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# THE ROLE OF KEMENY'S CONSTANT IN PROPERTIES OF MARKOV CHAINS

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# Andrei A Markov (1856 – 1922)

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# John G Kemeny (1926 – 1992)

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# Outline

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1. Preliminaries
2. Kemeny's constant
3. Expected time to mixing
4. Random surfer
5. Examples
6. Perturbation results
7. Mixing on directed graphs
8. Kirchhoff index
9. Variances of mixing times

# Introduction

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Let  $\{X_n\}$ , ( $n \geq 0$ ) be a finite irreducible (ergodic), discrete time Markov chain (MC).

Let  $S = \{1, 2, \dots, m\}$  be its state space.

Let  $p_{ij} = P[X_{n+1} = j \mid X_n = i]$  be the transition probability from state  $i$  to state  $j$ .

Let  $P = [p_{ij}]$  be the transition matrix of the MC.

$P$  stochastic  $\Rightarrow \sum_{j=1}^m p_{ij} = 1, \quad i \in S.$

Let  $\{p_j^{(n)}\} = \{P[X_n = j]\}$  be the probability distribution at the  $n$ -th trial.

# Limiting & stationary distrns

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When the MC is **regular** (finite, aperiodic & irreducible) a limiting distribution exists, that does not depend on the initial distribution and that the limiting distribution is the stationary distribution. ie.  $\{X_n\}$  has a unique stationary distribution  $\{\pi_j\}, j \in S$  and  $\lim_{n \rightarrow \infty} p_j^{(n)} = \pi_j$ .

When the MC is finite, irreducible and **periodic** a limiting distribution does not exist. However there is a unique stationary distribution.

# Stationary distributions

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**Irreducible** or **ergodic** MCs  $\{X_n\}$  have a unique stationary distribution  $\{\pi_j\}, j \in S$ .

The stationary probabilities are given as the solution of the stationary equations:

$$\pi_j = \sum_{i=1}^m \pi_i p_{ij} \quad (j \in S) \text{ with } \sum_{i=1}^m \pi_i = 1.$$

The "stationary probability vector" is  $\pi^T = (\pi_1, \pi_2, \dots, \pi_m)$ .

# Primer on g-inverses of $I - P$

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A 'one condition' g-inverse or an 'equation solving' g-inverse of a matrix  $A$  is any matrix  $A^-$  such that  $AA^-A = A$ .

Let  $P$  be the transition matrix of a finite irreducible MC with stationary probability vector  $\pi^T$ . Let  $\mathbf{t}$  and  $\mathbf{u}$  be any vectors.

$I - P + \mathbf{t}\mathbf{u}^T$  is non-singular  $\Leftrightarrow \pi^T \mathbf{t} \neq 0$  and  $\mathbf{u}^T \mathbf{e} \neq 0$ .

$\pi^T \mathbf{t} \neq 0$  and  $\mathbf{u}^T \mathbf{e} \neq 0 \Rightarrow [I - P + \mathbf{t}\mathbf{u}^T]^{-1}$  is a g-inverse of  $I - P$ .  
(Hunter, 1982)

# Use of g-inverses

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A necessary and sufficient condition for  $AXB = C$  to have a solution is that  $AA^-CB^-B = C$ .

If this consistency condition is satisfied the general solution is given by  $X = A^-CB^- + W - A^-AWBB^-$ , where  $W$  is an arbitrary matrix. (Rao, 1966)

$AX = C$  has a solution  $X = A^-C + (I - A^-A)W$ , where  $W$  is arbitrary, provided  $AA^-C = C$ .



# Special g-inverses of $I - P$

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If  $G$  is any g-inverse of  $I - P$  then there exists vectors  $\mathbf{f}, \mathbf{g}, \mathbf{t}$  and  $\mathbf{u}$  with  $\pi^T \mathbf{t} \neq 0$  and  $\mathbf{u}^T \mathbf{e} \neq 0$  such that

$$G = [I - P + \mathbf{t}\mathbf{u}^T]^{-1} + \mathbf{e}\mathbf{f}^T + \mathbf{g}\pi^T.$$

$Z = [I - P + \Pi]^{-1}$ , ( $\Pi \equiv \mathbf{e}\pi^T$ ) "fundamental matrix" of irreducible (ergodic) Markov chains. (Kemeny & Snell, 1960)  
 $(I - P)^\# = A^\# = Z - \Pi$ , "group inverse" of  $I - P$ . (Meyer, 1975)

If  $G$  is any generalized inverse of  $I - P$ ,  
 $(I - P)G(I - P)$  is invariant and  $= A^\#$ .  
(Meyer, 1975), (Hunter, 1982)



# First passage times in MCs

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Let  $T_{ij}$  be the first passage time r.v. from state  $i$  to state  $j$ ,

i.e.  $T_{ij} = \min\{n \geq 1 \text{ such that } X_n = j \text{ given that } X_0 = i\}$ ,

$T_{ii}$  is the "first return to state  $i$ ".

The irreducibility of the MC ensures that the  $T_{ij}$  are all proper random variables. Under the finite state space restriction, all the moments of  $T_{ij}$  are finite.

Let  $m_{ij}^{(k)}$  be the  $k$ -th moment of the first passage time from state  $i$  to state  $j$ .

i.e.  $m_{ij}^{(k)} = E[T_{ij}^k \mid X_0 = i]$  for all  $(i, j) \in S \times S$ .

# Mean first passage times

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Let  $m_{ij}^{(1)} = m_{ij}$ , the mean first passage time from state  $i$  to state  $j$ ,  $(i, j) \in S \times S$ .

For an irreducible finite MC with transition matrix  $P$ , let  $M = [m_{ij}]$  be the matrix of expected first passage times from state  $i$  to state  $j$ .

$M$  satisfies the matrix equation

$$(I - P)M = E - PM_d$$

where  $E = \mathbf{ee}^T = [1]$ ,  $M_d = [\delta_{ij}m_{ij}] = (\Pi_d)^{-1} \equiv D$ .

# Mean first passage times

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If  $G$  is any  $g$ -inverse of  $I - P$ , then

$$M = [G\Pi - E(G\Pi)_d + I - G + EG_d]D. \quad (\text{Hunter, 1982})$$

Under any of the following three equivalent conditions:

(i)  $G\mathbf{e} = g\mathbf{e}$ ,  $g$  a constant,

(ii)  $GE - E(G\Pi)_d D = 0$ ,

(iii)  $G\Pi - E(G\Pi)_d = 0$ ,

$$M = [I - G + EG_d]D. \quad (\text{Hunter, 2008})$$

Special cases:

$G = Z$ , Kemeny and Snell's fundamental matrix ( $g = 1$ )

$G = A^\# = Z - \Pi$ , Meyer's group inverse of  $I - P$ , ( $g = 0$ )

# Mean first passage times

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If  $G = [g_{ij}]$  is any generalized inverse of  $I - P$ ,

then  $m_{ij} = ([g_{jj} - g_{ij} + \delta_{ij}]/\pi_j) + (g_{i.} - g_{j.})$ , for all  $i, j$ .

Further, when  $Ge = ge$ ,

$$m_{ij} = [g_{jj} - g_{ij} + \delta_{ij}]/\pi_j, \text{ for all } i, j.$$

$$\text{Thus } m_{ij} = \begin{cases} \frac{z_{jj} - z_{ij}}{\pi_j} = \frac{a_{jj}^{\#} - a_{ij}^{\#}}{\pi_j}, & i \neq j, \\ \frac{1}{\pi_j} & i = j. \end{cases}$$

Using  $Z$  (Kemeny & Snell, 1960). Using  $A^{\#}$  (Meyer, 1975)

