6.2 Stochastic models of diffusion

MATHEMATICAL TECHNIQUES

- ♠ For the given probability that a molecule leaves a cell, write the discrete-time dynamical system for the probability that it remains inside (assuming it can never return) and find the solution. Compute the probability that the molecule remains inside after 10 seconds, and the time before it will have left with probability 0.9.
 - EXERCISE 6.2.1

The probability it leaves is 0.3 each second.

• EXERCISE **6.2.2**

The probability it leaves is 0.03 each second.

- \spadesuit The following probabilities describe molecules that can hop into and out of a cell. For each, find a discrete-time dynamical system for the probability that the molecule is inside. Find the probability that a molecule that begins inside at t=2, and the probability that a molecule that begins outside is inside at t=2. Compute the equilibrium, and use it to estimate how many out of 100 molecules would be inside after a long time.
 - EXERCISE **6.2.3**

The probability it leaves is 0.3 each second, and the probability it returns is 0.2 each second.

• EXERCISE 6.2.4

The probability it leaves is 0.03 each second, and the probability it returns is 0.1 each second.

- A Draw cobweb diagrams based on the discrete-time dynamical systems in the earlier exercise.
 - EXERCISE **6.2.5**

The molecule in exercise 6.2.1.

• EXERCISE 6.2.6

The molecule in exercise 6.2.2.

• EXERCISE 6.2.7

The molecule in exercise 6.2.3.

• EXERCISE 6.2.8

The molecule in exercise 6.2.4.

- ♠ Consider again the molecules in exercises 6.2.1–6.2.4. Suppose that we wish to consider 2 molecules instead of 1 molecule, both starting inside the cell. Find the following probabilities.
 - EXERCISE 6.2.9

What is the probability that both of the molecules in exercise 6.2.1 remain inside after 1 second?

 \bullet EXERCISE **6.2.10**

What is the probability that both of the molecules in exercise 6.2.2 have moved outside after 1 second?

• EXERCISE **6.2.11**

What is the probability that both of the molecules in exercise 6.2.3 are inside after 2 seconds?

• EXERCISE **6.2.12**

What is the probability that both of the molecules in exercise 6.2.4 are outside after 2 seconds?

- ♠ In many ways, probabilities act like fluids. For each of the following models of chemical exchange, let c_t represent the amount in container 1 and d_t the amount in container 2 at time t. Write a discrete-time dynamical system for the amount of chemical in each container. Define p_t to be the fraction of chemical in container 1 and write a discrete-time dynamical system giving p_{t+1} as a function of p_t . Find the equilibrium fraction of chemical in the first container.
 - EXERCISE **6.2.13**

Each second, 30% of the chemical in container 1 enters container 2 and 20% of the chemical in container 2 returns to container 1 (compare with exercise 6.2.3).

• EXERCISE **6.2.14**

Each second, 3% of the chemical in container 1 enters container 2 and 10% of the chemical in container 2 returns to container 1 (compare with exercise 6.2.4).

APPLICATIONS

♠ In each of the following circumstances, find the updating function describing the probability, find the solution, and use it to answer the question.

• EXERCISE **6.2.15**

A certain highly mutable gene has a 1.0% chance of mutating each time a cell divides. Suppose that there are 15 cell divisions between each pair of generations. What is the chance that the gene mutates in one generation? If there were 100 such genes, about how many would have mutated in one generation?

• EXERCISE **6.2.16**

A herd of lemmings is standing at the top of a cliff. Each jumps off with probability 0.2 each hour. What is the probability that a particular lemming remains on top of the cliff after 3 hours? If 5000 lemmings are standing around on top of the cliff, about how many will remain after 3 hours?

• EXERCISE **6.2.17**

A molecule has a 5.0% chance of binding to an enzyme each second and remains permanently attached thereafter. If the molecule starts out unbound, find the probability that it is bound after 10 seconds. How long would it take for the molecule to have bound with probability 0.95, or 95%?

• EXERCISE **6.2.18**

In tropical regions, caterpillars suffer extremely high predation, sometimes as high as 15% per day. In other words, a caterpillar is eaten with probability 0.15 each day. If a caterpillar takes 25 days to develop, what is the probability it survives? If a female lays 50 eggs, about how many would survive? How much lower would the predation rate have to be for the female to expect to replace herself by having 2 out of the 50 caterpillars survive?

♠ In each of the following circumstances, find the updating function describing the probability, find the solution, and use it to answer the question.

• EXERCISE **6.2.19**

Suppose that a mutant gene in exercise 6.2.15 has a 1.0% chance of correcting the mutation each division. Use the Markov chain approach to find the fraction of mutant genes after 15 generations. How much difference does the correction mechanism make?

