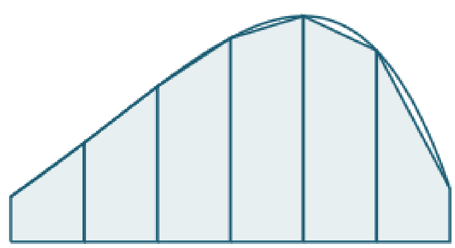
- Midpoint rule: uses the midpoint of each subinterval. mid(n) denotes the result obtained by using "midpoint rule" with n subintervals:

$$midrule(a, b, n) = h \sum_{i=0}^{n-1} f(\frac{t_i + t_{i+1}}{2}).$$

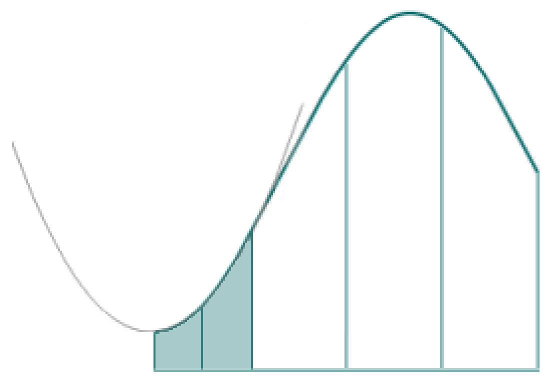


- Trapezoid rule:

$$traprule(a, b, n) = \frac{h}{2}\{f(t_0) + 2f(t_1) + ... + 2f(t_{n-1}) + f(t_n)\}.$$



- Simpson's Rules: In Simpson's Rule, we will use parabolas to approximate each part of the curve. This proves to be very efficient since it's generally more accurate than the other numerical methods we've seen. **In Simpson's Rule, n must be even.**



$$simprule(a,b,n) = \frac{h}{3}\{f(t_0)+4f(t_1)+2f(t_2)+4f(t_3)+...+2f(t_{n-2})+4f(t_{n-1})+f(t_n)\},$$

where we have used Lagrange polynomial interpolation through points $(t_0, f(t_0))$, $(t_1, f(t_1))$, $(t_2, f(t_2))$:

$$\begin{aligned} f(t) &\approx \frac{(t-t_1)(t-t_2)}{(t_0-t_1)(t_0-t_2)}f(t_0) + \frac{(t-t_0)(t-t_2)}{(t_1-t_0)(t_1-t_2)}f(t_1) + \frac{(t-t_0)(t-t_1)}{(t_2-t_0)(t_2-t_1)}f(t_2) \\ &= \frac{(t-t_1)(t-t_2)}{2h^2}f(t_0) + \frac{(t-t_0)(t-t_2)}{-h^2}f(t_1) + \frac{(t-t_0)(t-t_1)}{2h^2}f(t_2). \end{aligned}$$

The area of the small piece is

$$\int_{t_0}^{t_2} f(t) ft.$$

For example,

$$simprule(a,b,4) = \frac{h}{3}\{f(t_0)+4f(t_1)+2f(t_2)+4f(t_3)+f(t_4)\},$$

$$simprule(a,b,6) = \frac{h}{3}\{f(t_0)+4f(t_1)+2f(t_2)+4f(t_3)+2f(t_4)+4f(t_5)+f(t_6)\}.$$

Error = |true value - estimated value|

Maximum error:

$$|E_M| \le \frac{K(b-a)^3}{24n^2}, \qquad |E_T| \le \frac{K(b-a)^3}{12n^2}, \qquad |E_S| \le \frac{M(b-a)^5}{180n^4}.$$

Example 29 *Estimate* $I = \int_0^2 \sin(x^2)dx$ *by using midrule(0,2,4), traprule(0,2,4), simprule(0,2,2).*

Solution: 1) $h = \frac{b-a}{n} = 0.5, x_0 = 0, x_1 = 0.5, x_2 = 1, x_3 = 1.5, x_4 = 2.$

$$midrule(0,2,4) = 0.5\{f(0.25) + f(0.75) + f(1.25) + f(1.75)\}$$

$$traprule(0,2,4) = \frac{0.5}{2}\{f(0) + 2f(0.5) + 2f(1) + 2f(1.5) + f(2)\}$$

$$simprule(0,2,4) = \frac{0.5}{3}\{f(0) + 4f(0.5) + 2f(1) + 4f(1.5) + f(2)\}$$

Here is an M-file using the midpoint rule with n intervals:

```
function S=midrule(a,b,n)
h=(b-a)/n;
xx=zeros(1,n);
for i=1:n
        xx(i)=a+h/2+(i-1)*h;
end
S=0;
for i=1:n
        S=S+h*(sin(xx(i) ∧ 2));
end
```

Here is an M-file using the trapezoid rule with n intervals:

```
function S=traprule(a,b,n)
h=(b-a)/n;
x=zeros(1,n+1);
for i=1:n+1
        x(i)=a+h*(i-1);
end
S=0;
S=S+(h/2)*(sin(x(1) ∧ 2));
for i=2:n
        S=S+h*(sin(x(i) ∧ 2));
end
S=S+(h/2)*(sin(x(n+1) ∧ 2));
End
```

M-file using Simpson's rule with 2n intervals:

```
function S=simprule(a,b,n)
h=(b-a)/(2*n);
x=zeros(1,2*n+1);
for i=1:2*n+1
        x(i)=a+h*(i-1);
end
S=0;
S=S+(h/3)*(sin(x(1) ∧ 2));
for i=1:n-1
        S=S+(4*h/3)*(sin(x(2*i) ∧ 2));
S=S+(2*h/3)*(sin(x(2*i+1) ∧ 2));
end
S=S+(4*h/3)*(sin(x(2*n) ∧ 2));
S=S+(h/3)*(sin(x(2*n+1) ∧ 2));
end
```

Gaussian Quadrature

Gaussian Quadrature of $f(x)$:

$$\int_a^b f(x)dx \approx \sum_{i=1}^{n} w_i f(x_i),$$

where w_i are called weights, x_i are nodes. The above formula is exactly equal for any polynomial $f(x)$ of degree less than or equal to $2n-1$.

Example 30 *When $n = 2$, 2-point Gaussian formula is*

$$\int_{-1}^{1} f(x)dx \approx f(-\frac{1}{\sqrt{3}}) + f(\frac{1}{\sqrt{3}}).$$

Proof. By solving
$\int_{-1}^{1} 1dx = 2 = w_1 + w_2,$
$\int_{-1}^{1} xdx = 0 = w_1x_1 + w_2x_2,$
$\int_{-1}^{1} x^2dx = \frac{2}{3} = w_1x_1^2 + w_2x_2^2,$
$\int_{-1}^{1} x^3dx = 0 = w_1x_1^3 + w_2x_2^3,$
we imply that $w_1 = w_2 = 1$, $x_1 = -\frac{1}{\sqrt{3}}$, $x_2 = \frac{1}{\sqrt{3}}$.

Remark. By transformations,

$$\int_a^b f(x)dx = \frac{b-a}{2}\int_{-1}^{1} f\left(\frac{b-a}{2}x + \frac{a+b}{2}\right)dx.$$

Example 31 *Estimate* $\int_0^{1.2} \sin x dx$.

Solution. $\int_0^{1.2} \sin x dx = 0.6\int_{-1}^{1} \sin(0.6x + 0.6)dx = 0.6\int_{-1}^{1} \sin 0.6(x+1)dx$
$\approx 0.6\sin 0.6(-\frac{1}{\sqrt{3}} + 1) + \sin 0.6(\frac{1}{\sqrt{3}} + 1) \approx 0.6373216.$

Legendre's polynomials

Polynomial solution $P_n(x)$ of the Legendre's equation

$$(1-x^2)y'' - 2xy' + n(n+1)y = 0, \quad -1 < x < 1.$$

For example,

$$\begin{aligned} P_0(x) &= 1, \\ P_1(x) &= x, \\ P_2(x) &= \frac{1}{2}(3x^2-1), \\ P_3(x) &= \frac{1}{2}(5x^3-3x), \\ P_4(x) &= \frac{1}{8}(35x^4-30x^2+3), \\ P_5(x) &= \frac{1}{8}(63x^5-70x^3+15x). \end{aligned}$$

Legendre's polynomial can be obtained from the following Rodrigues formula

$$P_n(x) = \frac{1}{2^n n!}\frac{d^n}{dx^n}\left[(x^2-1)^n\right].$$

Orthogonality Relations for $P_n(x)$:

$$\int_{-1}^{1} P_m(x)P_n(x)\,dx = \begin{cases} 0, & m \neq n; \\ \frac{2}{2n+1}, & m = n. \end{cases}$$

Theorem 8

$$\int_a^b f(x)dx \approx \sum_{i=1}^{n} w_i f(x_i),$$

where x_i are the roots of the Legendre's polynomial of degree n,

$$w_i = \int_{-1}^{1} L_i(x)^2 dx, \quad L_i(x) = \Pi_{j=1,j\neq i}^{n}\frac{x-x_j}{x_i-x_j}.$$

```
function coefs = LegendrePoly(n)
if n == 0
  coefs = 1;
elseif n == 1
  coefs = [1 0];
else
  P_nm1 = 1;
  P_n = [1 0];

    for i=1:(n-1);
      P_np1 = ((2*i+1)*[P_n,0] - i*[0,0,P_nm1])/(i+1); % recurrence
      [P_nm1,P_n] = deal(P_n,P_np1); % shift
    end
    coefs = P_np1;
  end
```

Table 5.7. Nodes and Weights of Gaussian Quadrature Formulas

n	x_i	w_i
2	± 0.5773502692	1.0
3	± 0.7745966692	0.5555555556
	0.0	0.8888888889
4	± 0.8611363116	0.3478548451
	± 0.3399810436	0.6521451549
5	± 0.9061798459	0.2369268851
	± 0.5384693101	0.4786286705
	0.0	0.5688888889
6	± 0.9324695142	0.1713244924
	± 0.6612093865	0.3607615730
	± 0.2386191861	0.4679139346
7	± 0.9491079123	0.1294849662
	± 0.7415311856	0.2797053915
	± 0.4058451514	0.3818300505
	0.0	0.4179591837
8	± 0.9602898565	0.1012285363
	± 0.7966664774	0.2223810345
	± 0.5255324099	0.3137066459
	± 0.1834346425	0.3626837834

5.2 Generating Random Numbers

From previous section we see that, an important part of simulation is the generation of random numbers. The following method was developed by Newman etc.

Middle-Square Method:

1. Start with a four-digit number x_0, called the seed.
2. Square it to obtain an eight-digit number (add a leading zero if necessary).
3. Take the middle four digits as the next random number.

Continuing, we obtain a sequence that appears random over the integers from 0 to 9999. These integers can be scaled to any interval $[a, b]$.

Example 32

n	0	1	2	3	4	5
x_n	2041	1656	7423	1009	0180	0324
(x_n)^2	4165681	2742336	55100929	1018081	32400	

5.3 Simulating Probabilistic Behaviour

In this section we will simulate simple probabilistic behaviour.

Flipping a Fair Coin.

When we flip a coin, theoretically the probability of obtaining head or tail is $\frac{1}{2}$. Experimentally, in the long run, the ratio of the number of tails to the number of flips approaches $1:2$.

For any random number $x \in [0,1]$, define

$$f(x) = \begin{cases} head, & for \quad x \in [0, 0.5] \\ tail, & for \quad x \in (0.5, 1] \end{cases}$$

Monte Carlo Fair Coin Algorithm.

