



University
of Manitoba

Markov chains, Eigenvector centrality & PageRank

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Fall 2024

The University of Manitoba campuses are located on original lands of Anishinaabeg, Inineew, Anisinineew, Dakota and Dene peoples, and on the National Homeland of the Red River Métis.

We respect the Treaties that were made on these territories, we acknowledge the harms and mistakes of the past, and we dedicate ourselves to move forward in partnership with Indigenous communities in a spirit of Reconciliation and collaboration.

Outline

Markov chains

Eigenvector centrality

PageRank



What makes an important webpage?

In days of yore, the web was a small thing

Alta Vista was the search engine of choice

Google started in 1998, based on an algorithm (PageRank) described in a paper of Page, Brin, Motwani and Winograd ([link](#))

Overview

Give each page a rating (of its importance), a recursively defined measure whereby a page becomes important if important pages link to it

Recursive definition: the importance of a page refers back to the importance of other pages that link to it

Random surfer model: a random surfer on the web follows links from page to page. Page rank $\simeq \mathbb{P}$ random surfer lands on a particular page. Popular page \implies higher probability to go there. (\mathbb{P} stands for “probability”)

Example of a Markov chain

Markov chains

Eigenvector centrality

PageRank



Markov chain

A Markov chain is a *stochastic process* in which the evolution through time depends only on the current state of the system (we say the process is *memoryless*)

Markov chains are an interesting combination of matrix theory and graph theory

They form the theoretical foundation for Hidden Markov processes or Markov Chain Monte Carlo (MCMC) methods, are used in ML

Conduct an experiment with a set of n possible outcomes

$$S = \{S_1, \dots, S_n\}$$

Experiment repeated t times (with t large, potentially infinite)

System has *no memory*: the next state depends only on the present state

Probability of S_i occurring on the next step, given that S_j occurred on the last step, is

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

Suppose that S_i is the current state, then one of S_1, \dots, S_n must be the next state; so

$$p_{1i} + p_{2i} + \dots + p_{ni} = 1, \quad 1 \leq i \leq n$$

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

Definition 1

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

$$p_{ij} = \mathbb{P}(S_i \text{ on experiment } t + 1 \mid S_j \text{ on experiment } t)$$

Outcomes S_1, \dots, S_n are **states** and p_{ij} are **transition probabilities**. $P = [p_{ij}]$ the **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, $p_{ij} \leq 1$
- ▶ column sum 1, which we write

$$\sum_{i=1}^n p_{ij} = 1, \quad j = 1, \dots, n$$

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

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

Markov chains

Running example – Mendelian inheritance

Repetition of the process

Regular Markov chains

Absorbing Markov chains



(super simple) Mendelian genetics

A *phenotypic trait* (eye colour, hair colour, etc.) is determined by a specific pair of alleles, each of which may be two types, say G and g

Each individual can have

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

Individuals bearing GG or gg alleles are *homozygotes*, hybrids with Gg alleles are called *heterozygotes*

GG and gg combinations lead to different phenotypes, Gg combination leads to expressing the same phenotype as individuals bearing a GG combination, hence the name dominant given to GG

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

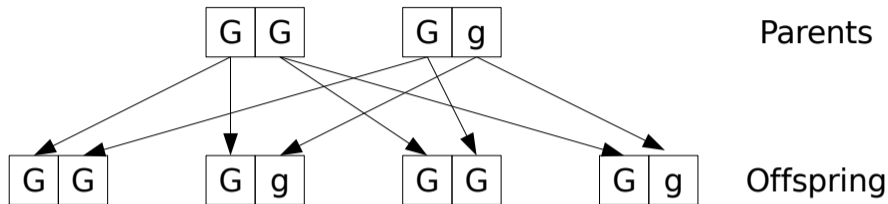
Alleles inherited from each parent are selected at random, independently of each other

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

Suppose one parent GG and the other Gg



		Parent 1	
		G	G
Parent 2	G	GG	GG
	g	Gg	Gg

To determine \mathbb{P} that offspring is of a certain type, count number of outcomes of each type (GG and Gg) and divide by 4

