Markov Chains and Monte–Carlo Simulation

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1 Introduction

- Markov chains
  - are a fundamental class of stochastic models for sequences of non–independent random variables, i.e. of random variables possessing a specific *dependency structure*.
  - have numerous applications e.g. in *insurance and finance*.
  - play also an important role in mathematical modelling and analysis in a variety of other fields such as *physics, chemistry*, *life sciences*, and *material sciences*.
- Questions of scientific interest often exhibit a degree of complexity resulting in great difficulties if the attempt is made to find an adequate mathematical model that is solely based on analytical formulae.
- In these cases Markov chains can serve as an alternative tool as they are crucial for the construction of *computer algorithms* for the Markov Chain Monte Carlo simulation (MCMC) of the mathematical models under consideration.

This course on Markov chains and Monte Carlo simulation will be based on the methods and models introduced in the course "Elementare Wahrscheinlichkeitsrechnung und Statistik". Further knowledge of probability theory and statistics can be useful but is not required.

- The main focus of this course will be on the following topics:
  - discrete–time Markov chains with finite state space
  - stationarity and ergodicity
  - Markov Chain Monte Carlo (MCMC)
  - reversibility and coupling algorithms
- Notions and results introduced in "Elementare Wahrscheinlichkeitsrechnung and Statistik" will be used frequently. References to these lecture notes will be labelled by the prefix "WR" in front of the number specifying the corresponding section, theorem, lemma, etc.
- The following list contains only a small collection of introductory texts that can be recommended for in–depth studies of the subject complementing the lecture notes.
  - E. Behrends (2000) *Introduction to Markov Chains.* Vieweg, Braunschweig
  - P. Bremaud (2008) *Markov Chains, Gibbs Fields, Monte Carlo Simulation, and Queues.* Springer, New York
  - B. Chalmond (2003) *Modeling and Inverse Problems in Image Analysis.* Springer, New York
  - D. Gamerman, H. Lopes (2006) *Markov Chain Monte Carlo: Stochastic Simulation for Bayesian Inference.* Chapman & Hall, London
  - O. Häggström (2002) *Finite Markov Chains and Algorithmic Applications.* Cambridge University Press, Cambridge
  - D. Levin, Y. Peres, E. Wilmer (2009) *Markov chains and mixing times.* Publications of the AMS, Riverside
  - S. Resnick (1992) *Adventures in Stochastic Processes.* Birkhäuser, Boston
  - C. Robert, G. Casella (2009) *Introducing Monte Carlo Methods with R.* Springer, Berlin
  - T. Rolski, H. Schmidli, V. Schmidt, J. Teugels (1999) *Stochastic Processes for Insurance and Finance.* Wiley, Chichester
  - Y. Suhov, M. Kelbert (2008) *Probability and Statistics by Example. Volume 2. Markov Chains: A Primer in Random Processes and their Applications.* Cambridge University Press, Cambridge
  - H. Thorisson (2002) *Coupling, Stationarity, and Regeneration.* Springer, New York
  - G. Winkler (2003) *Image Analysis, Random Fields and Dynamic Monte Carlo Methods.* Springer, Berlin

2 Markov Chains

- Markov chains can describe the (temporal) dynamics of objects, systems, etc.
  - that can possess one of *finitely* or *countably* many possible configurations at a given time,
  - where these configurations will be called the *states* of the considered object or system, respectively.
- Examples for this class of objects and systems are
  - the current prices of products like insurance policies, stocks or bonds, if they are observed on a discrete (e.g. integer) time scale,
  - the monthly profit of a business,
  - the current length of the checkout lines (so–called "queues") in a grocery store,
  - the vector of temperature, air pressure, precipitation and wind velocity recorded on an hourly basis at the meteorological office Ulm–Kuhberg,
  - digital maps, for example describing the momentary spatial dispersion of a disease.
  - microscopical 2D or 3D images describing the current state (i.e. structural geometrical properties) of biological tissues or technical materials such as polymers, metals or ceramics.

Remarks

- In this course we will focus on *discrete–time* Markov chains, i.e., the temporal dynamics of the considered objects, systems etc. will be observed *stepwise*, e.g. at integer points in time.
- The algorithms for Markov Chain Monte Carlo simulation we will discuss in part II of the course are based on exactly these discrete–time Markov chains.
- The number of potential states can be very high.
- For mathematical reasons it is therefore convenient to consider the case of infinitely many states as well. As long as the infinite case is restricted to *countably* many states, only slight methodological changes will be necessary.

2.1 Specification of the Model and Examples

2.1.1 State Space, Initial Distribution and Transition Probabilities

- The stochastic model of a discrete–time Markov chain with finitely many states consists of three components: state space, initial distribution and transition matrix.
  - The model is based on the (finite) set of all possible states called the *state space* of the Markov chain. W.l.o.g. the state space can be identified with the set $E = \{1, 2, \ldots, \ell\}$ where $\ell \in \mathbb{N} = \{1, 2, \ldots\}$ is an arbitrary but fixed natural number.
  - For each $i \in E$, let α_i be the probability of the system or object to be in state i at time $n = 0$, where it is assumed that
$$\alpha_i \in [0, 1]\,, \qquad \sum_{i=1}^{\ell} \alpha_i = 1\,. \tag{1}$$
The vector $\boldsymbol{\alpha} = (\alpha_1, \ldots, \alpha_\ell)^\top$ of the probabilities $\alpha_1, \ldots, \alpha_\ell$ defines the *initial distribution* of the Markov chain.
  - Furthermore, for each pair $i, j \in E$ we consider the (conditional) probability $p_{ij} \in [0, 1]$ for the transition of the object or system from state i to j within one time step.

– The $\ell \times \ell$ matrix $\mathbf{P} = (p_{ij})_{i,j=1,\ldots,\ell}$ of the transition probabilities p_{ij} where

$$p_{ij} \geq 0\,, \qquad \sum_{j=1}^{\ell} p_{ij} = 1\,, \tag{2}$$

is called one–step *transition matrix* of the Markov chain.

- For each set $E = \{1, 2, \ldots, \ell\}$, for any vector $\boldsymbol{\alpha} = (\alpha_1, \ldots, \alpha_\ell)^\top$ and matrix $\mathbf{P} = (p_{ij})$ satisfying the conditions (1) and (2) the notion of the corresponding Markov chain can now be introduced.

Definition

- Let $X_0, X_1, \ldots : \Omega \to E$ be a sequence of random variables defined on the probability space $(\Omega, \mathcal{F}, P)$ and mapping into the set $E = \{1, 2, \ldots, \ell\}$.
- Then $X_0, X_1, \ldots$ is called a (homogeneous) *Markov chain* with initial distribution $\boldsymbol{\alpha} = (\alpha_1, \ldots, \alpha_\ell)^\top$ and transition matrix $\mathbf{P} = (p_{ij})$, if

$$P(X_0 = i_0, X_1 = i_1, \ldots, X_n = i_n) = \alpha_{i_0} p_{i_0 i_1} \ldots p_{i_{n-1} i_n} \tag{3}$$

for arbitrary $n = 0, 1, \ldots$ and $i_0, i_1, \ldots, i_n \in E$.

Remarks

- A quadratic matrix $\mathbf{P} = (p_{ij})$ satisfying (2) is called a *stochastic matrix*.
- The following Theorem 2.1 reveals the intuitive meaning of condition (3). In particular the motivation for the choice of the words "initial distribution" and "transition matrix" will become evident.
- Furthermore, Theorem 2.1 states another (equivalent) definition of a Markov chain that is frequently found in literature.

Theorem 2.1 *The sequence $\{X_n\}$ of E–valued random variables is a Markov chain if and only if there is a stochastic matrix $\mathbf{P} = (p_{ij})$ such that*

$$P(X_n = i_n \mid X_{n-1} = i_{n-1}, \ldots, X_0 = i_0) = p_{i_{n-1} i_n} \tag{4}$$

for any $n = 1, 2, \ldots$ and $i_0, i_1, \ldots, i_n \in E$ such that $P(X_{n-1} = i_{n-1}, \ldots, X_0 = i_0) > 0$.

Proof

- Clearly condition (4) is necessary for $\{X_n\}$ to be a Markov chain as (4) follows immediately from (3) and the definition of the conditional probability; see Section WR–2.6.1.
- Let us now assume $\{X_n\}$ to be a sequence of E-valued random variables such that a stochastic matrix $\mathbf{P} = (p_{ij})$ exists that satisfies condition (4).
- For all $i \in E$ we define $\alpha_i = P(X_0 = i)$ and realize that condition (3) obviously holds for $n = 0$.
- Furthermore,
  – $P(X_0 = i_0) = 0$ implies $P(X_0 = i_0, X_1 = i_1) = 0$,
  – and in case $P(X_0 = i_0) > 0$ from (4) we can conclude that

$$P(X_0 = i_0, X_1 = i_1) = P(X_0 = i_0) P(X_1 = i_1 \mid X_0 = i_0) \overset{(4)}{=} \alpha_{i_0} p_{i_0 i_1}\,.$$

- Therefore

$$P(X_0 = i_0, X_1 = i_1) = \begin{cases} 0\,, & \text{if } \alpha_{i_0} = 0, \\ \alpha_{i_0} p_{i_0 i_1}\,, & \text{if } \alpha_{i_0} > 0, \end{cases}$$

i.e., we showed that (3) also holds for the case $n = 1$.

