From now on, I'll suppress the dependence of the process on θ in the notation.

Def. A discrete-time stochastic process is a (first-order) Markov chain if for $n = 1, 2, \ldots$; (b) any real number; and for all possible sequences of states $x_1, x_2, \ldots$

$$P(X_{n+1} \le b \mid X_1 = x_1, \ldots, X_n = x_n)$$

$$= P(X_{n+1} \le b \mid X_n = x_n).$$

In other words, the only thing you need to know to simulate where the Markov chain is going next is where it is now.

(Can define higher-order Markov chains with memory of 2 or more time periods; we won't pursue that here.)

Def.

The set of values a Markov chain can take on is called its state space S, which may be finite or infinite.

(Can also have Markov chains unfolding in continuous time, e.g. X_t = stock price at time t = seconds, milliseconds, microseconds, ...; we also won't pursue that here.)

It's easy to write down the joint PF of a Markov chain with finite S:

Consequences

① $(X_1, X_2, \ldots)$ finite Markov chain $\rightarrow$

$$P(X_1 = x_1, \ldots, X_n = x_n) =$$

$$P(X_1 = x_1) \cdot P(X_2 = x_2 \mid X_1 = x_1) \cdot$$

$$P(X_3 = x_3 \mid X_2 = x_2) \cdot \ldots$$

$$P(X_n = x_n \mid X_{n-1} = x_{n-1}).$$

Def. A Markov chain with a finite state space is called a finite Markov chain.

Def. Suppose you have a finite Markov chain with k possible states numbered $1, \ldots, k$

$(k \text{ integer} \geq 2) \rightarrow \{P(X_{n+1} = j \mid X_n = i),$

$i, j = 1, \ldots, k, \; n = 1, 2, \ldots\}$ is called the transition distribution of the Markov chain.

If $p(X_{n+1} = j \mid X_n = i)$ is the same for all n, the transition distribution is said to be stationary. If (DS) (bad name)

((time-homogeneous)

the Markov chain does have a ~~stationary~~ transition distribution, then the probabilities

$p_{ij} \triangleq p(X_{n+1} = j \mid X_n = i)$ completely characterize the Markov chain's behavior.

Can arrange the p_{ij} in a matrix called the transition matrix.

$$P = \begin{array}{c} \\ 1 \\ 2 \\ \vdots \\ k \end{array} \begin{array}{c} \begin{array}{cccc} 1 & 2 & \cdots & k \end{array} \\ \begin{bmatrix} p_{11} & p_{12} & \cdots & p_{1k} \\ \vdots & \vdots & & \vdots \\ p_{k1} & p_{k2} & \cdots & p_{kk} \end{bmatrix} \end{array}$$

$k = k$ (from) state k ; (to) state j

All of the elements of $\underline{\underline{P}}$ are non-negative (they're probabilities), and all of the row sums are 1 (because the chain has to go somewhere), i.e.

$$\sum_{j=1}^{k} p_{ij} = 1 \quad \text{for all } i = 1, \ldots, k.$$ Def.

matrix versus quaternion

A square matrix $\underset{k \times k}{P}$ with non-negative entries and all row sums equal to 1 is called a stochastic matrix.

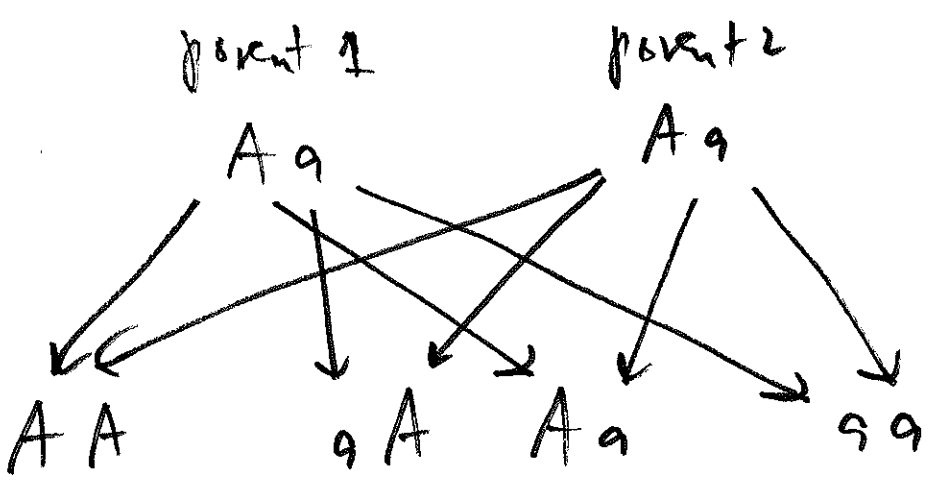
Example (~~dominant/recessive~~) Gene inheritance is Markovian: all we need to know to predict your genetic makeup at birth is the genetic story of your parents