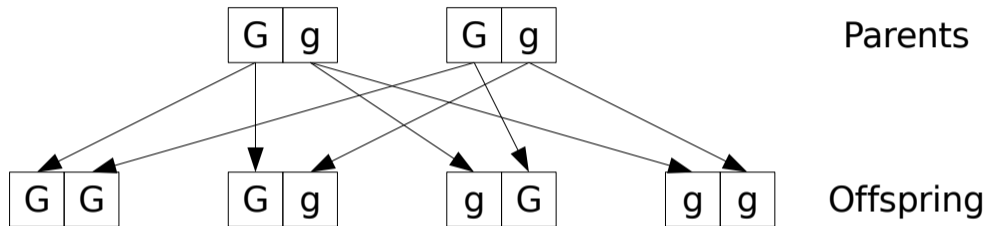
\implies offspring have probability

▶ 1/2 of being GG

▶ 1/2 of being Gg

Gg and Gg parents

Both parents are hybrid

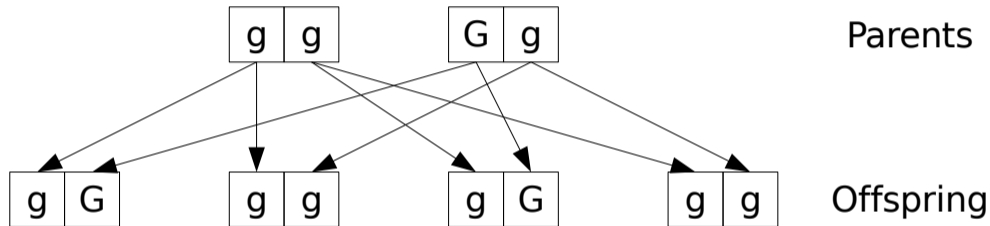


⇒ offspring have probability

- ▶ 1/4 of being GG
- ▶ 1/2 of being Gg
- ▶ 1/4 of being gg

gg and Gg parents

Recessive and hybrid parents



⇒ offspring have probability

- ▶ 1/2 of being Gg
- ▶ 1/2 of being gg

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General case

$p_i(t)$: probability that state S_i occurs on the t^{th} repetition of the experiment,
 $1 \leq i \leq n$

Since one the states S_i must occur on the t^{th} repetition

$$p_1(t) + p_2(t) + \cdots + p_n(t) = 1$$

$p_i(t+1)$: probability that state S_i , $1 \leq i \leq r$, occurs on $(t+1)^{\text{th}}$ repetition of the experiment

n ways to be in state S_i at step $t+1$:

1. Step t is S_1 . Probability of getting S_1 on t^{th} step is $p_1(t)$, and probability of having S_i after S_1 is p_{i1} . Therefore $P(S_i|S_1) = p_{i1}p_1(t)$
2. We get S_2 on step t and S_i on step $(t+1)$. Then $P(S_i|S_2) = p_{2i}p_2(t)$
- ..
- n . Probability of occurrence of S_i at step $t+1$ if S_n at step t is $P(S_i|S_n) = p_{in}p_n(t)$

$$\begin{aligned}\implies p_i(t+1) &= P(S_i|S_1) + \cdots + P(S_i|S_n) \\ &= p_{i1}p_1(t) + \cdots + p_{in}p_n(t)\end{aligned}$$

Therefore,

$$\begin{aligned}p_1(t+1) &= p_{11}p_1(t) + p_{12}p_2(t) + \cdots + p_{1n}p_n(t) \\ &\vdots \\ p_n(t+1) &= p_{n1}p_1(t) + p_{n2}p_2(t) + \cdots + p_{nn}p_n(t)\end{aligned}$$

In matrix form

$$p(t+1) = Pp(t), \quad n = 1, 2, 3, \dots$$

where $p(t) = (p_1(t), p_2(t), \dots, p_n(t))^T$ is a probability vector and $P = (p_{ij})$ is an $n \times n$ transition matrix,

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

So

$$\begin{pmatrix} p_1(t+1) \\ \vdots \\ p_n(t+1) \end{pmatrix} = \begin{pmatrix} p_{11} & p_{12} & \cdots & p_{1r} \\ p_{21} & p_{22} & \cdots & p_{2r} \\ \vdots & \vdots & \ddots & \vdots \\ p_{r1} & p_{r2} & \cdots & p_{rr} \end{pmatrix} \begin{pmatrix} p_1(t) \\ \vdots \\ p_n(t) \end{pmatrix}$$

Easy to check that this gives the same expression as before

Stochastic matrices

Definition 2 (Stochastic matrix)

The nonnegative $n \times n$ matrix M is **row-stochastic** (resp. **column-stochastic**) if $\sum_{j=1}^n a_{ij} = 1$ for all $i = 1, \dots, n$ (resp. $\sum_{i=1}^n a_{ij} = 1$ for all $j = 1, \dots, n$)

We often say **stochastic** and let the context determine whether we mean row- or column-stochastic