# Kemeny's constant

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**Key Result :**

$$M\pi = K\mathbf{e},$$

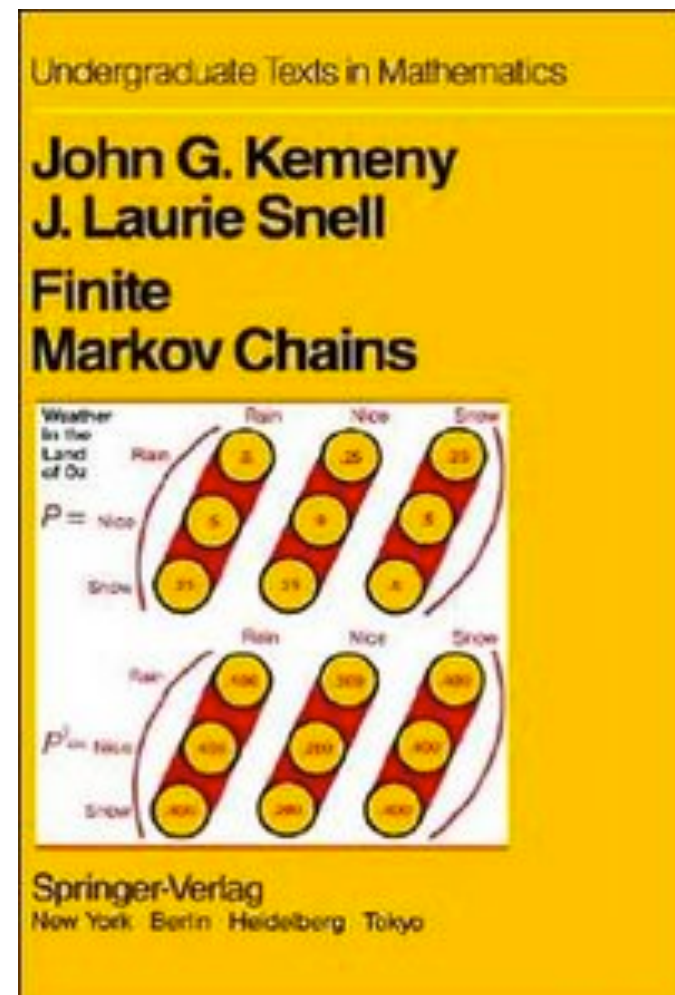
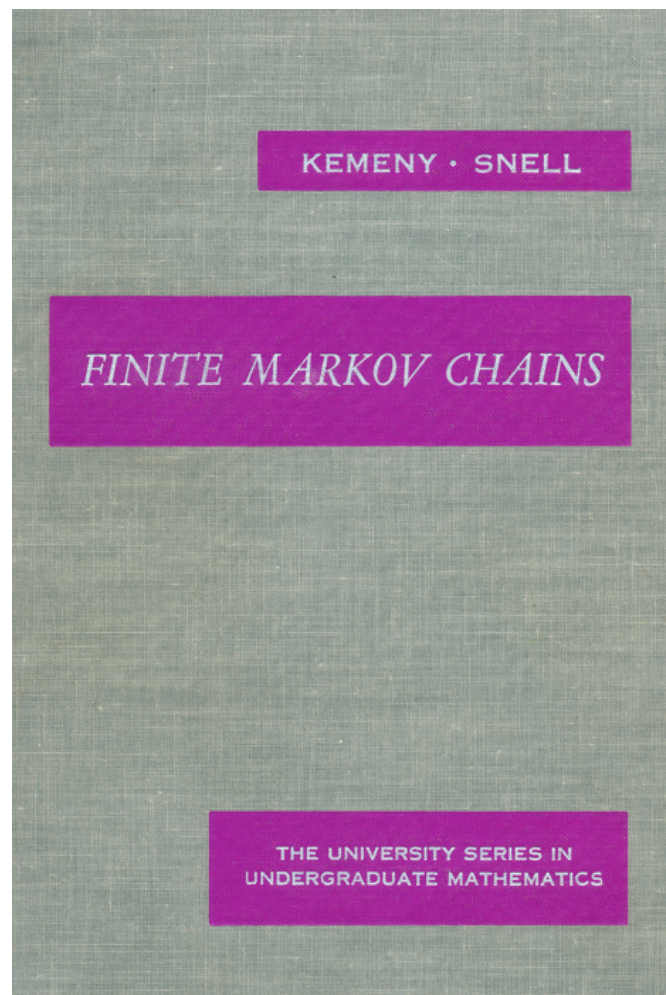
$$\sum_{j=1}^m m_{ij}\pi_j = K, \text{ "**Kemeny's constant**" for all } i \in S.$$

One of the simplest proofs is based upon  $Z$  :

$$\begin{aligned} M\pi &= [I - Z + EZ_d]D\pi \\ &= [I - Z + EZ_d]\mathbf{e} \\ &= \mathbf{e} - Z\mathbf{e} + \mathbf{e}\mathbf{e}^T Z_d \mathbf{e} = K\mathbf{e}, \end{aligned}$$

where  $K = \mathbf{e}^T Z_d \mathbf{e} = \text{tr}(Z)$ .

# Initial appearance - 1960



# Kemeny & Snell - Initial result

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SEC. 4

REGULAR MARKOV CHAINS

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**4.4.10 THEOREM.** *Let  $c = \sum_i z_{ii}$ . Then  $M\alpha^T = c\xi$ .*

PROOF.

$$\begin{aligned} M\alpha^T &= (I - Z + EZ_{\text{dg}})D\alpha^T \\ &= (I - Z + EZ_{\text{dg}})\xi \\ &= \xi(\eta Z_{\text{dg}}\xi) = c\xi. \end{aligned}$$

In terms of our notation:  $c = \text{tr}(Z)$ ,  $\alpha^T = \pi$ ,  $\eta = \mathbf{e}^T$ ,  $\xi = \mathbf{e}$  so that

$$M\pi = (\text{tr}(Z))\mathbf{e}.$$

(Kemeny & Snell, “Finite Markov Chains”, 1960)

# Kemeny's constant - Alternative

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Define  $\mathbf{k} = M\pi$ , where  $\mathbf{k}^T = (K_1, K_2, \dots, K_m)$ .

Since  $(I - P)M = E - PM_d$ ,

$$(I - P)\mathbf{k} = (I - P)M\pi = E\pi - PM_d\pi = \mathbf{e}\mathbf{e}^T\pi - P\mathbf{e} = \mathbf{e} - \mathbf{e} = \mathbf{0}.$$

i.e.  $P\mathbf{k} = \mathbf{k}$ , or  $\sum_{j=1}^m p_{ij}K_j = K_i$

The irreducibility of the MC implies that  $\mathbf{k}$  is the right eigenvector of  $P$  corresponding to the eigenvalue  $\lambda = 1$   
 $\Rightarrow k = Ke$ . i.e  $K_i = K$  for all  $i = 1, 2, \dots, m$ .

$$\text{i.e. } K_i = \sum_{j=1}^m m_{ij}\pi_j = K, \text{ "**Kemeny's constant**" for all } i \in S.$$

# Clarification of Kemeny's $K$

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$m_{ii}$  is typically defined as the mean time for the MC starting in state  $i$  to return to state  $i$ . It is well known that

$$m_{ii} = 1/\pi_i \text{ and thus } m_{ii}\pi_i = 1$$

Consequently "**Kemeny's constant**"

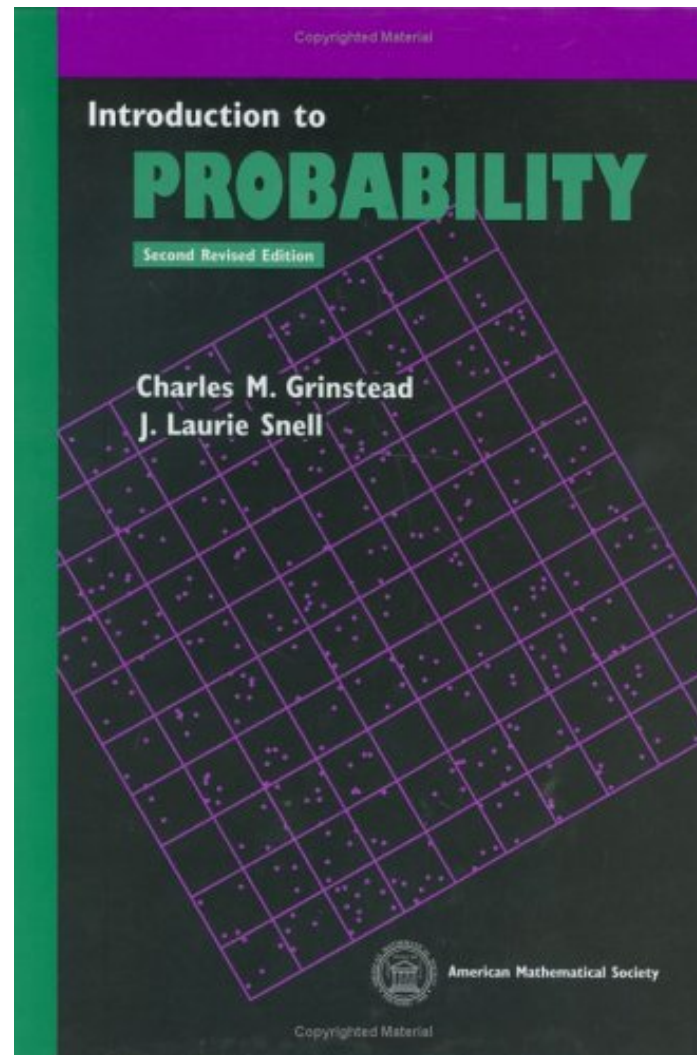
$$K = \sum_{j=1}^m m_{ij}\pi_j = m_{ii}\pi_i + \sum_{j \neq i} m_{ij}\pi_j = 1 + \sum_{j \neq i} m_{ij}\pi_j$$

Some authors (in particular, Grinstead and Snell, 2006) define, by convention, that  $m_{ii} = 0$  so that the expression for the mean first passage times as  $m_{ij} = (z_{jj} - z_{ij})/\pi_j$  holds for all  $i, j$ .