- Now assume that (3) holds for some $n = k - 1 \geq 1$.
  - By the monotonicity of probability measures (see statement 2 in Theorem WR–2.1) $P(X_0 = i_0, X_1 = i_1, \ldots, X_{k-1} = i_{k-1}) = 0$ immediately implies $P(X_0 = i_0, X_1 = i_1, \ldots, X_k = i_k) = 0$.
  - On the other hand if $P(X_0 = i_0, X_1 = i_1, \ldots, X_{k-1} = i_{k-1}) > 0$, then

$$\begin{aligned} & P(X_0 = i_0, X_1 = i_1, \ldots, X_k = i_k) \\ = \;& P(X_0 = i_0, X_1 = i_1, \ldots, X_{k-1} = i_{k-1}) P(X_k = i_k \mid X_{k-1} = i_{k-1}, \ldots, X_0 = i_0) \\ = \;& \alpha_{i_0} p_{i_0 i_1} \ldots p_{i_{k-2} i_{i-1}} p_{i_{k-1} i_k} \,. \end{aligned}$$

- Thus, (3) also holds for $n = k$ and hence for all $n \in \mathbb{N}$. □

Corollary 2.1 *Let $\{X_n\}$ be a Markov chain. Then,*

$$P(X_n = i_n \mid X_{n-1} = i_{n-1}, \ldots, X_0 = i_0) = P(X_n = i_n \mid X_{n-1} = i_{n-1}) \tag{5}$$

holds whenever $P(X_{n-1} = i_{n-1}, \ldots, X_0 = i_0) > 0$.

Proof

- Let $P(X_{n-1} = i_{n-1}, \ldots, X_0 = i_0)$ and hence also $P(X_{n-1} = i_{n-1})$ be strictly positive.
- In this case (3) yields

$$\begin{aligned} P(X_n = i_n \mid X_{n-1} = i_{n-1}) &= \frac{P(X_n = i_n, X_{n-1} = i_{n-1})}{P(X_{n-1} = i_{n-1})} \\ &= \frac{\sum\limits_{i_0, \ldots, i_{n-2} \in E} P(X_n = i_n, \ldots, X_0 = i_0)}{\sum\limits_{i_0, \ldots, i_{n-2} \in E} P(X_{n-1} = i_{n-1}, \ldots, X_0 = i_0)} \\ &\overset{(3)}{=} \frac{\sum\limits_{i_0, \ldots, i_{n-2} \in E} \alpha_{i_0} p_{i_0 i_1} \ldots p_{i_{n-2} i_{n-1}} p_{i_{n-1} i_n}}{\sum\limits_{i_0, \ldots, i_{n-2} \in E} \alpha_{i_0} p_{i_0 i_1} \ldots p_{i_{n-2} i_{n-1}}} = p_{i_{n-1} i_n} \,. \end{aligned}$$

- This result and (4) imply (5). □

Remarks

- Corollary 2.1 can be interpreted as follows:
  - The conditional distribution of the (random) state X_n of the Markov chain $\{X_n\}$ at "time" n is completely determined by the state $X_{n-1} = i_{n-1}$ at the preceding time $n - 1$.
  - It is *independent* from the states $X_{n-2} = i_{n-2}, \ldots, X_1 = i_1, X_0 = i_0$ observed in the earlier history of the Markov chain.
- The definition of the conditional probability immediately implies
  - the equivalence of (5) and

$$\begin{aligned} & P(X_n = i_n, X_{n-2} = i_{n-2} \ldots, X_0 = i_0 \mid X_{n-1} = i_{n-1}) \\ = \;& P(X_n = i_n \mid X_{n-1} = i_{n-1}) \; P(X_{n-2} = i_{n-2} \ldots, X_0 = i_0 \mid X_{n-1} = i_{n-1}) \,. \end{aligned} \tag{6}$$

  - The conditional independence (6) is called the *Markov property* of $\{X_n\}$.
- The definitions and results of Section 2.1.1 are still valid,
  - if instead of a finite state space $E = \{1, 2, \ldots, \ell\}$ a countably infinite state space such as the set of all integers or all natural numbers is considered.
  - It merely has to be taken into account that in this case $\boldsymbol{\alpha}$ and $\mathbf{P}$ possess an infinite number of components and entries, respectively.

2.1.2 Examples

1. *Weather Forecast*
   (see. O. Häggström (2002) *Finite Markov Chains and Algorithmic Applications.* CU Press, Cambridge)

   - We assume to observe the weather in an area whose typical weather is characterized by longer periods of rainy or dry days (denoted by rain and sunshine), where rain and sunshine exhibit approximately the same relative frequency over the entire year.
     - It is sometimes claimed that the best way to predict tomorrow's weather is simply to guess that it will be the same tomorrow as it is today.
     - If we assume that this way of predicting the weather will be correct in 75% of the cases (regardless whether today's weather is rain or sunshine), then the weather can be easily modelled by a Markov chain.
     - The state space consists of the two states 1 =rain and 2 = sunshine.
     - The transition matrix is given as follows:

$$\mathbf{P} = \begin{pmatrix} 0.75 & 0.25 \\ 0.25 & 0.75 \end{pmatrix} . \tag{7}$$

   - Note that a crucial assumption for this model is the perfect symmetry between rain and sunshine in the sense that the probability that today's weather will persist tomorrow is the same regardless of today's weather.
   - In areas where sunshine is much more common than rain a more realistic transition matrix would be the following:

$$\mathbf{P} = \begin{pmatrix} 0.5 & 0.5 \\ 0.1 & 0.9 \end{pmatrix} \tag{8}$$

2. *Random Walks; Risk Processes*

   - Classic examples for Markov chains are so–called *random walks*. The (unbounded) basic model is defined in the following way:
     - Let $Z, Z_1, Z_2, \ldots : \Omega \to \mathbb{Z}$ be a sequence of independent and identically distributed random variables mapping to $\mathbb{Z} = \{\ldots, -1, 0, 1, \ldots\}$.
     - Let $X_0 : \Omega \to \mathbb{Z}$ be an arbitrary random variable, which is independent from the increments $Z_1, Z_2, \ldots$, and define

$$X_n = X_{n-1} + Z_n \,, \qquad \forall\, n \geq 1 \,. \tag{9}$$

     - Then the random variables $X_0, X_1, \ldots$ form a Markov chain on the countably infinite state space $E = \mathbb{Z}$ with initial distribution $\boldsymbol{\alpha} = (\alpha_1, \alpha_2, \ldots)^\top$, where $\alpha_i = P(X_0 = i)$. The transition probabilities are given by $p_{ij} = P(Z = j - i)$.

   - Remarks
     - The Markov chain given in (9) can be used as a model for the temporal dynamics of the solvability reserve of insurance companies. X_0 will then be interpreted as the (random) initial reserve and the increments Z_n as the difference $Z_n = a - Z'_n$ between the risk–free premium income $a > 0$ and random expenses for the liabilities Z'_n in time period $n - 1$.
     - Another example for a random walk are the total winnings in n roulette games already discussed in Section WR–1.3. In this case we have $X_0 = 0$. The distribution of the random increment Z is given by $P(Z = i) = 1/2$ for $i = -1, 1$ and $P(Z = i) = 0$ for $i \in \mathbb{Z} \setminus \{-1, 1\}$.

3. *Queues*

   - The number of customers waiting in front of an arbitrary but fixed checkout desk in a grocery store can be modelled by a Markov chain in the following way:
     - Let $X_0 = 0$ be the number of customers waiting in the line, when the store opens.
     - By Z_n we denote the random number of new customers arriving while the cashier is serving the nth customer ($n = 1, 2, \ldots$).
     - We assume the random variables $Z, Z_1, Z_2, \ldots : \Omega \to \{0, 1, \ldots\}$ to be independent and identically distributed.
   - The recursive definition
   $$X_n = \max\{0, X_{n-1} + Z_n - 1\}\,, \qquad \forall\, n \geq 1\,, \tag{10}$$
   yields a sequence of random variables $X_0, X_1, \ldots \Omega \to \{0, 1, \ldots\}$ that is a Markov chain whose transition matrix $\mathbf{P} = (p_{ij})$ has the entries
   $$p_{ij} = \begin{cases} P(Z = j + 1 - i)\,, & \text{if } j + 1 \geq i > 0 \text{ or } j > i = 0, \\ P(Z = 0) + P(Z = 1)\,, & \text{if } j = i = 0, \\ 0\,, & \text{else} \end{cases}$$
   - X_n denotes the random number of customers waiting in the line right after the cashier has finished serving the nth customer, i.e., the customer who has just started checking out and hence already left the line is not counted any more.

