Genetics

Markov chains

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We conduct an experiment with a set of $r$ outcomes,

$$S = \{S_1, \ldots, S_r\}.$$

The experiment is repeated $n$ times (with $n$ large, potentially infinite).

The system has <u>no memory</u>: the next state depends only on the present state.

The probability of $S_j$ occurring on the next step, given that $S_i$ occurred on the last step, is

$$p_{ij} = p(S_j | S_i).$$

Suppose that $S_i$ is the current state, then one of $S_1, \ldots, S_r$ must be the next state; therefore,

$$p_{i1} + p_{i2} + \cdots + p_{ir} = 1, \quad 1 \leq i \leq r.$$

(Note that some of the $p_{ij}$ can be zero, all that is needed is that $\sum_{j=1}^{r} p_{ij} = 1$ for all $i$.)

# Markov chain

### Definition

An experiment with finite number of possible outcomes $S_1, \ldots, S_r$ is repeated. The sequence of outcomes is a *Markov chain* if there is a set of $r^2$ numbers $\{p_{ij}\}$ such that the conditional probability of outcome $S_j$ on any experiment given outcome $S_i$ on the previous experiment is $p_{ij}$, i.e., for $1 \le i, j \le r$, $n = 1, \ldots,$

$$p_{ij} = \Pr(S_j \text{ on experiment } n + 1 | S_i \text{ on experiment } n).$$

The outcomes $S_1, \ldots, S_r$ are the *states*, and the $p_{ij}$ are the *transition probabilities*. The matrix $P = [p_{ij}]$ is the *transition matrix*.

# Transition matrix

The matrix

$$P = \begin{pmatrix} p_{11} & p_{12} & \cdots & p_{1r} \\ p_{21} & p_{22} & \cdots & p_{2r} \\ \\ p_{r1} & p_{r2} & \cdots & p_{rr} \end{pmatrix}$$

has

- nonnegative entries, $p_{ij} \geq 0$
- entries less than 1, $p_{ij} \leq 1$
- row sum 1, which we write

$$\sum_{j=1}^{r} p_{ij} = 1, \quad i = 1, \ldots, r$$

or, using the notation $\mathbb{1}^T = (1, \ldots, 1)$,

$$P\mathbb{1} = \mathbb{1}$$

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# Simple Mendelian inheritance

A certain trait is determined by a specific pair of genes, each of which may be two types, say $G$ and $g$.

One individual may have:

- $GG$ combination (*dominant*)
- $Gg$ or $gG$, considered equivalent genetically (*hybrid*)
- $gg$ combination (*recessive*)

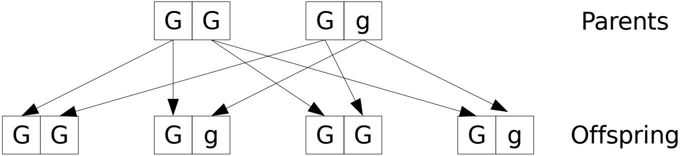
In sexual reproduction, offspring inherit one gene of the pair from each parent.

# Basic assumption of Mendelian genetics

Genes inherited from each parent are selected at random, independently of each other. This determines probability of occurrence of each type of offspring. The offspring

- of two $GG$ parents must be $GG$,
- of two $gg$ parents must be $gg$,
- of one $GG$ and one $gg$ parent must be $Gg$,
- other cases must be examined in more detail.

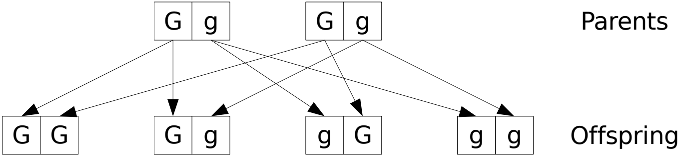
# $GG$ and $Gg$ parents




Offspring has probability

- $\frac{1}{2}$ of being $GG$
- $\frac{1}{2}$ of being $Gg$

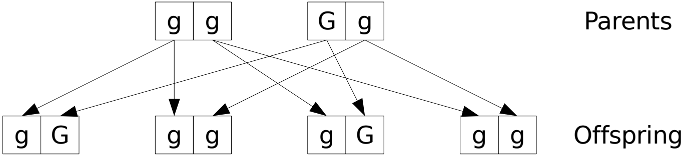
# $Gg$ and $Gg$ parents




Offspring has probability

- $\dfrac{1}{4}$ of being $GG$
- $\dfrac{1}{2}$ of being $Gg$
- $\dfrac{1}{4}$ of being $gg$

# *gg* and *Gg* parents




Offspring has probability

- $\dfrac{1}{2}$ of being $Gg$
- $\dfrac{1}{2}$ of being $gg$

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# General case

Let $p_i(n)$ be the probability that the state $S_i$ will occur on the $n^{th}$ repetition of the experiment, $1 \leq i \leq r$.