We will stay with the expression as defined above for  $K$ , bearing in mind that in some books and papers  $K$  is replaced by  $K - 1$ .

# Grinstead & Snell - 2006 - update

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# Grinstead & Snell - update

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**19** Show that, for an ergodic Markov chain (see Theorem 11.16),

$$\sum_j m_{ij} w_j = \sum_j z_{jj} - 1 = K .$$

By convention  $m_{ii} = 0$ .

The second expression above shows that the number  $K$  is independent of  $i$ . The number  $K$  is called *Kemeny's constant*. A prize was offered to the first person to give an intuitively plausible reason for the above sum to be independent of  $i$ . (See also Exercise 24.)

# Grinstead & Snell - update

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**24** In the course of a walk with Snell along Minnehaha Avenue in Minneapolis in the fall of 1983, Peter Doyle<sup>25</sup> suggested the following explanation for the constancy of *Kemeny's constant* (see Exercise 19). Choose a target state according to the fixed vector  $\mathbf{w}$ . Start from state  $i$  and wait until the time  $T$  that the target state occurs for the first time. Let  $K_i$  be the expected value of  $T$ . Observe that

$$K_i + w_i \cdot 1/w_i = \sum_j P_{ij} K_j + 1 ,$$

and hence

$$K_i = \sum_j P_{ij} K_j .$$

By the maximum principle,  $K_i$  is a constant. Should Peter have been given the prize?

# Peter Doyle – 2009 - update

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## The Kemeny constant of a Markov chain

Peter Doyle

Version 1.0 dated 14 September 2009

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$$M_{iw} = \sum_j P_i^j M_{jw}.$$

But now by the familiar *maximum principle*, any function  $f_i$  satisfying

$$\sum_j P_i^j f_j = f_i$$

must be constant: Choose  $i$  to maximize  $f_i$ , and observe that the maximum must be attained also for any  $j$  where  $P_i^j > 0$ ; push the max around until it is attained everywhere. So  $M_{iw}$  doesn't depend on  $i$ . ■

**Note.** The application of the maximum principle we've made here shows that the only column eigenvectors having eigenvalue 1 for the matrix  $P$  are the constant vectors—a fact that was stated not quite explicitly above.

This formula provides a computational verification that Kemeny's constant is constant, but doesn't explain *why* it is constant. Kemeny felt this keenly: A prize was offered for a more 'conceptual' proof, and awarded—rightly or wrongly—on the basis of the maximum principle argument outlined above.

# Expressions using g-inverses

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If  $G = [g_{ij}]$  is any g-inverse of  $I - P$ , then

$$K = 1 + \text{tr}(G) - \text{tr}(G\Pi) = 1 + \sum_{j=1}^m (g_{jj} - g_{j\cdot}\pi_j)$$

When  $G\mathbf{e} = g\mathbf{e}$ ,

$$K = 1 - g + \text{tr}(G) = 1 - g + \sum_{j=1}^m g_{jj}.$$

In particular,  $K = \text{tr}(Z) = \sum_{j=1}^m z_{jj}$

and  $K = 1 + \text{tr}(A^\#)$ .

"Classical result" (Hunter, 2006).

"Random target lemma" (with Z) (Lovasz & Winkler, 1998).

Book "Reversible MCs & RWs" (Aldous & Fill, 1999).

# Expressions using eigenvalues

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$P$  irreducible  $\Rightarrow$

The eigenvalues of  $P, \{\lambda_i\}$  ( $i = 1, 2, \dots, m$ )

are such that  $\lambda_1 = 1$ , with  $|\lambda_i| \leq 1$  and  $\lambda_i \neq 1$  ( $i = 2, \dots, m$ ).

$\Rightarrow$  The eigenvalues of  $Z = [I - P + \mathbf{e}\pi^T]^{-1}$  are

$$\lambda_i(Z) = 1 \quad (i = 1), \quad \frac{1}{1 - \lambda_i} \quad (i = 2, \dots, m).$$

$$\text{Thus } K = \text{tr}(Z) = \sum_{i=1}^m z_{ii}$$

$$= \sum_{i=1}^m \lambda_i(Z) = 1 + \sum_{i=2}^m \frac{1}{1 - \lambda_i}.$$

(Levene & Loizou, 2002), (Hunter, 2006), (Doyle, 2009)

# Bounds on $K$

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$K = 1 + \sum_{i=2}^m \frac{1}{1 - \lambda_i}$  and  $P$  is irreducible.

Hence  $\lambda_1 = 1$ , with  $|\lambda_i| \leq 1$  and  $\lambda_i \neq 1$  ( $i = 2, \dots, m$ ).

If any eigenvalue appears on the unit circle  $|\lambda| = 1$  must appear as a root of unity and be associated with a periodic chain (whose periodicity cannot exceed  $m$ ).

Any complex root  $\lambda = a + bi$  must be associated with its complex conjugate  $\bar{\lambda} = a - bi$ , with  $a^2 + b^2 \leq 1$ .

For this pair of conjugate roots

$$\frac{1}{1 - \lambda} + \frac{1}{1 - \bar{\lambda}} = \frac{2 - (\lambda + \bar{\lambda})}{(1 - \lambda)(1 - \bar{\lambda})} = \frac{2 - 2a}{1 - (\lambda + \bar{\lambda}) + \lambda\bar{\lambda}} = \frac{2 - 2a}{1 - 2a + a^2 + b^2} \geq 1.$$

# Bounds on $K$

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For conjugate pair of roots  $\frac{1}{1-\lambda} + \frac{1}{1-\bar{\lambda}} \geq 1$ . For any real roots,

$-1 \leq \lambda \leq 1 \Rightarrow \frac{1}{1-\lambda} \geq \frac{1}{2}$ . The only possible root at  $\lambda = -1$  occurs

with periodic chain with even period.

Thus taking the real roots individually and complex roots in pairs

$$K = 1 + \sum_{i=2}^m \frac{1}{1-\lambda_i} \geq 1 + \frac{m-1}{2} = \frac{m+1}{2}.$$

Hunter (2006) based on Styan (1964) when all  $\lambda_i$  are real.

If the MC is reversible (all the  $\lambda_i$  real) and regular (aperiodic)

then  $\frac{m-1}{2} \leq \sum_{i=2}^m \frac{1}{1-\lambda_i} \leq \frac{m-1}{1-\lambda_2}$ . (Levene & Loizou, 2002).

# Bounds on $K$

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Suppose the the MC is irreducible & reversible so that

$$1 = \lambda_1 > \lambda_2 \geq \dots \geq \lambda_m > -1. \text{ Note } K = 1 + \sum_{i=2}^m \frac{1}{1 - \lambda_i} = m + \sum_{i=2}^m \frac{\lambda_i}{1 - \lambda_i}$$

From Palacois & Remon (2010), the method of Lagrange multipliers

applied to the function  $f(x_2, \dots, x_m) = \sum_{i=2}^m \frac{x_i}{1 - x_i}$ , subject to the

condition  $1 + x_2 + \dots + x_m = 0$  on the domain  $1 > x_2 \geq \dots \geq x_m > -1$

$\Rightarrow$  minimum of  $f(x_1, x_2, \dots, x_m)$  attained at  $x_2 = \dots = x_m = \frac{-1}{m-1}$ .

$$\Rightarrow \frac{(m-1)^2}{m} \leq \sum_{i=2}^m \frac{1}{1 - \lambda_i} \leq \frac{m-1}{1 - \lambda_2}. \quad (\text{Palocois \& Remon, 2010}).$$

- an improvement on the earlier bounds of Levene & Loizou).

# Alternative representation of $K$

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$$K = \text{tr}(A_j^{-1}) - \frac{A_{jj}^{\#}}{\pi_j} + 1, \quad \text{where } A_j^{-1} \text{ is } (m-1) \times (m-1) \text{ principal}$$

submatrix of  $A$  obtained by deleting its  $j$  – th row and column. (Catral, Kirkland, Neumann, Sze, 2010)



The proof is based upon expressing  $A^{\#} = [a_{ij}^{\#}]$  in terms of  $A_n^{-1}$  and  $\pi^T$

Without loss of generality, take  $j = m$ . Use  $m_{ij}\pi_j = a_{jj}^{\#} - a_{ij}^{\#}$

and the result (Meyer, 1973) that if  $B$  is the leading  $(m-1) \times (m-1)$  principal submatrix of  $A^{\#}$ , then  $B = A_n^{-1} + \beta W - A_n^{-1}W - WA_n^{-1}$ ,

where  $\beta = \mathbf{u}^T A_n^{-1} \mathbf{e}$ ,  $W = \mathbf{e} \mathbf{u}^T$  and  $\pi^T = (\mathbf{u}^T, \pi_n)$ .