• EXERCISE **6.2.20**

Suppose that the lemmings in exercise 6.2.16 can sometimes crawl back up the cliff. In particular, suppose that a lemming at the bottom of the cliff climbs back up with probability 0.1 each hour. What is the probability that a particular lemming is on top of the cliff after 3 hours? If 5000 lemmings are standing around on top of the cliff to begin with, about how many will be there after 3 hours? How much difference does crawling back up make?

• EXERCISE **6.2.21**

Suppose that bound molecules in exercise 6.2.17 have a 2.0% chance of unbinding from the enzyme each second. Find the fraction of molecules that are bound in the long run. What is the probability that a molecule is bound after 10 seconds?

• EXERCISE **6.2.22**

Suppose that the caterpillars in exercise 6.2.18 are not being eaten by predators, but are having their bodies taken over by insects called parasitoids. After a parasitoid attack, there is some chance that the caterpillar will manage to eliminate it, becoming a caterpillar again. In particular, suppose that a caterpillar has a 0.03 chance of eliminating a parasitoid each day. Find the probability that a caterpillar is a caterpillar after 25 days. Is a 3% recovery rate enough for about 2 out of 50 eggs to end up as caterpillars?

 \spadesuit From each of the following sets of data, estimate the probability that a molecule that is inside a cell leaves during a given second. Write a discrete-time dynamical system for the probability that the molecule is inside and find the probability it is inside after three seconds. How does this probability compare with the fraction of molecule that actually were inside at t=3?

• EXERCISE **6.2.23**

10 molecules start inside a cell. They are first observed outside the cell in the given second.

Molecule	Time first	
	observed outside	
1	11	
2	1	
3	2	
4	3	
5	1	
6	2	
7	4	
8	7	
9	1	
10	4	

• EXERCISE **6.2.24**

10 molecules start inside a cell. They are first observed outside the cell in the given second.

Molecule	Time first		
	observed outside		
1	4		
2	16		
3	14		
4	10		
5	4		
6	1		
7	1		
8	11		
9	2		
10	12		

♠ From each of the following sets of data, estimate the probability that a molecule that is inside a cell leaves during a given second, and the probability that it returns. Write a discrete-time dynamical system for the probability that the molecule is inside and find the equilibrium probability. How does the equilibrium probability compare with the fraction of times the molecule actually was inside?

$\bullet \ \mathsf{EXERCISE} \ \mathbf{6.2.25}$

One molecule is observed for 20 seconds, and follows

Time	Location	Time	Location
1	In	11	Out
2	In	12	${ m In}$
3	Out	13	Out
4	Out	14	Out
5	${ m In}$	15	${ m In}$
6	${ m In}$	16	${ m In}$
7	Out	17	${ m In}$
8	${ m In}$	18	Out
9	In	19	${ m In}$
10	Out	20	Out

• EXERCISE **6.2.26**

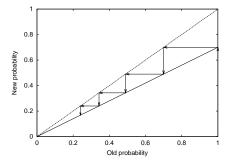
One molecule is observed for 20 seconds, and follows

Time	Location	Time	Location
1	In	11	Out
2	In	12	Out
3	In	13	Out
4	In	14	Out
5	Out	15	${ m In}$
6	Out	16	${ m In}$
7	Out	17	Out
8	In	18	Out
9	In	19	Out
10	In	20	In

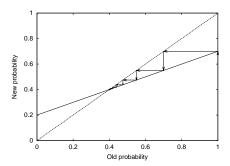
Chapter 7

Answers

6.2.1. The discrete-time dynamical system is $p_{t+1} = 0.7p_t$ because the probability it remains is 0.7 each second. The solution is $p_t = 0.7^t$. After 10 seconds, it remains with probability $p_{10} = 0.7^{10} = 0.028$. To find the time when it will have left with probability 0.9, we must solve $p_t = 0.1$ for t, or $0.7^t = 0.1$, $t = \ln(0.1)/\ln(0.7) = 6.45$. **6.2.3.** The discrete-time dynamical system is $p_{t+1} = 0.7p_t + 0.2(1-p_t)$. A molecule that starts inside has $p_0 = 1$, so $p_1 = 0.7$ and $p_2 = 0.7 \cdot 0.7 + 0.2 \cdot 0.3 = 0.55$. A molecule that starts outside has $p_0 = 0$, so $p_1 = 0.2$ and $p_2 = 0.7 \cdot 0.2 + 0.2 \cdot 0.8 = 0.30$. The equilibrium is where $p^* = 0.7p^* + 0.2(1-p^*)$, or $p^* = 0.2 + 0.5p^*$. This has solution $p^* = 0.4$. Out of 100 molecules, about 40 would be inside after a long time. **6.2.5.**



6.2.7.



