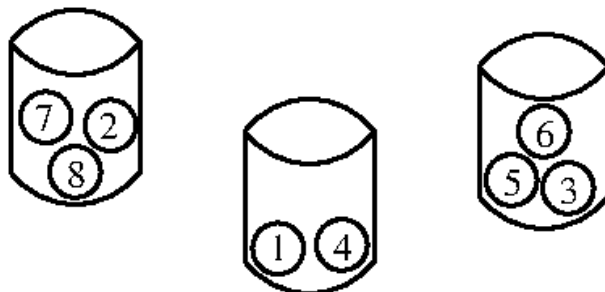## Solutions to Midterm Exam

Exercise 1. (20+2 points) There are $N \geq 2$ numbered balls divided into 3 urns:

We are interested in modelling the following process: at each time n, pick a number k uniformly at random in the set $\{1, \ldots, N\}$ (and independently from the previous picks); look then for the ball with this number, take it out of its urn and throw it uniformly at random in one of the other two urns.

We would like to keep track of the number of balls in one particular urn (say the first one) over time. Define X_n to be this number at time $n \geq 0$. The process $(X_n, n \geq 0)$ is then a Markov chain with state space $S = \{0, \ldots, N\}$.

a) Compute the transition matrix P of this chain.

Answer: If at time n the number of balls in the first urn is $i \in \{2, \ldots, N-1\}$ then, at time $n+1$, this number stays the same or is either increased or decreased by 1. We have

- $p_{i,i-1} = \frac{i}{N}$ (a ball is thrown out of the first urn in one of the other two);

- $p_{i,i} = \frac{N-i}{2N}$ (a ball is picked in one of the last two urns and is not thrown in the first urn);

- $p_{i,i+1} = \frac{N-i}{2N}$ (a ball is picked in one of the last two urns and is thrown in the first urn).

For $i = 0$ we have $p_{0,0} = p_{0,1} = 1/2$, and for $i = N$ we have $p_{N,N-1} = 1$.

b) Is the chain irreducible? aperiodic? Please justify.

Answer: Clearly we can go from a state i to a state $j > i$ in $j - i$ steps with non-zero probability (it corresponds to throwing $j - i$ times in a row the ball in the first urn) and vice-versa. So the chain is irreducible. Every state in the chain has a self-loop (except state N), so the chain is aperiodic too.

c) For a given state $i \in S$, define $T_i = \inf\{n \geq 1 : X_n = i\}$. What are the values of

$$f_{00} = \mathbb{P}(T_0 < +\infty \mid X_0 = 0) \quad \text{and} \quad f_{0N} = \mathbb{P}(T_N < +\infty \mid X_0 = 0) \quad ?$$

Answer: The chain is finite and irreducible, therefore it is positive-recurrent. For this reason $f_{00} = 1$ (it is the definition of recurrence) and $f_{0N} = 1$.

d) Without computing it, explain why the chain admits a unique stationary distribution π.

Answer: The chain is irreducible and positive-recurrent, therefore it has a unique stationary distribution π, by the theorem seen in class.

e) Compute π. Are the detailed balance equations satisfied?

Hint: You should remember here Newton's binomial formula, valid for any $a, b \in \mathbb{R}$:

$$(a+b)^N = \sum_{k=0}^{N} \binom{N}{k} a^k b^{N-k}, \quad \text{where} \quad \binom{N}{k} = \frac{N!}{k!\,(N-k)!}$$

Answer: If the detailed balance equations are satisfied then $\forall i \in \{1, \dots, N\} : p_{i,i-1}\pi_i = p_{i-1,i}\pi_{i-1}$, i.e. $\pi_i/\pi_{i-1} = p_{i-1,i}/p_{i,i-1} = (N+1-i)/2i$. We directly get

$$\pi_i = \pi_0 \prod_{j=1}^{i} \frac{(N+1-j)}{2j} = \pi_0 \frac{N(N-1)\cdots\cdot(N-i+1)}{2^i i!} = \frac{\pi_0}{2^i}\binom{N}{i}$$