4. *Branching Processes*

   - We consider the reproduction process of a certain population, where X_n denotes the total number of descendants in the nth generation; $X_0 = 1$.
   - We assume that
   $$X_n = \sum_{i=1}^{X_{n-1}} Z_{n,i}\,, \tag{11}$$
   where $\{Z_{n,i},\, n, i \in \mathbb{N}\}$ is a set of independent and identically distributed random variables mapping into the set $E = \{0, 1, \ldots\}$.
   - The random variable $Z_{n,i}$ is the random number of descendants of individual i in generation $(n - 1)$.
   - The sequence $X_0, X_1, \ldots : \Omega \to \{0, 1, \ldots\}$ of random variables given by $X_0 = 1$ and the recursion (11) is called a *branching process*.
   - One can show (see Section 2.1.3) that $X_0, X_1, \ldots$ is a Markov chain with transition probabilities
   $$p_{ij} = \begin{cases} P\Big(\sum\limits_{k=1}^{i} Z_{1,k} = j\Big)\,, & \text{if } i > 0, \\ 1\,, & \text{if } i = j = 0, \\ 0\,, & \text{else.} \end{cases}$$

5. *Cyclic random walks*

   - Further examples of Markov chains can be constructed as follows (see E. Behrends (2000) *Introduction to Markov Chains*. Vieweg, Braunschweig, p. 4).
     - We consider the finite state space $E = \{0, 1, \ldots, 999\}$, the initial distribution
     $$\boldsymbol{\alpha} = (1/16, 4/16, 6/16, 4/16, 1/16, 0, \ldots, 0)^\top \tag{12}$$

and the transition probabilities

$$p_{ij} = \begin{cases} \frac{1}{6}\,, & \text{if } (j+1000-i) \mod (1000) \in \{1,\ldots,6\}, \\ 0\,, & \text{else.} \end{cases}$$

– Let $X_0, Z_1, Z_2, \ldots : \Omega \to \{0,1,\ldots,999\}$ be independent random variables, where the distribution of X_0 is given by (12) and

$$P(Z_1 = i) = P(Z_2 = i) = \ldots = 1/6\,, \qquad \forall\, i = 1,\ldots,6\,.$$

– The sequence $X_0, X_1, \ldots \Omega \to \{0,1,\ldots,999\}$ of random variables defined by the recursion formula

$$X_n = (X_{n-1} + Z_n) \mod (1000) \tag{13}$$

for $n \geq 1$ is a Markov chain called *cyclic random walk*.

- Remarks
  - An experiment corresponding to the Markov chain defined above can be designed in the following way. First of all we toss a coin four times and record the frequency of the event "versus". The number x_0 of these events is regarded as realization of the random initial state X_0; see the *Bernoulli scheme* in Section WR–3.2.1.
  - Afterwards a dice is tossed n times. The outcome z_i of the ith experiment, is interpreted as a realization of the random "increment" Z_i; $i = 1,\ldots,n$.
  - The new state x_n of the system results from the update of the old state x_{n-1} according to (13) taking z_{n-1} as increment.
  - If the experiment is not realized by tossing a coin and a dice, respectively, but by a computer–based generation of *pseudo–random numbers* $x_0, z_1, z_2, \ldots$ the procedure is referred to as *Monte–Carlo simulation*.
  - Methods allowing the construction of *dynamic simulation algorithms* based on Markov chains will be discussed in the second part of this course in detail; see Chapter 3 below.

2.1.3 Recursive Representation

- In this section we will show
  - how Markov chains can be constructed from sequences of independent and identically distributed random variables,
  - that the recursive formulae (9), (10), (11) and (13) are special cases of a general principle for the construction of Markov chains,
  - that vice versa every Markov chain can be considered as solution of a recursive stochastic equation.
- As usual let $E = \{1,2,\ldots,\ell\}$ be a finite (or countably infinite) set.
  - Furthermore, let $(D, \mathcal{D})$ be a measurable space, e.g. $D = \mathbb{R}^d$ could be the d–dimensional Euclidian space and $\mathcal{D} = \mathcal{B}(\mathbb{R}^d)$ the Borel σ–algebra on $\mathbb{R}^d$, or $D = [0,1]$ could be defined as the unit interval and $\mathcal{D} = \mathcal{B}([0,1])$ as the Borel σ–algebra on $[0,1]$.
  - Let now $Z_1, Z_2, \ldots : \Omega \to D$ be a sequence of independent and identically distributed random variables mapping into D, and let $X_0 : \Omega \to E$ be independent of $Z_1, Z_2, \ldots$.

– Let the random variables $X_1, X_2, \ldots : \Omega \to E$ be given by the *stochastic recursion equation*

$$X_n = \varphi(X_{n-1}, Z_n)\,, \tag{14}$$

where $\varphi : E \times D \to E$ is an arbitrary measurable function.

Theorem 2.2

- *Let the random variables $X_0, X_1, \ldots : \Omega \to E$ be given by* (14).
- *Then*

$$P(X_n = i_n \mid X_{n-1} = i_{n-1}, \ldots, X_0 = i_0) = P(X_n = i_n \mid X_{n-1} = i_{n-1})$$

holds for any $n \geq 1$ and $i_0, i_1, \ldots, i_n \in E$ such that $P(X_{n-1} = i_{n-1}, \ldots, X_0 = i_0) > 0$.

Proof

- Formula (14) implies that

$$\begin{aligned} P(X_n = i_n \mid X_{n-1} = i_{n-1}, \ldots, X_0 = i_0) &= P(\varphi(X_{n-1}, Z_n) = i_n \mid X_{n-1} = i_{n-1}, \ldots, X_0 = i_0) \\ &= P(\varphi(i_{n-1}, Z_n) = i_n \mid X_{n-1} = i_{n-1}, \ldots, X_0 = i_0) \\ &= P(\varphi(i_{n-1}, Z_n) = i_n)\,, \end{aligned}$$

  – where the last equality follows from the transformation theorem for independent and identically distributed random variables (see Theorem WR–3.18),
  – as the random variables $X_0, \ldots, X_{n-1}$ are functions of $Z_1, \ldots, Z_{n-1}$ and hence independent of $\varphi(i_{n-1}, Z_n)$.
- In the same way one concludes that

$$\begin{aligned} P(\varphi(i_{n-1}, Z_n) = i_n) &= P(\varphi(i_{n-1}, Z_n) = i_n \mid X_{n-1} = i_{n-1}) \\ &= P(\varphi(X_{n-1}, Z_n) = i_n \mid X_{n-1} = i_{n-1}) \\ &= P(X_n = i_n \mid X_{n-1} = i_{n-1})\,. \end{aligned}$$

□

Remarks

- The proof of Theorem 2.2 yields that the conditional probability

$$p_{ij} = P(X_n = j \mid X_{n-1} = i)$$

is given by $p_{ij} = P(\varphi(i, Z_n) = j)$.
- p_{ij} does not dependent on n, as the "innovations" Z_n are identically distributed.
- Moreover, the joint probability $P(X_0 = i_0, X_1 = i_1, \ldots, X_n = i_n)$ is given by

$$P(X_0 = i_0, X_1 = i_1, \ldots, X_n = i_n) = \alpha_{i_0} p_{i_0 i_1} \ldots p_{i_{n-1} i_n}\,, \tag{15}$$

where $\alpha_{i_0} = P(X_0 = i_0)$.
- Consequently, the sequence $X_0, X_1, \ldots$ of random variables given by the recursive definition (14) is a Markov chain following the definition given in (3).

Our next step will be to show that vice versa, every Markov chain can be regarded as the solution of a recursive stochastic equation.