(your grandparents, ..., are irrelevant).

Suppose that A gene of interest to you has two alleles, A and a. Then a state in the Markov chain is of the form

$$\{\underset{\text{parent 1}}{\text{allele 1 from}}, \underset{\text{parent 1}}{\text{allele 2 from}}\}, \{\underset{\text{parent 2}}{\text{allele 1 from}}, \underset{\text{parent 2}}{\text{allele 2 from}}\},$$

for example $\{Aa, Aa\}$. Ignoring order (because it's irrelevant in inheritance), there are 6 possible states: $\{AA, AA\}$, $\{AA, Aa\}$, $\{AA, aa\}$, $\{Aa, Aa\}$, $\{Aa, aa\}$ and $\{aa, aa\}$.

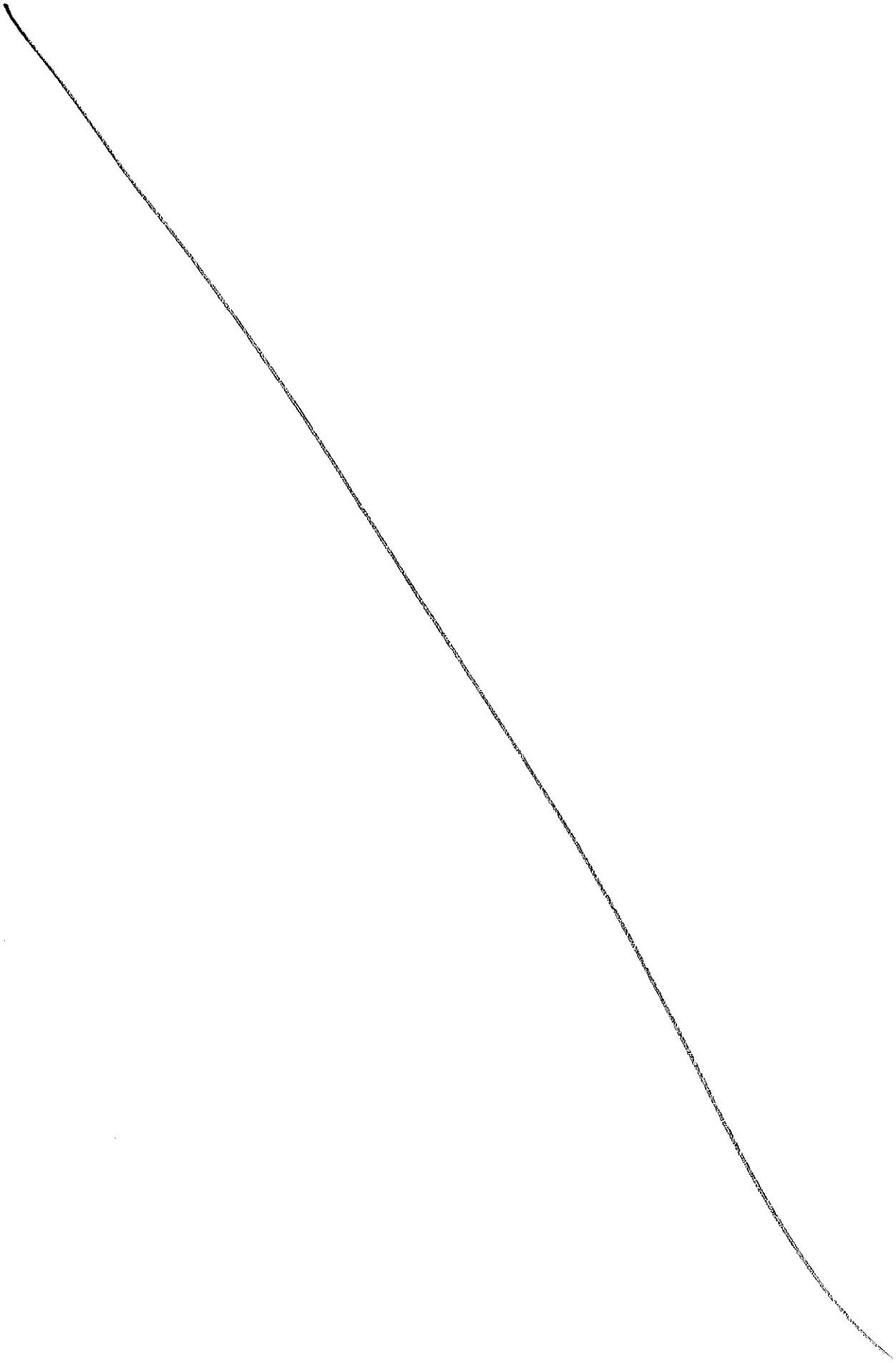


one possible inheritance sequence

offspring gets A or a from parent 1 and A or a (independently) from parent 2, each (A or a) with probability $\frac{1}{2}$.

Transition matrix

from ↓ to →	{AA, AA}	{AA, Aa}	{AA, aa}	{Aa, Aa}	{Aa, aa}	{aa, aa}
{AA, AA}	1	0	0	0	0	0
{AA, Aa}	$\frac{1}{4}$	$\frac{1}{2}$	0	$\frac{1}{4}$	0	0
{AA, aa}	0	0	0	1	0	0
{Aa, Aa}	$\frac{1}{16}$	$\frac{1}{4}$	$\frac{1}{8}$	$\frac{1}{4}$	$\frac{1}{4}$	$\frac{1}{16}$
{Aa, aa}	0	0	0	$\frac{1}{4}$	$\frac{1}{2}$	$\frac{1}{4}$
{aa, aa}	0	0	0	0	0	1