# Stationarity in Markov chains

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For all irreducible MCs (including periodic chains),  
if for some  $k \geq 0$ ,  $p_j^{(k)} = P[X_k = j] = \pi_j$  for all  $j \in S$ ,  
then  $p_j^{(n)} = P[X_n = j] = \pi_j$  for all  $n \geq k$  and all  $j \in S$ .

How many trials do we need to take so that  
 $P[X_n = j] = \pi_j$  for all  $j \in S$ ?

# Mixing times in Markov chains

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Let  $Y$  be a RV whose probability distribution is the stationary distribution  $\{\pi_j\}$ .

The MC  $\{X_n\}$ , achieves "mixing", at time  $T = k$ , when  $X_k = Y$  for the smallest such  $k \geq 1$ .

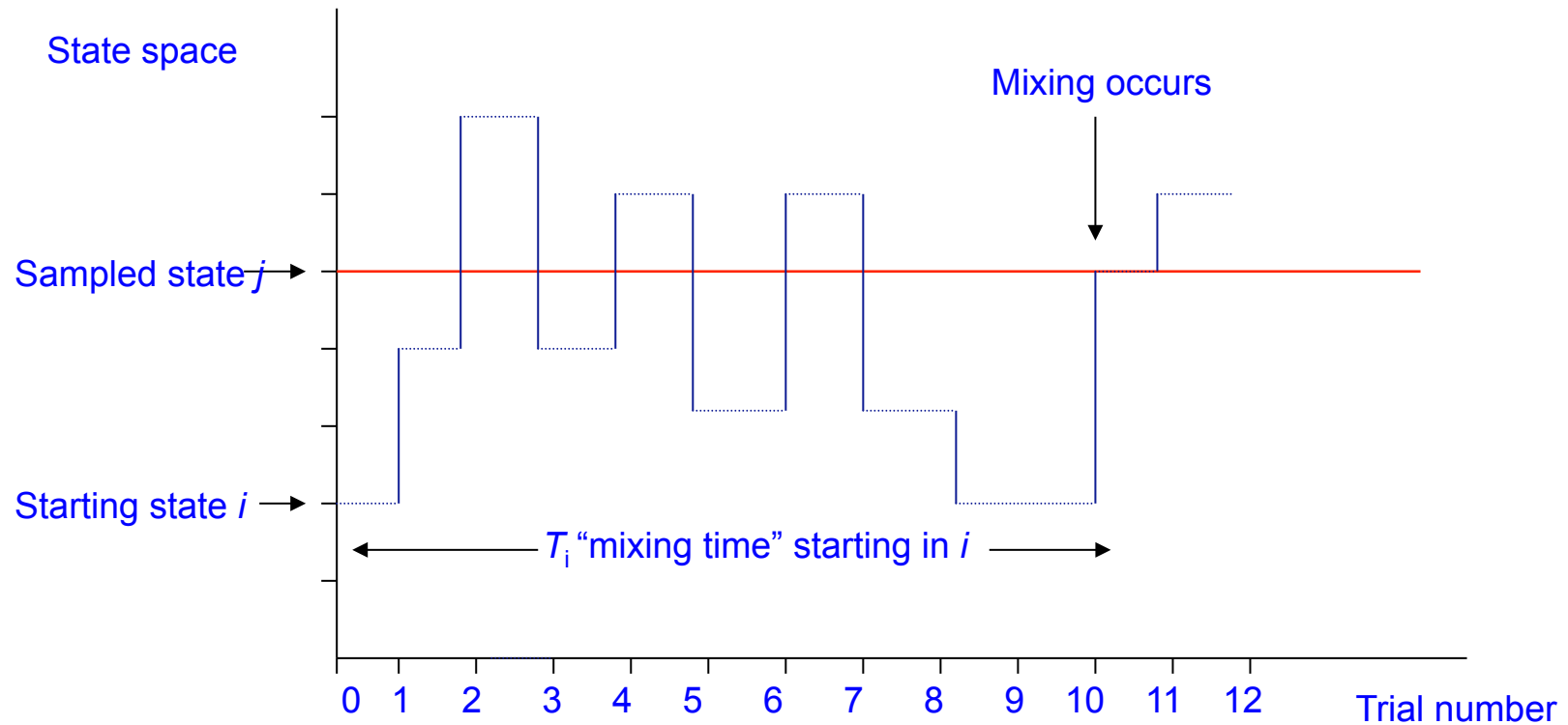
$T$  is the "time to mixing" in a Markov chain.

Thus, we first sample from the stationary distribution  $\{\pi_j\}$  to determine a value of the random variable  $Y$ , say  $Y = j$ .

Now observe the MC, starting at a given state  $i$ . We achieve "mixing" at time  $T = n$  when  $X_n = j$  for the first such  $n \geq 1$ .

# Expected time to mixing

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# Expected time to mixing in a MC

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The finite state space & irreducibility of the  $X_n$

$\Rightarrow T$  is finite (a.s), with finite moments.

Let  $\tau_{M,i}$  be the "*expected time to mixing*", starting at state  $i$ ,  
(assuming that mixing cannot occur at the first trial).

Conditional upon  $X_0 = i$ ,

$$E[T] = E_Y(E[T | Y]) = \sum_{j=1}^m E[T | Y = j] P[Y = j]$$

$$= \sum_{j=1}^m E[T_{ij} | X_0 = i] \pi_j = \sum_{j=i}^m m_{ij} \pi_j$$

$$\text{i.e. } \tau_{M,i} = E[T | X_0 = i] = \sum_{j=i}^m m_{ij} \pi_j = \sum_{j=1}^m m_{ij} \pi_j = \tau_M = K.$$

(Hunter, 2006)

# Expected mixing times

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Expected time to mixing, starting in any state, is constant

$$\tau_M = K.$$

If  $G = [g_{ij}]$  is any g-inverse of  $I - P$ , then

$$\tau_M = 1 + \text{tr}(G) - \text{tr}(G\Pi) = 1 + \sum_{j=1}^m (g_{jj} - g_{j \cdot} \pi_j)$$

When  $G\mathbf{e} = g\mathbf{e}$ ,

$$\tau_M = 1 - g + \text{tr}(G) = 1 - g + \sum_{j=1}^m g_{jj}$$

$$\tau_M = \text{tr}(Z) = \sum_{j=1}^m z_{jj}$$

and

$$\tau_M = 1 + \text{tr}(A^\#).$$

# Expected mixing times

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We have assumed that the MC  $\{X_n\}$ , achieves “mixing”, at time  $T = k$ , when  $X_k = Y$  for the smallest such  $k \geq 1$ .

If we assume that mixing might be possible at  $k = 0$  when the “mixing state”, sampled from  $\{\pi_j\}$ , *and* the “starting state”  $j$  are the same (say state  $i$ ) we would have “mixing” occurring at time  $T = 0$ , in which case the expected time to mixing would

be  $\sum_{j \neq i} m_{ij} \pi_j = K - 1$ , since  $m_{ii} \pi_i = 1$ .

(In our assumptions, mixing cannot occur initially and if the mixing state and the starting state are the same, mixing will not occur until a return to state  $i$  has occurred after a time  $T_{ii}$  ( $\geq 1$ ))

# Random surfer

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Note that  $K = \sum_{i=1}^m \pi_i \sum_{j=1}^m \pi_j m_{ij} = \sum_{i=1}^m \pi_i M_i$  where  $M_i = \sum_{j=1}^m \pi_j m_{ij}$ .

$M_i$  can represent the mean first passage time from state  $i$  when the destination state is unknown.

$K = \sum_{i=1}^m \pi_i M_i$  can be interpreted as the mean first passage time from an unknown starting state to an unknown destination state. Imagine a random surfer who is "lost" and doesn't know the state he is at and where he is heading.

$K$  can be interpreted as the mean number of links the random surfer follows before reaching his destination. Thus the random surfer is not "lost" anymore, he just has to follow  $K$  random links and he can expect to arrive at his final destination. (Levene & Loizou, 2002)

# Example – Two state MCs

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$$\text{Let } P = \begin{bmatrix} p_{11} & p_{12} \\ p_{21} & p_{22} \end{bmatrix} = \begin{bmatrix} 1-a & a \\ b & 1-b \end{bmatrix},$$

$(0 \leq a \leq 1, 0 \leq b \leq 1)$ . Let  $d = 1 - a - b$ .