Then $1 = \sum_{i=0}^{N} \pi_i = \pi_0 \sum_{i=0}^{N} \binom{N}{i}\frac{1}{2^i} = \pi_0 (3/2)^N$. In the end, we obtain $\pi_0 = (2/3)^N$ and for all $i \in \{1, \dots, N\}$, $\pi_i = \frac{2^{N-i}}{3^N}\binom{N}{i}$. It is a well-defined probability distribution, that satisfies the detailed balance equations by construction and is therefore the (unique) stationary distribution.

f) What is the value of $\mathbb{E}(T_0 \mid X_0 = 0)$? (with T_0 defined as in part c)

Answer: It is a known result that $\mathbb{E}(T_0 \mid X_0 = 0) = 1/\pi_0 = (3/2)^N$.

g) Do $\lim_{n\to\infty} \mathbb{P}(X_n = 0 \mid X_0 = 0)$ and $\lim_{n\to\infty} \mathbb{P}(X_n = N \mid X_0 = 0)$ exist? If yes, what are the values of these two limits? If no, explain why these two limits do not exist.

Answer: The chain is irreducible, positive-recurrent and aperiodic. Therefore it is an ergodic chain and the limits exist:

$$\lim_{n\to\infty} \mathbb{P}(X_n = 0 \mid X_0 = 0) = \pi_0 = (2/3)^N, \quad \lim_{n\to\infty} \mathbb{P}(X_n = N \mid X_0 = 0) = \pi_N = (1/3)^N$$

BONUS: h) What is the value of $\sum_{i\in S} i\,\pi_i$?

Answer: Let X_n, Y_n and Z_n be the number of balls in the first, second and third urns, respectively. Clearly $X_n + Y_n + Z_n = N$, hence

$$N = \lim_{n\to\infty} \mathbb{E}(X_n) + \mathbb{E}(Y_n) + \mathbb{E}(Z_n)$$

By ergodicity we know that $\lim_{n\to\infty} \mathbb{P}(X_n = i) = \pi_i$, therefore $\lim_{n\to\infty} \mathbb{E}(X_n) = \sum_{i=1}^{N} i\pi_i$. By symmetry the same limit applies for $\mathbb{E}(Y_n)$ and $\mathbb{E}(Z_n)$. It follows that $\sum_{i=1}^{N} i\pi_i = \frac{N}{3}$. A direct computation of the sum is also doable.

Exercise 2. (20 points) Let $0 \leq p \leq 1$ and $q = 1 - p$. We consider the Markov chain with the following transition graph:
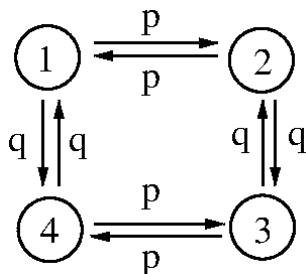
a) For what values of $0 \leq p \leq 1$ is the chain irreducible? Please justify.

Answer: The chain is irreducible for $0 < p < 1$: you can go from a state i to a state $i + 1 \bmod 4$ with non-zero probability and vice versa. This is not the case when $p = 0$ or $p = 1$.

b) For what values of $0 \leq p \leq 1$ is the chain aperiodic? Please justify.

Answer: The chain is never aperiodic. For $p = 0$ and $p = 1$ the chain has two equivalence classes that are both 2-periodic. For $0 < p < 1$ the chain has one equivalence class that is 2-periodic (you can leave one state and come back to it in an even number of steps only).

c) For what values of $0 \leq p \leq 1$ does the chain admit a *unique* stationary distribution π? Compute π for these values.

Answer: The chain is finite and, for $0 < p < 1$, it is irreducible. Therefore the chain is positive-recurrent and admits a unique stationary distribution for $0 < p < 1$. The transition matrix is doubly stochastic so the stationary distribution is the uniform distribution on the state space $\{1, 2, 3, 4\}$. For $p = 0$ or $p = 1$, any convex combination of the stationary distributions for the two equivalent classes is a stationary distribution and we don't have uniqueness.

d) Compute the eigenvalues $\lambda_0 \geq \lambda_1 \geq \lambda_2 \geq \lambda_3$ of the transition matrix P of the chain (as functions of the parameter p).

Hints: - You know already two of them!