If it is both row- and column-stochastic, the matrix is **doubly stochastic**

Theorem 3

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

Long time behaviour

Let $\rho(0)$ be the initial distribution vector. Then

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

Iterating, we get, for any t ,

$$\rho(t) = P^t\rho(0)$$

Therefore,

$$\begin{aligned}\lim_{t \rightarrow +\infty} \rho(t) &= \lim_{t \rightarrow +\infty} P^t\rho(0) \\ &= \left(\lim_{t \rightarrow +\infty} P^t \right) \rho(0)\end{aligned}$$

if this limit exists

$$\lim_{n \rightarrow +\infty} p(t) = \left(\lim_{t \rightarrow +\infty} P^t \right) p(0)$$

Does the limit exist?

Theorem 4

If M, N are nonsingular stochastic matrices, then MN is a stochastic matrix

Corollary 5

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

So P^t above is stochastic

Markov chains

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Regular Markov chains

Definition 6 (Regular Markov chain)

A **regular** Markov chain has P^k (entry-wise) positive for some integer $k > 0$, i.e., P^k has only positive entries

Definition 7 (Primitive matrix)

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

Theorem 8

Markov chain regular \iff transition matrix P primitive

Behaviour of a regular MC

Theorem 9

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

- 1. the powers P^t approach a stochastic matrix W*
- 2. each column of W is the same (column) vector $w = (w_1, \dots, w_n)^T$*
- 3. the components of w are positive*

So if the Markov chain is regular

$$\lim_{t \rightarrow +\infty} p(t) = \lim_{t \rightarrow +\infty} P^t p(0) = Wp(0)$$

Computing W

If $p(t)$ converges, then $p(t+1) = Pp(t)$ at the limit, so $w = \lim_{t \rightarrow \infty} p(t)$ is a **fixed point** of the system. Write

$$w = Pw$$

and solve for w , i.e., find w as a (right) eigenvector corresponding to the eigenvalue 1

w might have to be normalized (you want a probability vector). Check that the norm $\|w\|_1$ defined by

$$\|w\|_1 = |w_1| + \cdots + |w_n| = w_1 + \cdots + w_n$$

(since $w \geq 0$) is equal to one. If not, use

$$\tilde{w} = \frac{w}{\|w\|_1}$$

Back to genetics

Suppose we want to understand what it means to have hybrid individuals in the population

Investigate this using a process of continued matings

- ▶ Start with an individual of known or unknown genetic character (dominant, hybrid or recessive) and mate it with a hybrid
- ▶ Assume that the mating results in at least one offspring; choose one of the offspring at random and mate it with a hybrid
- ▶ Repeat this process through a number of generations

What can we expect in terms of the genetic composition of the population after a while?

⇒ consider MC with states GG , Gg and gg

3 states: $S_1 = GG$, $S_2 = Gg$ and $S_3 = gg$; we use GG , Gg and gg as well to name the states

\swarrow	GG	Gg	gg
GG	0.5	0.25	0
Gg	0.5	0.5	0.5
gg	0	0.25	0.5

The transition probabilities are thus

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

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

so

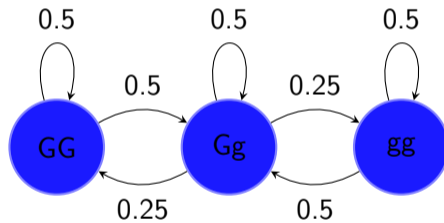
$$P^2 = \begin{pmatrix} \frac{3}{8} & \frac{1}{4} & \frac{1}{8} \\ \frac{1}{2} & \frac{1}{2} & \frac{1}{2} \\ \frac{1}{8} & \frac{1}{4} & \frac{3}{8} \end{pmatrix}$$

$\implies P$ primitive \implies Markov chain regular

Theorem 10

M primitive if the associated connection graph is strongly connected and there is at least one positive entry on the diagonal of M

This is checked directly on the transition graph



Compute (right) eigenvector associated to 1

$$\begin{pmatrix} 1/2 & 1/4 & 0 \\ 1/2 & 1/2 & 1/2 \\ 0 & 1/4 & 1/2 \end{pmatrix} \begin{pmatrix} w_1 \\ w_2 \\ w_3 \end{pmatrix} = \begin{pmatrix} w_1 \\ w_2 \\ w_3 \end{pmatrix}$$