MC irreducible  $\Leftrightarrow -1 \leq d < 1$ .

MC has a unique stationary probability vector

$$\pi^T = (\pi_1, \pi_2) = \left( \frac{b}{a+b}, \frac{a}{a+b} \right) = \left( \frac{b}{1-d}, \frac{a}{1-d} \right).$$

$-1 < d < 1 \Leftrightarrow$  MC is regular and the stationary distribution  
is the limiting distribution of the MC.

$d = -1 \Leftrightarrow$  MC is irreducible, periodic, period 2.

# Example – Two state MCs

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$$\tau_M = 1 + \frac{1}{a+b} = 1 + \frac{1}{1-d}.$$

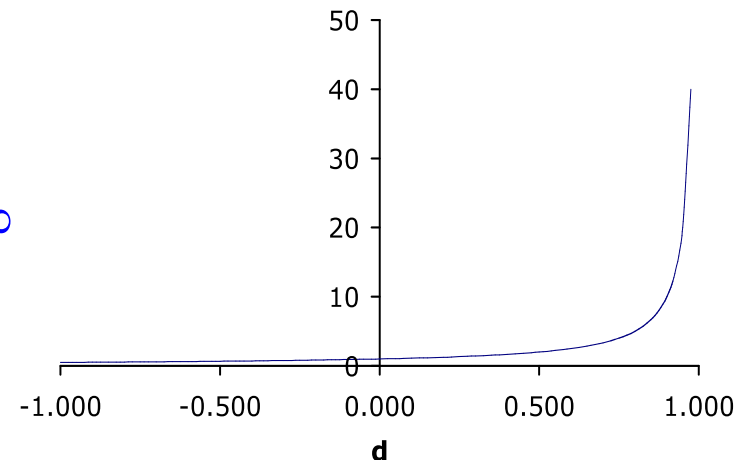
$d = 1 \Leftrightarrow$  Periodic, period 2, MC with  $a = 1$ ,  $b = 1$ .

$\Leftrightarrow \tau_M = 1.5$  (minimum value of  $\tau_M$ ).

$d = 0 \Leftrightarrow$  Independent trials  $\Leftrightarrow \tau_M = 2$ .

$d \rightarrow 1$  (both  $a \rightarrow 0$  and  $b \rightarrow 0$ )  $\Rightarrow$  arbitrarily large  $\tau_M$ .

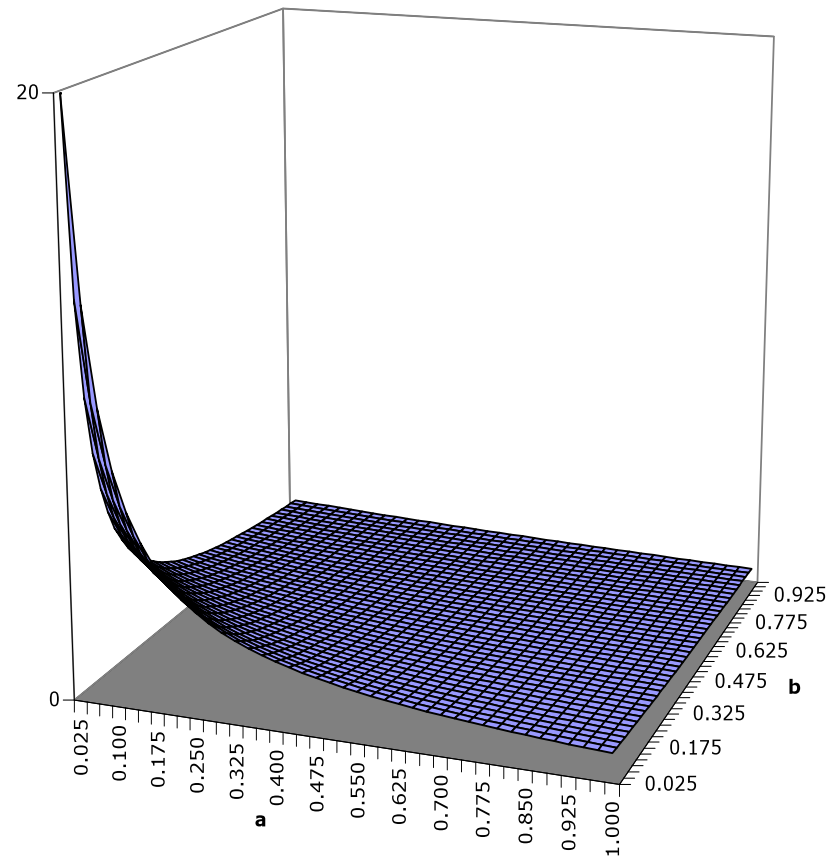
For all two state MCs:  $1.5 \leq \tau_M < \infty$



# Example – Two state MCs

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Plot of  $\tau_M = 1 + \frac{1}{a+b}$ .



# Example – Three state MCs

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$$P = [p_{ij}] = \begin{bmatrix} 1 - p_2 - p_3 & p_2 & p_3 \\ q_1 & 1 - q_1 - q_3 & q_3 \\ r_1 & r_2 & 1 - r_1 - r_2 \end{bmatrix}.$$

Six constrained parameters with

$0 < p_2 + p_3 \leq 1$ ,  $0 < q_1 + q_3 \leq 1$  and  $0 < r_1 + r_2 \leq 1$ .

Let  $\Delta_1 \equiv q_3 r_1 + q_1 r_2 + q_1 r_1$ ,

$\Delta_2 \equiv r_1 p_2 + r_2 p_3 + r_2 p_2$ ,

$\Delta_3 \equiv p_2 q_3 + p_3 q_1 + p_3 q_3$ ,

$\Delta \equiv \Delta_1 + \Delta_2 + \Delta_3$ .

# Example – Three state MCs

---

MC is irreducible

(and hence a stationary distribution exists)

$$\Leftrightarrow \Delta_1 > 0, \Delta_2 > 0, \Delta_3 > 0.$$

Stationary distribution given by

$$(\pi_1, \pi_2, \pi_3) = \frac{1}{\Delta} (\Delta_1, \Delta_2, \Delta_3).$$

# Example – Three state MCs

---

Let  $\tau_{12} = p_3 + r_1 + r_2$ ,  $\tau_{13} = p_2 + q_1 + q_3$ ,  $\tau_{21} = q_3 + r_1 + r_2$ ,

$\tau_{23} = q_1 + p_2 + p_3$ ,  $\tau_{31} = r_2 + q_1 + q_3$ ,  $\tau_{32} = r_1 + p_2 + p_3$ ,

Let  $\tau = p_2 + p_3 + q_1 + q_3 + r_1 + r_2$

$\Rightarrow \tau = \tau_{12} + \tau_{13} = \tau_{21} + \tau_{23} = \tau_{31} + \tau_{32}$ .

$$M = \begin{bmatrix} \Delta/\Delta_1 & \tau_{12}/\Delta_2 & \tau_{13}/\Delta_3 \\ \tau_{21}/\Delta_1 & \Delta/\Delta_2 & \tau_{23}/\Delta_3 \\ \tau_{31}/\Delta_1 & \tau_{32}/\Delta_2 & \Delta/\Delta_3 \end{bmatrix}$$

# Example – Three state MCs

---

Kemeny's constant:  $K = 1 + \frac{\tau}{\Delta} = \tau_M$

For all three-state irreducible MCs,  $\tau_M \geq 2$ .

$\tau_M = 2$  achieved in "the minimal period 3" case

when  $p_2 = q_3 = r_1$ , i.e. when  $P = \begin{bmatrix} 0 & 1 & 0 \\ 0 & 0 & 1 \\ 1 & 0 & 0 \end{bmatrix}$ .