Since one the states $S_i$ must occur on the $n^{th}$ repetition,

$$p_1(n) + p_2(n) + \cdots + p_r(n) = 1.$$

Let $p_i(n+1)$ be the probability that state $S_i$, $1 \leq i \leq r$, occurs on $(n+1)^{th}$ repetition of the experiment.

There are $r$ ways to be in state $S_i$ at step $n+1$:

1. Step $n$ is $S_1$. Probability of getting $S_1$ on $n^{th}$ step is $p_1(n)$, and probability of having $S_i$ after $S_1$ is $p_{1i}$. Therefore, by multiplication principle, $P(S_i|S_1) = p_{1i}p_1(n)$.
2. We get $S_2$ on step $n$ and $S_i$ on step $(n+1)$. Then $P(S_i|S_2) = p_{2i}p_2(n)$.

..

r. Probability of occurrence of $S_i$ at step $n+1$ if $S_r$ at step $n$ is $P(S_i|S_r) = p_{ri}p_r(n)$.

Therefore, $p_i(n+1)$ is sum of all these,

$$\begin{aligned} p_i(n+1) &= P(S_i|S_1) + \cdots + P(S_i|S_r) \\ &= p_{1i}p_1(n) + \cdots + p_{ri}p_r(n) \end{aligned}$$

Therefore,

$$
\begin{aligned}
p_1(n+1) &= p_{11}p_1(n) + p_{21}p_2(n) + \cdots + p_{r1}p_r(n) \\
&\vdots \\
p_k(n+1) &= p_{1k}p_1(n) + p_{2k}p_2(n) + \cdots + p_{rk}p_r(n) \qquad (1) \\
&\vdots \\
p_r(n+1) &= p_{1r}p_1(n) + p_{2r}p_2(n) + \cdots + p_{rr}p_r(n)
\end{aligned}
$$

In matrix form

$$p(n+1) = p(n)P, \quad n = 1, 2, 3, \ldots \tag{2}$$

where $p(n) = (p_1(n), p_2(n), \ldots, p_r(n))$ is a (row) probability vector and $P = (p_{ij})$ is a $r \times r$ *transition matrix*,

$$P = \begin{pmatrix} p_{11} & p_{12} & \cdots & p_{1r} \\ p_{21} & p_{22} & \cdots & p_{2r} \\ & & & \\ p_{r1} & p_{r2} & \cdots & p_{rr} \end{pmatrix}$$

So, what we have is

$$(p_1(n+1), \ldots, p_r(n+1)) = (p_1(n), \ldots, p_r(n)) \begin{pmatrix} p_{11} & p_{12} & \cdots & p_{1r} \\ p_{21} & p_{22} & \cdots & p_{2r} \\ & & & \\ p_{r1} & p_{r2} & \cdots & p_{rr} \end{pmatrix}$$

It is easy to check that this gives the same expression as (1).

# For our genetic model..

Consider a process of continued matings.

- Start with an individual of known or unknown genetic character and mate it with a hybrid.
- Assume that there is at least one offspring; choose one of them at random and mate it with a hybrid.
- Repeat this process through a number of generations.

The genetic type of the chosen offspring in successive generations can be represented by a Markov chain, with states $GG$, $Gg$ and $gg$. So there are 3 possibles states $S_1 = GG$, $S_2 = Gg$ and $S_3 = gg$.

We have

| $\nearrow$ | GG | Gg | gg |
|---|---|---|---|
| GG | 0.5 | 0.5 | 0 |
| Gg | 0.25 | 0.5 | 0.25 |
| gg | 0 | 0.5 | 0.5 |

The transition probabilities are thus

$$P = \begin{pmatrix} \frac{1}{2} & \frac{1}{2} & 0 \\ \frac{1}{4} & \frac{1}{2} & \frac{1}{4} \\ 0 & \frac{1}{2} & \frac{1}{2} \end{pmatrix}$$

# Stochastic matrices

### Definition (Stochastic matrix)

The nonnegative $r \times r$ matrix $M$ is *stochastic* if $\sum_{j=1}^{r} a_{ij} = 1$ for all $i = 1, 2, \ldots, r$.

