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

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Andrei A Markov (1856 – 1922)

John G Kemeny (1926 – 1992)

Outline

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Introduction

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

Let $S = \{1, 2, \ldots, m\}$ 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 $\Rightarrow \sum_{j=1}^{m} p_{ij} = 1, \; i \in S.$

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

Limiting & Stationary Distribns

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 $\lim_{n \to \infty} p_j^{(n)} = \pi_j$.

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

Stationary Distributions

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:

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

The "stationary probability vector" is $\boldsymbol{\pi}^T = (\pi_1, \pi_2, \ldots, \pi_m)$.

Primer on g-inverses of $I - P$

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 $\boldsymbol{\pi}^T$. Let $\boldsymbol{t}$ and $\boldsymbol{u}$ be any vectors. Let $\boldsymbol{e}^T = (1,1, \ldots, 1)$.

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

$\boldsymbol{\pi}^T\boldsymbol{t} \neq 0$ and $\boldsymbol{u}^T\boldsymbol{e} \neq 0 \Rightarrow$ $[I - P + \boldsymbol{t}\boldsymbol{u}^T]^{-1}$ is a g-inverse of $I - P$.

(Hunter, 1982)

Use of g-inverses

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 $I - P$

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

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

$Z = [I - P + \Pi]^{-1}$, $(\Pi \equiv \boldsymbol{e}\boldsymbol{\pi}^T)$ "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

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

i.e. $T_{ij} = \min\{n \geq 1$ such that $X_n = j$ 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} be the mean first passage time from state i to state j.

i.e. $m_{ij} = \mathrm{E}[T_{ij} \mid \mathrm{X}_0 = i]$ for all $(i, j) \in S \times S$.

Mean First Passage Times

For an irreducible finite MC with transition matrix P,

let $M = \left[m_{ij}\right]$ 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

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

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

Under any of the following three equivalent conditions:

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

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

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

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

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

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

then $m_{ij} = \left(\dfrac{g_{jj} - g_{ij} + \delta_{ij}}{\pi_j} \right) + (g_{i\bullet} - g_{j\bullet})$, for all i, j.

$\boldsymbol{Ge} = g\boldsymbol{e} \Rightarrow m_{ij} = \left(\dfrac{g_{jj} - g_{ij} + \delta_{ij}}{\pi_j} \right)$, for all i, j.

$$\text{Thus } m_{ij} = \begin{cases} \dfrac{z_{jj} - z_{ij}}{\pi_j} = \dfrac{a^{\#}_{jj} - a^{\#}_{ij}}{\pi_j}, & i \neq j, \\[2ex] \dfrac{1}{\pi_j} & i = j. \end{cases}$$

where Z = [z_{ij}] (Kemeny & Snell, 1960), A$^{\#} = [a^{\#}_{ij}]$ (Meyer, 1975)

Kemeny's constant

Key Result : For all $i \in S$,

$$\sum_{j=1}^{m} m_{ij}\pi_j = K, \text{ "}\textbf{\textit{Kemeny's constant}}\text{".}$$

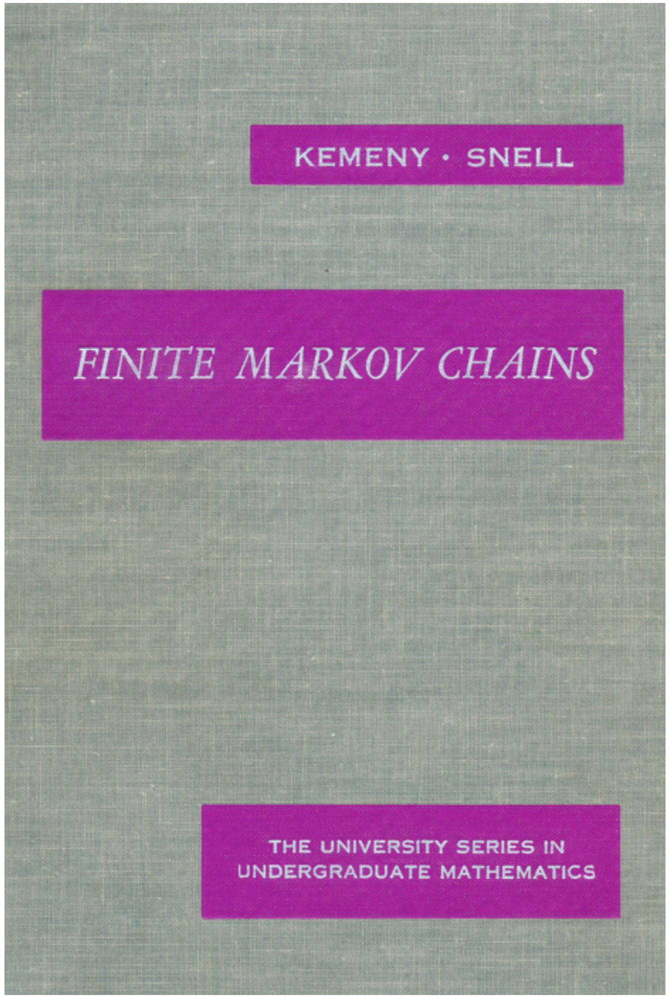
Equivalently, $\quad M\boldsymbol{\pi} = K\mathbf{e}.$