$$\frac{1}{2}w_1 + \frac{1}{4}w_2 = w_1$$

$$\frac{1}{2}w_1 + \frac{1}{2}w_2 + \frac{1}{2}w_3 = w_2$$

$$\frac{1}{4}w_2 + \frac{1}{2}w_3 = w_3$$

So $w_1 = w_2/2$, $w_3 = w_2/2$ and thus

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

that is, $w_2 = w_2$, i.e., w_2 can take any value

$$\implies w = \left(\frac{1}{4}, \frac{1}{2}, \frac{1}{4} \right)$$

```
# Total population
nb_states = 10
# Parameters
proba_left = 0.5
proba_right = 0.5
proba_stay = 1-(proba_left+proba_right)
# Make the transition matrix
T = mat.or.vec(nr = nb_states, nc = nb_states)
for (row in 2:(nb_states-1)) {
  T[row,(row-1)] = proba_left
  T[row,(row+1)] = proba_right
  T[row, row] = proba_stay
}
T[1,2] = 1 # First row only moves right
T[nb_states, (nb_states-1)] = 1 # Last row only moves left
```


Create the MC object

```
# Library: markovchain  
mcRW <- new("markovchain",  
            states = sprintf("S_%d", 1:nb_states),  
            transitionMatrix = T,  
            name = "RW_reg")
```

Show some information about the chain

```
summary(mcRW)

## RW_reg Markov chain that is composed by:
## Closed classes:
## S_1 S_2 S_3 S_4 S_5 S_6 S_7 S_8 S_9 S_10
## Recurrent classes:
## {S_1,S_2,S_3,S_4,S_5,S_6,S_7,S_8,S_9,S_10}
## Transient classes:
## NONE
## The Markov chain is irreducible
## The absorbing states are: NONE
```

The equilibrium distribution

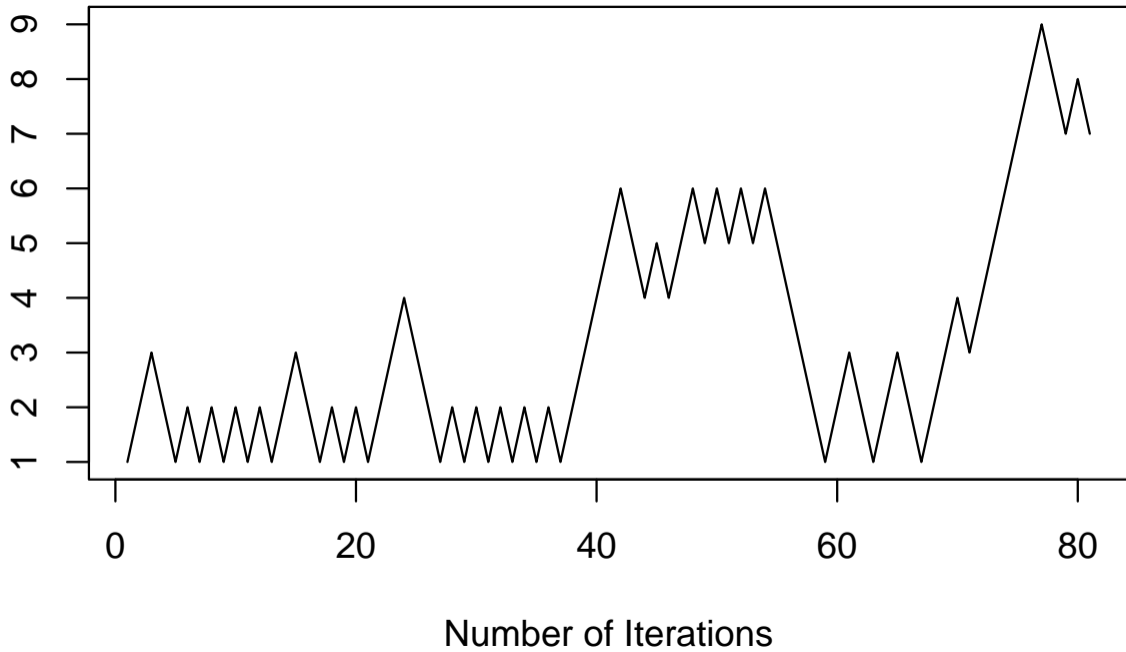
```
steadyStates(mcRW)
```

```
##           S_1           S_2           S_3           S_4           S_5           S_6
## [1,] 0.05555556 0.11111111 0.11111111 0.11111111 0.11111111 0.11111111 0.11111111 0.11111111
##           S_8           S_9           S_10
## [1,] 0.11111111 0.11111111 0.05555556
```

Showing a realisation

```
# Library: DTMCpack  
IC = rep(0, nb_states)  
IC[1] = 1  
sol = DTMC(T, IC, 81, trace=TRUE)  
  
## NULL
```