Input: Total number n of random flips of a fair coin to be generated in the simulation.

Output: Probability of getting tails when we flip a fair coin.

Step 1: Initialize COUNTER=0.

Step 2: for $i = 1, ..., n$, generate a random number x_i between 0 and 1.

Step 3: if $0.5 < x_i \leq 1$, then COUNTER=COUNTER+1.

Step 4: Calculate P(tails) = COUNTER/n.

Step 5: Output P(tails), the probability of tails.

Monte Carlo Roll of a Fair Die Algorithm: Theoretically, rolling a fair die, $P(i) = \frac{1}{6}$ for ant $1 \leq i \leq 6$.

Input: Total number n of random rolls of a die to be generated in the simulation.

Output: Probability of rolling a [1,2,3,4,5,6].

Step 1: Initialize COUNTER1=0,..., COUNTER6=0.

Step 2: for $i = 1, ..., n$, generate a random number x_i between 0 and 1.

Step 3:
1. If $0 \leq x_i \leq 1/6$, then COUNTER1=COUNTER1+1.
2. If $1/6 < x_i \leq 2/6$, then COUNTER2=COUNTER2+1.
3. If $2/6x_i \leq 3/6$, then COUNTER3=COUNTER3+1.

4. If $3/6 < x_i \leq 4/6$, then COUNTER4=COUNTER4+1.
5. If $4/6x_i \leq 5/6$, then COUNTER5=COUNTER5+1.
6. If $5/6 < x_i \leq 6/6$, then COUNTER6=COUNTER6+1.

Step 4: Calculate P(k) = COUNTERk/n, $1 \leq k \leq n$.

Step 5: Output P(k), the probability to get the face k.

Traffic Simulation

https://en.wikipedia.org/wiki/Traffic_simulation

Simulating Blackjack with MATLAB

http://www.mathworks.com/company/newsletters/articles/simulating-blackjack-with-matlab.html

Linear Congruence Generator

Linear congruence: a linear rule for generating the next element of a sequence from previous elements:

$$x_{n+1} = ax_n + b \pmod{c},$$

where a, b, c are constants.

Example 33 *Generate the sequence with the model:*

$$x_{n+1} = 7x_n + 2 \quad (mod\ 10).$$

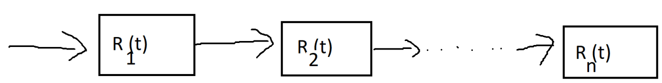
Solution: If we take $x_0 = 3$, then we get a sequence 3, 3, 3, 3, ...
If we take $x_0 = 5$, then we get a sequence 5, 7, 1, 9, 5, 7, 1, 9, ...

6.2 Modelling Component and System Reliability

Reliability of a component or system is the probability that it will not failure over a specified period of time t. Let $f(t)$ be the failure rate over time t, $F(t)$ be the cumulative distribution function corresponding $f(t)$, we define the reliability by

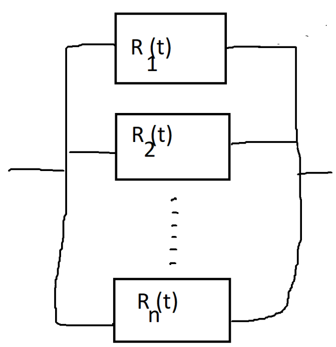
$$R(t) = 1 - F(t).$$

- **Series system** is one that performs well as long as all of the components are fully functional.



$$R_s(t) = R_1(t) \cdots R_n(t).$$

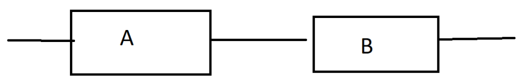
- **Parallel system** is one that performs well as long as a single one of its components remains functional.



$$R_s(t) = 1 - \Pi_{i=1}^{n}[1 - R_i(t)].$$

If $n = 2$, then $R_s(t) = R_1(t) + R_2(t) - R_1(t)R_2(t)$.

Example 34 *A system contains two components, A and B, connected in series as shown in the following diagram:*

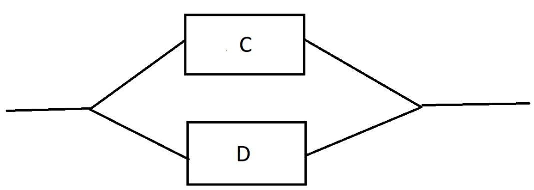


The system will function only if both components function. The probability that A functions is given by P(A) = 0.98, and the probability that B functions is given by P(B) = 0.95. Assume that A and B function independently. Find the probability that the system functions.

Solution:

$$P(system\ functions) = P(A \cap B) = P(A) \times P(B) = 0.95 \times 0.98 = 0.931$$

Example 35 *A system contains two components, C and D, connected in parallel as shown in the following diagram:*



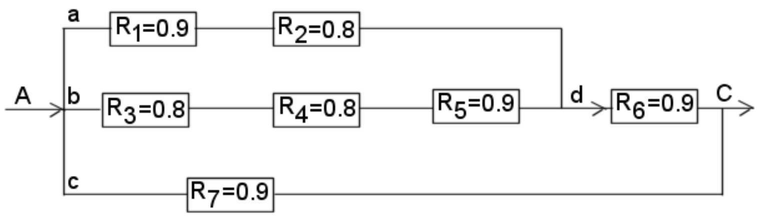
The system will function if either C or D functions. The probability that C functions is 0.90, and the probability that D functions is 0.85. Assume C and D function independently. Find the probability that the system functions.

Solution: Since the system will function so long as either of the two components functions, it follows that

$$P(systemfunctions) = P(C \cup D) = P(C) + P(D) - P(C \cap D)$$

$$= P(C) + P(D) - P(C) \times P(D) = 0.90 + 0.85 - 0.90 \times 0.85 = 0.985.$$

Example 36 *Most practical equipments and systems are combinations of series and parallel components. For example,*



Find the reliability of the combined network, i.e., R_{AC}.

Solution: To solve this network, one merely uses series and parallel relationships to decompose and recombine the network step by step.

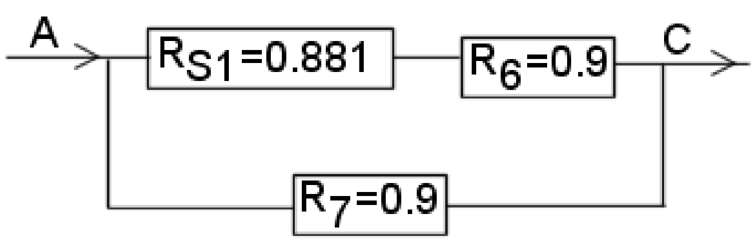
$$R_{ad} = R_1 \cdot R_2 = (0.9)(0.8) = 0.72$$

$$R_{bd} = R_3 \cdot R_4 \cdot R_5 = (0.8)(0.8)(0.9) = 0.576$$

but R_{ad} and R_{bd} are in parallel; thus,

$$R_{S1} = R_{abd} = 1 - (1 - 0.72)(1 - 0.576) = 1 - (0.28)(0.424) = 0.88128.$$

Now the network has been decomposed to



$$R_{S1,6} = R_{S1} \cdot R_6 = (0.88128)(0.9) = 0.793152$$

Since the last system is in parallel, the total system reliability is

$$R_{AC} = 1 - (1 - 0.793152)(1 - 0.9)1 - (0.206848)(0.1) = 0.9793152.$$

Thus, the reliability of the combined network is 0.9793152.

6.1 Probabilistic Modeling with Discrete Systems

In this section we will study the systems of difference equations, where coefficients can vary in a probabilistic manner. A special case is Markov chain.

Markov chain

- A Markov chain is a process in which there are the same finite number of states (or outcomes) that can be occupied at any given time.
- The states do not overlap and cover all possible outcomes.
- The system moves from one state to another, one for each time step. There is a probability associated with this transition for each possible outcome.
- The sum of the probabilities for transitioning from one state to the next is 1.

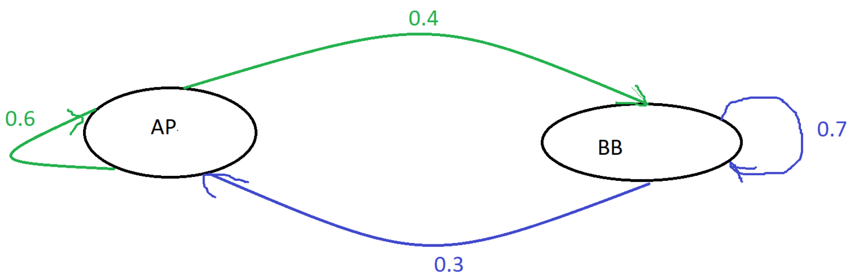
Probability vector: a vector with non-negative entries that add up to one.

Example 37 *(Two-state Markov chain) MATH3800 Tutoring Ottawa has two branches in Ottawa: Andrew Park, and Billings Bridge, with market portion* a_0 *and* b_0 *respectively. According to market statistics, due to variety of tutors, after each year, 40% of AP's customers will switch to BB's, while 30% of BB's customers will switch to AP's.*

We can array the data as following, which is **transition matrix**:

		Next state	
		AP	BB
Present state	AP	0.6	0.4
	BB	0.3	0.7

Markov chain graph:

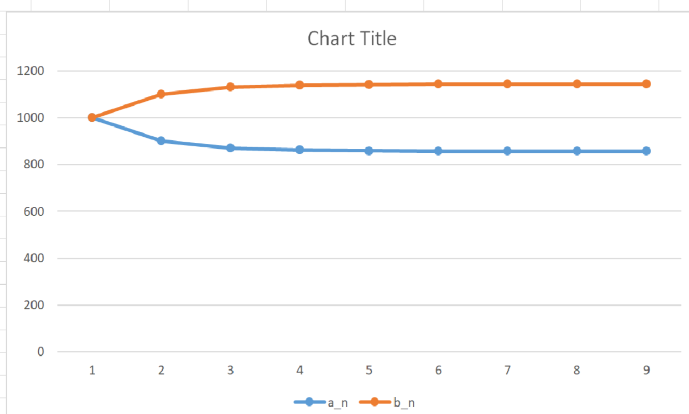


Let
a_n = the number of customers at the branch Andrew Park , at the end of year n.
b_n = the number of customers at the branch Billings Bridge, at the end of year n.
Then

$$\begin{aligned} a_{n+1} &= 0.6a_n + 0.3b_n \\ b_{n+1} &= 0.4a_n + 0.7b_n \end{aligned}$$

Numerical method:

a_n	b_n
1000	1000
900	1100
870	1130
861	1139
858.3	1141.7
857.49	1142.51
857.247	1142.753
857.1741	1142.8259
857.15223	1142.84777



$$a_n \to \frac{3}{7}, \qquad b_n \to \frac{4}{7}.$$

Algebra method: Let T be the transition matrix, i.e., $x_{k+1} = Tx_k, k = 0, 1, 2, \cdots$ where $x_k = \begin{bmatrix} a_k \\ b_k \end{bmatrix}$ Then Steady-State Vector $\vec{q}$ (which gives long-term distribution) is a probability vector such that

$$T\vec{q} = \vec{q}, \Rightarrow (T - I)\vec{q} = \vec{0}.$$

Now

$$T = \begin{bmatrix} 0.6 & 0.3 \\ 0.4 & 0.7 \end{bmatrix}, T - I = \begin{bmatrix} -0.4 & 0.3 \\ 0.4 & -0.3 \end{bmatrix} \sim \begin{bmatrix} 1 & -3/4 \\ 0 & 0 \end{bmatrix}.$$

By solving the system $q_1 - 3/4q_2 = 0, \quad q_1 + q_2 = 1$, $q_1 = 3/7$, $q_2 = 4/7$.