### Theorem

*Let $M$ be a stochastic matrix $M$. Then all eigenvalues $\lambda$ of $M$ are such that $|\lambda| \leq 1$. Furthermore, $\lambda = 1$ is an eigenvalue of $M$.*

To see that 1 is an eigenvalue, write the definition of a stochastic matrix, i.e., $M$ has row sums 1. In vector form, $M\mathbb{1} = \mathbb{1}$. Now remember that $\lambda$ is an eigenvalue of $M$, with associated eigenvector $v$, iff $Mv = \lambda v$. So, in the expression $M\mathbb{1} = \mathbb{1}$, we read an eigenvector, $\mathbb{1}$, and an eigenvalue, 1.

# Long "time" behavior

Let $p(0)$ be the initial distribution (row) vector. Then

$$\begin{aligned} p(1) &= p(0)P \\ p(2) &= p(1)P \\ &= (p(0)P)P \\ &= p(0)P^2 \end{aligned}$$

Iterating, we get that for any $n$,

$$p(n) = p(0)P^n$$

Therefore,

$$\lim_{n\to+\infty} p(n) = \lim_{n\to+\infty} p(0)P^n = p(0) \lim_{n\to+\infty} P^n$$

# Additional properties of stochastic matrices

**Theorem**

*If $M, N$ are stochastic matrices, then $MN$ is a stochastic matrix.*

**Theorem**

*If $M$ is a stochastic matrix, then for any $k \in \mathbb{N}$, $M^k$ is a stochastic matrix.*

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# Regular Markov chain

### Definition (Regular Markov chain)

A regular Markov chain is one in which $P^k$ is positive for some integer $k > 0$, i.e., $P^k$ has only positive entries, no zero entries.

### Definition

A nonnegative matrix $M$ is primitive if, and only if, there is an integer $k > 0$ such that $M^k$ is positive.

### Theorem

*A Markov chain is regular if, and only if, the transition matrix $P$ is primitive.*

# Important result for regular Markov chains

Theorem

*If $P$ is the transition matrix of a regular Markov chain, then*

1. *the powers $P^n$ approach a stochastic matrix $W$,*
2. *each row of $W$ is the same (row) vector $w = (w_1, \ldots, w_r)$,*
3. *the components of $w$ are positive.*

So if the Markov chain is regular,

$$\lim_{n \to +\infty} p(n) = p(0) \lim_{n \to +\infty} P^n = p(0)W$$

# Left and right eigenvectors

Let $M$ be an $r \times r$ matrix, $u, v$ be two column vectors, $\lambda \in \mathbb{R}$. Then, if

$$Mu = \lambda u,$$

$u$ is the (right) eigenvector corresponding to $\lambda$, and if

$$v^T M = \lambda v^T$$

then $v$ is the left eigenvector corresponding to $\lambda$. Note that to a given eigenvalue there corresponds one left and one right eigenvector.

The vector $w$ is in fact the left eigenvector corresponding to the eigenvalue 1 of $P$. (We already know that the (right) eigenvector corresponding to 1 is $\mathbb{1}$.)

To see this, remark that, if $p(n)$ converges, then $p(n+1) = p(n)P$, so $w$ is a fixed point of the system. We thus write

$$wP = w$$

and solve for $w$, which amounts to finding $w$ as the left eigenvector corresponding to the eigenvalue 1.

Alternatively, we can find $w$ as the (right) eigenvector associated to the eigenvalue 1 for the transpose of $P$,

$$P^T w^T = w^T$$

Now remember that when you compute an eigenvector, you get a result that is the eigenvector, to a multiple.

So the expression you obtain for $w$ might have to be normalized (you want a probability vector). Once you obtain $w$, check that the norm $\|w\|$ defined by

$$\|w\| = w_1 + \cdots + w_r$$

is equal to one. If not, use

$$\frac{w}{\|w\|}$$

# Back to genetics..

The Markov chain is here regular. Indeed, take the matrix $P$,

$$P = \begin{pmatrix} \frac{1}{2} & \frac{1}{2} & 0 \\ \frac{1}{4} & \frac{1}{2} & \frac{1}{4} \\ 0 & \frac{1}{2} & \frac{1}{2} \end{pmatrix}$$

and compute $P^2$:

$$P^2 = \begin{pmatrix} \frac{3}{8} & \frac{1}{2} & \frac{1}{8} \\ \frac{1}{4} & \frac{1}{2} & \frac{1}{4} \\ \frac{1}{8} & \frac{1}{2} & \frac{3}{8} \end{pmatrix}$$

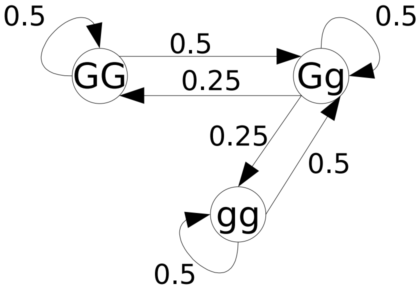
As all entries are positive, $P$ is primitive and the Markov chain is regular.