Example (random walk) You're watching a particle move around on the integers $S = \{\dots, -2, -1, 0, 1, 2, \dots\}$ over time: here are the rules: wherever it is at time $t = n$, it moves left 1 unit with prob p_1, ——— right 1 unit ——— p_3, and it stays where it is with prob p_2, where $0 < p_i < 1$ and $\sum_{i=1}^{3} p_i = 1$. This is clearly a Markov chain (why?); what is its transition matrix?

from ↓ \ to →	⋯	−2	−1	0	1	2	⋯
⋮	⋱	⋮	⋮	⋮	⋮	⋮	⋮
−2	⋯	p_2	p_3	0	0	0	⋯
−1	⋯	p_1	p_2	p_3	0	0	⋯
0	⋯	0	p_1	p_2	p_3	0	⋯
1	⋯	0	0	p_1	p_2	p_3	⋯
2	⋯	0	0	0	p_1	p_2	⋯
⋮	⋰	⋮	⋮	⋮	⋮	⋮	⋱

$= \underline{\underline{P}}$

This is an example of a band matrix, in which the only non-zero entries are on the main diagonal and 1 diagonal either way from the main diagonal; since there are only 3 non-zero diagonals, $\underline{\underline{P}}$ is said to be tridiagonal.

Moreover, all of the main diagonal entries are the same (p_2); all of the entries 1 diagonal below are also the same (p_1); and all of the entries 1 diagonal above are also the same (p_3).

Such matrices are called Toeplitz (named after Otto Toeplitz, (1881-1940) (died of tuberculosis at 58) a German mathematician who was fired by the Nazis from his university position in 1935 for being Jewish!)

Q: Start this process, which is called a random walk, at 0 & let it go; where is the particle likely to be at time n, n large?