- Let $X_0, X_1, \ldots : \Omega \to E$ be a Markov chain with state space $E = \{1, 2, \ldots, \ell\}$, initial distribution $\boldsymbol{\alpha} = (\alpha_1, \ldots, \alpha_\ell)^\top$ and transition matrix $\mathbf{P} = (p_{ij})$.
- Based on a recursive equation of the form (14) we will construct a Markov chain $X_0', X_1', \ldots$ with initial distribution $\boldsymbol{\alpha}$ and transition matrix $\mathbf{P}$ such that

$$P(X_0 = i_0, \ldots, X_n = i_n) = P(X_0' = i_0, \ldots, X_n' = i_n)\,, \qquad \forall\, i_0, \ldots, i_n \in E \tag{16}$$

for all $n \geq 0$:

1. We start with a sequence $Z_0, Z_1, \ldots$ of independent random variables that are uniformly distributed on the interval $(0, 1]$.
2. First of all the E–valued random variable X_0' is defined as follows:

$$X_0' = k \qquad \text{if and only if} \qquad Z_0 \in \Big(\sum_{i=1}^{k-1} \alpha_i, \sum_{i=1}^{k} \alpha_i\Big]\,,$$

for all $k = 1, \ldots, \ell$, i.e.

$$X_0' = \sum_{k=1}^{\ell} k \mathbb{1}\Big(\sum_{i=1}^{k-1} \alpha_i < Z_0 \leq \sum_{i=1}^{k} \alpha_i\Big)\,. \tag{17}$$

3. The random variables $X_1', X_2', \ldots$ are defined by the recursive equation

$$X_n' = \varphi(X_{n-1}', Z_n)\,, \tag{18}$$

where the function $\varphi : E \times (0, 1] \to E$ is given by

$$\varphi(i, z) = \sum_{k=1}^{\ell} k \mathbb{1}\Big(\sum_{j=1}^{k-1} p_{ij} < z \leq \sum_{j=1}^{k} p_{ij}\Big)\,. \tag{19}$$

- It is easy to see that the probabilities $P(X_0' = i_0, X_1' = i_1, \ldots, X_n' = i_n)$ for the sequence $\{X_n'\}$ defined by (17)–(18) are given by (3), i.e., $\{X_n'\}$ is a Markov chain with initial distribution $\boldsymbol{\alpha}$ and transition matrix $\mathbf{P}$.

Remarks

- If (16) holds for two sequences $\{X_i\}$ and $\{X_i'\}$ of random variables, these sequences are called *stochastically equivalent*.
- The construction principle (17)–(19) can be exploited for the Monte–Carlo simulation of Markov chains with given initial distribution and transition matrix.
- Markov chains on a countably infinite state space can be constructed and simulated in the same way. However, in this case (17)–(19) need to be modified by considering vectors $\boldsymbol{\alpha}$ and matrices $\mathbf{P}$ of infinite dimensions.

2.1.4 The Matrix of the n–Step Transition Probabilities

- Let $X_0, X_1, \ldots : \Omega \to E$ be a Markov chain on the state space $E = \{1, 2, \ldots, \ell\}$ with initial distribution $\boldsymbol{\alpha} = (\alpha_1, \ldots, \alpha_\ell)^\top$ and transition matrix $\mathbf{P} = (p_{ij})$.
- For arbitrary but fixed $n \geq 1$ and $i, j \in E$ the product $p_{ii_1} p_{i_1 i_2} \ldots p_{i_{n-1} j}$ can be interpreted as the probability of the path $i \to i_1 \to \ldots \to i_{n-1} \to j$.

- Consequently, the probability of the transition from state i to state j within n steps is given by the sum

$$p_{ij}^{(n)} = \sum_{i_1,\ldots,i_{n-1}\in E} p_{ii_1}p_{i_1i_2}\cdots p_{i_{n-1}j}, \tag{20}$$

where

$$p_{ij}^{(n)} = P(X_n = j \mid X_0 = i) \qquad \text{if } P(X_0 = i) > 0. \tag{21}$$

Remarks

- The matrix $\mathbf{P}^{(n)} = (p_{ij}^{(n)})_{i,j=1,\ldots,\ell}$ is called the *n–step transition matrix* of the Markov chain $\{X_n\}$.
- If we introduce the convention $\mathbf{P}^{(0)} = \mathbf{I}$, where $\mathbf{I}$ denotes the $\ell \times \ell$–dimensional identity matrix, then $\mathbf{P}^{(n)}$ has the following representation formulae.

Lemma 2.1 *The equation*

$$\mathbf{P}^{(n)} = \mathbf{P}^n \tag{22}$$

holds for arbitrary $n = 0, 1, \ldots$ and thus for arbitrary $n, m = 0, 1, \ldots$

$$\mathbf{P}^{(n+m)} = \mathbf{P}^{(n)}\mathbf{P}^{(m)}. \tag{23}$$

Proof Equation (22) is an immediate consequence of (20) and the definition of matrix multiplication. □

Example (*Weather Forecast*)

- Consider $E = \{1, 2\}$, and let

$$\mathbf{P} = \begin{pmatrix} 1-p & p \\ p' & 1-p' \end{pmatrix}$$

be an arbitrarily chosen transition matrix, i.e. $0 < p, p' \leq 1$.

- One can show that the n–step transition matrix $\mathbf{P}^{(n)} = \mathbf{P}^n$ is given by the formula

$$\mathbf{P}^n = \frac{1}{p+p'}\begin{pmatrix} p' & p \\ p' & p \end{pmatrix} + \frac{(1-p-p')^n}{p+p'}\begin{pmatrix} p & -p \\ -p' & p' \end{pmatrix}.$$

Remarks

- The matrix identity (23) is called the *Chapman-Kolmogorov equation* in literature.
- Formula (23) yields the following useful inequalities.

Corollary 2.2 *For arbitrary $n, m, r = 0, 1, \ldots$ and $i, j, k \in E$,*

$$p_{ii}^{(n+m)} \geq p_{ij}^{(n)} p_{ji}^{(m)} \tag{24}$$

and

$$p_{ij}^{(r+n+m)} \geq p_{ik}^{(r)} p_{kk}^{(n)} p_{kj}^{(m)}. \tag{25}$$

Furthermore, Lemma 2.1 allows the following representation of the distribution of X_n. Recall that X_n denotes the state of the Markov chain at step n.

Theorem 2.3

- *Let $X_0, X_1, \ldots$ be a Markov chain with state space $E = \{1, \ldots, \ell\}$, initial distribution $\boldsymbol{\alpha}$ and one–step transition matrix $\mathbf{P}$.*
- *Then the vector $\boldsymbol{\alpha}_n = (\alpha_{n1}, \ldots, \alpha_{n\ell})^\top$ of the probabilities $\alpha_{ni} = P(X_n = i)$ is given by the equation*

$$\boldsymbol{\alpha}_n^\top = \boldsymbol{\alpha}^\top \mathbf{P}^n. \tag{26}$$

Proof

- From the formula of total probability (see Theorem WR–2.6) and (21) we conclude that

$$P(X_n = j) = \sum_{i \in E} \alpha_i \, P(X_n = j \mid X_0 = i) = \sum_{i \in E} \alpha_i p_{ij}^{(n)} \,,$$

  where we define $P(X_n = j \mid X_0 = i) = 0$ if $\alpha_i = P(X_0 = i) = 0$.
- Now statement (26) follows from Lemma 2.1. □

Remarks

- Due to Theorem 2.3 the probabilities $\alpha_{ni} = P(X_n = i)$ can be calculated via the nth power $\mathbf{P}^n$ of the transition matrix $\mathbf{P}$.
- In this context it is often useful to find a so–called *spectral representation* of $\mathbf{P}^n$. It can be constructed by using the eigenvalues and a basis of eigenvectors of the transition matrix as follows. Note that there are matrices having no spectral representation.

- *A short recapitulation*
  - Let $\mathbf{A}$ be a (not necessarily stochastic) $\ell \times \ell$ matrix, let $\boldsymbol{\phi}, \boldsymbol{\psi} \neq \mathbf{0}$ be two ℓ–dimensional (column–) vectors such that for each of them at least one of their components is different from 0, and let θ be an arbitrary (real or complex) number.
  - If

$$\mathbf{A}\boldsymbol{\phi} = \theta\boldsymbol{\phi} \qquad \text{and} \qquad \boldsymbol{\psi}^\top \mathbf{A} = \theta\boldsymbol{\psi}^\top \,, \text{ respectively,} \tag{27}$$

    then θ is an *eigenvalue* of $\mathbf{A}$ and $\boldsymbol{\phi}$ and $\boldsymbol{\psi}$ are left and right *eigenvectors* (for θ).
  - As (27) is equivalent to

$$(\mathbf{A} - \theta\mathbf{I})\boldsymbol{\phi} = \mathbf{0} \qquad \text{and} \qquad \boldsymbol{\psi}^\top(\mathbf{A} - \theta\mathbf{I}) = \mathbf{0}^\top \,, \text{ respectively,}$$

    θ is an eigenvalue of $\mathbf{A}$ if and only if θ is a solution of the so-called *characteristic equation*

$$\det(\mathbf{A} - \theta\mathbf{I}) = 0 \,. \tag{28}$$

  - Note that the determinant in (28) is a polynomial of order ℓ. Thus, the algebraic equation (28) has ℓ possibly complex solutions $\theta_1, \ldots, \theta_\ell$. These solutions might not be all different from each other.
  - W.l.o.g. we may assume the eigenvalues $\theta_1, \ldots, \theta_\ell$ to be ordered such that

$$|\theta_1| \geq |\theta_2| \geq \ldots \geq |\theta_\ell| \,.$$

  - For every eigenvalue θ_i left and right eigenvectors $\boldsymbol{\phi}_i$ and $\boldsymbol{\psi}_i$, respectively, can be found.