Another way to check regularity:

### Theorem

*A matrix $M$ is primitive if the associated connection graph is strongly connected, i.e., that there is a path between any pair $(i, j)$ of states, and that there is at least one positive entry on the diagonal of $M$.*

This is checked directly on the transition graph



Compute the left eigenvector associated to 1 by solving

$$(w_1, w_2, w_3) \begin{pmatrix} \frac{1}{2} & \frac{1}{2} & 0 \\ \frac{1}{4} & \frac{1}{2} & \frac{1}{4} \\ 0 & \frac{1}{2} & \frac{1}{2} \end{pmatrix} = (w_1, w_2, w_3)$$

$$\frac{1}{2}w_1 + \frac{1}{4}w_2 = w_1 \tag{3a}$$
$$\frac{1}{2}w_1 + \frac{1}{2}w_2 + \frac{1}{2}w_3 = w_2 \tag{3b}$$
$$\frac{1}{4}w_2 + \frac{1}{2}w_3 = w_3 \tag{3c}$$

From (3a), $w_1 = w_2/2$, and from (3c), $w_3 = w_2/2$. Substituting these values into (3b),

$$\frac{1}{4}w_2 + \frac{1}{2}w_2 + \frac{1}{4}w_2 = w_2,$$

that is, $w_2 = w_2$, i.e., $w_2$ can take any value. So $w = (\frac{1}{4}, \frac{1}{2}, \frac{1}{4})$.

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# Mating with a *GG* individual

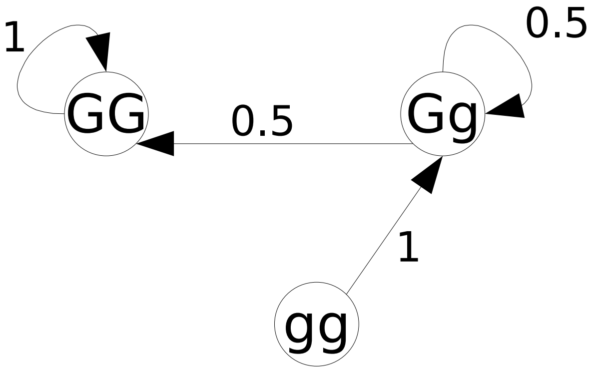
Suppose now that we conduct the same experiment, but mate each new generation with a *GG* individual instead of a *Gg* individual. Transition table is

| $\nearrow$ | GG | Gg | gg |
|---|---|---|---|
| GG | 1 | 0 | 0 |
| Gg | 0.5 | 0.5 | 0 |
| gg | 0 | 1 | 0 |

The transition probabilities are thus

$$P = \begin{pmatrix} 1 & 0 & 0 \\ \frac{1}{2} & \frac{1}{2} & 0 \\ 0 & 1 & 0 \end{pmatrix}$$

# New transition graph




Clearly:

- we leave $gg$ after one iteration, and can never return,
- as soon as we leave $Gg$, we can never return,
- can never leave $GG$ as soon as we get there.

# Absorbing states, absorbing chains

## Definition

A state $S_i$ in a Markov chain is *absorbing* if whenever it occurs on the $n^{th}$ generation of the experiment, it then occurs on every subsequent step. In other words, $S_i$ is absorbing if $p_{ii} = 1$ and $p_{ij} = 0$ for $i \neq j$.

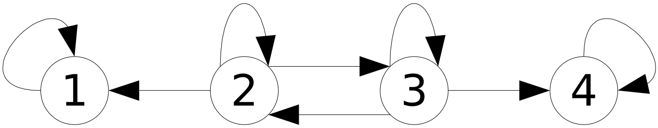
## Definition

A Markov chain is said to be absorbing if it has at least one absorbing state, and if from every state it is possible to go to an absorbing state.

In an absorbing Markov chain, a state that is not absorbing is called *transient*.

# Some questions on absorbing chains

Suppose we have a chain like the following:




1. Does the process eventually reach an absorbing state?
2. Average number of times spent in a transient state, if starting in a transient state?
3. Average number of steps before entering an absorbing state?
4. Probability of being absorbed by a given absorbing state, when there are more than one, when starting in a given transient state?