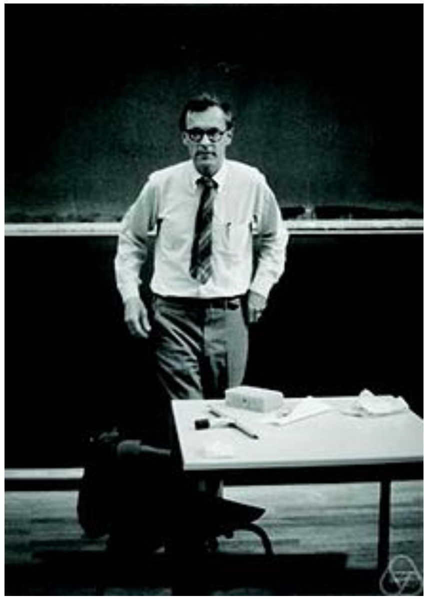
One of the simplest proofs is based upon Z :

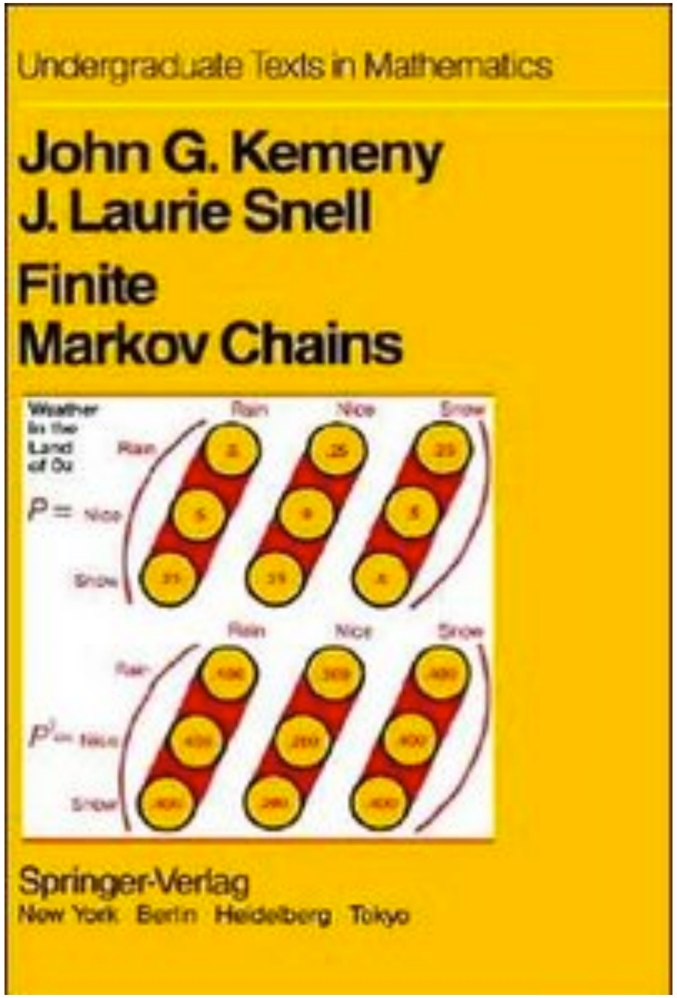
$$\begin{aligned} M\boldsymbol{\pi} &= [I - Z + EZ_d]D\boldsymbol{\pi} \\ &= [I - Z + EZ_d]\mathbf{e} \\ &= \mathbf{e} - Z\mathbf{e} + \mathbf{e}\mathbf{e}^T Z_d \mathbf{e} = K\mathbf{e}, \end{aligned}$$

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

Initial appearance - 1960







Kemeny & Snell - Initial result

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

PROOF.

