Mathematical Modeling
Lia Vas

Discrete Dynamical Systems. Difference Equations

Recall that the change can be modeled using the formula

$$\text{change} = \text{future value} - \text{present value}.$$

If values that we monitor changes during discrete periods (for example, in discrete time intervals), the formula above leads to a difference equation or a dynamical system. In this case, we are dealing with a function that depends on discrete integer values – a sequence.

Recall that a sequence of real numbers (indexed by nonnegative integers) can be given by listing its terms (for example, $1, \frac{1}{2}, \frac{1}{3}, \ldots$) or by the formula for its n-th term (for example $a_n = \frac{1}{n}$). Alternatively, a sequence of real numbers $\{a_n\}$ can be represented by a recursive equation

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

with some initial value a_0. This relationship between terms of a sequence is called a **dynamical system**.

A dynamical system allows us to describe the change from one state of the system to the next. At n-th stage, the change is described by

$$\text{change at stage } n = \text{future } (n+1)\text{-st state} - \text{present } n\text{-th state} = a_{n+1} - a_n$$

The difference $a_{n+1} - a_n$ is frequently denoted by Δa_n and is called a **change** or **n-th first difference**.

A **difference equation** is an equation of the form

$$\Delta a_n = g(a_n)$$

A **solution** of a difference equation is a sequence a_n. The solution can be given analytically (i.e. by the formula of a_n in terms of n), graphically, or numerically (i.e. as a table of a_n values for various values of n).

Every dynamical system $a_{n+1} = f(a_n)$ **determines a difference equation** obtained by subtracting a_n from both sides of the equation. We obtain $a_{n+1} - a_n = f(a_n) - a_n$. Note that the left side is Δa_n. If we denote the right side by $g(a_n)$, we obtain the difference equation $\Delta a_n = g(a_n)$.

Conversely, **every difference equation** $\Delta a_n = g(a_n)$ **determines a dynamical system** by writing the left side as $a_{n+1} - a_n$ and solving for a_{n+1}. We obtain that $a_{n+1} = g(a_n) + a_n$. Denoting the right side by $f(a_n)$, we obtain the dynamical system $a_{n+1} = f(a_n)$.

The difference equation $\Delta a_n = g(a_n)$ is a discrete analogue of the autonomous differential equation $y' = g(y)$. The stable equilibrium solutions of differential equation $y' = g(y)$ correspond to the accumulation points of the sequence a_n that is the solution of difference equation $\Delta a_n = g(a_n)$ with the initial value a_0. Recall that the equilibrium solutions were obtained by solving $g(y) = 0$ for y. Analogously, **we obtain the limiting values by solving** $g(a) = 0$ **for** a.

This fact can be explained also by the following argument. Note that if $\lim_{n\to\infty} a_n = a$, then the values of a_{n+1} and of a_n will be close to each other for large values of n. Thus, $\Delta a_n =$

$a_{n+1} - a_n = g(a_n)$ is close to 0. So, when $n \to \infty$, $g(a_n) \to 0$. Thus, if a is the limiting value $\lim_{n\to\infty} a_n$, a **can be obtained as a solution of the equation** $g(a) = 0$.

Let us consider a dynamical system $a_{n+1} = f(a_n)$. If a is the limiting value $\lim_{n\to\infty} a_n$, then $\lim_{n\to\infty} a_{n+1}$ is equal to a as well. Thus, a **can be obtained as a solution of the equation** $a = f(a)$.

Note that a limit of sequence a_n also corresponds to the values of the sequence satisfying $a_{n+1} = f(a_n)$ with initial value $a_0 = a$. Namely, if a is such that $a = f(a)$ and we consider a dynamical system given by $a_{n+1} = f(a_n)$ and $a_0 = a$, then

$$a_1 = f(a_0) = f(a) = a, \quad a_2 = f(a_1) = f(a) = a, \quad \ldots \quad a_{n+1} = f(a_n) = f(a) = a \ldots$$

We obtain a constant sequence with all terms equal to a. Because of this, the limiting value a of a dynamical system $a_{n+1} = f(a_n)$ is also called a **fixed point,** a **steady state** or, using the same terminology as in continuous case, **equilibrium solution**. Thus, a is a fixed point of $a_{n+1} = f(a_n)$ if and only if $a = f(a)$ when $a_0 = a$. The same terminology regarding stability is used as in the case of autonomous differential equations. To determine the stability, sketch the graph according to the sign of $f(a) - a$.