# Reaching an absorbing state

Answer to question 1:

### Theorem

*In an absorbing Markov chain, the probability of reaching an absorbing state is 1.*

# Standard form of the transition matrix

For an absorbing chain with $k$ absorbing states and $r-k$ transient states, the transition matrix can be written as

$$P = \begin{pmatrix} \mathbb{I}_k & \mathbf{0} \\ R & Q \end{pmatrix}$$

with following meaning,

| | Absorbing states | Transient states |
|---|---|---|
| Absorbing states | $\mathbb{I}_k$ | $\mathbf{0}$ |
| Transient states | $R$ | $Q$ |

with $\mathbb{I}_k$ the $k \times k$ identity matrix, $\mathbf{0}$ an $k \times (r-k)$ matrix of zeros, $R$ an $(r-k) \times k$ matrix and $Q$ an $(r-k) \times (r-k)$ matrix.

The matrix $\mathbb{I}_{r-k} - Q$ is invertible. Let

- $N = (\mathbb{I}_{r-k} - Q)^{-1}$ be the *fundamental matrix* of the Markov chain
- $T_i$ be the sum of the entries on row $i$ of $N$
- $B = NR$.

Answers to our remaining questions:

2. $N_{ij}$ is the average number of times the process is in the $j$th transient state if it starts in the $i$th transient state.
3. $T_i$ is the average number of steps before the process enters an absorbing state if it starts in the $i$th transient state.
4. $B_{ij}$ is the probability of eventually entering the $j$th absorbing state if the process starts in the $i$th transient state.

# Back to genetics..

The matrix is already in standard form,

$$P = \begin{pmatrix} 1 & 0 & 0 \\ \frac{1}{2} & \frac{1}{2} & 0 \\ 0 & 1 & 0 \end{pmatrix} = \begin{pmatrix} \mathbb{I}_1 & \mathbf{0} \\ R & Q \end{pmatrix}$$

with $\mathbb{I}_1 = 1$, $\mathbf{0} = (0 \;\; 0)$ and

$$R = \begin{pmatrix} \frac{1}{2} \\ 0 \end{pmatrix} \qquad Q = \begin{pmatrix} \frac{1}{2} & 0 \\ 1 & 0 \end{pmatrix}$$

We have

$$\mathbb{I}_2 - Q = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} - \begin{pmatrix} \frac{1}{2} & 0 \\ 1 & 0 \end{pmatrix} = \begin{pmatrix} \frac{1}{2} & 0 \\ -1 & 1 \end{pmatrix}$$

so

$$N = (\mathbb{I}_2 - Q)^{-1} = 2 \begin{pmatrix} 1 & 0 \\ 1 & \frac{1}{2} \end{pmatrix} = \begin{pmatrix} 2 & 0 \\ 2 & 1 \end{pmatrix}$$

Then

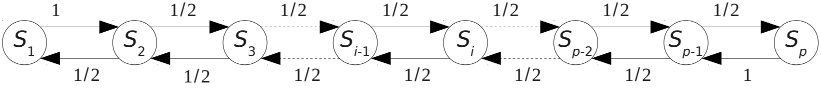
$$T = N\mathbb{1} = \begin{pmatrix} 2 \\ 3 \end{pmatrix}$$

and

$$B = NR = \begin{pmatrix} 2 & 0 \\ 2 & 1 \end{pmatrix} \begin{pmatrix} \frac{1}{2} \\ 0 \end{pmatrix} = \begin{pmatrix} 1 \\ 1 \end{pmatrix}$$

# The drunk man's walk, 1.0

- chain of states $S_1, \ldots, S_p$
- if in state $S_i$, $i = 2, \ldots, p-1$, probability $1/2$ of going left (to $S_{i-1}$) and $1/2$ of going right (to $S_{i+1}$)
- if in state $S_1$, probability 1 of going to $S_2$
- if in state $S_p$, probability 1 of going to $S_{p-1}$



# The transition matrix for DMW 1.0

$$P = \begin{pmatrix} 0 & 1 & 0 & 0 & 0 & \cdots & 0 \\ 1/2 & 0 & 1/2 & 0 & & & \\ 0 & 1/2 & 0 & 1/2 & & & \\ \vdots & & \ddots & \ddots & \ddots & & \vdots \\ & & & & & & \\ & & & & 1/2 & 0 & 1/2 \\ & & & & 0 & 1 & 0 \end{pmatrix}$$

Clearly a primitive matrix, so this is an regular Markov chain.