State



Markov chains

Running example – Mendelian inheritance

Repetition of the process

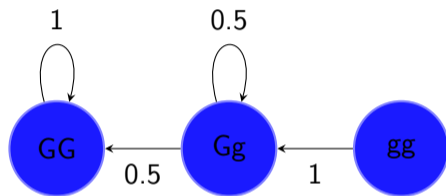
Regular Markov chains

Absorbing Markov chains



Changing the setting of the genetic experiment

Suppose now the same type of experiment, but mate each new generation with a GG individual instead of a Gg individual



↙	GG	Gg	gg
GG	1	0.5	0
Gg	0	0.5	1
gg	0	0	0

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

- ▶ leave gg after 1 iteration and can never return
- ▶ when we leave Gg, we can never return
- ▶ we can never leave GG when we get there

Absorbing Markov chains

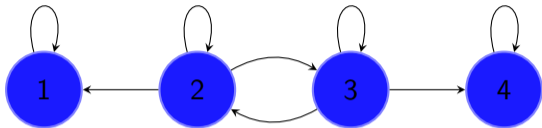
Definition 11 (Absorbing state)

A state S_i in a Markov chain is **absorbing** if whenever it occurs on the t^{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 12 (Absorbing chain)

A Markov chain is **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**

Suppose we have a chain like the following



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

The answer to the first question (“Does the process eventually reach an absorbing state?”) is given by the following result

Theorem 13

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

To answer the other questions, write the transition matrix in **standard** form

For an absorbing chain with k absorbing states and $r - k$ transient states, write transition matrix as

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

with following meaning

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

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

- ▶ $N = (\mathbb{I}_{r-k} - Q)^{-1}$ the **fundamental matrix** of the MC
- ▶ T_i sum of the entries on row i of N
- ▶ $B = RN$

Answers to our remaining questions:

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

Back to the genetic example

The matrix is already in standard form

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

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

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

We have

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

so

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

We have

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

So

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

and

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

2. N_{ij} average number of times the process is in the j th transient state if it starts in the i th transient state

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

3. T_i average number of steps before the process enters an absorbing state if it starts in the i th transient state

$$T = \begin{pmatrix} 2 \\ 3 \end{pmatrix}$$

4. B_{ij} probability of eventually entering the i th absorbing state if the process starts in the j th transient state

$$B = \begin{pmatrix} 1 & 1 \end{pmatrix}$$

Make an absorbing random walk

```
# Total population
nb_states = 7
proba_left = 0.5 # Probability of moving left
proba_right = 0.5 # Probability of moving right
proba_stay = 1-(proba_left+proba_right)
# Make the transition matrix
T = mat.or.vec(nr = nb_states, nc = nb_states)
for (row in 2:(nb_states-1)) {
  T[row,(row-1)] = proba_left
  T[row,(row+1)] = proba_right
  T[row, row] = proba_stay
}
T[1,1] = 1 # First state is absorbing
T[nb_states, nb_states] = 1 # Last too
```


Create MC object

```
mcRW <- new("markovchain",  
            states = sprintf("S_%d", 1:nb_states),  
            transitionMatrix = T,  
            name = "RW_abs")
```

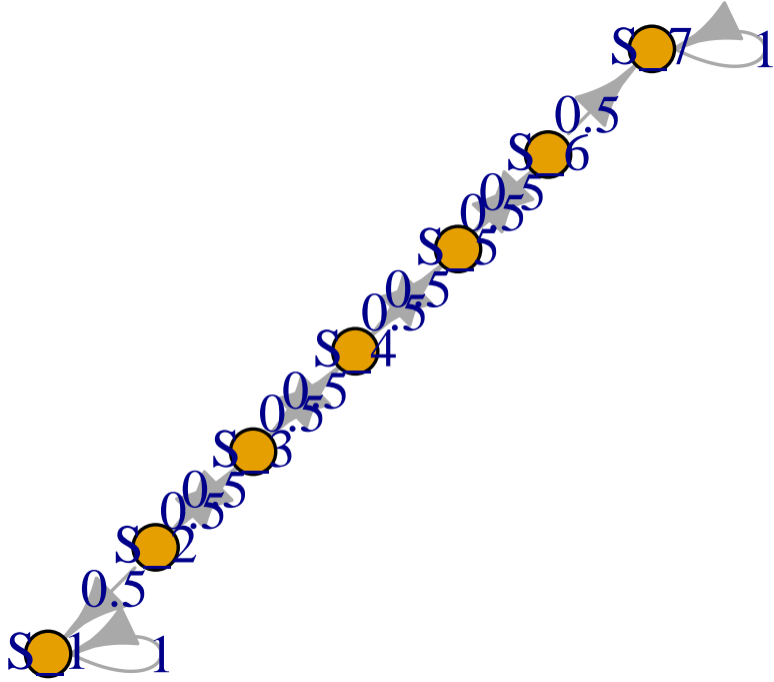
Show some info about the chain

```
summary(mcRW)

## RW_abs Markov chain that is composed by:
## Closed classes:
## S_1
## S_7
## Recurrent classes:
## {S_1},{S_7}
## Transient classes:
## {S_2,S_3,S_4,S_5,S_6}
## The Markov chain is not irreducible
## The absorbing states are: S_1 S_7
```