Example 1. Consider the dynamical system given by $a_{n+1} = \sqrt{6 + a_n}$. Find the fixed points and check their stability. Using the graph, determine the limit of solutions with initial conditions $a_0 = -3$, $a_0 = 0$, and $a_0 = 5$ respectively.

Solution. The fixed points can be obtained from the equation $a = \sqrt{6+a} \longrightarrow a^2 = 6 + a \longrightarrow a^2 - a - 6 = 0 \longrightarrow a = 3$ and $a = -2$. Plugging $a = -2$ in the original equation, we conclude that it is an extraneous root, ($\sqrt{6-2} = 2$, not -2) so $a = 3$ is the only fixed point. Considering the sign of $\sqrt{6+a} - a$, we conclude the following.

- The solutions with initial value with $a_0 > 3$ decrease towards 3. If the initial value $a_0 = 3$, we obtain a constant solution with fixed point 3.
- The solutions with initial value such that $-6 \leq a_0 < 3$, increase towards 3. Thus 3 is a stable equilibrium solution.
- The formula describing the dynamical system is not defined for the initial values with $a_0 < -6$.

Finally, from this analysis we can conclude that the solutions with initial conditions $a_0 = -3$ and $a_0 = 0$ will increase to 3, and the solution with initial condition $a_0 = 5$ will decrease to 3.

The relationship between terms of a sequence can be such that the next term depends on more than one of the previous terms of the sequence. Thus, a dynamical system can be a function of more than one variable. The most general recursive formula has the form

$$a_{n+1} = f(a_0, a_1, \ldots a_n)$$

Example 2. Fibonacci numbers are terms of the following recursive sequence.

$$f_0 = 0, f_1 = 1 \text{ and } f_n = f_{n-1} + f_{n-2}$$

in other words: one starts with 0 and 1, and then produces the next Fibonacci number by adding the two previous Fibonacci numbers. The following sequence is obtained

$$0, 1, 1, 2, 3, 5, 8, 13, 21, 34, 55, 89, 144, 233, 377, 610, 987, 1597, 2584, 4181, 6765, \ldots$$

This sequence is clearly divergent. However, sometimes one is interested in a sequence determined by the **quotient of two consecutive terms of the Fibonacci sequence**. So, let us denote $a_n = \frac{f_n}{f_{n-1}}$. Dividing the equation $f_n = f_{n-1} + f_{n-2}$ by f_{n-1}, we obtain $\frac{f_n}{f_{n-1}} = 1 + \frac{f_{n-2}}{f_{n-1}} \longrightarrow a_n = 1 + \frac{1}{a_{n-1}}$. Multiplying by a_{n-1}, we obtain $a_n a_{n-1} = a_{n-1} + 1$.

The fix point of this sequence is the solution of $a^2 = a + 1$. Solving this equation gives us $\frac{1 \pm \sqrt{5}}{2} \approx 1.618$ and -0.618. The positive solution is called the **golden ratio** and is a stable equilibrium value (consider the sign of $a + 1 - a^2$). In particular, the sequence a_n with initial condition 1 decreases and converges to $\frac{1+\sqrt{5}}{2}$.

The golden ratio is defined as the ratio that results when a line segment is divided so that the whole segment has the same ratio to the larger segment as the larger segment has to the smaller segment. If we start with a line such that the larger part has length 1, and if x denotes the length of the line segment, this gives us $\frac{1}{x} = \frac{x-1}{1}$. Cross multiplying gives us $1 = x^2 - x$ which is the same quadratic equation as the one producing the fix point of the sequence defined by quotients of consecutive terms of Fibonacci sequence.

Exponential growth or decay. Let k be a positive number. A frequently used dynamical system is obtained when assuming that a certain quantity is **changing by a multiple of** k in every time unit. Thus, this process can be modeled by the dynamical system

$$a_{n+1} = ka_n$$

or, alternatively by the difference equation $\Delta a_n = (k-1)a_n$. If r denotes $k-1$, the difference equation becomes

$$\Delta a_n = ra_n.$$

The quantity $r = k - 1$ can be interpreted as the **percent change**.