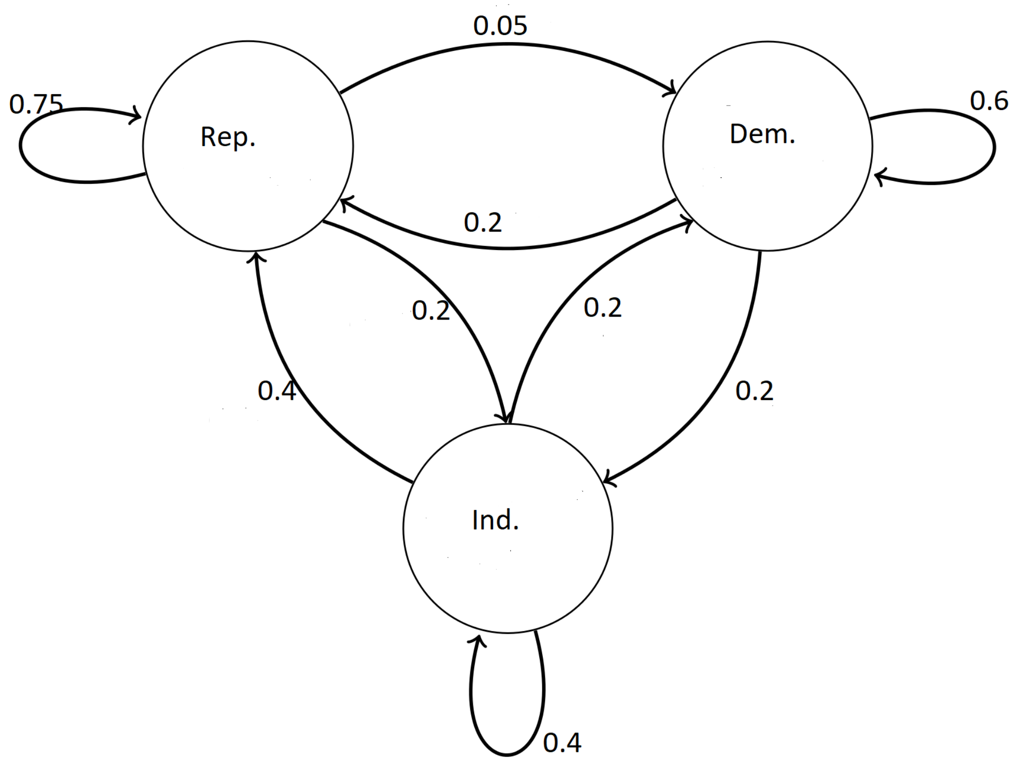
Example 38 *(Three-state Markov chain) Presidential voting tendencies are of interest every 4 years.*

Problem Identification: Can we find the long-term behavior of voters in a presidential election?

Assumptions: The data for past decades are arranged in the following **transition matrix**:

		Next state		
		Republicans	Democrats	Independents
Present state	Republicans	0.75	0.05	0.2
	Democrats	0.2	0.6	0.2
	Independents	0.4	0.2	0.4

Markov chain graph:

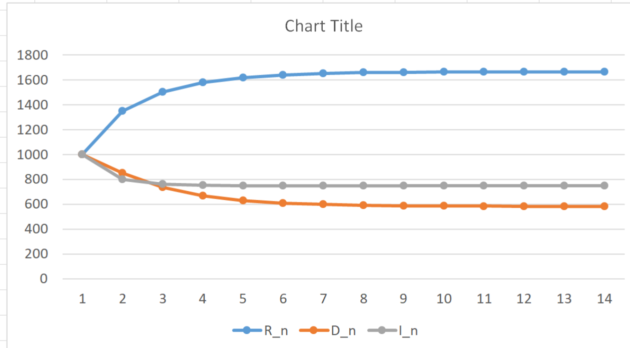


Model Formulation: Let

R_n = percentage of voters to vote Republican in period n.
D_n = percentage of voters to vote Democratic in period n.
I_n = percentage of voters to vote Independent in period n.

$$
\begin{aligned}
R_{n+1} &= 0.75R_n + 0.20D_n + 0.40I_n \\
D_{n+1} &= 0.05R_n + 0.60D_n + 0.20I_n \\
I_{n+1} &= 0.20R_n + 0.20D_n + 0.40I_n.
\end{aligned}
$$

	R_n	D_n	I_n
	1000	1000	1000
	1350	850	800
	1502.5	737.5	760
	1578.375	669.625	752
	1618.506	631.09375	750.4
	1640.258	609.66156	750.08
	1652.158	597.82586	750.02
	1658.69	591.30662	750
	1662.28	587.71912	750
	1664.254	585.74561	750
	1665.34	584.66011	750
	1665.937	584.06306	750
	1666.265	583.73469	750
	1666.446	583.55408	750
%	0.555482	0.194518	0.25



Algebra method:

$$T = \begin{bmatrix} 0.75 & 0.2 & 0.4 \\ 0.05 & 0.6 & 0.2 \\ 0.2 & 0.2 & 0.4 \end{bmatrix}, \quad T - I = \begin{bmatrix} -0.25 & 0.2 & 0.4 \\ 0.05 & -0.4 & 0.2 \\ 0.2 & 0.2 & -0.6 \end{bmatrix} \sim \begin{bmatrix} 1 & 0 & -20/9 \\ 0 & 1 & -7/9 \\ 0 & 0 & 0 \end{bmatrix}.$$

Thus $q_1 = \dfrac{5}{9}, q_2 = \dfrac{7}{36}, q_3 = \dfrac{1}{4}$.

Matrix Computations

LU Decomposition.

To solve $Ax = b$, one way is to use row reduction, another way is to use LU-decomposition.

1. Write $A = LU$, where L is an lower triangular matrix, the entries on the main diagonal are 1 only, U is an upper triangular matrix.

2. Solve $Ly = b$.

3. Solve $Ux = y$.

Example 39 *Let*

$$A = \begin{bmatrix} a_{11} & a_{12} & a_{13} \\ a_{21} & a_{22} & a_{23} \\ a_{31} & a_{32} & a_{33} \end{bmatrix}, \quad L = \begin{bmatrix} 1 & 0 & 0 \\ m_{21} & 1 & 0 \\ m_{31} & m_{32} & 1 \end{bmatrix}, \quad U = \begin{bmatrix} u_{11} & u_{12} & u_{13} \\ 0 & u_{22} & u_{23} \\ 0 & 0 & u_{33} \end{bmatrix}.$$

Then

$$LU = \begin{bmatrix} u_{11} & u_{12} & u_{13} \\ m_{21}u_{11} & m_{21}u_{12} + u_{22} & m_{21}u_{13} + u_{23} \\ m_{31}u_{11} & m_{31}u_{12} + m_{32}u_{22} & m_{31}u_{13} + m_{32}u_{23} + u_{33} \end{bmatrix} = \begin{bmatrix} a_{11} & a_{12} & a_{13} \\ a_{21} & a_{22} & a_{23} \\ a_{31} & a_{32} & a_{33} \end{bmatrix}.$$

Example 40 *Solve $Ax = b$ by LU-decomposition, where* $A = \begin{bmatrix} 1 & 2 & 4 \\ 3 & 8 & 14 \\ 2 & 6 & 13 \end{bmatrix}$, $b = \begin{bmatrix} 3 \\ 13 \\ 4 \end{bmatrix}$.

Solution. Step 1:

$$\begin{bmatrix} u_{11} & u_{12} & u_{13} \\ m_{21}u_{11} & m_{21}u_{12} + u_{22} & m_{21}u_{13} + u_{23} \\ m_{31}u_{11} & m_{31}u_{12} + m_{32}u_{22} & m_{31}u_{13} + m_{32}u_{23} + u_{33} \end{bmatrix} = \begin{bmatrix} 1 & 2 & 4 \\ 3 & 8 & 14 \\ 2 & 6 & 13 \end{bmatrix}.$$

$$L = \begin{bmatrix} 1 & 0 & 0 \\ 3 & 1 & 0 \\ 2 & 1 & 1 \end{bmatrix}, \quad U = \begin{bmatrix} 1 & 2 & 4 \\ 0 & 2 & 2 \\ 0 & 0 & 3 \end{bmatrix}.$$

Step 2: Solve $Ly = b$, $y = \begin{bmatrix} 3 \\ 4 \\ -6 \end{bmatrix}$.

Step 3: Solve $Ux = y$, $x = \begin{bmatrix} 3 \\ 4 \\ -2 \end{bmatrix}$.

Cholesky Decomposition.

Positive definite matrix A: if $x^T Ax > 0$ for any nonzero vector x. We denote this by $A > 0$.

- $A > 0$ iff all of its principle minors are positive, i.e., $a_{11} > 0$, $det \begin{bmatrix} a_{11} & a_{12} \\ a_{21} & a_{22} \end{bmatrix} > 0$, ..., $det(A) > 0$.
- $A > 0$ iff all eigenvalues are positive.
- If A is diagonally dominant with positive diagonal entries, then $A > 0$. Here a matrix A is diagonally dominant if
$$|a_{ii}| \geq \sum_{j \neq i} |a_{ij}|, \ all\ i.$$
- If A is symmetric positive definite, then A has special LU-decomposition:
$$A = GG^T,$$
which is called Cholesky decomposition, where G is lower triangular matrix.

Example 41 *Solve $Ax = b$ by Cholesky decomposition, where* $A = \begin{bmatrix} 4 & 2 & 14 \\ 2 & 17 & -5 \\ 14 & -5 & 83 \end{bmatrix}$, $b = \begin{bmatrix} 14 \\ -101 \\ 155 \end{bmatrix}$.

Solution. Step 1: $A = GG^T$,

$$\begin{bmatrix} g_{11} & 0 & 0 \\ g_{21} & g_{22} & 0 \\ g_{31} & g_{32} & g_{33} \end{bmatrix} \begin{bmatrix} g_{11} & g_{21} & g_{31} \\ 0 & g_{22} & g_{32} \\ 0 & 0 & g_{33} \end{bmatrix} = \begin{bmatrix} g_{11}^2 & g_{11}g_{21} & g_{11}g_{31} \\ g_{21}g_{11} & g_{21}^2 + g_{22}^2 & g_{21}g_{31} + g_{22}g_{32} \\ g_{31}g_{11} & g_{31}g_{21} + g_{32}g_{22} & g_{31}^2 + g_{32}^2 + g_{33}^2 \end{bmatrix}$$

$$\begin{bmatrix} g_{11}^2 & g_{11}g_{21} & g_{11}g_{31} \\ g_{21}g_{11} & g_{21}^2+g_{22}^2 & g_{21}g_{31}+g_{22}g_{32} \\ g_{31}g_{11} & g_{31}g_{21}+g_{32}g_{22} & g_{31}^2+g_{32}^2+g_{33}^2 \end{bmatrix} = \begin{bmatrix} 4 & 2 & 14 \\ 2 & 17 & -5 \\ 14 & -5 & 83 \end{bmatrix}.$$

We imply that $G = \begin{bmatrix} 2 & 0 & 0 \\ 1 & 4 & 0 \\ 7 & -3 & 5 \end{bmatrix}$.

Step 2: Solve $Gy = b$, $y = \begin{bmatrix} 7 \\ -27 \\ 5 \end{bmatrix}$.