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

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

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

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

Kemeny's constant

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

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

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

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

The irreducubility of the MC implies that $\boldsymbol{k}$ is the right eigenvector of P corresponding to the eigenvalue $\lambda = 1$

$\Rightarrow k = Ke.\ \ i.e\ K_i = K\ for\ all\ i\ =\ 1,\ 2,\ \ldots,\ m.$

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

Kemeny's *K* - Clarification

Note that m_{ii} is the "mean recurrence time for state i".

It is well known that $m_{ii} = 1/\pi_i$ and thus $m_{ii}\pi_i = 1$.

Consequently "***Kemeny's constant***"

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

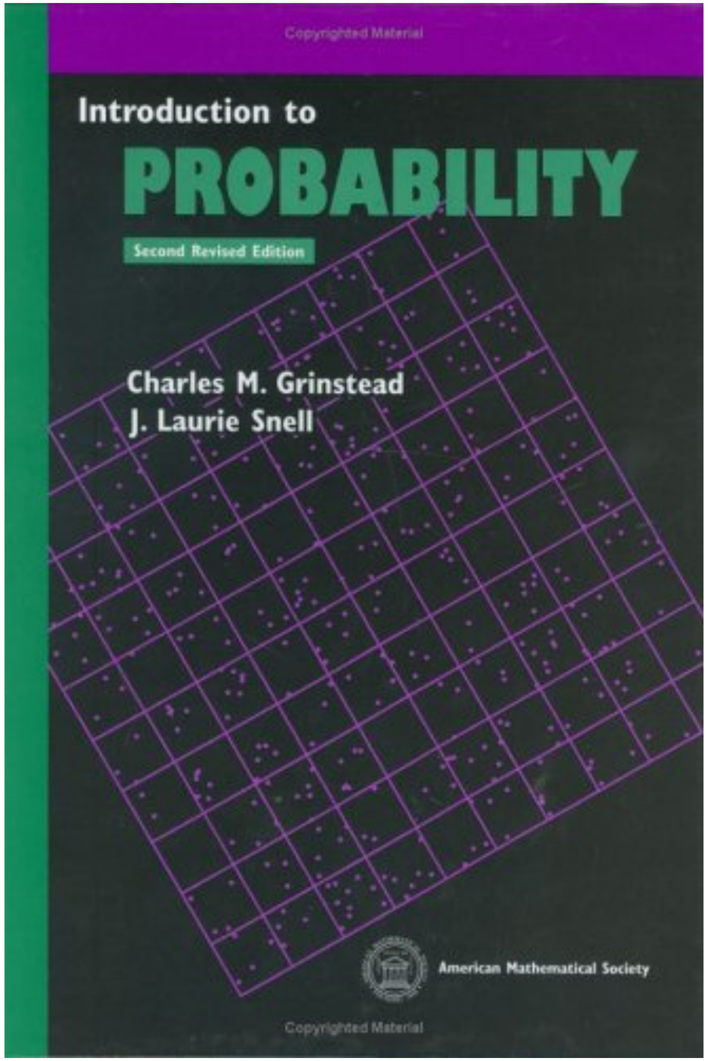
Some authors define, by convention, that $m_{ii} = 0$

so that the expression for the mean first passage times

taken 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



Grinstead & Snell - Update

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

24 In the course of a walk with Snell along Minnehaha Avenue in Minneapolis in the fall of 1983, Peter Doyle[25] 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

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.

Kemeny's constant: G-inverses

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

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

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

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

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

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

"Classical result" (Hunter, 2006).

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

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

Kemeny's constant: Eigenvalues

P irreducible $\Rightarrow$

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

are such that $\lambda_1 = 1$, with $|\lambda_i| \le 1$ and $\lambda_i \ne 1$ $(i = 2, \ldots, m)$.

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

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

Thus $K = tr(Z) = \sum_{i=1}^{m} z_{ii} = \sum_{i=1}^{m} \lambda_i(Z) = 1 + \sum_{i=2}^{m} \frac{1}{1 - \lambda_i}.$

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

Kemeny's constant: Bounds

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

Hence $\lambda_1 = 1$, with $|\lambda_i| \le 1$ and $\lambda_i \ne 1$ $(i = 2, \ldots, m)$.