A: Suppose, for example, that $(p_1, p_2, p_3) = (0.1, 0.3, 0.6)$. Then you would expect the particle to drift off to $+\infty$. Similarly, $(p_1, p_2, p_3) = (0.5, 0.25, 0.25)$ should yield a drift to $-\infty$. $(p_1, p_2, p_3) = (\frac{1}{3}, \frac{1}{3}, \frac{1}{3})$?

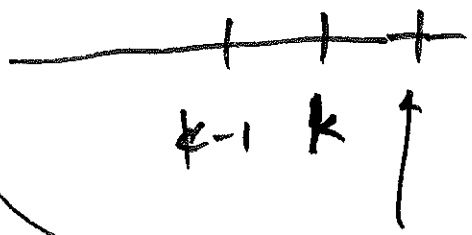
Can show that as $n \to \infty$ every integer is visited infinitely many times, and the expected time you must wait for the chain to return to 0 (having started there) is also infinite.

The infinite random walk evidently has "too much freedom" to move around to get interesting results; let's bound it.

Bounded random walk

Restrict the Markov chain to $S = \{-k, -k+1, \ldots, -1, 0, 1, \ldots, k-1, k\}$ for some integer $k \geq 1$.

Q: what to do at the boundaries?



one idea would be to wrap around: if you try to move to $(k+1)$, interpret that as a move to $-k$; if you try to move to $-(k+1)$, move to $+k$.

(move 2)

Transition matrix with $k=2$

from \ to	-2	-1	0	1	2
-2	p_2	p_3	0	0	p_1
-1	p_1	p_2	p_3	0	0	(hit $-k$)
0	0	p_1	p_2	p_3	0
1	0	0	p_1	p_2	p_3
2	p_3	0	0	p_1	p_2

(move 2)

R demo

Another idea: keep trying until you make a legal move

(move 1)

Back to a general finite Markov chain

Let $p_{ij}^{(m)} = P(\text{chain moves from } i \text{ to } j \text{ in } m \text{ steps})$

Theorem $= P(X_{n+m} = j \mid X_n = i)$

Finite Markov chain with stationary transition distributions & transition matrix $\underline{\underline{P}} \to p_{ij}^{(m)}$ is just the (i,j) entry of the matrix $\underline{\underline{P}}^m$ which is called the m-step transition matrix of the Markov chain.

Genetic example, continued

$\{AA, Aa\}$ has the property that once the chain is in that state, it can't

p_{ij} anywhere else; so does $\{99, 99\}$

This occurs for a state i when $p_{ii} = 1$.

Def. Any state with $p_{ii} = 1$ is called an absorbing state. Notice that in this genetic Markov chain, states 2, 3 all have positive probability of moving to state 1 in 2 steps, and the same is true of moving to state 4 in 2 steps. It follows that, if the chain is run long enough (simulating many generations), it will either end up

in state {AA, AA} or in state {aa, aa} (341)

Markov chains that settle down to a single stable long-run distribution are especially important in contemporary Bayesian computation; the long-run stable distribution is called the equilibrium distribution of the chain.

Important note on terminology

We call this distribution the stationary dist. of the chain, but this choice is unfortunate because we've already used stationary to mean something else:

DS: If $P(X_{n+1} = j \mid X_n = i)$ is the same for all n, DS say that the transition distribution is stationary; other people call this time-homogeneous.

I'll use equilibrium distribution for the long-run behavior of Markov chains that settle down into a stable long-run story.

Where should the Markov chain start?

You can either initialize a Markov chain to a deterministic value, or you can start it off by making a random draw from what's called the initial distribution of the Markov chain:

Def Any vector $\underset{\sim}{v}$ of non-negative numbers that add up to 1 is called a probability vector; any such vector whose components specify that a Markov chain will be in each possible state at time 1 is referred to as the initial distribution of the chain.

So: After 1 timestep (iteration), the probability dist. over the Markov chain's possible states is $\underset{\sim}{v}$; after 2 iterations the chain's dist. is $\underset{\sim}{v}\underset{=}{P}$; after $(m+1)$ iterations its dist. is $\underset{\sim}{v}\underset{=}{P}^m$; it would be nice if $\underset{\sim}{v}\underset{=}{P}^m$ converged to a unique dist. as $m \to \infty$: this would

be its equilibrium distribution.