We need to solve $w^T P = w^T$, that is,

$$\begin{aligned}
\frac{1}{2}w_2 &= w_1 \\
w_1 + \frac{1}{2}w_3 &= w_2 \\
\frac{1}{2}w_2 + \frac{1}{2}w_4 &= w_3 \\
\frac{1}{2}w_3 + \frac{1}{2}w_5 &= w_4 \\
&\vdots \\
\frac{1}{2}w_{p-3} + \frac{1}{2}w_{p-1} &= w_{p-2} \\
\frac{1}{2}w_{p-2} + w_p &= w_{p-1} \\
\frac{1}{2}w_{p-1} &= w_p
\end{aligned}$$

Express everything in terms of $w_1$:

$$
\begin{aligned}
w_2 &= 2w_1 \\
w_1 + \frac{1}{2}w_3 &= w_2 \Leftrightarrow w_3 = 2(w_2 - w_1) = 2w_1 \\
\frac{1}{2}w_2 + \frac{1}{2}w_4 &= w_3 \Leftrightarrow w_4 = 2(w_3 - \frac{1}{2}w_2) = 2(w_3 - w_1) = 2w_1 \\
\frac{1}{2}w_3 + \frac{1}{2}w_5 &= w_4 \Leftrightarrow w_5 = 2(w_4 - \frac{1}{2}w_3) = 2(w_4 - w_1) = 2w_1 \\
&\vdots \\
\frac{1}{2}w_{p-3} + \frac{1}{2}w_{p-1} &= w_{p-2} \Leftrightarrow w_{p-1} = 2w_1 \\
\frac{1}{2}w_{p-2} + w_p &= w_{p-1} \Leftrightarrow w_p = w_{p-1} - \frac{1}{2}w_{p-2} = w_1 \\
\frac{1}{2}w_{p-1} &= w_p \qquad \text{(confirms that } w_p = w_1\text{)}
\end{aligned}
$$

So we get

$$w^T = (w_1, 2w_1, \ldots, 2w_1, w_1)$$

We have

$$\begin{aligned}
\sum_{i=1}^{p} w_i &= w_1 + \left(\sum_{i=2}^{p-1} 2w_1\right) + w_1 \\
&= 2w_1 + \sum_{i=2}^{p-1} 2w_1 \\
&= \sum_{i=1}^{p-1} 2w_1 \\
&= 2w_1 \sum_{i=1}^{p-1} 1 \\
&= 2w_1(p-1)
\end{aligned}$$

Since

$$\sum_{i=1}^{p} w_i = 2w_1(p-1)$$

to get a probability vector, we need to take

$$w_1 = \frac{1}{2(p-1)}$$

So

$$w^T = \left(\frac{1}{2(p-1)}, \frac{1}{p-1}, \dots, \frac{1}{p-1}, \frac{1}{2(p-1)}\right)$$

Now assume we take an initial condition with $p(0) = (1, 0, \ldots, 0)$, i.e., the walker starts in state 1. Then

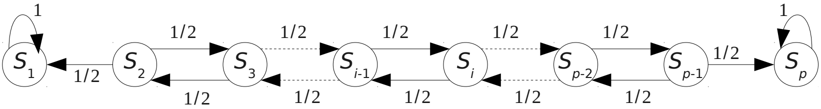
$$\lim_{t\to\infty} p(t) = p(0)W = p(0)w = p(0) \cdot w^T$$

so

$$\lim_{t\to\infty} p(t) = (1, 0, \ldots, 0) \cdot \left(\frac{1}{2(p-1)}, \frac{1}{p-1}, \ldots, \frac{1}{p-1}, \frac{1}{2(p-1)}\right)$$

# The drunk man's walk, 2.0

- chain of states $S_1, \ldots, S_p$
- if in state $S_i$, $i = 2, \ldots, p-1$, probability $1/2$ of going left (to $S_{i-1}$) and $1/2$ of going right (to $S_{i+1}$)
- if in state $S_1$, probability 1 of going to $S_1$
- if in state $S_p$, probability 1 of going to $S_p$



# The transition matrix for DMW 2.0

$$P = \begin{pmatrix} 1 & 0 & 0 & 0 & 0 & \cdots & 0 \\ 1/2 & 0 & 1/2 & 0 & & & \\ 0 & 1/2 & 0 & 1/2 & & & \\ \vdots & & \ddots & \ddots & \ddots & & \vdots \\ & & & & & & \\ & & & & 1/2 & 0 & 1/2 \\ & & & & 0 & 0 & 1 \end{pmatrix}$$

# Put $P$ in standard form

Absorbing states are $S_1$ and $S_p$, write them first, then write other states.