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 $a^2 + b^2 \le 1$.

For this pair of conjugate roots

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

Bounds on K

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 a periodic MC 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)) Proof based on results of Styan (1964) with λ_i real.

If the **MC is reversible** (all the λ_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).

Improved Bounds on K

Suppose the the MC is irreducible & reversible so that

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

Apply the method of Lagrange multipliers to the function

$f(x_2, \ldots, x_m) = \sum_{i=2}^{m} \frac{x_i}{1-x_i},$

subject to $1 + x_2 + \ldots + x_m = 0$ on the domain $1 > x_2 \geq \ldots \geq x_m > -1$

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

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

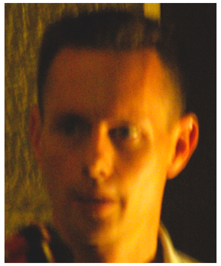
- an improvement on the earlier bounds of Levene & Loizoiu).

Alternative representation of *K*

$$K = tr(A_j^{-1}) - \frac{A_{jj}^{\#}}{\pi_j} + 1,$$

where A_j^{-1} is $(m-1)\times(m-1)$ principal submatrix of $A = I - P$ obtained by deleting 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 $\boldsymbol{\pi}^T$

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 $B = A^{-1}{}_n + \beta W - A_n^{-1}W - WA_n^{-1}$,

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

Stationarity in Markov chains

For all irreducible MCs (including periodic chains),

if for some $k \geq 0$, $p_j^{(k)} = \mathrm{P}[X_k = j] = \pi_j$ for all $j \in S$,

then $p_j^{(n)} = \mathrm{P}[X_n = j] = \pi_j$ 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

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

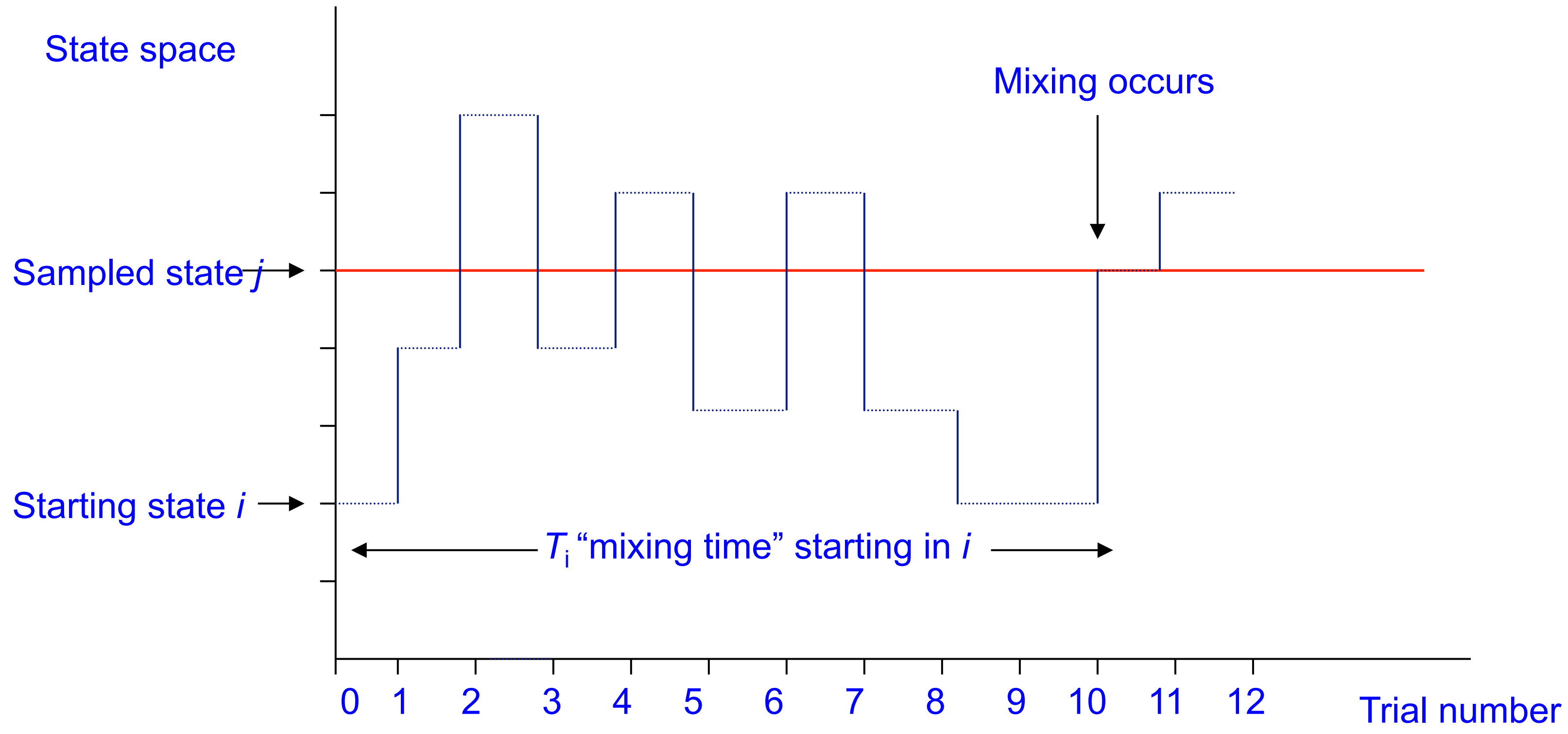
The MC $\{X_n\}$, achieves "mixing", at time $T = k$, when $X_k = Y$ for the smallest such $k \geq 1$.