Step 3: Solve $G^T x = y$, $x = \begin{bmatrix} 3 \\ -6 \\ 1 \end{bmatrix}$.

Gauss Seidel Iteration

In numerical linear algebra, the GaussSeidel method, also known as the Liebmann method or the method of successive displacement, is an iterative method used to solve a linear system of equations.
To solve $Ax = b$,

1. Write $A = L + U$, where L is the lower triangular matrix, U is the strict upper triangular matrix:

$$\begin{bmatrix} a_{11} & a_{12} & \cdots & a_{1n} \\ a_{21} & a_{22} & \cdots & a_{2n} \\ \cdots & \cdots & \cdots & \cdots \\ a_{n1} & a_{n2} & \cdots & a_{nn} \end{bmatrix} = \begin{bmatrix} a_{11} & 0 & \cdots & 0 \\ a_{21} & a_{22} & \cdots & 0 \\ \cdots & \cdots & \cdots & \cdots \\ a_{n1} & a_{n2} & \cdots & a_{nn} \end{bmatrix} + \begin{bmatrix} 0 & a_{12} & \cdots & a_{1n} \\ 0 & 0 & \cdots & a_{2n} \\ \cdots & \cdots & \cdots & \cdots \\ 0 & 0 & \cdots & 0 \end{bmatrix} = L + U.$$

2. Solve the recursion $x^{(n+1)} = L^{-1}(b - Ux^{(n)})$.

Example 42 *Solve $Ax = b$ by Gauss Seidel Iteration, where* $A = \begin{bmatrix} 16 & 3 \\ 7 & -11 \end{bmatrix}$, $b = \begin{bmatrix} 11 \\ 13 \end{bmatrix}$.

Solution: $A = \begin{bmatrix} 16 & 3 \\ 7 & -11 \end{bmatrix} = L + U$, where $L = \begin{bmatrix} 16 & 0 \\ 7 & -11 \end{bmatrix}$, $U = \begin{bmatrix} 0 & 3 \\ 0 & 0 \end{bmatrix}$. We imply that

$$x^{(n+1)} = L^{-1}(b - Ux^{(n)}) = \begin{bmatrix} 0.0625 & 0 \\ 0.0398 & -0.0909 \end{bmatrix} \left(\begin{bmatrix} 11 \\ 13 \end{bmatrix} - \begin{bmatrix} 0 & 3 \\ 0 & 0 \end{bmatrix} x^{(n)} \right)$$

$$x^{(n+1)} = \begin{bmatrix} 0 & -0.1875 \\ 0 & -0.1194 \end{bmatrix} x^{(n)} + \begin{bmatrix} 0.6875 \\ -0.7439 \end{bmatrix}$$

$$x^{(1)} = \begin{bmatrix} 0.000 & -0.1875 \\ 0.000 & -0.1193 \end{bmatrix} \times \begin{bmatrix} 1.0 \\ 1.0 \end{bmatrix} + \begin{bmatrix} 0.6875 \\ -0.7443 \end{bmatrix} = \begin{bmatrix} 0.5000 \\ -0.8636 \end{bmatrix}.$$

$$x^{(2)} = \begin{bmatrix} 0.000 & -0.1875 \\ 0.000 & -0.1193 \end{bmatrix} \times \begin{bmatrix} 0.5000 \\ -0.8636 \end{bmatrix} + \begin{bmatrix} 0.6875 \\ -0.7443 \end{bmatrix} = \begin{bmatrix} 0.8494 \\ -0.6413 \end{bmatrix}.$$

$$x^{(3)} = \begin{bmatrix} 0.000 & -0.1875 \\ 0.000 & -0.1193 \end{bmatrix} \times \begin{bmatrix} 0.8494 \\ -0.6413 \end{bmatrix} + \begin{bmatrix} 0.6875 \\ -0.7443 \end{bmatrix} = \begin{bmatrix} 0.8077 \\ -0.6678 \end{bmatrix}.$$

$$x^{(4)} = \begin{bmatrix} 0.000 & -0.1875 \\ 0.000 & -0.1193 \end{bmatrix} \times \begin{bmatrix} 0.8077 \\ -0.6678 \end{bmatrix} + \begin{bmatrix} 0.6875 \\ -0.7443 \end{bmatrix} = \begin{bmatrix} 0.8127 \\ -0.6646 \end{bmatrix}.$$

$$x^{(5)} = \begin{bmatrix} 0.000 & -0.1875 \\ 0.000 & -0.1193 \end{bmatrix} \times \begin{bmatrix} 0.8127 \\ -0.6646 \end{bmatrix} + \begin{bmatrix} 0.6875 \\ -0.7443 \end{bmatrix} = \begin{bmatrix} 0.8121 \\ -0.6650 \end{bmatrix}.$$

$$x^{(6)} = \begin{bmatrix} 0.000 & -0.1875 \\ 0.000 & -0.1193 \end{bmatrix} \times \begin{bmatrix} 0.8121 \\ -0.6650 \end{bmatrix} + \begin{bmatrix} 0.6875 \\ -0.7443 \end{bmatrix} = \begin{bmatrix} 0.8122 \\ -0.6650 \end{bmatrix}.$$

$$x^{(7)} = \begin{bmatrix} 0.000 & -0.1875 \\ 0.000 & -0.1193 \end{bmatrix} \times \begin{bmatrix} 0.8122 \\ -0.6650 \end{bmatrix} + \begin{bmatrix} 0.6875 \\ -0.7443 \end{bmatrix} = \begin{bmatrix} 0.8122 \\ -0.6650 \end{bmatrix}.$$

The actual solution is

$$x = A^{-1}b = \frac{1}{-197} \begin{bmatrix} -11 & -3 \\ -7 & 16 \end{bmatrix} \begin{bmatrix} 11 \\ 13 \end{bmatrix} = \frac{1}{-197} \begin{bmatrix} -160 \\ 131 \end{bmatrix} = \begin{bmatrix} 0.8122 \\ -0.6650 \end{bmatrix}$$

For any vector $\vec{x} = [x_1\ x_2\ ...\ x_n]^T$, we define

l_1-norm: $||x||_1 = |x_1| + ... + |x_n|$.

l_2-norm: $||x||_2 = \sqrt{|x_1|^2 + ... + |x_n|^2}$.

l_∞-norm: $||x||_\infty = max\{|x_1|, ..., |x_n|\}$.

For any matrix A, we define norms as follows:

$||A||_1 = max_{1 \le j \le n}\{|a_{1j}| + ... + |a_{nj}|\}$.

$||A||_2 = max_i \sqrt{\sigma_i}$, where σ_i is an eigenvalue of $A^T A$, which represents the largest singular value of matrix A .

$||A||_\infty = max_{1 \le i \le n}\{|a_{i1}| + ... + |a_{in}|\}$.

$$||A||_F = \sqrt{\sum_{i=1}^{\infty} \sum_{j=1}^{\infty} |a_{ij}|}.$$

Least Squares Fit of a line to Data, Algebraic method: Suppose we have n points $(x_i, y_i) : i = 1, ..., n$. We want to find the "best" straight line $y = c + dx = \begin{bmatrix} 1 & x \end{bmatrix} \begin{bmatrix} c \\ d \end{bmatrix}$.

1. Let $A = \begin{bmatrix} 1 & x_1 \\ 1 & x_2 \\ \vdots & \vdots \\ 1 & x_n \end{bmatrix}$, $\vec{x} = \begin{bmatrix} c \\ d \end{bmatrix}$, $\vec{b} = \begin{bmatrix} y_1 \\ \vdots \\ y_n \end{bmatrix}$. We hope to solve $A\vec{x} = \vec{b}$. But usually not possible.
2. Solve $A^T A\vec{x} = A^T\vec{b}$, i.e., $\begin{bmatrix} n & \sum x_i \\ \sum x_i & \sum x_i^2 \end{bmatrix} \vec{x} = \begin{bmatrix} \sum y_i \\ \sum x_i y_i \end{bmatrix}$.
3. The error $E = ||A\vec{x} - \vec{b}||$ is minimum.

Example 43 *Find the least square fit of a line by Algebraic method to the points* $(-2, 1), (0, 2), (2, 4)$.

Solution: $A = \begin{bmatrix} 1 & -2 \\ 1 & 0 \\ 1 & 2 \end{bmatrix}$, $\vec{x} = \begin{bmatrix} c \\ d \end{bmatrix}$, $\vec{b} = \begin{bmatrix} 1 \\ 2 \\ 4 \end{bmatrix}$.

$$A^T A = \begin{bmatrix} 3 & 0 \\ 0 & 8 \end{bmatrix}, \quad A^T\vec{b} = \begin{bmatrix} 7 \\ 6 \end{bmatrix}.$$

$$\vec{x} = (A^T A)^{-1}(A^T\vec{b}) = \frac{1}{24}\begin{bmatrix} 56 \\ 18 \end{bmatrix}.$$

$y = \frac{7}{3} + \frac{3}{4}x$.

Least Squares Fit of quadratic to Data, Algebraic method: Suppose we have n points $(x_i, y_i) : i = 1, ..., n$. We want to find the "best" quadratic $y = c_0 + c_1 x + c_2 x^2$.

1. Let $A = \begin{bmatrix} 1 & x_1 & x_1^2 \\ 1 & x_2 & x_2^2 \\ \vdots & \vdots & \vdots \\ 1 & x_n & x_n^2 \end{bmatrix}$, $\vec{x} = \begin{bmatrix} c_1 \\ c_2 \\ c_3 \end{bmatrix}$, $\vec{b} = \begin{bmatrix} y_1 \\ \vdots \\ y_n \end{bmatrix}$.
2. Solve $A^T A\vec{x} = A^T\vec{b}$, i.e., $\begin{bmatrix} n & \sum x_i & \sum x_i^2 \\ \sum x_i & \sum x_i^2 & \sum x_i^3 \\ \sum x_i^2 & \sum x_i^3 & \sum x_i^4 \end{bmatrix} \vec{x} = \begin{bmatrix} \sum y_i \\ \sum x_i y_i \\ \sum x_i^2 y_i \end{bmatrix}$.

3. The error $E = ||A\vec{x} - \vec{b}||$ is minimum.

Example 44 *Find the least square fit of a line by Algebraic method to the points* $(0, 6), (1, 0), (2, 0)$.

Solution: $y = 6 - 9x + 3x^2$.

Estimate eigenvalues: The eigenvalues of the matrix A are the solutions of the characteristic equation

$$\det(A - \lambda I) = 0.$$

Abel's Impossibility Theorem. There is no general algebraic solution for solving a polynomial equation of degree ≥ 5.

Method to estimate eigenvalue λ (Gershgorin circle theorem):

$$|a_{ii} - \lambda| \leq \sum_{j \neq i, j=1}^{n} |a_{ij}|, \quad 1 \leq i \leq n.$$

Example 45 *Estimate eigenvalues of* $A = \begin{bmatrix} 5 & -2 & 2 \\ 2 & 0 & 4 \\ 4 & 2 & 7 \end{bmatrix}$.

Solution:
$|5 - \lambda_1| \leq |-2| + |2|$, $1 \leq \lambda_1 \leq 9$;
$|0 - \lambda_1| \leq |2| + |4|$, $-6 \leq \lambda_1 \leq 6$;
$|7 - \lambda_1| \leq |4| + |2|$, $1 \leq \lambda_1 \leq 13$.
Actual eigenvalues are 4, $6 \pm \sqrt{17}$.