Notice something interesting: if we choose $\underset{\sim}{v}$ so that $\underset{\sim}{v}\underline{\underline{P}} = \underset{\sim}{v}$, then

$\underset{\sim}{v}\underline{\underline{P}}^2 = (\underset{\sim}{v}\underline{\underline{P}})\underline{\underline{P}} = \underset{\sim}{v}\underline{\underline{P}} = \underset{\sim}{v}$, $\underset{\sim}{v}\underline{\underline{P}}^3 = (\underset{\sim}{v}\underline{\underline{P}}^2)\underline{\underline{P}}$

$= \underset{\sim}{v}\underline{\underline{P}} = \underset{\sim}{v}$; and so $\lim_{m\to\infty} \underset{\sim}{v}\underline{\underline{P}}^m = \underset{\sim}{v}$

Def. Markov chain with transition matrix $\underline{\underline{P}}$ + any probability vector $\underset{\sim}{v}$ such that $\underset{\sim}{v}\underline{\underline{P}} = \underset{\sim}{v}$ is (an) equilibrium dist. for the Markov chain

(an) ← under additional conditions on $\underline{\underline{P}}$, such an equilibrium dist. will be unique (we won't fully pursue that here).

How find $\underset{\sim}{v}$ so that $\underset{\sim}{v}\,\underline{\underline{P}} = \underset{\sim}{v}$?

In linear algebra this is an example of an eigenvalue/eigenvector problem:

Def. Given a square matrix $\underset{k=k}{P}$, any vector $\underset{k\,1}{\underset{\sim}{v}_R}$ satisfying $\underset{k=k}{P}\,\underset{\sim 1}{v_R} = \lambda_R \underset{k\,1}{\underset{\sim}{v}_R}$ is called a right eigenvector of $\underline{\underline{P}}$ with eigenvalue λ_R, and any vector $\underset{1\,k}{\underset{\sim}{v}_L}$ satisfying $\underset{1\,k}{\underset{\sim}{v}_L}\,\underset{=k}{P} = \lambda_L \underset{1}{\lambda_L}\,\underset{\sim}{v}_L$ is called a left eigenvector of $\underline{\underline{P}}$ with eigenvalue λ_L.

So, given a transition matrix $\underset{k=k}{P}$ for a Markov chain, an equilibrium dist. for the chain can be found by computing the left eigenvector $\underset{1\sim L_k}{V}$ where eigenvalue is 1, if such a vector exists. Most computer routines for eigenanalysis only give you right eigenvectors, but notice that if

$$\underset{1\sim L}{V}\underset{k=k}{P} = \underset{1\sim L}{V}$$

then $\left(\underset{1\sim L}{V}\underset{k=k}{P}\right)^T = \underset{k\sim 1}{V^T}$ ← transpose

$$= \underset{k=k}{P^T}\underset{k\sim 1}{V^T} = \underset{k\sim 1}{V^T}$$

so we can just eigendecompose $\underset{=}{P}^T$ instead of $\underset{=}{P}$.

Genetic example, continued

R's routine eigen gives the following results: P^T has two eigenvectors whose eigenvalues are 1: $\begin{pmatrix}1\\0\\0\\0\\0\\0\end{pmatrix}$ and $\begin{pmatrix}0\\0\\0\\0\\0\\1\end{pmatrix}$, corresponding to the two absorbing states.

This suggests that there's an entire family of equilibrium distributions of the form $(p, 0, 0, 0, 0, 1-p)^T$ for $0 \le p \le 1$; and Wa can be used to verify this conjecture.

So the earlier guess is also correct: after many generations either one of {AA, AA} or {aa, aa} will be absorbing.

There is a special case in which a unique stationary distribution exists.

Theorem If you can find a positive integer $m \geq 1$ such that every element of $\underline{\underline{P}}^m$ is strictly positive, then $\lim_{n \to \infty} \underline{\underline{P}}^n$ is a matrix with all rows equal to the unique stationary dist $\underline{v}$, and no matter what the chain's initial distribution is, its distribution after n steps converges to $\underline{v}$ as $n \to \infty$.