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



Expected Time to Mixing

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 $X_0 = i$,

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

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

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

i.e. Expected time to mixing, starting in any state, is K.

(Hunter, 2006)

Mixing or Hitting Times

Suppose the sampled stationary state ("mixing state") is j and the initial "starting state" is i.

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

Suppose however we allow mixing to be possible when $k = 0$ when i = j. i.e. we permit "mixing" to occur at time $T = 0$, when state i is the "hitting" state (rather than "returned state")

The expected time to mixing in this situation would be

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

(Hunter - 2010 preprint - considers the distribution of the time to mixing and time to hitting in each of the above situations.)

Random surfer

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 doesnt know the state he is at and where he is heading.

K can be intrepeted 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)

Ex: Two state Markov Chains

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

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

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

MC has a unique stationary probability vector

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

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

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

Ex: Two state Markov Chains

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

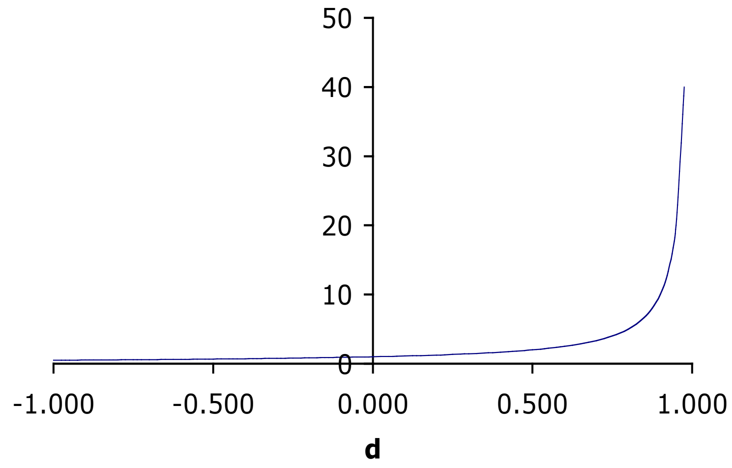
$d = 1 \Leftrightarrow$ Periodic, period 2, MC with $a = 1,\ b = 1.$