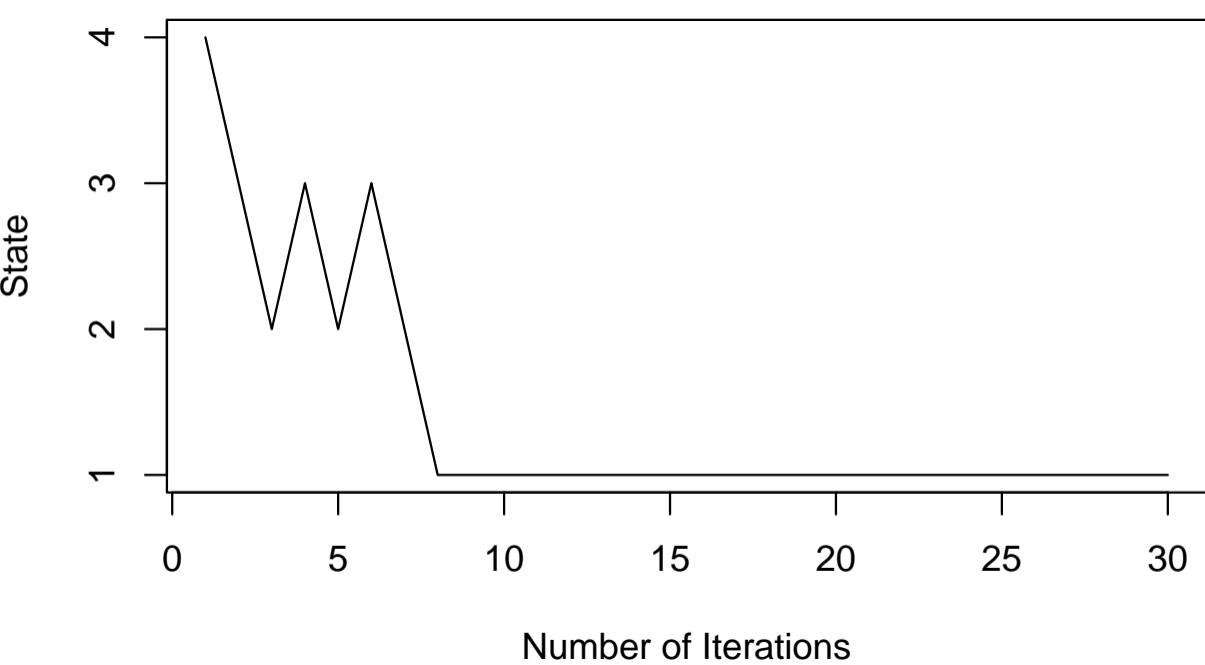
Plotting the chain

```
plot(mcRW)
```



Showing a realisation

```
# Library: DTMCpack  
IC = rep(0, nb_states)  
IC[4] = 1  
sol = DTMC(T, IC, 30, trace=TRUE)  
  
## NULL
```



Additional information about absorbing chains

`canonicForm(mcRW)`

`meanAbsorptionTime(mcRW)`

`absorptionProbabilities(mcRW)`

`hittingProbabilities(mcRW)`

Canonical form

```
canonicForm(mcRW)

## RW_abs
## A 7 - dimensional discrete Markov Chain defined by the following states
## S_1, S_7, S_2, S_3, S_4, S_5, S_6
## The transition matrix (by rows) is defined as follows:
##      S_1 S_7 S_2 S_3 S_4 S_5 S_6
## S_1 1.0 0.0 0.0 0.0 0.0 0.0 0.0
## S_7 0.0 1.0 0.0 0.0 0.0 0.0 0.0
## S_2 0.5 0.0 0.0 0.5 0.0 0.0 0.0
## S_3 0.0 0.0 0.0 0.5 0.0 0.5 0.0
## S_4 0.0 0.0 0.0 0.0 0.5 0.0 0.5
## S_5 0.0 0.0 0.0 0.0 0.0 0.5 0.0 0.5
## S_6 0.0 0.5 0.0 0.0 0.0 0.0 0.5 0.0
```