The equilibrium solution is obtained from equation $ra = 0$ and is $a = 0$. We distinguish the following cases.

- If $r > 0$ ($k > 1$), the equilibrium solution is unstable. The sequences with positive initial values are increasing without bounds.

- If $r < 0$ ($0 < k < 1$), the equilibrium solution is stable. The sequences with positive initial values are decreasing towards 0.

- If $r = 0$ ($k = 1$) the sequence is constant - every term is equal to the initial value.

It is not hard to determine the explicit formula describing the terms of the sequence. Let a_0 denote the initial value. Then $a_1 = ka_0$, $a_2 = ka_1 = k^2 a_0$, $a_3 = ka_2 = k^3 a_0, \ldots$ Thus $a_n = k^n a_0$ or

$$a_n = a_0(r+1)^n$$

Discrete versus continuous. Let us compare the system from previous example (quantity changing by factor k in each time interval) with the system that is changing by factor k **continuously** throughout the time unit. The continuous analogue of the difference equation $\Delta a_n = ra_n$, with initial value a_0 is the differential equation $y' = ry$, $y(0) = a_0$. Note that this is an autonomous differential equation with equilibrium solution $y = 0$ that is unstable for $r > 0$ and stable for $r < 0$.

The differential equation $y' = ry$ has solution $y = a_0e^{rt}$. If we consider n as a measure of time elapsed in the discrete case, the solution $a_n = a_0(r+1)^n$ of difference equation corresponds to the exponential function $y = a_0(1+r)^t$. Thus, if a_0 is the initial size, we have that:

- A quantity increasing by percent r in discrete time intervals has the size given

$$y = a_0(1+r)^t.$$

- A quantity increasing by percent r continuously, has the size given by

$$y = a_0e^{rt} = a_0\left(e^r\right)^t.$$

Both of these functions are exponential functions. The first one has base $1+r$ and the second base e^r. Note that the values of $1+r$ and e^r are close for small values of r (compare the graphs of these two functions near $r = 0$). That is $1+r \approx e^r$. Note also that $1+r$ are the first two terms of the Taylor series of e^r centered at zero ($e^r = \sum_{n=0}^{\infty} \frac{r^n}{n!} = 1 + r + \frac{r^2}{2} + \frac{r^3}{6} + \ldots \approx 1 + r$.)

Example 3. If one invests 1000 dollars to an account with annual interest rate of 5 percent, find the amount on the account after 3 years if the interest is computed a) annually, b) continuously.

Solution. a) $1000 \cdot 1.05^3 = 1157.625$ b) $1000e^{.05 \cdot 3} = 1161.834$. Note that .05 is pretty close to 0 so the difference between two values is not that large. Also note that the amounts would differ by more if either the number of years in question was larger, or the annual interest rate was larger.

Consider now a dynamical system with the positive initial value a_0 that is defined by the equation

$$a_{n+1} = ka_n + b$$

where k is a positive proportionality constant. Let us again denote $k-1$ with r. The difference equation describing this system is $\Delta a_n = a_{n+1} - a_n = ka_n + b - a_n = (k-1)a_n + b = ra_n + b$. The equilibrium solution is $a = -b/r$. The stability will depend on the sign of r again. We distinguish two cases.

1. If $r > 0$ ($k > 1$) the equilibrium solution is unstable. The sequence is increasing without bounds.

   An example of the situation that can be modeled by such dynamical system is a bank account with a monthly interest rate $r > 0$ (so $k = 1 + r > 1$) on which a fixed amount b is deposited each month.

2. If $r < 0$ ($0 < k < 1$) the equilibrium solution is stable. The sequence is decreasing towards $\frac{b}{-r} = \frac{b}{1-k}$.

   An example of the situation that can be modeled by such dynamical system is the following: a person is given the same dose b of a medicine at equally spaced time intervals. The body metabolizes some of the drug so that, after some time, only a portion k of the original amount remains.