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

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

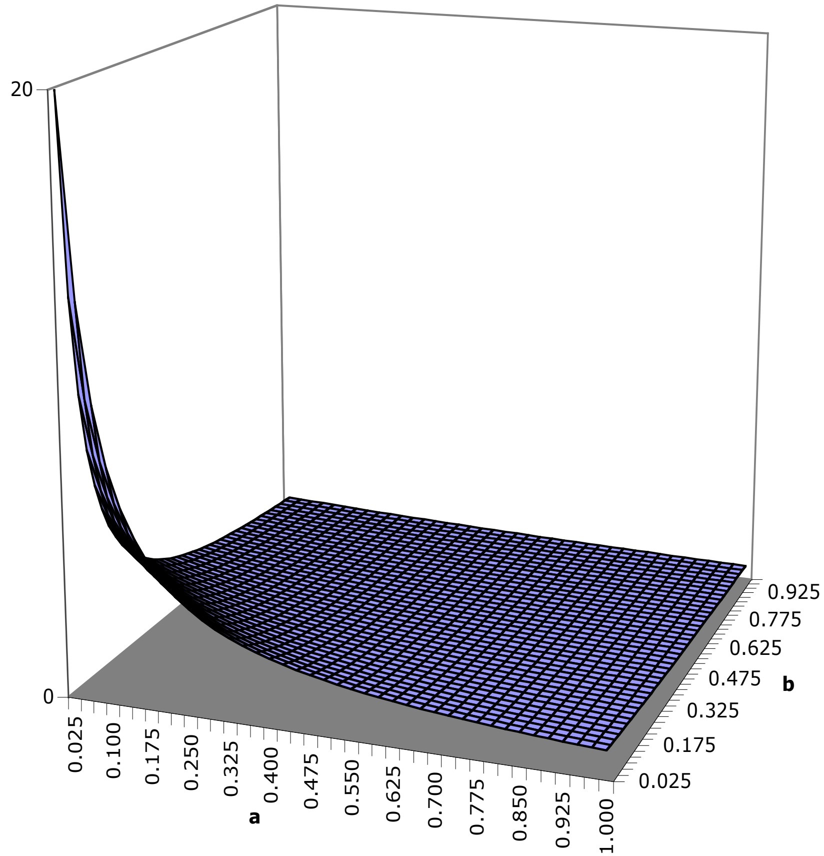
$d \to 1$ (both a $\to 0$ and b $\to 0$) $\Rightarrow$ arbitrarily large K.

For all two state MCs: $1.5 \le K < \infty$



Ex: Two state Markov Chains

Plot of $K = 1 + \dfrac{1}{a+b}$.



Ex: Three state Markov Chains

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

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

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

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

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

Ex: Three state Markov Chains

MC is irreducible

(and hence a stationary distribution exists)

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

Stationary distribution given by

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

Ex: Three state Markov Chains

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

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

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

Ex: Three state Markov Chains

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

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

$K = 2$ achieved in "the minimal period 3" case

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

Ex: Three state Markov Chains

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

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

"Constant movement" case:

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

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

General *m* - state MCs

Periodic, period-m chain $K = \dfrac{m+1}{2}$.

Independent trials with m possible outcomes: $K = m$.

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

(Hunter, 2006)

Perturbation results

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

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

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

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

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

(Hunter, 2006)

Elementary perturbations

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

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

Then $\quad \overline{m_{ir}} = m_{ir}$ for all $i \neq r$,

$\overline{m_{ij}} \geq m_{ij} \Leftrightarrow \overline{\pi_j} \leq \pi_j$ for all $i, j \neq r$.

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

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

Then $K = \overline{K}$. (Catral, Kirkland, Neumann, Sze, 2010)

Extended perturbations

Extensions:

1. Let P be a symmetric stochastic, irreducible matrix

$\overline{P} = P - \boldsymbol{E}$ where $\boldsymbol{E}$ is a positive semi definite matrix with

$\overline{P}$ stochastic.

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

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

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

Then $\overline{K} \le K$.

(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) $i \in \mathcal{V} = \{1, \ldots, m\}$ and directed edges or arcs $(i \to j) \in \mathcal{E}$.

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 $(i \to j)$ and $a_{ij} = 0$ if $(i \to j) \notin \mathcal{E}$.

A digraph $\mathcal{G}$ is strongly connected or a strong digraph if there is a path $i = i_0 \to i_1 \to \ldots \to i_k = j$ for any pair of nodes where each link $i_{r-1} \to i_r \in \mathcal{E}$. 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 $D = Diag(A\mathbf{e}) = Diag(\mathbf{d})$.
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.

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

The graph is undirected $\Rightarrow$ the associated MC is reversible, and the stationary probability vector $\boldsymbol{\pi}^T = \mathbf{d}/\mathbf{d}^T\mathbf{e}$.

Mixing on Directed Graphs

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

For a strongly connected graph D on m vertices define the class

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

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

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

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

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

Electric networks and graphs

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

On a connected graph G with vertex set $V = \{1, 2,\ ..., m\}$ 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 RW on G to be a MC with transition probabilities $p_{ij} = C_{ij} / C_i$ with $C_i = \sum_j C_{ij}$.