– Let $\mathbf{\Phi} = (\boldsymbol{\phi}_1, \ldots, \boldsymbol{\phi}_\ell)$ be the $\ell \times \ell$ matrix consisting of the right eigenvectors $\boldsymbol{\phi}_1, \ldots, \boldsymbol{\phi}_\ell$ and let

$$\mathbf{\Psi} = \begin{pmatrix} \boldsymbol{\psi}_1^\top \\ \vdots \\ \boldsymbol{\psi}_\ell^\top \end{pmatrix}$$

be the $\ell \times \ell$ matrix formed by the left eigenvectors $\boldsymbol{\psi}_1, \ldots, \boldsymbol{\psi}_\ell$.

– By definition of the eigenvectors

$$\mathbf{A}\mathbf{\Phi} = \mathbf{\Phi}\ \mathrm{diag}(\boldsymbol{\theta})\,, \tag{29}$$

where $\boldsymbol{\theta} = (\theta_1, \ldots, \theta_\ell)^\top$ and $\mathrm{diag}(\boldsymbol{\theta})$ denotes the diagonal matrix with diagonal elements $\theta_1, \ldots, \theta_\ell$.

- If the eigenvectors $\boldsymbol{\phi}_1, \ldots, \boldsymbol{\phi}_\ell$ are linearly independent,
  – the inverse $\mathbf{\Phi}^{-1}$ exists and we can set $\mathbf{\Psi} = \mathbf{\Phi}^{-1}$.
  – Moreover, in this case (29) implies

$$\mathbf{A} = \mathbf{\Phi}\ \mathrm{diag}(\boldsymbol{\theta})\mathbf{\Phi}^{-1} = \mathbf{\Phi}\ \mathrm{diag}(\boldsymbol{\theta})\mathbf{\Psi}$$

and hence

$$\mathbf{A}^n = \mathbf{\Phi}(\,\mathrm{diag}(\boldsymbol{\theta}))^n\mathbf{\Phi}^{-1} = \mathbf{\Phi}(\,\mathrm{diag}(\boldsymbol{\theta}))^n\mathbf{\Psi}\,.$$

  – This yields the *spectral representation* of $\mathbf{A}$:

$$\mathbf{A}^n = \sum_{i=1}^{\ell} \theta_i^n \boldsymbol{\phi}_i \boldsymbol{\psi}_i^\top\,. \tag{30}$$

Remarks

- An application of (30) for the transition matrix $\mathbf{A} = \mathbf{P}$ results in a simple algorithm calculating the nth power $\mathbf{P}^n$ of (26).
- For the necessary calculation of the eigenvalues and eigenvectors of $\mathbf{P}$ standard software like MAPLE, MATLAB or MATHEMATICA can be used.
- A striking advantage of the spectral representation (30) can be seen in the fact that the complexity of the numerical calculation for $\mathbf{P}^n$ stays constant if n is increased.
- However, the derivation of (30) requires the eigenvectors $\boldsymbol{\phi}_1, \ldots, \boldsymbol{\phi}_\ell$ to be linearly independent. The next lemma gives a sufficient condition for the linear independence of eigenvectors.

Lemma 2.2

- *If all eigenvalues $\theta_1, \ldots, \theta_\ell$ of $\mathbf{A}$ are pairwise distinct, every family of corresponding right eigenvectors $\boldsymbol{\phi}_1, \ldots, \boldsymbol{\phi}_\ell$ is linearly independent.*
- *Furthermore, if the left eigenvectors $\boldsymbol{\psi}_1, \ldots, \boldsymbol{\psi}_\ell$ are given by $\mathbf{\Psi} = \mathbf{\Phi}^{-1}$ it holds that*

$$\boldsymbol{\psi}_i^\top \boldsymbol{\phi}_j = \begin{cases} 1 & \text{if } i = j, \\ 0 & \text{if } i \neq j. \end{cases} \tag{31}$$

Proof

- The first statement will be proved by complete induction.
  – As every eigenvector $\boldsymbol{\phi}_1$ has at least one non–zero component, $a_1\boldsymbol{\phi}_1 = \mathbf{0}$ implies $a_1 = 0$.

- Let now all eigenvalues $\theta_1, \ldots, \theta_\ell$ of $\mathbf{A}$ be pairwise different and let the eigenvectors $\boldsymbol{\phi}_1, \ldots, \boldsymbol{\phi}_{k-1}$ be linearly independent for a certain $k \leq \ell$.
- In order to show the independence of $\boldsymbol{\phi}_1, \ldots, \boldsymbol{\phi}_k$ it suffices to show that

$$\sum_{j=1}^{k} a_j \boldsymbol{\phi}_j = \mathbf{0} \tag{32}$$

  implies $a_1 = \ldots = a_k = 0$.
- Let $a_1, \ldots, a_k$ be such that (32) holds. This also implies

$$\mathbf{0} = \mathbf{A}\,\mathbf{0} = \sum_{j=1}^{k} a_j \mathbf{A}\boldsymbol{\phi}_j = \sum_{j=1}^{k} a_j \theta_j \boldsymbol{\phi}_j \,.$$

- The same argument yields

$$\mathbf{0} = \theta_k\,\mathbf{0} = \theta_k \sum_{j=1}^{k} a_j \boldsymbol{\phi}_j = \sum_{j=1}^{k} \theta_k a_j \boldsymbol{\phi}_j$$

  and thus

$$\mathbf{0} = \sum_{j=1}^{k-1} (\theta_k - \theta_j) a_j \boldsymbol{\phi}_j \,.$$

- As the eigenvectors $\boldsymbol{\phi}_1, \ldots, \boldsymbol{\phi}_{k-1}$ are linearly independent

$$(\theta_k - \theta_1)a_1 = (\theta_k - \theta_2)a_2 = \ldots = (\theta_k - \theta_{k-1})a_{k-1} = 0$$

  and hence $a_1 = a_2 = \ldots = a_{k-1} = 0$ as $\theta_k \neq \theta_j$ for $1 \leq j \leq k-1$.
- Now (32) immediately implies $a_k = 0$.

• If the eigenvalues $\theta_1, \ldots, \theta_\ell$ of $\mathbf{A}$ are pairwise distinct,
- the $\ell \times \ell$ matrix $\boldsymbol{\Phi}$ consists of ℓ linearly independent column vectors,
- and thus $\boldsymbol{\Phi}$ is invertible.
- Consequently, the matrix $\boldsymbol{\Psi}$ of the left eigenvectors is simply the inverse $\boldsymbol{\Psi} = \boldsymbol{\Phi}^{-1}$. This immediately implies (31). □

2.2 Ergodicity and Stationarity

2.2.1 Basic Definitions and Quasi-positive Transition Matrices

• If the Markov chain $X_0, X_1, \ldots$ has a very large number ℓ of possible states, the spectral representation (30) of the n-step transition matrix $\mathbf{P}^{(n)} = \mathbf{P}^n$ discussed in Section 2.1.4 turns out to be inappropriate in order to calculate
- the conditional probabilities $p_{ij}^{(n)} = P(X_n = j \mid X_0 = i)$ of the random state X_n
- as well as the (unconditional) probabilities $P(X_n = j) = \sum_{i=1}^{\ell} \alpha_i p_{ij}^{(n)}$ of X_n

after $n \gg 1$ (time-) steps.

• However, there are certain conditions
- ensuring the existence of the limits $\lim_{n\to\infty} p_{ij}^{(n)}$ and $\lim_{n\to\infty} P(X_n = j)$, respectively, as well as their equality and independence of i,

– thus justifying to consider the limit $\pi_j = \lim_{n\to\infty} p_{ij}^{(n)} = \lim_{n\to\infty} P(X_n = j)$ as *approximation* of $p_{ij}^{(n)}$ and $P(X_n = j)$ if $n \gg 1$.

This serves as a motivation to formally introduce the notion of the *ergodicity* of Markov chains.

Definition The Markov chain $X_0, X_1, \ldots$ with transition matrix $\mathbf{P} = (p_{ij})$ and the corresponding n-step transition matrices $\mathbf{P}^{(n)} = (p_{ij}^{(n)})$ $(= \mathbf{P}^n)$ is called *ergodic* if the limits

$$\pi_j = \lim_{n\to\infty} p_{ij}^{(n)} \tag{33}$$

1. exist for all $j \in E$
2. are positive and independent of $i \in E$
3. form a probability function $\boldsymbol{\pi} = (\pi_1, \ldots, \pi_\ell)^\top$, i.e. $\sum_{j\in E} \pi_j = 1$.