- Reminder for computing the determinant of an $n \times n$ matrix A: for any $1 \leq i \leq n$, we have

$$\det(A) = \sum_{j=1}^{n} (-1)^{i+j} a_{ij} \det(A(i,j))$$

where $A(i,j)$ denotes the $(n-1) \times (n-1)$ matrix A with deleted row i and column j.

Answer: P is a transition matrix, so $\lambda_0 = 1$, and it describes a periodic Markov chain, so $\lambda_3 = -1$. Therefore, the trace and the determinant of P satisfy $\operatorname{Tr}(P) = \lambda_0 + \lambda_1 + \lambda_2 + \lambda_3 = \lambda_1 + \lambda_2$ and $\det(P) = \lambda_0 \lambda_1 \lambda_2 \lambda_3 = -\lambda_1 \lambda_2$, respectively. We find $\operatorname{Tr}(P) = 0$ and $\det(P) = (2p-1)^2$. Hence λ_1 and λ_2 are the roots of the degree-2 polynomial $X^2 - (\lambda_1 + \lambda_2)X + \lambda_1 \lambda_2 = X^2 - (2p-1)^2$, i.e.,

$$\lambda_1 = |2p - 1| \quad \lambda_2 = -|2p - 1|$$

Note that a direct computation of the 4 eigenvalues of P (i.e., solving $\det(P - \lambda I) = 0$) is also possible here.

Consider now the Markov chain with added self-loops:
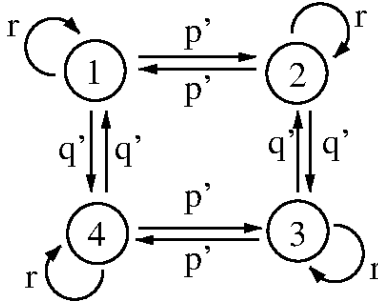
where $0 < r < 1$, $p' = (1-r)p$ and $q' = (1-r)q$ [so that $p' + q' + r = 1$].

e) Compute the eigenvalues $\lambda_0' \geq \lambda_1' \geq \lambda_2' \geq \lambda_3'$ of this new chain (as functions of the parameters p and r).

Answer: The new Markov chain has transition matrix $P' = rI + (1-r)P$ and for $i \in \{1, \ldots, 4\}$ we have $\lambda_i' = r + (1-r)\lambda_i$. More precisely:

$$\lambda_0' = 1, \quad \lambda_1' = r + (1-r)|2p-1|, \quad \lambda_2' = r - (1-r)|2p-1|, \quad \lambda_3' = 2r - 1$$

f) For any given value of $0 < p < 1$, find the value of $r(p)$ that maximizes the spectral gap of this new chain.

Answer: We have $\lambda^* = \max_{1 \leq i \leq 3} |\lambda_i'| = \max\{-\lambda_3', \lambda_1'\}$. When $r = 0$, λ^* is $-\lambda_3'$. Increasing r from 0, λ^* decreases and stays equal to $-\lambda_3'$ until r reaches some value $r(p)$ for which $\lambda^* = -\lambda_3' = \lambda_1'$. For r increasing from $r(p)$ to 1, λ^* is now equal to λ_1' and increases. Therefore λ^* is minimized, and the spectral gap is maximized, for the value of r that gives $\lambda_1' = -\lambda_3'$.

For $0 \leq p \leq \frac{1}{2}$ we have $\lambda_1' = 1 - 2p$. We easily find the solution $r(p) = \frac{p}{1+p} = 1 - \frac{1}{1+p}$.

For $\frac{1}{2} \leq p \leq 1$ we have $\lambda_1' = 2p - 1$. We easily find the solution $r(p) = \frac{1-p}{2-p} = 1 - \frac{1}{2-p}$.

g) For what value of the triple (p', q', r) is the spectral gap the largest as possible?

Answer: For $0 \leq p \leq 1$, the spectral gap is the largest for $r = r(p)$, in which case it equals $\gamma(p) = 1 - (-\lambda_3') = 2r(p)$. As $r(p)$ increases on $(0, 1/2]$ and decreases on $[1/2, 1)$, the spectral gap is the largest for $p = 1/2$ and $r = r(1/2) = 1/3$. In that case $p' = q' = r = 1/3$.