The graph is connected $\Rightarrow$ MC is ergodic with a stationary probability vector $\boldsymbol{\pi}^T = (\pi_1, ..., \pi_m)$ 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 $p_{ii} \neq 0$ the resulting network will need a conductance from i to i.)

Electric networks and graphs

For a network of resistors assigned to the edges of a connected graph 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 π_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

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

Kirchhoff index

Let G be a simple connected graph with vertex set

$V = \{1, 2, \ldots, m\}$.

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

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

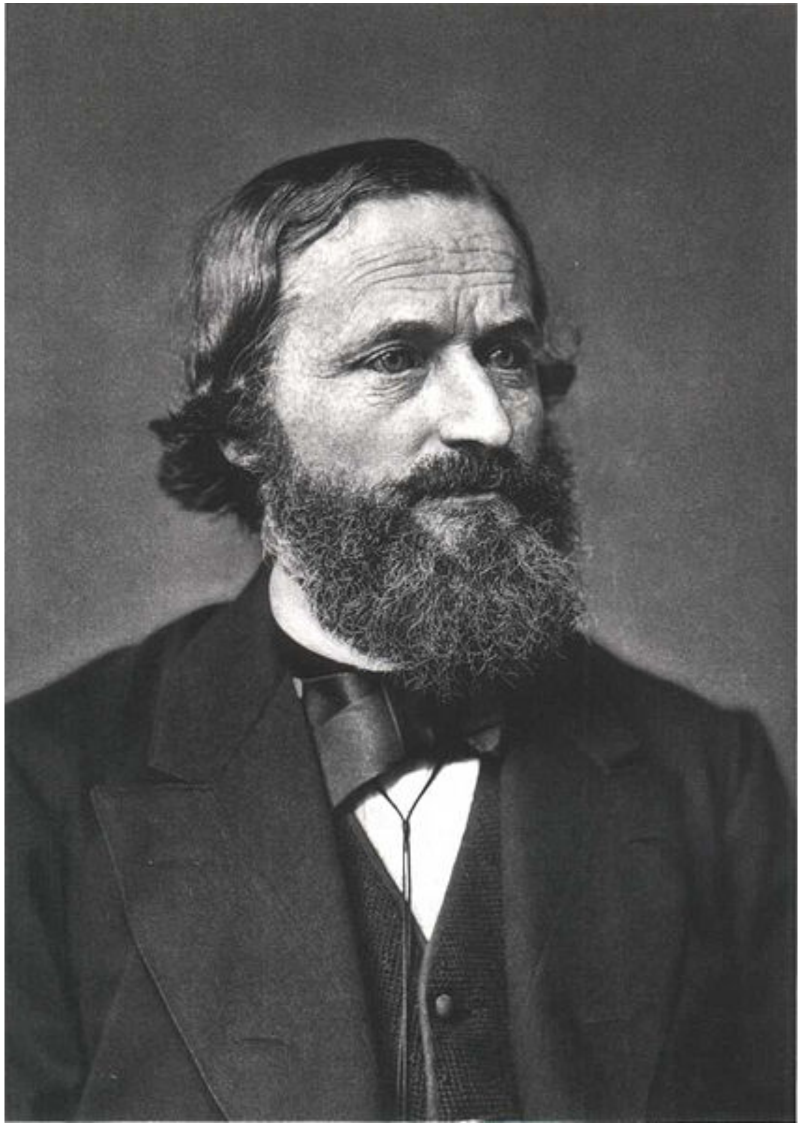
$$Kf(G) = \sum_{i<j} R_{ij}. \qquad \text{(Klein \& Randic,1993)}$$

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)



Kirchhoff index

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

We use the relations between electric networks and RWs 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 RW 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

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

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 μ_i's (i = 1, 2, ..,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 Trinajstic, 2009). They also found bounds in terms of the eigenvalues of the normalised Laplacian $\mathrm{L} = \mathrm{D}^{-1/2}L\mathrm{D}^{-1/2}$.

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 $\boldsymbol{\pi}^T$ 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 is *K*,
a constant independent of the starting state.
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.* $m_{ij}^{(2)} = \mathrm{E}[T_{ij}^2 \mid \mathrm{X}_0 = i]$ for all $(i, j) \in S \times S$;
and let $M^{(2)} = \left[m_{ij}^{(2)} \right]$.

Variances of the Mixing Times

Let T be the mixing time variable and let

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

We have seen that $\boldsymbol{\eta}^{(1)T} = K\mathbf{e}$, i.e the expected mixing times, starting at i, is constant.