Example (*Weather Forecast*)

- In order to illustrate the notion of an ergodic Markov chain we return to the simple example of weather forecast already discussed in Sections 2.1.2 and 2.1.4.
- Let $E = \{1, 2\}$ and
$$\mathbf{P} = \begin{pmatrix} 1-p & p \\ p' & 1-p' \end{pmatrix}$$
be an arbitrary transition matrix such that $0 < p, p' \leq 1$.
- The n-step transition matrix $\mathbf{P}^{(n)} = \mathbf{P}^n$ is given by
$$\mathbf{P}^n = \frac{1}{p+p'} \begin{pmatrix} p' & p \\ p' & p \end{pmatrix} + \frac{(1-p-p')^n}{p+p'} \begin{pmatrix} p & -p \\ -p' & p' \end{pmatrix}.$$
- If $p + p' < 2$, this and (26) imply
$$\lim_{n\to\infty} \mathbf{P}^n = \frac{1}{p+p'} \begin{pmatrix} p' & p \\ p' & p \end{pmatrix}$$
and
$$\boldsymbol{\pi} = \lim_{n\to\infty} \boldsymbol{\alpha}_n = \Big(\frac{p'}{p+p'}\ ,\ \frac{p}{p+p'}\Big)^\top, \tag{34}$$
respectively. Note that the limit distribution $\boldsymbol{\pi}$ in (34) does *not* depend on the choice of the initial distribution $\boldsymbol{\alpha}$ $(= \boldsymbol{\alpha}_0)$.
- However, if $p + p' = 2$, then
$$\mathbf{P}^n = \begin{cases} \mathbf{P} & \text{if } n \text{ is odd,} \\ \mathbf{I} & \text{if } n \text{ is even.} \end{cases}$$

The ergodicity of Markov chains on an arbitrary finite state space can be characterized by the following notion from the theory of positive matrices.

Definition

- The $\ell \times \ell$ matrix $\mathbf{A} = (a_{ij})$ is called *non-negative* if all entries a_{ij} of $\mathbf{A}$ are non-negative.
- The non-negative matrix $\mathbf{A}$ is called *quasi-positive* if there is a natural number $n_0 \geq 1$ such that all entries of $\mathbf{A}^{n_0}$ are positive.

Remark If $\mathbf{A}$ is a stochastic matrix and we can find a natural number $n_0 \geq 1$ such that all entries of $\mathbf{A}^{n_0}$ are positive, then it is easy to see that for all natural numbers $n \geq n_0$ all entries of $\mathbf{A}^n$ are positive.

Theorem 2.4 *The Markov chain $X_0, X_1, \ldots$ with state space $E = \{1, \ldots, \ell\}$ and transition matrix $\mathbf{P}$ is ergodic if and only if $\mathbf{P}$ is quasi-positive.*

Proof

- First of all we show that the condition
$$\min_{i,j \in E} p_{ij}^{(n_0)} > 0 \tag{35}$$
for some $n_0 \in \mathbb{N}$ is sufficient for the ergodicity of $\{X_n\}$.
  - Let $m_j^{(n)} = \min_{i \in E} p_{ij}^{(n)}$ and $M_j^{(n)} = \max_{i \in E} p_{ij}^{(n)}$. The Chapman–Kolmogorov equation (23) yields
$$p_{ij}^{(n+1)} = \sum_{k \in E} p_{ik} p_{kj}^{(n)}$$
and thus
$$m_j^{(n+1)} = \min_i p_{ij}^{(n+1)} = \min_i \sum_k p_{ik} p_{kj}^{(n)} \geq \min_i \sum_k p_{ik} \min_l p_{lj}^{(n)} = m_j^{(n)},$$
i.e., $m_j^{(n)} \leq m_j^{(n+1)}$ for all $n \geq 0$, where we define $\mathbf{P}^{(0)} = \mathbf{I}$. A similar argument shows that $M_j^{(n)} \geq M_j^{(n+1)}$ for all $n \geq 0$.
  - Consequently, in order to show the existence of the limits π_j in (33) it suffices to show that for all $j \in E$
$$\lim_{n \to \infty} (M_j^{(n)} - m_j^{(n)}) = 0\,. \tag{36}$$
  - For this purpose we consider the sets $E' = \{k \in E : p_{i_0 k}^{(n_0)} \geq p_{j_0 k}^{(n_0)}\}$ and $E'' = E \setminus E'$ for arbitrary but fixed states $i_0, j_0 \in E$.
  - Let $a = \min_{i,j \in E} p_{ij}^{(n_0)} > 0$. Then
$$\sum_{k \in E'} \left(p_{i_0 k}^{(n_0)} - p_{j_0 k}^{(n_0)}\right) = 1 - \sum_{k \in E''} p_{i_0 k}^{(n_0)} - \sum_{k \in E'} p_{j_0 k}^{(n_0)} \leq 1 - \ell a$$
and
$$\sum_{k \in E''} \left(p_{i_0 k}^{(n_0)} - p_{j_0 k}^{(n_0)}\right) = -\sum_{k \in E'} \left(p_{i_0 k}^{(n_0)} - p_{j_0 k}^{(n_0)}\right).$$

– By another application of the Chapman–Kolmogorov equation (23) this yields for arbitrary $n \geq 0$ and $j \in E$

$$\begin{aligned} p_{i_0 j}^{(n_0+n)} - p_{j_0 j}^{(n_0+n)} &= \sum_{k\in E} \big(p_{i_0 k}^{(n_0)} - p_{j_0 k}^{(n_0)}\big) p_{kj}^{(n)} \\ &= \sum_{k\in E'} \big(p_{i_0 k}^{(n_0)} - p_{j_0 k}^{(n_0)}\big) p_{kj}^{(n)} + \sum_{k\in E''} \big(p_{i_0 k}^{(n_0)} - p_{j_0 k}^{(n_0)}\big) p_{kj}^{(n)} \\ &\leq \sum_{k\in E'} \big(p_{i_0 k}^{(n_0)} - p_{j_0 k}^{(n_0)}\big) M_j^{(n)} + \sum_{k\in E''} \big(p_{i_0 k}^{(n_0)} - p_{j_0 k}^{(n_0)}\big) m_j^{(n)} \\ &= \sum_{k\in E'} \big(p_{i_0 k}^{(n_0)} - p_{j_0 k}^{(n_0)}\big) M_j^{(n)} - \sum_{k\in E'} \big(p_{i_0 k}^{(n_0)} - p_{j_0 k}^{(n_0)}\big) m_j^{(n)} \\ &= \sum_{k\in E'} \big(p_{i_0 k}^{(n_0)} - p_{j_0 k}^{(n_0)}\big) \big(M_j^{(n)} - m_j^{(n)}\big) \\ &\leq (1-\ell a)\big(M_j^{(n)} - m_j^{(n)}\big)\,. \end{aligned}$$

– As a consequence, $M_j^{(n_0+n)} - m_j^{(n_0+n)} \leq (M_j^{(n)} - m_j^{(n)})(1-\ell a)$ and by induction one shows that for any $k \geq 1$

$$M_j^{(kn_0+n)} - m_j^{(kn_0+n)} \leq (M_j^{(n)} - m_j^{(n)})(1-\ell a)^k\,. \tag{37}$$

– This ensures the existence of an (unbounded) sequence $n_1, n_2, \ldots$ such that for all $j \in E$

$$\lim_{k\to\infty} (M_j^{(n_k)} - m_j^{(n_k)}) = 0\,. \tag{38}$$

– By the monotonicity of the differences $M_j^{(n)} - m_j^{(n)}$ in n, (38) holds for *every* sequence $n_1, n_2, \ldots$ of natural numbers.

– This proves (36).

- The limits π_j are positive because

$$\pi_j = \lim_{n\to\infty} p_{ij}^{(n)} \geq \lim_{n\to\infty} m_j^{(n)} \geq m_j^{(n_0)} \geq a > 0\,.$$

- Furthermore, $\sum_{j\in E} \pi_j = \sum_{j\in E} \lim_{n\to\infty} p_{ij}^{(n)} = \lim_{n\to\infty} \sum_{j\in E} p_{ij}^{(n)} = 1$ as the sum consists of *finitely* many summands.
- It follows immediately from $\min_{j\in E} \pi_j > 0$ and (33) that the condition (35) is necessary for ergodicity if one takes into account that the state space E is finite. □

Remarks

- As the limits $\pi_j = \lim_{n\to\infty} p_{ij}^{(n)}$ of ergodic Markov chains do not depend on i and the state space $E = \{1, \ldots, \ell\}$ is finite, clearly

$$\lim_{n\to\infty} \boldsymbol{\alpha}_n^\top = \boldsymbol{\alpha}^\top \lim_{n\to\infty} \mathbf{P}^{(n)} = \boldsymbol{\pi}^\top\,.$$

- The proof of Theorem 2.4 does not only show the existence of the limits $\pi_j = \lim_{n\to\infty} p_{ij}^{(n)}$ but also yields the following *estimate for the rate of convergence*: The inequality (37) implies

$$\sup_{i,j\in E} |p_{ij}^{(n)} - \pi_j| \leq \sup_{j\in E} \big(M_j^{(n)} - m_j^{(n)}\big) \leq (1-\ell a)^{\lfloor n/n_0 \rfloor} \tag{39}$$

and hence

$$\sup_{j\in E} |\alpha_{nj} - \pi_j| \leq (1-\ell a)^{\lfloor n/n_0 \rfloor}\,, \tag{40}$$

where $\lfloor n/n_0 \rfloor$ denotes the integer part of n/n_0.