11.1 Population Growth

Population Growth. To model populations, a popular assumption is: the population growth is proportional to the size of the population:

$$\frac{dP}{dt} \propto P, \quad or, \quad \frac{dP}{dt} = kP.$$

By separating variables, we get the solution:

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

If k is positive, then the population increases. If k is negative, then the population decreases.

Example 46 *A bacteria culture growth at a rate proportional to its size. After 2 hours there are 40 bacteria and after 4 hours the count is 120. Find an expression for the population after t hours.*

Solution: We measure the time t in hours. Let $P(t)$ be the population at t hours, then we have

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

The solution of the equation is

$$P(t) = P(0)e^{kt}.$$

Note that $P(2) = 40$ and $P(4) = 120$, we obtain

$$40 = P(0)e^{2k}, \quad 120 = P(0)e^{4k}.$$

These imply that

$$P(0) = \frac{40}{3}$$

and

$$e^{2k} = 3, \quad \text{or} \quad k = \ln 3/2.$$

We thus have

$$P(t) = \frac{40}{3}3^{t/2} = \frac{40}{3}\sqrt{3}^t = \frac{40}{3}e^{(\ln 3/2)t}.$$

Example 47 *The half-life of Sodium-24 is 15 hours. Suppose you have 100 grams of Sodium-24. How many grams remaining after 27 minutes (keep three decimals)?*

Solution: Assume $m(t)$ be the amount after t hours. Then

$$m(t) = m(0)(\frac{1}{2})^{t/H},$$

where $m(0) = 100$, $H = 15$ hours. Note that 27 minutes = 27/60=0.45 hours. Thus

$$m(0.45) = 100(\frac{1}{2})^{0.45/15} = 100(\frac{1}{2})^{0.03} = 97.942g.$$

Limited Growth Model (logistic model). If the population is limited by maximum M, we have a simple submodel

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

where r is a constant. Then the equation becomes:

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

By separating variables,

$$\ln \frac{P}{M - P} = rMt + C.$$

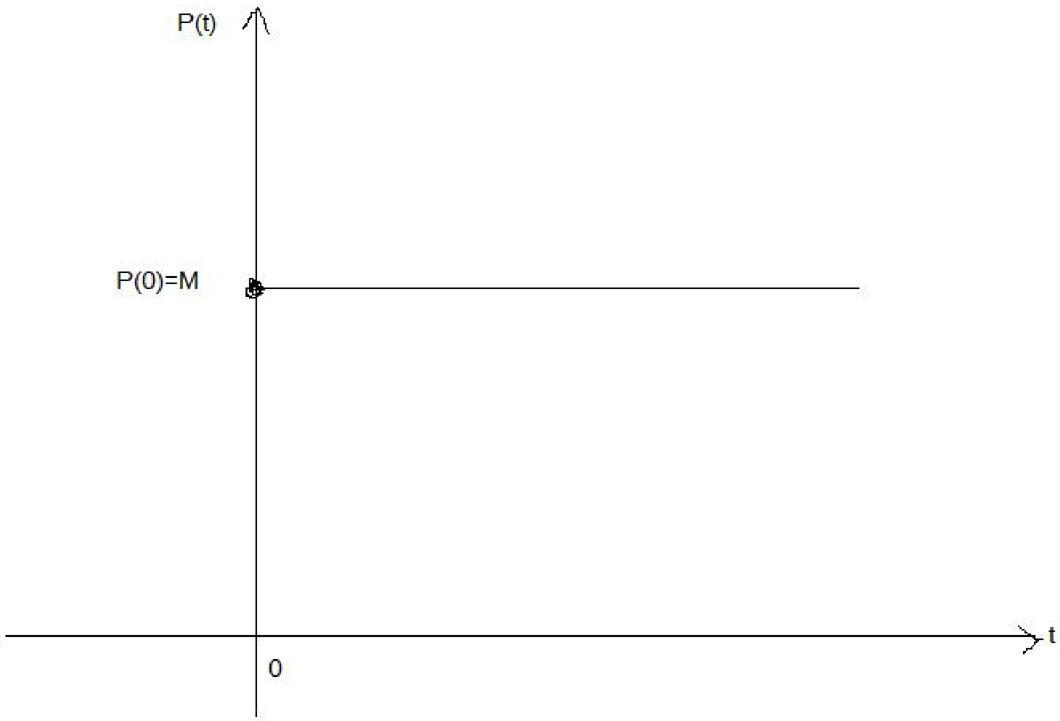
$$P(t) = \frac{MP(t_0)}{P(t_0) + (M - P(t_0))e^{-rM(t-t_0)}}.$$

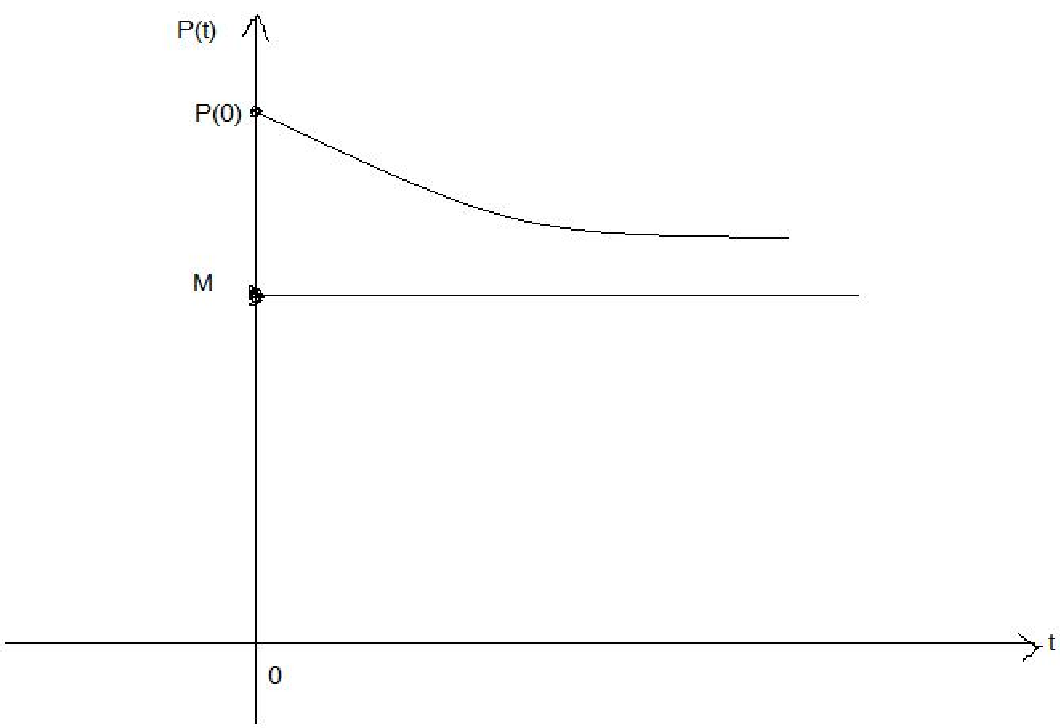
$$P(t) = \frac{M}{1 + [(M - P(t_0))/P(t_0)]e^{-rM(t-t_0)}} = \frac{M}{1 + de^{-rMt}}, \quad d = \frac{M - P(t_0)}{P(t_0)}e^{rMt_0}.$$

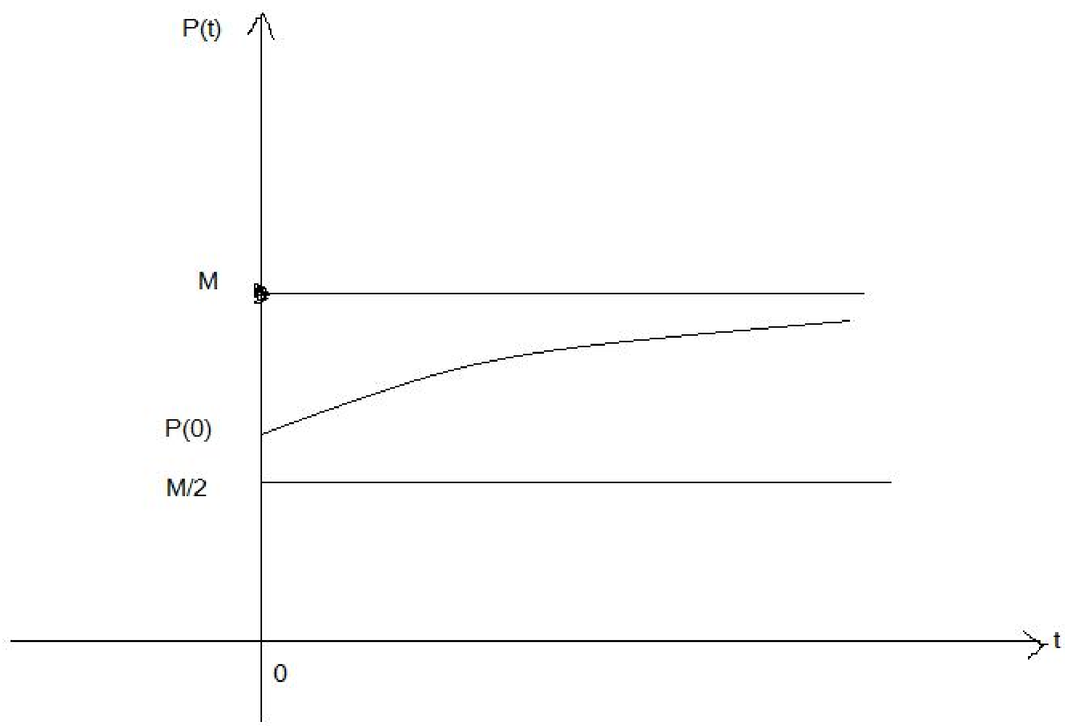
Let t^* be the time such that $P(t^*) = \frac{M}{2}$. Then

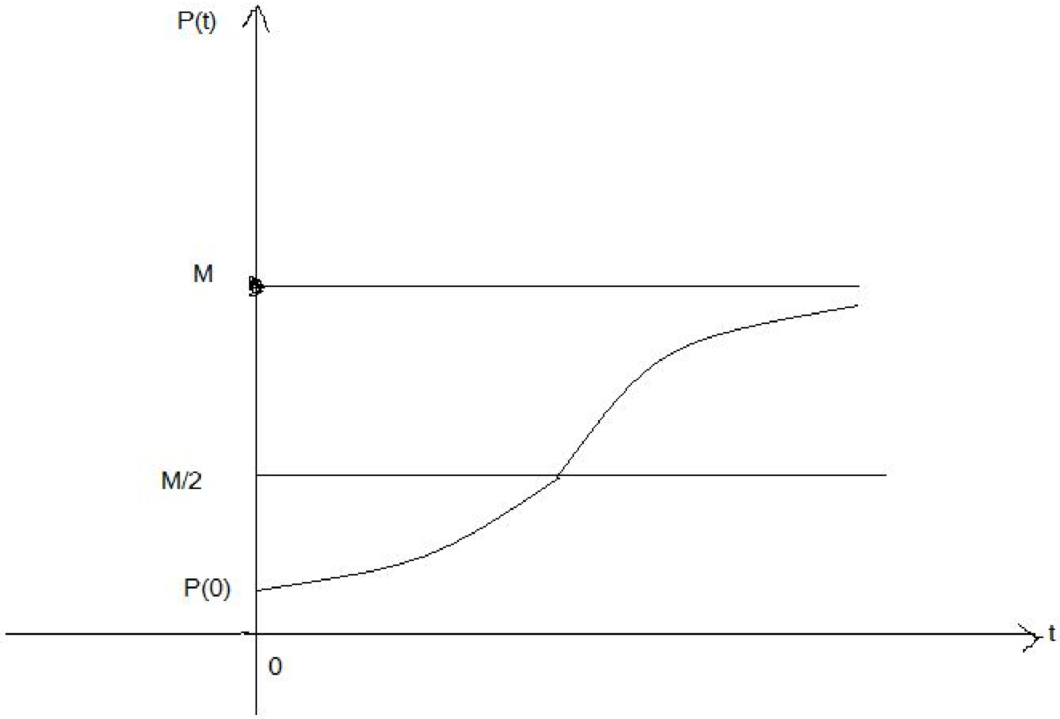
$$t^* = t_0 - \frac{1}{rM} \ln \frac{P_0}{M - P_0}, \quad or \quad t^* = -\frac{C}{rM}.$$