Example 4. Determine the explicit formula of the sequence in the case when $k < 1$. If the dynamical system describes the amount of drug given in the same dose b of a medicine at equally spaced time intervals, the body metabolizes some of the drug so that, after some time, only a portion k of the original amount remains. Find the formula describing the amount of drug right before and after the n-th dose. Sketch the graph of the concentration as function of time.

Solution. After the each dose, the amount of the drug in the body is equal to the amount of the given dose b plus the amount remnant from the previous dose. The dynamical system $a_{n+1} = ka_n + b$ with initial value b describes this situation. Let us calculate the first few terms of the sequence.

Step 0 Size $= b$.

Step 1 Amount remaining of previous step: kb. Amount added: b. Total amount $= b + kb$

Step 2 Amount remaining of previous step: $k(b + kb) = kb + k^2b$. Amount added: b. Total amount $=b + kb + k^2b$.

...

Step n Amount remaining of previous step: $k(b+kb+\ldots+k^{n-1}b)$. Amount added: b. Total amount $= b + kb + k^2b + \ldots + k^nb$.

Consider the n-th term

$$a_n = b + kb + k^2b + \ldots + k^nb = b(1 + k + \ldots + k^n) = \frac{b(1 - k^{n+1})}{1 - k}.$$

Here we used the fact that $(1-k^{n+1})$ factors as $(1-k)(1+k+\ldots+k^n)$ and so $1+k+\ldots+k^n = \frac{1-k^{n+1}}{1-k}$. This formula describes the amount of the drug present in the body right after the n-th dose.

Letting $n \to \infty$, and noting that $k < 1$ and so $k^{n+1} \to 0$, we obtain that

$$\lim_{n\to\infty} a_n = \lim_{n\to\infty} \frac{b(1 - k^{n+1})}{1 - k} = \frac{b(1 - 0)}{1 - k} = \frac{b}{1 - k}$$

The value $\frac{b}{1-k}$ is the same limiting value we obtained earlier as fixed point of $a_{n+1} = ka_n + b.$. Note also that the limit $\frac{b}{1-k}$ is the sum of the geometric series $b\sum_{n=0}^{\infty} k^n = b+bk+bk^2+\ldots = \frac{b}{1-k}$.

Thus, the amount of the drug in the body present after the new dose in the long run is $A = \frac{b}{1-k}$ and the amount of the drug present before the new dose is $A - b$. The amount A is sometimes called the **steady state**.

Elimination rate. In some cases, the elimination rate $p = 1 - k$ will be of interest instead of the retention rate k. In this case, $p = -r$ is positive since r is negative and the equilibrium value is $\frac{b}{-r} = \frac{b}{p}$.

Discrete versus continuous. In continuous case, the value r is approximated by $r = r + 1 - 1 \approx e^r - 1$. Thus, the value p is approximated by $p = -r \approx 1 - e^r = 1 - e^{-p}$. Also, substituting that $1 - k = p$ we obtain that $1 - k = p \approx 1 - e^{-p} = 1 - e^{k-1}$. In this case, the equilibrium value is

$$A = \frac{b}{1 - e^r} = \frac{b}{1 - e^{-p}} = \frac{b}{1 - e^{k-1}}.$$

Highest safe and lowest effective levels. Determining dose schedule. Above analysis may be needed when determining the optimal time between the doses, called the dose schedule. This can be determined by considering that:

- The concentration should not exceed the highest safe level H.

- The concentration should not drop below the lowest effective level L.

Thus, we are interested in solutions that remain in the interval $[L, H]$. This gives us that $A-b \geq L$ and $A \leq H$.

In case when we want to maximize the time between the drug doses for patients convenience, we might require that $A - b = L$ and $A = H$. This way, we can determine the dose schedule and the safe time between the doses to guarantees the effectiveness without compromising the safety. Assuming that the new dose is given every T time units (in analysis above it was assumed that $T = 1$), e^{k-1} in the previous analysis should be replaced by $e^{(k-1)T}$. Thus $A = \frac{b}{1-e^{(k-1)T}}$. Considering the elimination rate $p = 1 - k$ instead of retention rate k, we obtain that $A = \frac{b}{1-e^{-pT}}$.