| | $S_1$ | $S_p$ | $S_2$ | $S_3$ | $S_4$ | $\cdots$ | $S_{p-2}$ | $S_{p-1}$ |
|---|---|---|---|---|---|---|---|---|
| $S_1$ | 1 | 0 | 0 | 0 | 0 | $\cdots$ | 0 | 0 |
| $S_p$ | 0 | 1 | 0 | 0 | 0 | $\cdots$ | 0 | 0 |
| $S_2$ | 1/2 | 0 | 0 | 1/2 | 0 | $\cdots$ | 0 | 0 |
| $S_3$ | 0 | 0 | 1/2 | 0 | 1/2 | $\cdots$ | 0 | 0 |
| $\vdots$ | | | | | | | | |
| $S_{p-2}$ | 0 | 0 | 0 | 0 | 0 | $\cdots$ | 0 | 1/2 |
| $S_{p-1}$ | 0 | 1/2 | 0 | 0 | 0 | $\cdots$ | 1/2 | 0 |

So we find

$$P = \begin{pmatrix} \mathbb{I}_2 & \mathbf{0} \\ R & Q \end{pmatrix}$$

where $\mathbf{0}$ a $2 \times (p-2)$-matrix, $R$ a $(p-2) \times 2$ matrix and $Q$ a $(p-2) \times (p-2)$ matrix

$$R = \begin{pmatrix} 1/2 & 0 \\ 0 & 0 \\ \vdots & \vdots \\ 0 & 0 \\ 0 & 1/2 \end{pmatrix}$$

and

$$Q = \begin{pmatrix} 0 & 1/2 & 0 & & & \\ 1/2 & 0 & 1/2 & & & \\ 0 & 1/2 & 0 & & & \\ & & \ddots & \ddots & \ddots & \\ & & & & & \\ 0 & & & 1/2 & 0 & 1/2 \\ 0 & & & & 1/2 & 0 \end{pmatrix}$$

$$\mathbb{I}_{p-2} - Q = \begin{pmatrix} 1 & -1/2 & 0 & & & \\ -1/2 & 1 & -1/2 & & & \\ 0 & -1/2 & 1 & & & \\ & & \ddots & \ddots & \ddots & \\ & & & & & \\ 0 & & & -1/2 & 1 & -1/2 \\ 0 & & & & -1/2 & 1 \end{pmatrix}$$

This is a *tridiagonal symmetric Toeplitz* matrix

# Inverting a symmetric tridiagonal matrix

We want to use the following result (found for example in some slides of Gérard Meurant about Tridiagonal matrices): if

$$J_k = \begin{pmatrix} \alpha_1 & \beta_1 & & & \\ \beta_1 & \alpha_2 & \beta_2 & & \\ & \ddots & \ddots & \ddots & \\ & & \beta_{k-2} & \alpha_{k-1} & \beta_{k-1} \\ & & & \beta_{k-1} & \alpha_k \end{pmatrix}$$

$$\delta_1 = \alpha_1, \quad \delta_j = \alpha_j - \frac{\beta_{j-1}^2}{\delta_{j-1}}, j = 2, \dots, k$$

$$d_k^{(k)} = \alpha_k, \quad d_j^{(k)} = \alpha_j - \frac{\beta_j^2}{d_{j+1}^{(k)}}, j = k-1, \dots, 1$$

then we have the result on the next slide

# Inverse of a symmetric tridiagonal Toeplitz matrix

### Theorem

*The inverse of the symmetric tridiagonal Toeplitz matrix $J_k$ is given by*

$$(J_k^{-1})_{ij} = (-1)^{j-i}\beta_i \cdots \beta_{j-1}\frac{d_{j+1}^{(k)} \cdots d_k^{(k)}}{\delta_i \cdots \delta_k},\ \forall i, \forall j > i$$

$$(J_k^{-1})_{ii} = \frac{d_{i+1}^{(k)} \cdots d_k^{(k)}}{\delta_i \cdots \delta_k},\ \forall i$$

Note that $\alpha_1 = \cdots = \alpha_k = 1$ and $\beta_1 = \cdots = \beta_{k-1} = -1/2$. Write $\alpha := \alpha_i = 1$ and $\beta := \beta_i = -1/2$. We have $\delta_1 = \alpha = 1$, and the general term takes the form

$$\delta_j = \alpha - \frac{\beta^2}{\delta_{j-1}} = 1 - \frac{1}{4\delta_{j-1}}, \quad j = 2, \ldots, k$$