- Estimates like (39) and (40) are referred to as *geometric bounds* for the rate of convergence in literature.

Now we will show that the limits $\pi_j = \lim_{n\to\infty} p_{ij}^{(n)}$ can be regarded as solution of a system of linear equations.

Theorem 2.5

- *Let $X_0, X_1, \ldots$ be an ergodic Markov chain with state space $E = \{1, \ldots, \ell\}$ and transition matrix $\mathbf{P} = (p_{ij})$.*
- *In this case the vector $\boldsymbol{\pi} = (\pi_1, \ldots, \pi_\ell)^\top$ of the limits $\pi_j = \lim_{n\to\infty} p_{ij}^{(n)}$ is the uniquely determined (positive) solution of the linear equation system*

$$\pi_j = \sum_{i\in E} \pi_i p_{ij}\,, \qquad j \in E, \tag{41}$$

when additionally the condition $\sum_{j\in E} \pi_j = 1$ is imposed.

Proof

- The definition (33) of the limits π_j and the Chapman–Kolmogorov equation (23) imply by changing the order of limit and sum that

$$\pi_j \overset{(33)}{=} \lim_{n\to\infty} p_{kj}^{(n)} \overset{(23)}{=} \lim_{n\to\infty} \sum_{i\in E} p_{ki}^{(n-1)} p_{ij} = \sum_{i\in E} \lim_{n\to\infty} p_{ki}^{(n-1)} p_{ij} \overset{(33)}{=} \sum_{i\in E} \pi_i p_{ij}\,.$$

- Suppose now that there is another solution $\boldsymbol{\pi}' = (\pi'_1, \ldots, \pi'_\ell)^\top$ of (41) such that $\pi'_j = \sum_{i\in E} \pi'_i p_{ij}$ for all $j \in E$ and $\sum_{j\in E} \pi'_j = 1$.
- By induction one easily shows

$$\pi'_j = \sum_{i\in E} \pi'_i p_{ij}^{(n)}, \qquad j \in E\,, \tag{42}$$

for all $n = 1, 2, \ldots$.

- In particular (42) implies

$$\pi'_j \overset{(42)}{=} \lim_{n\to\infty} \sum_{i\in E} \pi'_i p_{ij}^{(n)} = \sum_{i\in E} \pi'_i \lim_{n\to\infty} p_{ij}^{(n)} \overset{(33)}{=} \pi_j\,.$$

□

Remarks

- In matrix notation the linear equation system (41) is of the form $\boldsymbol{\pi}^\top = \boldsymbol{\pi}^\top \mathbf{P}$.
- If the number ℓ of elements in the state space is reasonably small this equation system can be used for the numerical calculation of the probability function $\boldsymbol{\pi}$; see Section 2.2.5.
- In case $\ell \gg 1$, Monte–Carlo simulation turns out to be a more efficient method to determine $\boldsymbol{\pi}$; see Section 3.3.

2.2.2 Estimates for the Rate of Convergence; Perron–Frobenius–Theorem

- Recall:
  - If $\{X_n\}$ is a Markov chain whose 1-step transition matrix $\mathbf{P}$ has only strictly positive entries p_{ij},

– then the geometric bound for the rate of convergence to the limit distribution $\boldsymbol{\pi} = (\pi_1, \ldots, \pi_\ell)^\top$ derived in (40) is given as follows:

$$\max_{j \in E} |\alpha_{nj} - \pi_j| = O((1 - \ell a)^n)\,, \tag{43}$$

where $a = \min_{i,j \in E} p_{ij} > 0$.

- Whenever the minimum a of the entries p_{ij} of the transition matrix $\mathbf{P}$ is close to 0 the bound in (43) is not very useful.
- However, in some cases the basis $1 - \ell a$ of the convergence estimate (43) can be improved.

Example (*Weather Forecast*)

- Let $E = \{1, 2\}$ and

$$\mathbf{P} = \begin{pmatrix} 1-p & p \\ p' & 1-p' \end{pmatrix}\,, \qquad \text{where } 0 < p, p' < 1.$$

- In Section 2.2.1 we showed that
  - the n-step transition matrix $\mathbf{P}^{(n)} = \mathbf{P}^n$ is given by

$$\mathbf{P}^n = \frac{1}{p+p'} \begin{pmatrix} p' & p \\ p' & p \end{pmatrix} + \frac{(1-p-p')^n}{p+p'} \begin{pmatrix} p & -p \\ -p' & p' \end{pmatrix}$$

  - and thus

$$\Big(\mathbf{P}^\infty = \Big) \quad \lim_{n \to \infty} \mathbf{P}^n = \frac{1}{p+p'} \begin{pmatrix} p' & p \\ p' & p \end{pmatrix}\,.$$

  - Consequently

$$\mathbf{P}^n - \mathbf{P}^\infty = \frac{(1-p-p')^n}{p+p'} \begin{pmatrix} p & -p \\ -p' & p' \end{pmatrix} \qquad \Big(= O(|1-p-p'|^n)\Big)\,, \tag{44}$$

  where $p + p' > 2a = 2 \min_{i,j \in E} p_{ij}$ and hence $|1 - p - p'| < 1 - 2a$ if $p \neq p'$.
- Remarks
  - The basis $|\theta_2| = |1 - p - p'|$ of the rate of convergence in (44) is the absolute value of the second largest eigenvalue θ_2 of the transition matrix $\mathbf{P}$,
  - as the characteristic equation

$$\Big(\det(\mathbf{P} - \theta \mathbf{I}) = \Big) \quad (1-p-\theta)(1-p'-\theta) - pp' = 0$$

  of $\mathbf{P}$ has the two solutions $\theta_1 = 1$ and $\theta_2 = 1 - p - p'$.

In general geometric estimates of the form (44) for the rate of convergence can be derived by means of the following so–called *Perron–Frobenius theorem* for quasi-positive matrices.

Theorem 2.6

- *Let* $\mathbf{A}$ *be a quasi-positive* $\ell \times \ell$ *matrix with eigenvalues* $\theta_1, \ldots, \theta_\ell$ *such that* $|\theta_1| \geq \ldots \geq |\theta_\ell|$.
- *Then the following holds:*

(a) *The eigenvalue* θ_1 *is real and positive.*

(b) $\theta_1 > |\theta_i|$ *for all* $i = 2, \ldots, \ell$,

(c) *The right and left eigenvectors* $\boldsymbol{\phi}_1$ *and* $\boldsymbol{\psi}_1$ *of* θ_1 *are uniquely determined up to a constant factor and can be chosen such that all components of* $\boldsymbol{\phi}_1$ *and* $\boldsymbol{\psi}_1$ *are positive.*

A *proof* of Theorem 2.6 can be found in Chapter 1 of E. Seneta (1981) *Non-Negative Matrices and Markov Chains*, Springer, New York.

Corollary 2.3 *Let* $\mathbf{P}$ *be a quasi-positive transition matrix. Then*

- $\theta_1 = 1, \boldsymbol{\phi}_1 = \mathbf{e}$ *and* $\boldsymbol{\psi}_1 = \boldsymbol{\pi}$, *where* $\mathbf{e} = (1, \ldots, 1)^\top$ *and* $\boldsymbol{\pi} = (\pi_1, \ldots, \pi_\ell)^\top$.
- $|\theta_i| < 1$ *for all* $i = 2, \ldots, \ell$.

Proof

- As $\mathbf{P}$ is a stochastic matrix, obviously $\mathbf{Pe} = \mathbf{e}$ and (41) implies $\boldsymbol{\pi}^\top \mathbf{P} = \boldsymbol{\pi}^\top$.
- Thus 1 is an eigenvalue of $\mathbf{P}$ and $\mathbf{e}$ and $\boldsymbol{\pi}$ are right and left eigenvectors of this eigenvalue, respectively.
- Let now θ be an arbitrary eigenvalue of $\mathbf{P}$ and let $\boldsymbol{\phi} = (\phi_1, \ldots, \phi_\ell)^\top$ be an eigenvector corresponding to θ.
- By definition (27) of θ and $\boldsymbol{\phi}$

$$|\theta|\,|\phi_i| \le \sum_{j=1}^{\ell} p_{ij}|\phi_j| \le \max_{j\in E} |\phi_j|\,, \qquad \forall\, i \in E\,.$$

- Consequently $|\theta| \le 1$ and therefore $\theta_1 = 1$ is the largest eigenvalue of $\mathbf{P}$.
- Theorem 2.6 now implies $|\theta_i| < 1$ for $i = 2, \ldots, \ell$. □

Corollary 2.3 yields the following geometric convergence estimate.