Thus,

$$H = A = \frac{b}{1 - e^{-pT}} = \frac{A - L}{1 - e^{-pT}} = \frac{H - L}{1 - e^{-pT}}.$$

Solving for T gives us $1 - e^{-pT} = \frac{H-L}{H} = 1 - \frac{L}{H}$. Thus, $-pT = \ln \frac{L}{H}$ and so $pT = \ln \frac{H}{L}$. This gives us the dose schedule

$$T = \frac{1}{p} \ln \frac{H}{L}.$$

Similar methods can be used to compute the amount of herbicides or pesticides accumulated in humans, the time that the natural resources will last assuming that the current usage levels increase at a constant rate, and other phenomena.

Example 5. Assume that a company is monitoring how the production level impact the profit.

1. The profit becomes zero if it falls below a minimum effective level of \$150,000.

2. If the profit is above the minimum effective level, then the growth is limited by \$3,000,000.

3. If the profit is above \$3,000,000 then it will decrease to the value of \$3,000,000.

Consider the profit P to be a function of the number of items produced n (thus it depends on the production level). Although this system could be modeled with a differential equation, a discrete model is more realistic just due to the fact that the number of items produced is a positive integer. Thus, we can describe this situation by a difference equation. Let $P = P_n$ denote the profit when n items are produced. We can use an autonomous difference equation with equilibrium solutions $P_n = 15,000$ and $P = 3,000,000$. The conditions determine that

1. If $P_0 < 15,000$, P_n is to decrease towards 0. Thus $\Delta P_n < 0$.

2. If $15,000 < P_0 < 3,000,000$, P_n is to increase towards $3,000,000$. Thus $\Delta P_n > 0$.

3. If $P_0 > 3,000,000$, P_n is to decrease towards $3,000,000$. Thus $\Delta P_n < 0$.

These conditions are satisfied for the product $(3,000,000 - P)(P - 15,000)$. Thus the difference equations

$$\Delta P_n = k(3,000,000 - P)(P - 15,000,000)$$

where k is a positive constant, models the given situation. Note that the continuous analogue is a differential equation $y' = k(3,000,000 - y)(y - 15,000)$.

Example 6. In Analytical Chemistry, the following notation is frequently used:

- [X] = equilibrium concentration = molarity of X at equilibrium. C_X = analytical concentration of X = number of moles of X added to the solution per liter. $pX = -\log[X]$.

- K_w = water's autoprotolysis constant = $1.01 \cdot 10^{-14}$ at 25 degrees Centigrade. It is usually rounded to 10^{-14}. K_a = acid dissociation constant. K_b = base dissociation constant. Recall that $K_b = K_w / K_a$.

When calculating the hydrogen ion concentration $[H^+]$ in a acid-base system, the problem frequently boils down to finding the equilibrium value of a dynamical system.

For example [1], when hydrochloric acid HCl is dissolved in water, we have

$$HCl \rightarrow H^+ + Cl^- \quad \text{and} \quad H_2O \rightleftharpoons H^+ + OH^-$$

$[H^+]$ coming from the first equation is equal to C_{HCl}. To obtain the total concentration of H^+, we can use the successive approximations.

1st approximation: $[H^+]_1 = C_{\text{HCl}}$, 2nd approximation: $[H^+]_2 = C_{\text{HCl}} + K_w/[H^+]_1$,

3rd approximation: $[H^+]_3 = C_{\text{HCl}} + K_w/[H^+]_2$ etc.

This creates the dynamical system $[H^+]_{n+1} = C_{\text{HCl}} + K_w/[H^+]_n$ with the initial value C_{HCl}. The fixed point can be found by solving the equation $[H^+] = C_{\text{HCl}} + K_w/[H^+]$ for $[H^+]$. For example, for values of $C_{\text{HCl}} = 10^{-7}$ and $K_w = 10^{-14}$, we obtain $[H^+] = 1.618 \cdot 10^{-7}$, with pH value of 6.7910.

Practice Problems.

1. Consider the following dynamical systems. Find the fixed points and check their stability. Using the graph, determine the limit of solutions with initial conditions $a_0 = 0$.

   a) $a_{n+1} = \sqrt{2 + a_n}$ b) $a_{n+1} = 1/(1 + a_n)$

2. A person with an ear infection takes 200 mg ampicillin tablet once every 4 hours. About 12% of the drug in the body at the start of a four hour period is still there at the end of that period. What quantity of ampicillin is in the body

   a) Right after taking the third tablet? b) Right after taking the sixth tablet?

   c) At the steady state level right after taking a tablet?

   d) At the steady state level right before taking a tablet?