$$P(t) = \frac{M}{1 + e^{-rM(t-t^*)}}.$$


P(t)
P(0)=M
t
0

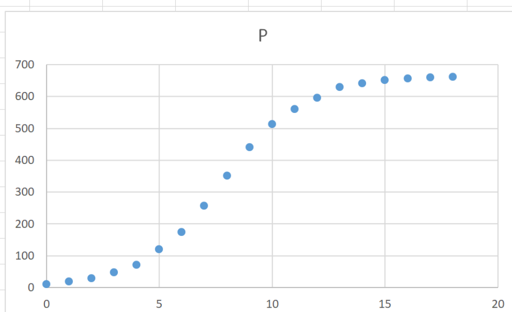

P(t)
P(0)
M
t
0


P(t)
M
P(0)
M/2
t
0



Example 48 *Yeast Culture: Given the data and scatterplot are as follows:*

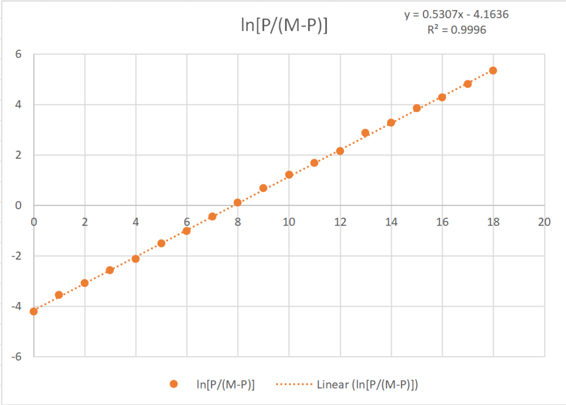
n	P
0	9.6
1	18.3
2	29
3	47.2
4	71.1
5	119.1
6	174.6
7	257.3
8	350.7
9	441
10	513.3
11	559.7
12	594.8
13	629.4
14	640.8
15	651.1
16	655.9
17	659.6
18	661.8



(1) Estimate M: $M \approx 665$.

(2) Plot $\ln[P/(M-P)]$ against t.

n	P	ln[P/(M-P)]
0	9.6	-4.223482638
1	18.3	-3.564981449
2	29	-3.087902733
3	47.2	-2.571770888
4	71.1	-2.122623618
5	119.1	-1.522472332
6	174.6	-1.032723741
7	257.3	-0.460288891
8	350.7	0.109583213
9	441	0.677398824
10	513.3	1.218955583
11	559.7	1.670587507
12	594.8	2.136876904
13	629.4	2.872421347
14	640.8	3.276364763
15	651.1	3.8467744
16	655.9	4.277733925
17	659.6	4.805234637
18	661.8	5.331812586



(3) Estimate r, t^*.

Solution:

$$rM = 0.5307, r = 0.5307/665 = 0.000798045.$$

$$t^* = -\frac{C}{rM} = -\frac{-4.1636}{0.5307} = 7.845487093.$$

11.4 Graphical Solutions of Autonomous Differential Equations

- $y' = f(y)$ is called **autonomous differential equation**.
- The solutions of $y' = f(y) = 0$ are called **equilibrium values (points)** or **rest points**.
- An equilibrium point is **stable** if solutions that begin near the equilibrium approach the equilibrium; An equilibrium point is **unstable** if solutions that begin near the equilibrium move away from the equilibrium.
- **Phase line** is the plot on the y axis with equilibrium values and intervals where y' and y'' are positive and negative.

Theorem 9 *(Stability Theorem). Consider the autonomous equation*

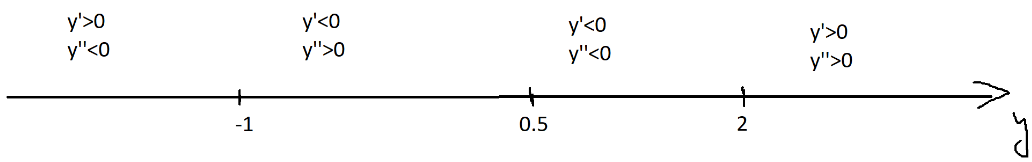
$$\frac{dy}{dt} = f(y)$$

with an equilibrium $y*$. If $f'(y*) < 0$, then $y*$ is stable; If $f'(y*) > 0$, then $y*$ is unstable.

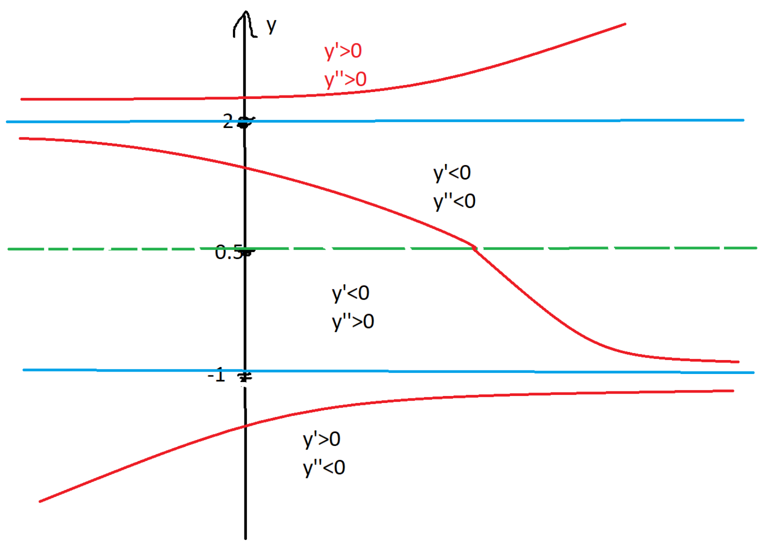
Example 49 *Consider the equation*

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

(1) Find the equilibrium values (points).
Solution: $y = -1, 2$.
(2) Identify intervals where y' and y'' are positive and negative.
Solution:
$y' = y^2 - y - 2$,
$y'' = 2yy' - y' = (2y-1)(y+1)(y-2)$.



(3) Graphic solution curves.



(4) Study the stability of the equilibrium points.

Solution: $y = -1$ is stable, $y = 2$ is unstable.

Example 50 *Newton's Law of Cooling:*

$$\frac{dT}{dt} = k(A - T),$$

where k is a positive constant, A is a constant, the temperature of the surrounding area.

Use Newton's Law of Cooling to determine the time of death of a healthy man.

- *He died in his room some time before noon;*
- *At noon, his body temperature was found to be 70 degrees;*
- *His body cooled another 5 degrees in 1 hour after noon;*
- *The room temperature was a constant 60 degrees;*
- *Normal temperature of people's body is 98.6 degree.*

Solution: Let $T(t)$ be the temperature of the body at time t. Taking noon as $t = 0$, we have $T(0) = 70$. Note that $T_s = 60$, we have

$$\frac{dT}{dt} = -k(T - 60),$$

this equation is separable. We obtain

$$\frac{dT}{T - 60} = -kdt, \Rightarrow T(t) = 60 + Ce^{-kt}.$$

From $T(0) = 70$ we get $70 = 60 + C$, $C = 10$ and

$$T(t) = 60 + 10e^{-kt}.$$

At 1:00pm, his body temperature is $70 - 5 = 65$. Hence $T(1) = 65$.

$$65 = 60 + 10e^{-k(1)}, \Rightarrow 5 = 10e^{-k}, \Rightarrow k = \ln 2, \Rightarrow T(t) = 60 + 10e^{-t\ln 2}.$$

Thus

$$98.6 = 60 + 10e^{-t\ln 2}, \Rightarrow t = -\ln 3.86/\ln 2 = -1.95,$$

which means 1 hour and 0.95(60) minutes before noon, or 1 hour and 57 minutes before noon. Or the time of death is 10:03AM.

Example 51 *Consider the logistic equation*

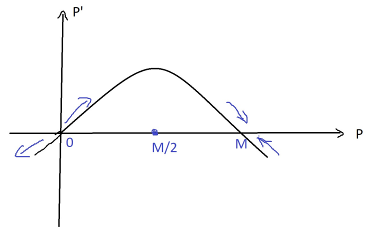
$$\frac{dP}{dt} = r(M - P)P.$$

Analyse the equilibria.

Solution: The equilibrium points are $0, M$. Let

$$f(P) = rP(M - P).$$

Then $f'(P) = rM - 2rP = r(M - 2P)$. $f'(0) = rM > 0$, $f'(M) = -rM < 0$.



- If $0 < P < M$, then $dP/dt > 0$ and thus, population grows (the point in the graph moves to the right).
- If $P < 0$ or $P > M$ (of course, $N < 0$ has no biological sense), then population declines (the point in the graph moves to the left).

The arrows show that the equilibrium $P = 0$ is unstable, whereas the equilibrium $P = M$ is stable. From the biological point of view, this means that after small deviation of population numbers from $P = 0$ (e.g., immigration of a small number of organisms), the population never returns back to this equilibrium. Instead, population numbers increase until they reach the stable equilibrium $P = M$. After any deviation from $P = M$ the population returns back to this stable equilibrium.

12.1 Graphical Solutions of Autonomous Systems of First-Order Differential Equations

Autonomous Systems of First-Order Differential Equations :

$$\begin{cases} \frac{dx}{dt} &= f(x,y) \\ \frac{dy}{dt} &= g(x,y). \end{cases}$$

- A solution is a pair $x = x(t)$, $y = y(t)$ satisfying the system.
- The solution curve whose coordinates are $(x(t), y(t))$ is called a **trajectory, path, orbit** of the system.
- The xy-plane is referred to as **phase plane**.
- The point(x, y) satisfying both $f(x, y) = 0$ and $g(x, y) = 0$ is called **equilibrium point** or **rest point**.
- An equilibrium point (x_0, y_0) is
  - **stable** if any trajectory that starts close to the point stays close to it for all future time;
  - **asymptotically stable** it it is stable and if any trajectory that starts close to (x_0, y_0) approaches that point as $t \to \infty$;
  - **unstable** if (x_0, y_0) is not stable.

Properties:

1. There is at most one trajectory through any point in the phase plane.
2. A trajectory that starts at a point other than an equilibrium point can not reach an equilibrium point in a finite amount of time.
3. No trajectory can cross itself unless it is a closed curve. If it is a closed curve, it is a periodic solution.

4. A particle along a trajectory behaves in one of three possible ways: (a) the particle approaches an equilibrium point; (b) the particle moves along or approaches asymptotically a closed path; (c) either $x(t) \to \infty$ or $y(t) \to \infty$ as $t \to \infty$.