$$\delta_2 = 1 - \frac{1}{4} = \frac{3}{4}$$

$$\delta_3 = 1 - \frac{1}{4\frac{3}{4}} = \frac{2}{3}$$

$$\delta_4 = 1 - \frac{1}{4\frac{2}{3}} = 1 - \frac{3}{8} = \frac{5}{8}$$

$$\delta_5 = 1 - \frac{1}{4\frac{5}{8}} = 1 - \frac{2}{5} = \frac{3}{5}$$

$$\delta_6 = 1 - \frac{1}{4\frac{3}{5}} = 1 - \frac{5}{12} = \frac{7}{12}$$

$$\delta_7 = 1 - \frac{1}{4\frac{7}{12}} = 1 - \frac{3}{7} = \frac{4}{7}$$

Taking a look at the few terms in the sequence, we get the feeling that

$$\delta_{2n} = \frac{2n+1}{4n} \text{ and } \delta_{2n+1} = \frac{n+1}{2n+1}$$

A little induction should confirm this. Induction hypothesis (changing indices for odd $\delta$):

$$\mathcal{P}_n : \begin{cases} \delta_{2n-1} & = \frac{n}{2n-1} \\ \delta_{2n} & = \frac{2n+1}{4n} \end{cases}$$

$\mathcal{P}_1$ is true. Assume $\mathcal{P}_j$. Then

$$\delta_{2j+1} = 1 - \frac{1}{4\delta_{2j}} = 1 - \frac{1}{4\frac{2j+1}{4j}} = 1 - \frac{j}{2j+1} = \frac{j+1}{2j+1}$$

$$\delta_{2j+2} = 1 - \frac{1}{4\delta_{2j+1}} = 1 - \frac{1}{4\frac{j+1}{2j+1}} = 1 - \frac{2j+1}{4(j+1)} = \frac{2(j+1)+1}{4(j+1)}$$

So $\mathcal{P}_{j+1}$ holds true

In fact, we can go further, by expressing

$$\delta_{2n} = \frac{2n+1}{4n} \text{ and } \delta_{2n+1} = \frac{n+1}{2n+1}$$

in terms of odd and even $j$. If $j$ is even,

$$\delta_j = \frac{j+1}{2j}$$

while if $j$ is odd,

$$\delta_j = \frac{(j+1)/2}{j}$$

But the latter gives

$$\delta_j = \frac{j+1}{2j}$$

so this formula holds for all $j$'s

For the $d_j^{(k)}$'s, we have $d_k^{(k)} = 1$ and

$$d_j^{(k)} = 1 - \frac{1}{4d_{j+1}^{(k)}}$$

So $d_k^{(k)} = \delta_1$ and

$$d_{k-j+1}^{(k)} = \delta_j = \frac{j+1}{2j}, \quad j = 2, \ldots, k$$

The form

$$d_j^{(k)} = \delta_{k-j+1}$$

will also be useful. In summary,

| $\delta_1$ | $\delta_2$ | $\cdots$ | $\delta_j$ | $\cdots$ | $\delta_{k-1}$ | $\delta_k$ |
|---|---|---|---|---|---|---|
| $d_k^{(k)}$ | $d_{k-1}^{(k)}$ | $\cdots$ | $d_{k-j+1}^{(k)}$ | $\cdots$ | $d_2^{(k)}$ | $d_1^{(k)}$ |
| $1$ | $\frac{3}{4}$ | $\cdots$ | $\frac{j+1}{2j}$ | $\cdots$ | $\frac{k}{2(k-1)}$ | $\frac{k+1}{2k}$ |

In $J^{-1}$, the following terms appear

$$\frac{d_{j+1}^{(k)} \cdots d_k^{(k)}}{\delta_i \cdots \delta_k}, \ \forall i, \forall j > i$$

and

$$\frac{d_{i+1}^{(k)} \cdots d_k^{(k)}}{\delta_i \cdots \delta_k}, \ \forall i$$

We have, $\forall i$,

$$\begin{aligned}
\frac{d_{i+1}^{(k)} \cdots d_k^{(k)}}{\delta_i \cdots \delta_k} &= \frac{\delta_{k-(i+1)+1} \cdots \delta_{k-k+1}}{\delta_i \cdots \delta_k} \\
&= \frac{\delta_{k-i} \cdots \delta_1}{\delta_i \cdots \delta_k} \\
&= \frac{\delta_1 \cdots \delta_{k-i}}{\delta_i \cdots \delta_k} \\
&= \frac{\prod_{j=1}^{k-i} \frac{j+1}{2j}}{\prod_{j=i}^{k} \frac{j+1}{2j}} \\
&= \prod_{j=1}^{k-i} \frac{j+1}{2j} \prod_{j=i}^{k} \frac{2j}{j+1}
\end{aligned}$$