3. A person takes 100 mg of a drug at regular time intervals. About 15% of the drug in the body at the start of a new time period is still there at the end of that period. What quantity of the drug is in the body a) right after taking the fourth dose; b) in the long run right after taking a dose; c) in the long run right before taking a dose?

[1] The following examples are taken from "Analytical Chemistry" by A. L. Soli and E. College.

4. Every day person consumes 5 micrograms of a toxin which leaves the body at a rate of 2% per day. How much toxin is accumulated in the body in the long run?

5. Dioxin is used in the treatment of heart patients. If 90% of the dose is eliminated from the body during a day and if the highest effective level is 3 mg/ml and the lowest effective level is .5 mg/ml, find the dose schedule.

6. A yeast culture initially has the biomass of 9.6 grams. It has the carrying capacity (the limiting value of the population) of 665 g and the increase in size in each hour is proportional to the size of population and the difference between the current size and the carrying capacity. Assuming that the proportionality constant is 0.00082, write a difference equation that models the size of the yeast culture. Sketch the graph of the solution.

7. Write the dynamical system that models the value $[\mathrm{H}^+]$ of a weak base HA using the following approximations.

   1st approx. $[\mathrm{H}^+]_1 = \sqrt{\mathrm{K}_a C_{\mathrm{HA}}}$, 2nd approx. $[\mathrm{H}^+]_2 = \sqrt{\mathrm{K}_a (C_{\mathrm{HA}} - [\mathrm{H}^+]_1)}$,

   3rd approx. $[\mathrm{H}^+]_3 = \sqrt{\mathrm{K}_a (C_{\mathrm{HA}} - [\mathrm{H}^+]_2)}$ etc.

   Find the fixed value of the system for the hydrofluoric acid HF using the values $\mathrm{K}_a = 6.8 \times 10^{-4}$ and C_{HF} =.01 M. Compute the pH value also.

Solutions

1. a) The equation $\sqrt{2+a} - a = 0$ has only one solution $a = 2$. By analyzing the sign of $\sqrt{2+a} - a$, we obtain that 2 is a stable equilibrium solution. Thus, the solution with initial condition 0 will increase towards 2.

   b) The equilibriums solutions can be obtained from the equation $\frac{1}{1+a} - a = 0 \longrightarrow \frac{1-a-a^2}{1+a} = 0 \longrightarrow a = -1.618$ and $a = .618$. The dynamical system is not defined for $a = -1$. Analyzing the sign of $\frac{1-a-a^2}{1+a}$, we obtain that both $a = -1.618$ and $a = .618$ are stable. Thus, the solution with initial condition 0 will converge towards .618.

2. $b = 200$ and $k = .12$. a) $b + kb + k^2 b$ or $\frac{b(1-k^3)}{1-k} = 226.88$ mg; b) $\frac{b(1-k^6)}{1-k} = 227.27$ mg; c) $\frac{b}{1-k} = 227.27$ mg; d) $A - b = 27.27$ mg.

3. $b = 100$ and $k = .15$. a) $\frac{b(1-k^4)}{1-k} = 117.59$ mg b) $\frac{b}{1-k} = 117.65$ mg c) $A - b = 17.65$ mg.

4. $b = 5$ and $k = .98$ (so $p = 0.2$). Then $A = \frac{5}{1-.98} = 250$ micrograms. If using continuous model (arguably more realistic in this case), get $A = \frac{b}{1-e^{-p}} = 252.51$ micrograms.

5. $p = 0.9$, $H = 3$ and $L = 0.5$ so $T = \frac{1}{p} \ln \frac{H}{L} = \frac{1}{0.9} \ln \frac{3}{0.5} = 1.9991 \approx 2$ days.

6. $\Delta a_n = 0.00082 a_n (665 - a_n)$. This equation has two equilibrium solutions, 0 and 665. 0 is unstable and 665 is stable. Thus the solution with initial value 9.6 is increasing to 665 g.

7. $[\mathrm{H}^+]$ value is .00229. pH value is 2.64.