# Example – Three state MCs

---

"Period-2 case": Transitions between {1,3} and {2}

$$P = \begin{bmatrix} 0 & 1 & 0 \\ q_1 & 0 & q_3 \\ 0 & 1 & 0 \end{bmatrix}, (q_1 + q_3 = 1) \Rightarrow \tau_M = 2.5$$

"Constant movement" case:

$$P = \begin{bmatrix} 0 & p_2 & p_3 \\ q_1 & 0 & q_3 \\ r_1 & r_2 & 0 \end{bmatrix}, (p_2 + p_3 = q_1 + q_3 = r_1 + r_2 = 1)$$

$$\tau_M = 1 + \frac{3}{3 - q_3 r_2 - r_1 p_3 - p_2 q_1} \Rightarrow 2 \leq \tau_M \leq 2.5$$

Period-3 case :  $\tau_M = 2$ .      Period-2 case :  $\tau_M = 2.5$

# Example – Three state MCs

---

"Cyclic drift" case:

$$P = \begin{bmatrix} 1-a & a & 0 \\ 0 & 1-b & b \\ c & 0 & 1-c \end{bmatrix}, \Rightarrow \tau_M = 1 + \frac{a+b+c}{bc+ca+ab}.$$

$$a+b+c \rightarrow 3 \Rightarrow \tau_M \rightarrow 2; a=b=c=\varepsilon \Rightarrow \tau_M = 1 + \frac{1}{\varepsilon} \rightarrow \infty \text{ as } \varepsilon \rightarrow 0$$

"Constant probability state selection" case:

$$P = \begin{bmatrix} 1-a & a/2 & a/2 \\ b/2 & 1-b & b/2 \\ c/2 & c/2 & 1-c \end{bmatrix} \Rightarrow \tau_M = 1 + \frac{4(a+b+c)}{3(bc+ca+ab)}$$

$$a=b=c=\varepsilon \Rightarrow \tau_M = 1 + \frac{4}{3\varepsilon} \Rightarrow 2\frac{1}{3} < \tau_M < \infty$$

# Summary of general results

---

Periodic, period- $m$  chain  $\tau_M = \frac{m+1}{2}$ .

Independent trials with  $m$  possible outcomes:  $\tau_M = m$ .

For all irreducible  $m$  - state MCs:  $\frac{m+1}{2} \leq \tau_M < \infty$ .

$\tau_M$  could be interpreted as the expected time to "stationarity"

(Hunter, 2006)

# Perturbation results

---

Consider perturbing  $P = [p_{ij}]$  (where  $P$  associated with an ergodic,  $m$ -state MC, to  $\bar{P} = [\bar{p}_{ij}] = P + \mathbf{E}$  where  $\mathbf{E} = [\varepsilon_{ij}]$ , ( $\sum_{j=1}^m \varepsilon_{ij} = 0$ ).

Let  $\pi^T = (\pi_1, \pi_2, \dots, \pi_m)$  and  $\bar{\pi}^T = (\bar{\pi}_1, \bar{\pi}_2, \dots, \bar{\pi}_m)$  be the associated stationary probability vectors.

For all irreducible  $m$ -state MCs undergoing a perturbation  $\mathbf{E} = [\varepsilon_{ij}]$

$$\|\pi^T - \bar{\pi}^T\|_1 \leq (K - 1) \|\mathbf{E}\|_\infty$$

$$\text{i.e.} \quad \sum_{j=1}^m |\pi_j^T - \bar{\pi}_j^T| \leq (K - 1) \max_{1 \leq i \leq m} \sum_{k=1}^m |\varepsilon_{ki}|.$$

(Hunter, 2006)

# Perturbation results

---

Special cases:

$$\begin{aligned} \|\pi^T - \bar{\pi}^T\|_1 &\leq (\text{tr}(Z) - 1) \|\mathbf{E}\|_\infty \\ \text{and } \|\pi^T - \bar{\pi}^T\|_1 &\leq (\text{tr}((I - P)^\#)) \|\mathbf{E}\|_\infty \end{aligned}$$

These were new bounds and a comparison was given with earlier results

$$\begin{aligned} \|\pi^T - \bar{\pi}^T\|_1 &\leq \|Z\|_\infty \|\mathbf{E}\|_\infty \quad (\text{Schweitzer, 1968}) \\ \text{and } \|\pi^T - \bar{\pi}^T\|_1 &\leq \|(I - P)^\#\|_\infty \|\mathbf{E}\|_\infty \quad (\text{Meyer, 1980}) \end{aligned}$$

# Elementary perturbations

---

Let  $M$  and  $\bar{M}$  be the mean first passage matrices and  $K$  and  $\bar{K}$  be the Kemeny constants associated with  $P$  and  $\bar{P}$

Type 1 perturbation: Let  $\bar{P} = P + \mathbf{E}$  where  $\mathbf{E} = \mathbf{e}_r \mathbf{h}^T$ .

Then  $\bar{m}_{ir} = m_{ir}$  for all  $i \neq r$ ,  
 $\bar{m}_{ij} \geq m_{ij} \Leftrightarrow \bar{\pi}_j \leq \pi_j$  for all  $i, j \neq r$ .

and  $K \leq \bar{K} \Leftrightarrow \sum_{i \neq r} (\bar{\pi}_i - \pi_i) m_{ir} \geq 0$ .

Type 2 perturbation: Let  $\bar{P} = P + \mathbf{E}$  where  $\mathbf{E} = \mathbf{e} \mathbf{h}^T$ .

Then  $K = \bar{K}$

(Catral, Kirkland, Neumann, Sze, 2010)

# Extended perturbations

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Extensions:

1. Let  $P$  be a symmetric stochastic, irreducible matrix

$\bar{P} = P - E$  where  $E$  is a positive semi definite matrix with  $\bar{P}$  stochastic.

Then  $\sum_{j=1}^m \bar{m}_{ij} \leq \sum_{j=1}^m m_{ij}$ , and  $\bar{K} \leq K$ .

2. Let  $P$  be a stochastic, irreducible matrix and suppose  $0 \leq \alpha \leq 1$ .

$\bar{P} = \alpha P + (1 - \alpha)\mathbf{e}\mathbf{v}^T$  where  $\mathbf{v}^T$  is a positive probability vector,

Then  $\bar{K} \leq K$ .

(Catral, Kirkland, Neumann, Sze, 2010)

# Directed graphs

---

A directed graph, or digraph,  $\mathcal{G} = (\mathcal{V}, \mathcal{E})$  is a collection of vertices (or nodes)  $i \in \mathcal{V} = \{1, \dots, m\}$  and directed edges or arcs  $(i \rightarrow j) \in \mathcal{E}$ . One can assign weights to each directed edge, making it a weighted digraph.

An unweighted digraph has common edge weight 1.

$\mathcal{G}$  can be represented by its  $m \times m$  **adjacency** matrix  $A = [a_{ij}]$  where  $a_{ij} \neq 0$  is the weight on arc  $(i \rightarrow j)$  and  $a_{ij} = 0$  if  $(i \rightarrow j) \notin \mathcal{E}$ .

A digraph  $\mathcal{G}$  is strongly connected or a strong digraph if there is a path  $i = i_0 \rightarrow i_1 \rightarrow \dots \rightarrow i_k = j$  for any pair of nodes where each link  $i_{r-1} \rightarrow i_r \in \mathcal{E}$ . We focus on strong digraphs.

# Random walks over a graph

---

A random walk over a graph can be represented as a MC with transition matrix  $P = D^{-1}A$  where  $D = \text{Diag}(A\mathbf{e}) = \text{Diag}(\mathbf{d})$ .

We assume that every node has at least one out-going edge, which can include self loops. Note that  $D_{ii} = d_i$ , the degree of node  $i$ .

If the graph is strongly connected the associated MC is irreducible with  $p_{ij} = 1/d_j$  for those states  $j$  such that  $i \rightarrow j$ , 0 otherwise.

If the graph were undirected the associated MC would be reversible, and the stationary probability vector  $\boldsymbol{\pi}^T = \mathbf{d}/\mathbf{d}^T \mathbf{e}$ .

# Mixing on directed graphs

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For any stochastic matrix  $P$  of order  $m$ , the *directed graph associated with  $P$* ,  $D(P)$  is the directed graph on vertices labelled  $1, 2, \dots, m$  such that for each  $i, j = 1, 2, \dots, m$ ,  $i \rightarrow j$  is an arc on  $D(P)$  if and only if  $p_{ij} > 0$ .

For a strongly connected graph  $D$  on  $m$  vertices define

$\sum_D = \{P \mid P \text{ is stochastic and } m \times m \text{ and for each } i, j = 1, 2, \dots, m,$   
 $i \rightarrow j \text{ is an arc on } D(P) \text{ only if } i \rightarrow j \text{ is an arc in } D\}$

Define  $K(P)$  with the convention that  $m_{ii} = 0$ .

Let  $\mu(D) = \inf\{K(P) \mid P \in \sum_D \text{ and } P \text{ has } 1 \text{ as a simple eigenvalue}\}$

Let  $k$  = the length of the longest cycle in  $D$ , (i.e. period  $m \Rightarrow d = m$ )

then 
$$\mu(D) = \frac{2m - k - 1}{2}. \quad (\text{Kirkland, 2010})$$

# Electric networks and graphs

---

There is a connection between electric networks and random walks and graphs. (Doyle & Snell, 1984).

On a connected graph  $G$  with vertex set  $V = \{1, 2, \dots, m\}$  assign to the edge  $(i, j)$  a resistance  $r_{ij}$ . The conductance of an edge

$(i, j)$  is  $C_{ij} = 1 / r_{ij}$ . Define a random walk on  $G$  to be a MC with transition probabilities  $p_{ij} = C_{ij} / C_i$  with  $C_i = \sum_j C_{ij}$ .