Example 52 *Consider the system:*

$$\begin{cases} \frac{dx}{dt} &= -x + y \\ \frac{dy}{dt} &= -x - y. \end{cases}$$

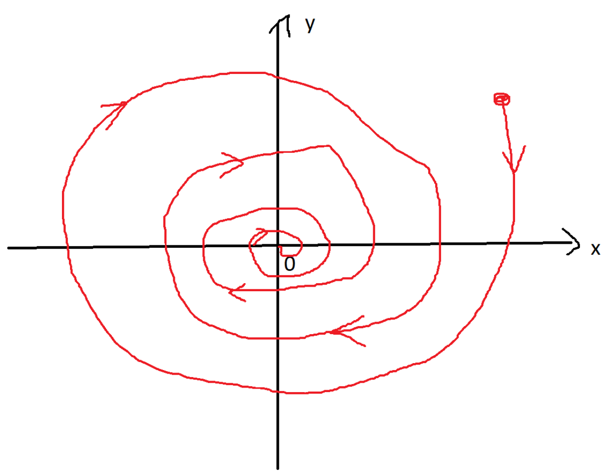
(a) Verify that The solution of the system is $x = e^{-t}\sin t$, $y = e^{-t}\cos t$.
(b) Find the equilibrium points and study the stability of the system

Solution:
(b) Solve the system

$$\begin{cases} -x + y &= 0 \\ -x - y &= 0. \end{cases}$$

The equilibrium point is $(x, y) = (0, 0)$. Note that

$$x^2 + y^2 = e^{-2t} \to 0 \quad as \quad t \to \infty.$$



The equilibrium point is asymtotically stable.

12.2 A Competitive Hunter Model

Consider fish species in Ontario Rideau Lake.

- Let $x(t)$ be the pike-fish population.
- Let $y(t)$ be the bass-fish population..

Then we have the following Competitive Hunter model:

$$\begin{aligned} dx/dt &= (a - by)x, \\ dy/dt &= (m - nx)y, \end{aligned}$$

where a, b, m, n are positive constants.

Equilibrium points:

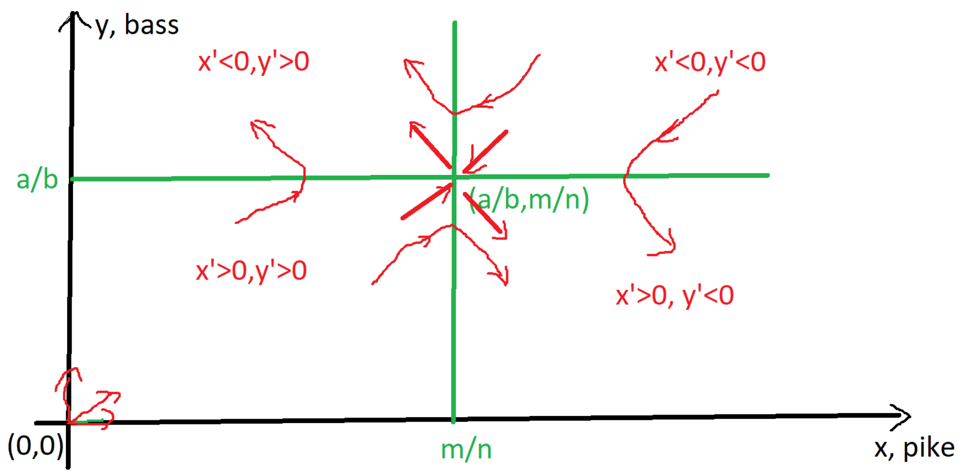
1. $x'(t) = 0 \Leftrightarrow y = \frac{a}{b}$.
2. $y'(t) = 0 \Leftrightarrow x = \frac{m}{n}$.

Thus equilibria: $(x, y) = (0, 0), (\frac{m}{n}, \frac{a}{b})$ in the phase plane.

- Along the vertical line $x = \dfrac{m}{n}$ and the x axis in the phase plane, the growth in the bass population is zero;
- Along the horizontal line $y = \dfrac{a}{b}$ and the y axis in the phase plane, the growth in the pike population is zero.

Graphical Analysis of the Model:

- Whenever $x'(t) > 0$, the component $x(t)$ of the trajectory is increasing and the trajectory is moving toward the right; whenever $x'(t) < 0$ is negative, the trajectory is moving to the left.
- Whenever $y'(t) > 0$, the component $y(t)$ of the trajectory is increasing and the trajectory is moving upward; whenever $y'(t) < 0$, the trajectory is moving downward.
- The directions of the associated trajectories are indicated in the following phase plane figure.



Stability of equilibria: both $(x, y) = (0, 0), (\frac{m}{n}, \frac{a}{b})$ are unstable.

Analytic Solution of the Model:

$$\frac{dy}{dx} = \frac{(m - nx)y}{(a - by)x},$$
$$\left(\frac{a}{y} - b\right) dy = \left(\frac{m}{x} - n\right) dx,$$
$$a \ln y - by = m \ln x - nx + K.$$

12.3 A Predator-Prey Model

Consider fish species in Ontario Rideau Lake. It's reasonable to assume that:

- The predator species (such as pike, walleye, bass, muskie) is totally dependent on the prey species as their only food supply.
- The prey species (such as sunfish, perch) has an unlimited food supply and no threat to their growth other than the specific predator.

Lotka-Volterra Model . The mass action approach to modelling trophic interactions was pioneered, independently, by the American physical chemist Lotka (1925) and Italian mathematician Volterra (1926). These authors argued that consumer and resource populations could be treated like particles interacting in a homogeneously mixed gas or liquid.

Principle of Mass Action: The (reaction) rate of encounter between consumers and resources would be proportional to the product of their masses.

- $x(t)$ = resource population (bacteria, prey)n.
- $y(t)$ = consumer population (amoebas, predator) .

The dynamics of the interaction between them is then described by the differential equations (system):

$$\begin{aligned} dx/dt &= (a - by)x, \\ dy/dt &= (nx - m)y, \quad n = cb, \end{aligned}$$

where a, b, m, n are positive constants, a represents the per-capita rate of change of the resource in the absence of consumers, b the consumption rate of the consumer, c the constant of conversion of resources into consumer offspring, and m the per-capita mortality rate of consumers in the absence of resources. The terms in the equations have the following meaning:

1. ax = the growth rate of the resource population in the absence of predators. Thus, in the absence of predators, the resource population grows according to the equation $dx/dt = ax$, i.e., $x(t) = x(0)e^{at}$, exponential growth.

2. byx = the rate of consumption of resources, or their death rate due to attack by predators.

3. $cbxy$ = the rate of production of predator offspring, which is directly related to the number of prey consumed.

4. my = the death rate of consumers in the absence of food (prey). Thus, in the absence of prey, predators die according to $dy/dt = -my$, i.e., $y(t) = y(0)e^{-mt}$, exponential decay.

Equilibrium points: $(x, y) = (0, 0), (\frac{m}{n}, \frac{a}{b})$.

Graphical Analysis of the Model:

1. Find the nullcline of x, i.e., the set of points where $dx/dt = 0$, or equivalently $f(x, y) = 0$.

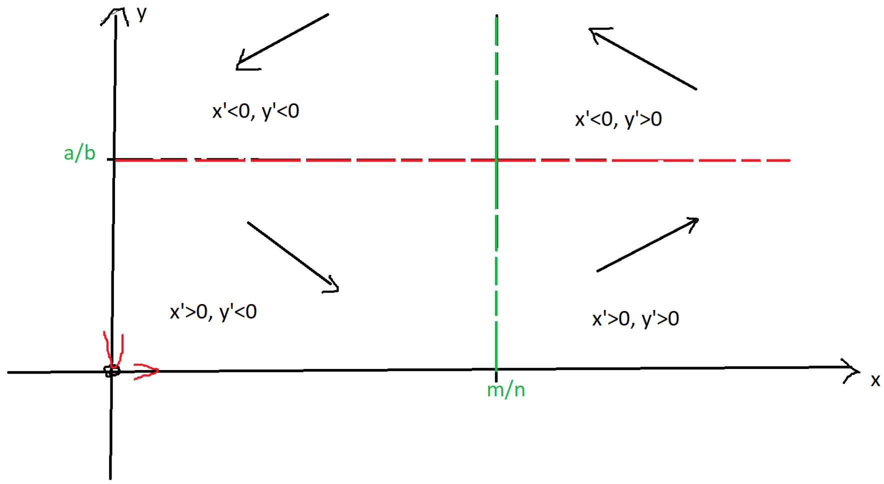
2. Find the nullcline of y, i.e., the set of points where $dy/dt = 0$, or equivalently $g(x, y) = 0$.

3. Draw these two sets in the phase plane: xy-plane.

4. The intersection of the nullclines are equilibrium points (or steady states, or rest points).

5. On each of the nullclines, draw the direction arrows.

6. In each of the regions in space in between the nullclines, draw the direction arrows.



Stability of equilibria: The equilibrium $(x, y) = (0, 0)$ is unstable.

Sketch trajectories (solution curves):

For a given initial condition, draw a solution into the phase plane. Then plot the two components of the solution as a function of time.

Analytic Solution of the Model:

$$\frac{dy}{dx} = \frac{(nx - m)y}{(a - by)x},$$

$$\left(\frac{a}{y} - b\right) dy = \left(n - \frac{m}{x}\right) dx,$$

$$a \ln y - by = nx - m \ln x + K.$$

Example 53 *Find the equilibrium points, study stabilities, and sketch trajectories (solution curves).*

$$\begin{aligned} dx/dt &= x(0.33 - 0.2y), \\ dy/dt &= y(0.1x - 0.5). \end{aligned}$$

11.5 Numerical Approximation Methods

Euler's method: Consider the initial value problem

$$\frac{dy}{dx} = f(x, y), \quad y(x_0) = y_0, \quad x_0 \leq x \leq b.$$

If $h = \Delta x$ is the step size, then

$$y_{n+1} = y_n + hf(x_n, y_n), \quad x_{n+1} = x_n + h.$$

Example 54 *Let $y(x)$ be the solution of the initial value problem $y' = x + y$, $y(0) = 0$.*

(a) Use Euler's method with step size 0.1 to estimate $y(0.4)$;
(b) Verify that the exact solution is $y = -x - 1 + 2e^x$.
(c) Calculate the error in (a).

Solution:
(a)

i	x_i	y_i
0	0	0
1	0.1	0
2	0.2	0.01
3	0.3	0.031
4	0.4	0.0641

(b) The actual value at 0.4 is $y(0.4) = 0.091825$.
(c) Absolute Error=$|0.091825 - 0.0641| = 0.027725$.

Remark. It is not true that by taking h sufficiently small one can obtain any desired level of precision.

Euler's Method to a system:

$$\begin{aligned} dx/dt &= f(x,y), \\ dy/dt &= g(x,y). \end{aligned}$$

Let $h = \Delta t$.

$$\begin{cases} t_{n+1} = t_n + h, \\ x_{n+1} = x_n + hf(x_n, y_n), \\ y_{n+1} = y_n + hg(x_n, y_n). \end{cases}$$

Example 55 *Consider the system*

$$\begin{aligned} dx/dt &= (3-y)x, \\ dy/dt &= (x-2)y, \end{aligned}$$

with $t_0 = 0$, $h = 0.1$, $x_0 = 1, y_0 = 2$. *Find* t_3, x_3, y_3.

i	t_i	x_i	y_i
0	0	1	2
1	0.1	1.1	1.8
2	0.2	1.232	1.638
3	0.3	1.3997984	1.5122016

Improved Euler's Method. Use Euler's method to get 'predicted' value (**predictor**), then use improved formula to get 'corrected' value (**corrector**):

$$\begin{aligned} y_{n+1}^p &= y_n^c + hf(x_n, y_n^c) \\ y_{n+1}^c &= y_n^c + \frac{1}{2}h\left[f(x_n, y_n^c) + f(x_{n+1}, y_{n+1}^p)\right] \end{aligned}$$

Example 56 *Let $y(x)$ be the solution of the initial value problem $y' = x + y$, $y(0) = 0$. Use step size 0.1 to estimate $y(0.4)$ and calculate the error.*

Solution:

i	x_i	y_i^p	y_i^c
0	0	0	0
1	0.1	0	0.005
2	0.2	0.0155	0.021025
3	0.3	0.043128	0.049233
4	0.4	0.084156	0.090902

The actual value at 0.4 is $y(0.4) = 0.091825$.
Absolute Error=$|0.091825 - 0.090902| = 0.000923$.