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

$\nu_i = \eta_i^{(2)} - \eta^2$. If $\boldsymbol{\nu}^T = (\nu_1, \nu_2, \ldots, \nu_m)$ then $\boldsymbol{\nu} = \boldsymbol{\eta}^{(2)} - \eta^2\mathbf{e}$.

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

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

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

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

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

Variances Mixing Times, 2-states

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

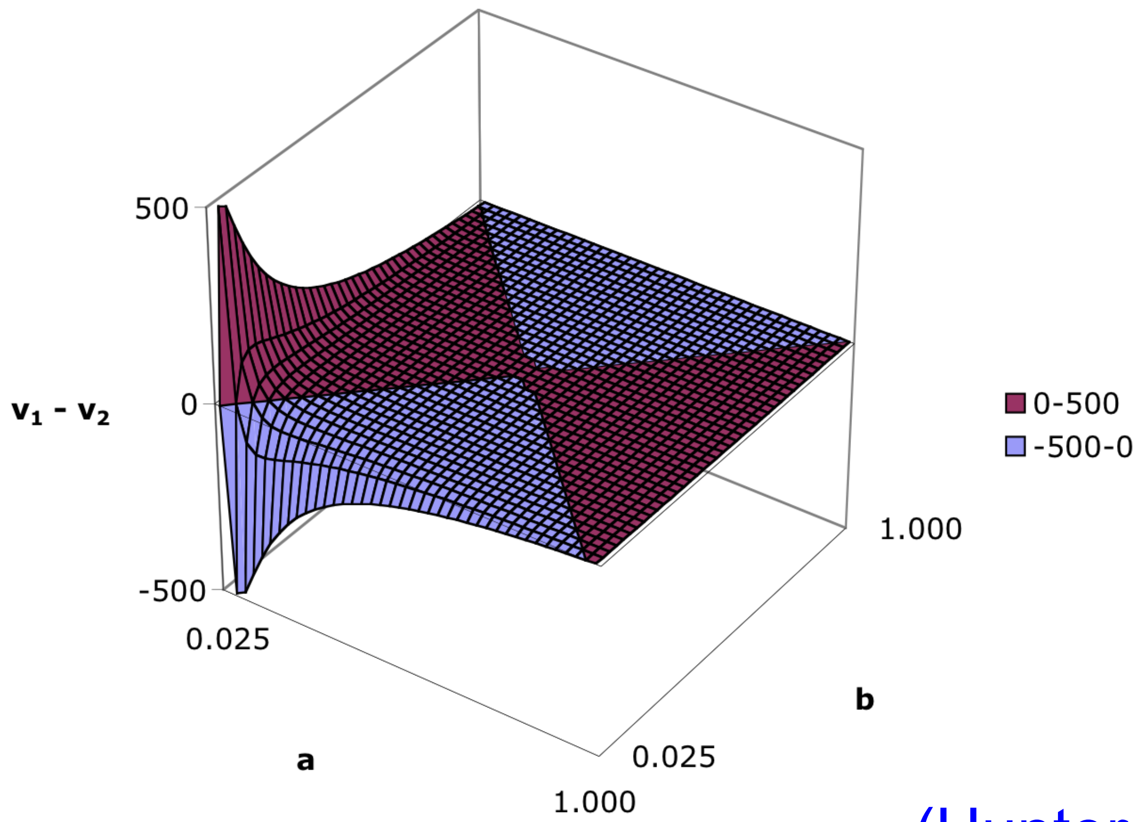
$$\boldsymbol{\nu} = \begin{bmatrix} \nu_1 \\ \nu_2 \end{bmatrix} = \frac{1}{ab(1-d)^2} \begin{bmatrix} (2a^2+2b-3ab)(a+b)-ab \\ (2b^2+2a-3ab)(a+b)-ab \end{bmatrix}$$

Lines $a = b$ & $a + b = 1$ partition the parameter space (a,b) to give regions where $\nu_1 = \nu_2, \nu_1 < \nu_2$ and $\nu_1 > \nu_2$.

$\nu_1 < \nu_2$ if $p_{21} < p_{11} < p_{22}$ *or* $p_{22} < p_{11} < p_{21}$.

Variances Mixing Times, 2-states

Graph of $\nu_1 - \nu_2$:



(Hunter, 2008)

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