Since the graph is connected the MC is ergodic with a stationary probability vector  $\pi^T = (\pi_1, \dots, \pi_m)$  where  $\pi_j = C_j / C$  with  $C = \sum_i C_i$ .

The MC is in fact reversible.

On the electric network we define  $C_{ij} = \pi_i p_{ij}$ .

(If  $p_{ij} \neq 0$  the resulting network will need a conductance from  $i$  to  $j$ .)

# Electric networks and graphs

---

For a network of resistors assigned to the edges of a connected graph we choose two points  $a$  and  $b$  and put a 1-volt battery across these points establishing a voltage  $v_a = 1, v_b = 0$ .

We are interested in finding the voltages  $v_i$  and the currents  $I_{ij}$  in the circuit and to give a probabilistic interpretation.

By Ohm's Law  $I_{ij} = (v_i - v_j)/r_{ij} = (v_i - v_j)C_{ij}$ . Note  $I_{ij} = -I_{ji}$ .

By Kirchhoff's current law  $\sum_j I_{ij} = 0$  for  $i \neq a, b$ .

i.e if  $\sum_j (v_i - v_j)C_{ij} = 0 \Rightarrow v_i = \sum_j v_j p_{ij}$  for  $i \neq a, b$ .

Let  $h_i$  be the probability of starting at  $i$ , that state  $a$  is reached before  $b$ . Then  $h_i$  also satisfies above equations with  $v_a = h_a = 1$  and  $v_b = h_b = 0$ . i.e. interpret the voltage as a "hitting probability".

# Electric networks and graphs

---

Let  $E_a T_b$  be the expected value, starting from the vertex  $a$ , of the hitting time  $T_b$  of the vertex  $b$ .

Let  $\pi_i$  be the stationary probability of the MC at vertex  $i$ .

When we impose a voltage  $v$  between points  $a$  and  $b$  a voltage  $v_a = v$  is established at  $a$  and  $v_b = 0$  and a current  $I_a = \sum_x I_{ax}$  will flow into the circuit from outside the source.

We define the effective resistance between  $a$  and  $b$  as

$R_{ab} = v_a / I_a$ , as calculated using Ohm's Law.

Then

$$E_a T_b = \frac{1}{2} \sum_i C_i \{R_{ab} + R_{bi} - R_{ai}\} \quad (\text{Palacios \& Tetali, 1996})$$

# Kirchhoff index

---

Let  $G$  be a simple connected graph with vertex set  $V = \{1, 2, \dots, m\}$ .

Let  $R_{ij}$  be the *effective resistance* between  $i$  and  $j$ .

The ***Kirchhoff index*** is defined as

$$Kf(G) = \sum_{i < j} R_{ij}. \quad (\text{Klein \& Randic, 1993})$$

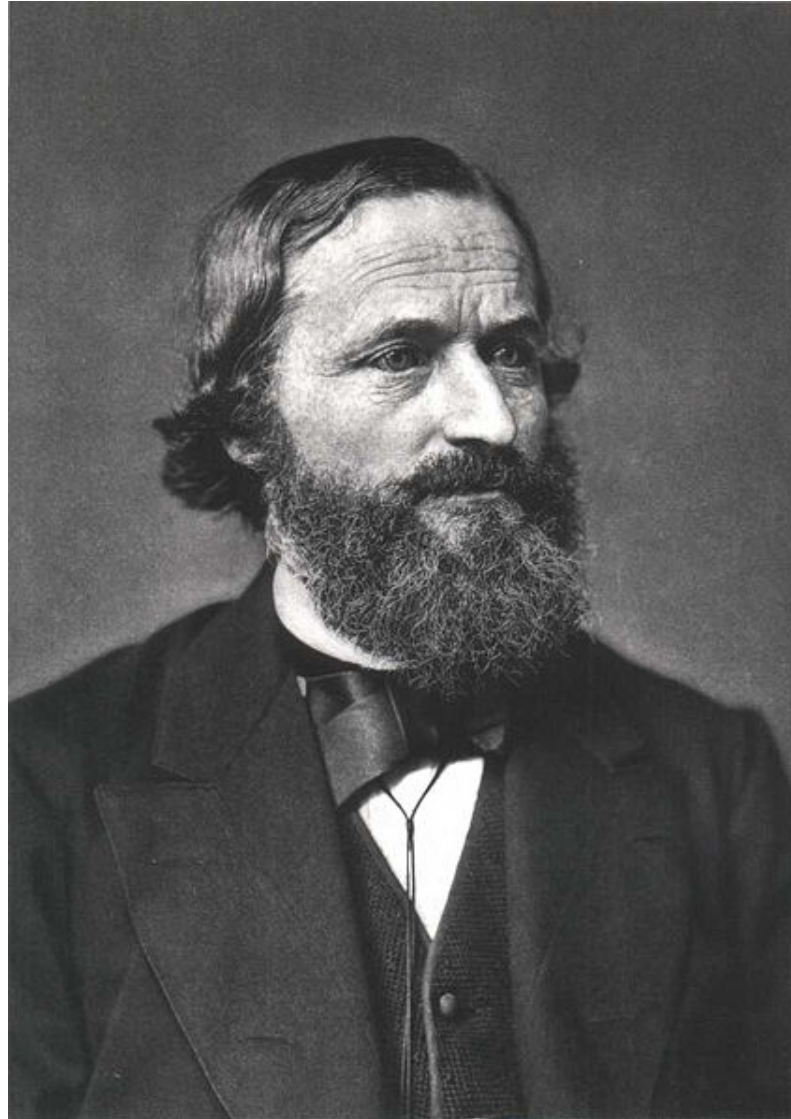
Since  $R_{ij} = R_{ji}$  and  $R_{ii} = 0$ ,  $Kf(G) = \frac{1}{2} \sum_{i,j} R_{ij}$ .

(Used in Chemistry to discriminate between different molecules with similar shapes and cycle structures.)

A lot of interest in recent years - graph theory, Laplacian and normalised Laplacians, electric networks, hitting times.

# Gustav R Kirchhoff (1824 – 1887)

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# Kirchhoff index

---

$$Kf(G) = \sum_{i < j} R_{ij}.$$

We use the relations between electric networks and random walks on graphs.

For a graph of  $m$  vertices computing  $Kf(G)$  entails finding  $O(m^2)$  values of the  $R_{ij}$  which is equivalent to finding  $O(m^2)$  values of the  $E_i T_j$  for the random walk on the graph.

$Kf(G)$  can be characterised as (Palacois & Renom, 2010)

$$Kf(G) = \frac{1}{2|E|} \sum_{i,j} E_i T_j$$

- based on the fact that the "commute times" can be expressed as

$$E_i T_j + E_j T_i = 2|E| R_{ij} \quad (\text{Aldous \& Fill, 2002})$$

# Kirchhoff index

---

$Kf(G)$  can also be characterised as  $Kf(G) = m \sum_{i=1}^{m-1} \frac{1}{\mu_i}$

(Zhu, Klein, Lukovits, 1996) (Gutman, Mohar, 1996)

where the  $\mu_i$ 's ( $i = 1, 2, \dots, m$ ) with  $\mu_m = 0$ , are the eigenvalues of the (ordinary or combinatorial) Laplacian matrix  $L$  of  $G$ ,  
i.e.  $L = D - A = D(I - P)$ .

Using the above characterisation, upper and lower bounds for  $Kf$  have been found (Zhou and Trinajstić, 2009). They also found bounds in terms of the eigenvalues of the normalised Laplacian

$$L = D^{-1/2} L D^{-1/2}.$$

# Kirchhoff index and $Z$

---

In the case of  $d$ -regular graphs, (where all vertices have exactly  $d$  neighbours) using the characterisation of the Kirchhoff index as

$$Kf(G) = \frac{1}{d} \sum_j E_1 T_j$$

it was shown (Palacois, 2010) that

$$Kf(G) = \frac{m}{d} [tr(Z) - 1]$$

where  $Z = (I - P + \mathbf{e}\pi^T)^{-1}$ , with  $P$  the transition matrix of the random walk and  $\pi^T$  its stationary probability vector.

Thus we have a connection between the Kirchhof index and Kemeny's constant  $K = tr(Z) - 1$ .

# Variances of mixing times

---

The expected time to mixing starting in any state,  $\tau_M$ , is constant independent of the starting state;  $\tau_M = K = \sum_{j=1}^m m_{ij} \pi_j$ .

What about the variance of the mixing times?

Do these depend on the starting state?

If so, can we choose a desirable starting state?

We explore some results on the second moments of the first passage time variables.