- **6.2.9.** The probability that both molecules remain inside matches the probability that one molecule remains inside for two consecutive seconds, or $0.7 \cdot 0.7 = 0.49$.
- **6.2.11.** The probability that both molecules are inside is the product of the probability that the first is inside with the probability that the second is inside. These probabilities can be found by finding p_2 from the discrete-time dynamical system $p_{t+1} = 0.7p_t + 0.2(1 p_t)$ with $p_0 = 1$. Then $p_1 = 0.7$, and $p_2 = 0.55$. The probability that both molecules are inside is $0.55 \cdot 0.55 = 0.3025$.

6.2.13. The discrete-time dynamical systems for c and d are $c_{t+1} = 0.7c_t + 0.2d_t$, $d_{t+1} = 0.3c_t + 0.8d_t$. Then

$$p_{t+1} = \frac{c_{t+1}}{c_{t+1} + d_{t+1}}$$

$$= \frac{0.7c_t + 0.2d_t}{0.7c_t + 0.2d_t + 0.3c_t + 0.8d_t}$$

$$= \frac{0.7c_t + 0.2d_t}{c_t + d_t} = 0.7p_t + 0.2(1 - p_t).$$

The equilibrium fraction solves $p^* = 0.7p^* + 0.2(1-p^*)$, with solution $p^* = 0.4$. This describes the same process as in exercise 6.2.3 but is about fluids, which are effectively infinite numbers of molecules. There is nothing random about the results of this discrete-time dynamical system.

- **6.2.15.** The discrete-time dynamical system is $p_{t+1} = 0.99p_t$, with solution $p_t = 0.99^t$. After 15 divisions, the probability that a gene has not mutated is $0.99^{15} = 0.86$. The probability that it has mutated is therefore 0.14, or about 14%. Out of 100 genes, about 14 would have mutated in one generation.
- **6.2.17.** The discrete-time dynamical system is $p_{t+1} = 0.95p_t$, with solution $p_t = 0.95^t$. After 10 seconds, the probability that a molecule is unbound is $0.95^{10} = 0.599$. The probability that it is bound is therefore 0.401, or about 40%. It has a 95% of being bound when it has a 5% or 0.05 chance of remaining unbound. We solve $p_t = 0.95^t = 0.05$ for t as $t = \ln(0.05)/\ln(0.95) = 58.4$, or nearly one minute.
- **6.2.19.** The updating function for the fraction of normal genes is $p_{t+1} = 0.99p_t + 0.01(1 p_t)$. Iterating this function 15 times starting from $p_0 = 1$ gives 0.869. The correction mechanism hardly makes any difference.
- **6.2.21.** The updating function is $p_{t+1} = 0.95p_t + 0.02(1 p_t)$. The equilibrium solves $p^* = 0.95p^* + 0.02(1 p^*)$, which has solution $p^* = 0.286$. After 10 seconds, an initially unbound molecule has a 63.1% chance of being bound, or a 36.9% chance of being bound.
- **6.2.23.** One way to estimate the probability is to note that 3 of the 10 molecules left during the first second, or an estimated probability of leaving of 0.3. The probability of remaining is then 0.7, so the updating function is $p_{t+1} = 0.7p_t$. The probability of being inside after 3 seconds is $0.7^3 = 0.343$, so we expect 3 or 4 to still be inside at time 3. In fact, 5 out of 10 remain inside, slightly more than we expected. An alternative, and more accurate, way to estimate the probability is to note that the first molecule, for example, remained in between t = 0 and t = 1, between t = 1 and t = 2 for 10 times, and left once. Adding all these up, there are 26 observations of a molecule remaining inside, and 10 of it leaving. We thus estimate that molecules remain with probability 26/36 = 0.72. Then $0.72^3 = 0.37$, giving pretty much the same result as the simpler estimate.
- **6.2.25.** It was "In" 11 times. After being "In", it remained "In" 5 times, for a probability of remaining "In" of about 5/11 = 0.45. It was "Out" 9 times, but we don't know what happened after time 20. Of the other 8, it jumped "In" 5 times, for a probability of 5/8 = 0.625. The discrete-time dynamical system is

$$p_{t+1} = 0.45p_t + 0.625(1 - p_t). (9.1)$$

The equilibrium probability is $p^* = 0.53$. The observed fraction "In" is similar, 11/20 = 0.55.