Runge-Kutta Method

Euler's Method gave us one possible approach for solving differential equations numerically. The problem with Euler's Method is that you have to use a small interval size to get a reasonably accurate result. That is, it's not very efficient.

The Runge-Kutta Method of 4th order (RK4), Multi-step Predictor-corrector Method , produces a better result in fewer steps.

We wish to approximate the solution to a first order differential equation given by

$$\frac{dy}{dx} = f(x, y), \quad y(x_n) = y_n.$$

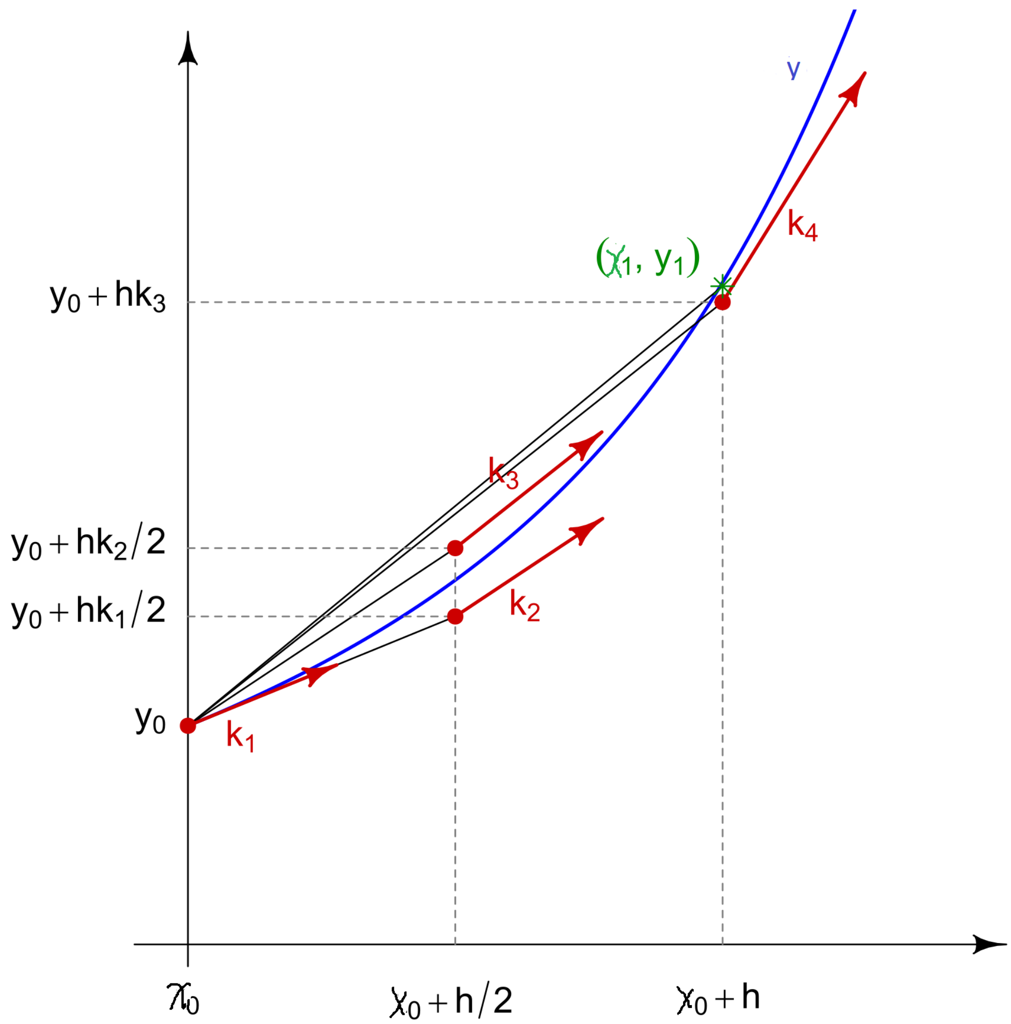
We will use the following slope approximations to estimate $y_{n+1} = y(x_n+h)$ at $x_{n+1} = x_n+h$ with step size h.

$$\begin{aligned} k_1 &= hf(x_n, y_n) \\ k_2 &= hf(x_n + \frac{1}{2}h, y_n + \frac{1}{2}k_1) \\ k_3 &= hf(x_n + \frac{1}{2}h, y_n + \frac{1}{2}k_2) \\ k_4 &= hf(x_n + h, y_n + \frac{1}{2}k_3) \end{aligned}$$

$$y_{n+1} = y_n + \frac{1}{6}(k_1 + 2k_2 + 2k_3 + k_4).$$

Each of these estimates can be described verbally.

- k_1 is the increment based on the slope at the beginning of the interval, using y (Euler's method);
- k_2 is the increment based on the slope at the midpoint of the interval, using y and k_1;
- k_3 is the increment based on the slope at the midpoint of the interval, using y and k_2;
- k_4 is the increment based on the slope at the end of the interval, using y and k_3.



Example 57 *Use Runge-Kutta method of order 4 to solve the following equation, using the step size $h = 0.1$ for $0 \le x \le 1$:*

$$\frac{dy}{dx} = (5x^2 - y)e^{-(x+y)}, \quad y(0) = 1.$$

Solution:

Step 1:

$k_1 = hf(x_0, y_0) = 0.1f(0, 1) = 0.03678794411.$

$k_2 = hf(x_0 + \frac{1}{2}h, y_0 + \frac{1}{2}k_1) = 0.1f(0.05, 0.98160602794) = 0.03454223937.$

$k_3 = hf(x_0 + \frac{1}{2}h, y_0 + \frac{1}{2}k_2) = 0.1f(0.05, 0.98272888031) = 0.03454345267.$

$k_4 = hf(x_0 + \frac{1}{2}h, y_0 + \frac{1}{2}k_3) = 0.1f(0.05, 0.96545654732) = 0.03154393258.$
We take those 4 values and substitute them into the Runge-Kutta RK4 formula:

$$y_1 = y(x_0 + h) = y(0.1) = y(0) + \frac{1}{6}(k_1 + 2k_2 + 2k_3 + k_4)$$

$$= 1 + \frac{1}{6}(0.03678794411 - 2 \times 0.03454223937 - 2 \times 0.03454223937 - 0.03154393258)$$

$$= 0.9655827899$$

Steps 2-10: Repeat Step 1 with initial values $(x_1, y_1) = (0.1, 0.9655827899)$.

x	y	K1	K2	K3	K4
0	1	- 0.0367879441	- 0.0345422394	- 0.0345434527	- 0.0315439326
0.1	0.9655827899	- 0.0315443	- 0.0278769283	- 0.0278867954	- 0.023647342
0.2	0.937796275	- 0.023648185	- 0.0189267761	- 0.0189548088	- 0.0138576597
0.3	0.9189181059	- 0.0138588628	- 0.0084782396	- 0.0085314167	- 0.0029773028
0.4	0.9104421929	- 0.0029786344	0.0026604329	0.002580704	0.0082022376
0.5	0.913059839	0.0082010354	0.013727301	0.0136258867	0.018973147
0.6	0.9267065986	0.0189722976	0.0240794197	0.0239658709	0.0287752146
0.7	0.9506796142	0.0287748718	0.0332448616	0.0331305132	0.0372312889
0.8	0.9838057659	0.0372315245	0.0409408747	0.0408359751	0.0441484563
0.9	1.024628046	0.0441492608	0.0470593807	0.0469712279	0.0494916177
1	1.0715783953				

Example 58 *Use Runge-Kutta method of order 4 to solve the following equation, using the step size $h = 0.5$ for $0 \le t \le 2$:*

$$\frac{dy}{dt} = y - t^2 + 1, \quad y(0) = 0.5.$$

Given that the exact solution is

$$y(t) = t^2 + 2t + 1 - \frac{1}{2}e^t,$$

estimate the error.

Solution:

Step 1:

$k_1 = hf(t_0, y_0) = 0.5f(0, 0.5).$

$k_2 = hf(t_0 + \frac{1}{2}h, y_0 + \frac{1}{2}k_1) = 0.5f(0.25, 0.5 + k_1/2).$

$k_3 = hf(t_0 + \frac{1}{2}h, y_0 + \frac{1}{2}k_2) = 0.5f(0.25, 0.5 + k_2/2).$

$k_4 = hf(t_0 + \frac{1}{2}h, y_0 + \frac{1}{2}k_3) = 0.5f(0.25, 0.5 + k_3/2).$

We take those 4 values and substitute them into the Runge-Kutta RK4 formula:

$$y_1 = y(t_0 + h) = y(0.5) = y(0) + \frac{1}{6}(k_1 + 2k_2 + 2k_3 + k_4)$$

Steps 2-4: Repeat Step 1 with initial values (t_1, y_1).

t_n	Exact solution $y(t_n)$	Numerical solution y_n	Error $\lvert y(t_n) - y_n\rvert$
0.0	0.5	0.5	0
0.5	1.425639364649936	1.425130208333333	0.000509156316603
1.0	2.640859085770477	2.639602661132812	0.001256424637665
1.5	4.009155464830968	4.006818970044454	0.002336494786515
2.0	5.305471950534675	5.301605229265987	0.003866721268688

If we take step size $h = 0.2$, then the solution is:

t_n	Exact solution $y(t_n)$	Numerical solution y_n	Error $\lvert y(t_n) - y_n\rvert$
0.0	0.5	0.5	0
0.2	0.829298620919915	0.829293333333333	0.000005287586582
0.4	1.214087651179365	1.214076210666667	0.000011440512698
0.6	1.648940599804746	1.648922017041600	0.000018582763146
0.8	2.127229535753766	2.127202684947944	0.000026850805823
1.0	2.640859085770477	2.640822692728752	0.000036393041726
1.2	3.179941538631726	3.179894170232231	0.000047368399496
1.4	3.732400016577663	3.732340072854980	0.000059943722683
1.6	4.283483787802442	4.283409498318406	0.000074289484036
1.8	4.815176267793527	4.815085694579435	0.000090573214092
2.0	5.305471950534674	5.305363000692655	0.000108949842019

All this can be done by using Matlab:

```
function rungekutta
    h = 0.5;
    t = 0;
    w = 0.5;
    fprintf('Step 0: t = %12.8f, y = %12.8f\n', t, y);
    for i=1:4
        k1 = h*f(t,y);
        k2 = h*f(t+h/2, y+k1/2);
        k3 = h*f(t+h/2, y+k2/2);
        k4 = h*f(t+h, y+k3);
        y = y + (k1+2*k2+2*k3+k4)/6;
        t = t + h;
        fprintf('Step %d: t = %6.4f, y = %18.15f\n', i, t, y);
    end
%%%%%%%%%%%%%%%%%%
function v = f(t,y)
v = y-t^2+1;
```