Let  $m_{ij}^{(2)}$  be the 2-nd moment of the first passage time

from state  $i$  to state  $j$ . i.e.  $m_{ij}^{(2)} = E[T_{ij}^2 \mid X_0 = i]$  for all  $(i, j) \in S \times S$ ;

and let  $M^{(2)} = [m_{ij}^{(2)}]$ .

# 2<sup>nd</sup> moments first passage times

---

$M^{(2)}$  satisfies the matrix equation

$$(I - P)M^{(2)} = E + 2P(M - M_d) - PM_d^{(2)}.$$

$$M_d^{(2)} = 2D(\Pi M)_d - D.$$

If  $G$  is any  $g$ -inverse of  $I - P$

$$M_d^{(2)} = D + 2D\{(I - \Pi)G(I - \Pi)\}_d D.$$

$$\text{If } Ge = ge, \quad M_d^{(2)} = D + 2D\{(I - \Pi)G\}_d D.$$

In particular,

$$M_d^{(2)} = D + 2DT_d D = 2DZ_d D - D$$

# 2<sup>nd</sup> moments first passage times

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If  $G$  is any g-inverse of  $I - P$

$$\begin{aligned} M^{(2)} &= 2[GM - E(GM)_d] + [I - G + EG_d][M_d^{(2)} + D] - M, \\ &= 2[GM - E(GM)_d] + 2[I - G + EG_d]D(\Pi M)_d - M. \end{aligned}$$

(Hunter, 2006)

If  $Ge = ge$ , then

$$M^{(2)} = 2[GM - E(GM)_d] + MD^{-1}M_d^{(2)} \quad (\text{Hunter, 2006})$$

$$\begin{aligned} \text{In particular, } M^{(2)} &= 2[ZM - E(ZM)_d] + M(2Z_dD - I) \\ &= 2[A^\#M - E(A^\#M)_d] + M(2A_d^\#D + I). \end{aligned}$$

# Elemental expressions

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If  $G = [g_{ij}]$  then

$$m_{ij}^{(2)} = 2 \sum_{k=1}^m (g_{ik} - g_{jk}) m_{kj} - m_{ij} + (\delta_{ij} - g_{ij} + g_{jj})(m_{jj}^{(2)} + m_{jj}).$$

If  $Ge = ge$

$$m_{ij}^{(2)} = 2 \sum_{k=1}^m (g_{ik} - g_{jk}) m_{kj} + \frac{m_{ij} m_{jj}^{(2)}}{m_{jj}}.$$

Also  $m_{jj}^{(2)} + m_{jj} = 2m_{jj} \sum_{i=1}^m \pi_i m_{ij}.$

(Hunter, 2006)

# Variances of the mixing times

---

Let  $T$  be the mixing time variable and let

$$\eta_i^{(k)} = E[T^k \mid X_0 = i] = \sum_{j=1}^m m_{ij}^{(k)} \pi_j \text{ and } \boldsymbol{\eta}^{(k)T} = (\eta_1^{(k)}, \eta_2^{(k)}, \dots, \eta_m^{(k)}).$$

We have seen that  $\boldsymbol{\eta}^{(1)T} = (\tau_{M,1}, \tau_{M,2}, \dots, \tau_{M,m}) = \boldsymbol{\eta} \mathbf{e} = \mathbf{K} \mathbf{e}$ ,

showing that the expected mixing time, starting at  $i$ , is constant.

The variance of the mixing time, starting at  $i$ , is given by

$$v_i = \eta_i^{(2)} - \eta^2. \text{ If } \mathbf{v}^T = (v_1, v_2, \dots, v_m) \text{ then } \mathbf{v} = \boldsymbol{\eta}^{(2)} - \eta^2 \mathbf{e}.$$

From (Hunter, 2006), if  $G$  is any g-inverse of  $I - P$ , such that  $G\mathbf{e} = \mathbf{e}$

$$\boldsymbol{\eta}^{(2)} = [2\text{tr}(G^2) - 3\text{tr}(G) - (1 - 2g)(1 - g)]\mathbf{e} + 2L\boldsymbol{\alpha},$$

$$\mathbf{v} = [2\text{tr}(G^2) - (\text{tr}(G))^2 - (5 - 2g)\text{tr}(G) - (1 - g)(2 - 3g)]\mathbf{e} + 2L\boldsymbol{\alpha},$$

where  $L = I - G + EG_d$  and  $\boldsymbol{\alpha} = \mathbf{e} - (\Pi G)_d D\mathbf{e} + G_d D\mathbf{e}$ .

$v_i = v$  for all  $i \Leftrightarrow L\boldsymbol{\alpha} = l\mathbf{e}$ . A sufficient condition is  $\boldsymbol{\alpha} = \alpha\mathbf{e}$ .

# Variances mixing times, 2-states

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For the 2-state case,  $P = \begin{bmatrix} 1-a & a \\ b & 1-b \end{bmatrix}$  and  $d = 1 - a - b$ .

$$\mathbf{v} = \begin{bmatrix} v_1 \\ v_2 \end{bmatrix} = \frac{1}{ab(1-d)^2} \begin{bmatrix} (2a^2 + 2b - 3ab)(a+b) - ab \\ (2b^2 + 2a - 3ab)(a+b) - ab \end{bmatrix}$$

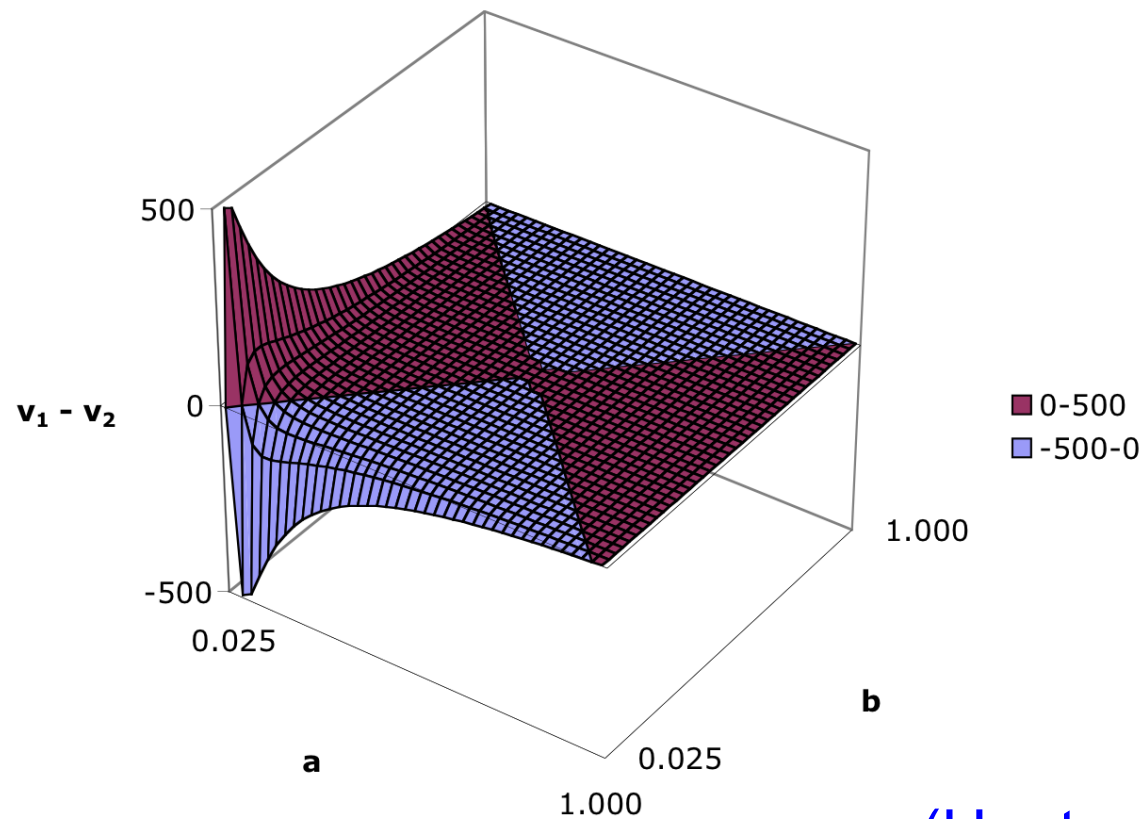
Lines  $a = b$  &  $a + b = 1$  partition the parameter space  $(a,b)$  to give regions where  $v_1 = v_2$ ,  $v_1 < v_2$  and  $v_1 > v_2$ .

$v_1 < v_2$  if  $p_{21} < p_{11} < p_{22}$  or  $p_{22} < p_{11} < p_{21}$ .

# Variances mixing times, 2-states

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Graph of  $v_1 - v_2$  :



(Hunter, 2008)

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