Mean absorption time

```
meanAbsorptionTime(mcRW)
```

```
## S_2 S_3 S_4 S_5 S_6
```

```
## 5 8 9 8 5
```

Absorption probabilities

```
absorptionProbabilities(mcRW)
```

```
##           S_1           S_7
## S_2 0.8333333 0.1666667
## S_3 0.6666667 0.3333333
## S_4 0.5000000 0.5000000
## S_5 0.3333333 0.6666667
## S_6 0.1666667 0.8333333
```

Hitting probabilities

```
hittingProbabilities(mcRW)
```

```
##           S_1 S_2   S_3           S_4   S_5 S_6           S_7
## S_1 1.0000000 0.0 0.000 0.0000000 0.000 0.0 0.0000000
## S_2 0.8333333 0.4 0.500 0.3333333 0.250 0.2 0.1666667
## S_3 0.6666667 0.8 0.625 0.6666667 0.500 0.4 0.3333333
## S_4 0.5000000 0.6 0.750 0.6666667 0.750 0.6 0.5000000
## S_5 0.3333333 0.4 0.500 0.6666667 0.625 0.8 0.6666667
## S_6 0.1666667 0.2 0.250 0.3333333 0.500 0.4 0.8333333
## S_7 0.0000000 0.0 0.000 0.0000000 0.000 0.0 1.0000000
```



Markov chains

Eigenvector centrality

PageRank

Constructing a stochastic matrix from an adjacency matrix

Let A be the adjacency matrix of a simple graph $G = (V, E)$ and D its degree matrix, i.e., the diagonal matrix $D = (d_{ij})$ with diagonal entries

$$d_{ii} = \sum_{j=1}^n a_{ji} = \sum_{j=1}^n a_{ij}$$

(Recall that A symmetric since G nondirected.) Then the matrix AD^{-1} is column stochastic

Indeed, write entries in D^{-1} as d_{ij}^{-1} . Of course, $d_{ii}^{-1} = 1/d_{ii}$, $1 \leq i \leq n$ and $d_{ij}^{-1} = 0$ if $i \neq j$

Then

$$AD^{-1} = \sum_{k=1}^n a_{ik} d_{kj}^{-1} = a_{ij} d_{jj}^{-1}, \quad i, j = 1, \dots, n$$

So the sum of column j of AD^{-1} is

$$\begin{aligned} \sum_{i=1}^n a_{ij} d_{jj}^{-1} &= d_{jj}^{-1} \sum_{i=1}^n a_{ij} \\ &= d_{jj}^{-1} \sum_{i=1}^n a_{ji} \\ &= d_{jj}^{-1} d_{jj} \\ &= 1 \end{aligned}$$

and the matrix is column-stochastic

Eigenvector centrality (undirected graph)

Let \mathbf{x} be an eigenvector corresponding to the largest eigenvalue λ of the non-negative adjacency matrix A of the undirected graph $G = (V, E)$

(We often call λ the **Perron root** of A and \mathbf{x} a **Perron eigenvector**)

The **eigenvector centrality** (or **prestige score**) of vertex i is the i th component of the eigenvector \mathbf{x} of the (column) stochastic matrix $N := AD^{-1}$ corresponding to the eigenvalue 1:

$$N\mathbf{x} = \mathbf{x}$$

Consider a particular vertex i with its neighbouring vertices $\mathcal{N}(i)$:

$$x_i = \sum_{j \in \mathcal{N}(i)} x_j = \sum_j A_{ij} x_j$$

The eigenvector centrality defined this way depends both on the number of neighbours $|\mathcal{N}(i)|$ and the quality of its connections x_j , $j \in \mathcal{N}(i)$

Let $A = (a_{ij})$ be the adjacency matrix of a graph. The eigenvector centrality x_i of vertex i is given by

$$x_i = \frac{1}{\lambda} \sum_k a_{ki} x_k$$

where $\lambda \neq 0$ is a constant. In matrix form

$$\mathbf{x}^T A = \lambda \mathbf{x}^T$$

Hence the centrality vector \mathbf{x} is the left eigenvector of the adjacency matrix A associated with the eigenvalue λ

Power method to solve eigenvector centrality

$m(v)$: signed component of maximal magnitude of vector v ; if more than one maximal component, let $m(v)$ be the first one. E.g., $m(-3, 3, 2) = -3$

Let $x^{(0)}$ be an arbitrary vector. For $k \geq 1$

- ▶ repeatedly compute $x^{(k)} = x^{(k-1)}A$
- ▶ normalize $x^{(k)} = x^{(k)} / m(x^{(k)})$

until desired precision is achieved

Then $x^{(k)}$ converges to the dominant eigenvector of A and $m(x^{(k)})$ converges to the dominant eigenvalue of A

If matrix A is sparse, each vector-matrix product can be performed in linear time in the size of the graph.

Power method converges when the dominant (largest) and the sub-dominant (second largest) eigenvalues of A λ_1 and λ_2 are separated, i.e., are different in absolute value, i.e., when $|\lambda_1| > |\lambda_2|$

Rate of convergence is rate at which $(\lambda_2/\lambda_1)^k$ goes to 0. Hence, if the sub-dominant eigenvalue is small compared to the dominant one, the method converges quickly

Why use the leading eigenvector?

We want a nonnegative measure, so we want a vector in \mathbb{R}_+

We know from the Perron-Frobenius Theorem that the eigenvector corresponding to the dominant eigenvalue of a nonnegative matrix is nonnegative

Furthermore, if the graph is strongly connected, the matrix is irreducible and the eigenvector corresponding to the dominant eigenvalue is *positive*

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PageRank

Variant of the Eigenvector centrality measure for directed network

Basic PageRank

- ▶ Whenever a vertex i has no outgoing link, we add a self-loop to i such that $k_i^{in} = k_i^{out} = 1$. Therefore $A_{ii} = 1$ for such vertices in the adjacency matrix
- ▶ Let D^+ be the diagonal matrix of outdegrees where each element $D_{ii}^+ = k_i^{out}$
- ▶ Define a column stochastic matrix $N = A(D^+)^{-1}$
- ▶ The PageRank centrality of node i is equal to the eigenvector x_i of matrix N (The leading eigenvalue is 1): $x = Nx$

Problem

Given n interlinked webpages, rank them in order of “importance”

Assign the pages importance scores $x_1, x_2, \dots, x_n \geq 0$

Key insight: use the existing link structure of the web to determine importance. A link to a page “is” a vote for its importance

How does this help with web searches?

First attempt: let x_k equal the number of links to page k

Criticism: a link from an “important” page (like Google) should carry more weight than a link from some random blog!

Second attempt: let x_k equal the sum of the importance scores of all pages linking to page k

Criticism 1: a webpage gets more “votes” (exerts more influence) if it has many outgoing links

Criticism 2: this system only has the trivial solution!

Third attempt (Brin and Page, late 90s): let x_k equal the sum of x_j/n_j , where the sum is taken over all the pages j that link to page k , and n_j is the number of outgoing links on page j

A page's number of votes is then its importance score, and gets split evenly among the pages it links to

Summary: given a web with n pages, construct an $n \times n$ matrix A as

$$a_{ij} = \begin{cases} 1/n_j & \text{if page } j \text{ links to page } i \\ 0 & \text{otherwise} \end{cases}$$

where n_j is number of outgoing links on page j

Sum of j th column is $n_j/n_j = 1$, so A is a stochastic matrix

The ranking vector \tilde{x} solves $A\tilde{x} = \tilde{x}$

Possible issues: existence of solution with nonnegative entries? Non-unique solutions?

PF Theorem guarantees a unique steady-state vector if entries of A are strictly positive or A irreducible. But irreducible $\not\Rightarrow \lambda_1$ and λ_2 separated, so make it primitive

Brin-Page: replace A with

$$B = 0.85A + \frac{0.15}{n}\mathbb{J}$$

where \mathbb{J} is the matrix of all ones

$B > 0$ is primitive \implies PF Theorem says B has a unique steady-state vector, x . So x can be used for rankings!

The Random Surfer

Why Markov chains?

Brin and Page

PageRank can be thought of as a model of user behavior. We assume there is a “random surfer” who is given a web page at random and keeps clicking on links, never hitting “back” but eventually gets bored and starts on another random page

Surfer clicks on a link on the current page with probability 0.85; opens up a random page with probability 0.15

A page's rank is the probability the random user will end up on that page, OR, equivalently the fraction of time the random user spends on that page in the long run

In practice

Estimates of the number of web pages vary.. 4.77×10^9 to more than 50×10^9

Computing stationary distribution is **hard** computationally

Instead, use power method, i.e., an iterative method, starting with initial distribution $(1/n, \dots, 1/n)$