Corollary 2.4 *Let* $\mathbf{P}$ *be a quasi-positive transition matrix such that all eigenvalues* $\theta_1, \ldots, \theta_\ell$ *of* $\mathbf{P}$ *are pairwise distinct. Then*

$$\sup_{j\in E} |\alpha_{nj} - \pi_j| = O(|\theta_2|^n)\,. \tag{45}$$

Proof

- Corollary 2.3 implies

$$\lim_{n\to\infty} \sum_{i=2}^{\ell} \theta_i^n \boldsymbol{\phi}_i \boldsymbol{\psi}_i^\top = \mathbf{0}\,, \tag{46}$$

  as $|\theta_i| < 1$ for all $i = 2, \ldots, \ell$.
- Furthermore, Corollary 2.3 implies $\theta_1 = 1$ as well as $\boldsymbol{\phi}_1 = (1, \ldots, 1)^\top$ and $\boldsymbol{\psi}_1 = \boldsymbol{\pi}$ being the right and left eigenvectors of θ_1, respectively.
- Taking into account the spectral representation (30) of $\mathbf{P}^n$, i.e.,

$$\mathbf{P}^n = \sum_{i=1}^{\ell} \theta_i^n \boldsymbol{\phi}_i \boldsymbol{\psi}_i^\top\,,$$

  it is easy to see that

$$\mathbf{P}^n - \begin{pmatrix} \boldsymbol{\pi}^\top \\ \vdots \\ \boldsymbol{\pi}^\top \end{pmatrix} = \mathbf{P}^n - \theta_1^n \boldsymbol{\phi}_1 \boldsymbol{\psi}_1^\top = \sum_{i=2}^{\ell} \theta_i^n \boldsymbol{\phi}_i \boldsymbol{\psi}_i^\top\,.$$

- As $\boldsymbol{\alpha}_n^\top = \boldsymbol{\alpha}^\top \mathbf{P}^n$ (see Theorem 2.3) this together with (46) shows (45). □

Example (*Reaching a Consensus*)
see C. Hesse (2003) *Angewandte Wahrscheinlichkeitstheorie*. Vieweg, Braunschweig, p. 349

- A committee consisting of ℓ members has the mandate to project a certain (economical) parameter $\mu \in \mathbb{R}$, one could think of the German Council of Economic Experts projecting economic growth for the next year.
  - In a first step each of the ℓ experts gives a personal projection for μ, where the single projection results are denoted by $\widehat{\mu}_1^{(0)}, \ldots, \widehat{\mu}_\ell^{(0)}$.
  - What could be a method for the experts to settle on a *common* projection, i.e. reach a *consensus*?
  - A simple approach would be to calculate the arithmetic mean $(\widehat{\mu}_1^{(0)} + \ldots + \widehat{\mu}_\ell^{(0)})/\ell$, thus ignoring the different levels of expertise within the group.
- Alternatively, every committee member could modify his own projection based on the projections by his $\ell - 1$ colleagues and his personal assessment of their authors expertise.
  - For arbitrary $i, j \in \{1, \ldots, \ell\}$ the expert i attributes the „trust probability" p_{ij} to the expert j such that
$$p_{ij} > 0 \qquad \text{and} \qquad \sum_{j=1}^{\ell} p_{ij} = 1\,, \qquad \forall\, i, j \in \{1, \ldots, \ell\}$$
  - and expert i modifies his original projection $\widehat{\mu}_i^{(0)}$ replacing it by
$$\widehat{\mu}_i^{(1)} = \sum_{j=1}^{\ell} p_{ij} \widehat{\mu}_j^{(0)}\,.$$
  - In most cases the modified projections $\widehat{\mu}_1^{(1)}, \ldots, \widehat{\mu}_\ell^{(1)}$ will still be different from each other. Therefore the procedure is repeated until the differences are sufficiently small.
- Theorem 2.4 ensures
  - that this can be achieved if the modification procedure is repeated often enough,
  - as according to Theorem 2.4 the limits
$$\lim_{n\to\infty} \widehat{\mu}_i^{(n)} = \sum_{j=1}^{\ell} \pi_j \widehat{\mu}_j^{(0)} \tag{47}$$
    exist and do not depend on i,
  - where the vector $\boldsymbol{\pi} = (\pi_1, \ldots, \pi_\ell)^\top$ of the limits $\pi_j = \lim_{n\to\infty} p_{ij}^{(n)}$ is the (uniquely determined) solution of the linear equation system (41), i.e. $\boldsymbol{\pi}^\top = \boldsymbol{\pi}^\top \mathbf{P}$ with $\mathbf{P} = (p_{ij})$.
- The equality (47) can be seen as follows:
$$\begin{aligned} \lim_{n\to\infty} \widehat{\mu}_i^{(n)} &= \lim_{n\to\infty} \sum_{j=1}^{\ell} p_{ij}\, \widehat{\mu}_j^{(n-1)} = \lim_{n\to\infty} \sum_{j=1}^{\ell} p_{ij}^{(n)}\, \widehat{\mu}_j^{(0)} \\ &= \sum_{j=1}^{\ell} \lim_{n\to\infty} p_{ij}^{(n)}\, \widehat{\mu}_j^{(0)} = \sum_{j=1}^{\ell} \pi_j\, \widehat{\mu}_j^{(0)}\,. \end{aligned}$$
- The consensus, i.e. the common projection of the unknown parameter μ, reached by the committee is given by
$$\widehat{\mu} = \sum_{j=1}^{\ell} \pi_j \widehat{\mu}_j^{(0)}\,. \tag{48}$$

Remarks

- For large ℓ the algebraic solution of the linear equation system (41) can be difficult.
- In this case the estimates for the rate of convergence in (47) become relevant for the practical implementation of the method to reach a consensus described in (47).
- We consider the following numerical example.
  - Let $\ell = 3$ and

$$\mathbf{P} = \begin{pmatrix} \frac{2}{6} & \frac{1}{6} & \frac{3}{6} \\ \frac{1}{4} & \frac{1}{4} & \frac{2}{4} \\ \frac{2}{8} & \frac{1}{8} & \frac{5}{8} \end{pmatrix} . \tag{49}$$

  - The entries of this stochastic matrix imply that the third expert has a particularly high reputation among his colleagues.
  - The solution $\boldsymbol{\pi} = (\pi_1, \pi_2, \pi_3)^\top$ of the corresponding linear equation system (41) is given by

$$\pi_1 = \frac{21}{77} , \qquad \pi_2 = \frac{12}{77} , \qquad \pi_3 = \frac{44}{77} ,$$

    i.e. the projection $\widehat{\mu}_3^{(0)}$ of the third expert with the outstanding reputation is most influential.
- The eigenvalues of the transition matrix given in (49) are $\theta_1 = 1$, $\theta_2 = 1/8$ and $\theta_3 = 1/12$.
- The „basis" in the rate of convergence given by (43) is

$$1 - 3a = 1 - 3 \min_{i,j=1,2,3} p_{ij} = 1 - \frac{3}{8} = \frac{5}{8} ,$$

  whereas Corollary 2.4 yields the following substantially improved geometric rate of convergence

$$\max_{i \in \{1,\ldots,\ell\}} \left| \widehat{\mu} - \widehat{\mu}_i^{(n)} \right| = O(|\theta_2|^n)$$

  where $\theta_2 = 1/8$ denotes the second largest eigenvalue of the stochastic matrix $\mathbf{P}$ given by (49).

2.2.3 Irreducible and Aperiodic Markov Chains

- Recall that in Theorem 2.4 we characterized the ergodicity of the Markov chain $X_0, X_1, \ldots$ by the quasi-positivity of its transition matrix $\mathbf{P}$.
- However, it can be difficult to show this property of $\mathbf{P}$ directly, especially if $\ell \gg 1$.
- Therefore, we will derive another (probabilistic) way to characterize the ergodicity of a Markov chain with finite state space. For this purpose we will need the following notion.
  - For arbitrary but fixed states $i, j \in E$ we say that the state j is *accessible* from state i if $p_{ij}^{(n)} > 0$ for some $n \geq 0$ where $\mathbf{P}^{(0)} = \mathbf{I}$. (notation: $i \to j$)
  - Another (equivalent) definition for accessibility of states is the following:
  - Let $\tau_j = \min\{n \geq 0 : X_n = j\}$ be the number of steps until the Markov chain $\{X_n\}$ reaches the state $j \in E$ for the first time. We define $\tau_j = \infty$ if $X_n \neq j$ for all $n \geq 0$.

Theorem 2.7 *Let $i \in E$ be such that $P(X_0 = i) > 0$. In this case j is accessible from $i \in E$ if and only if $P(\tau_j < \infty \mid X_0 = i) > 0$.*

Proof

- The condition is obviously necessary because

$$\{X_n = j\} \subset \{\tau_j \le n\} \subset \{\tau_j < \infty\} \qquad \text{and thus} \qquad 0 < p_{ij}^{(n)} \le P(\tau_j < \infty \mid X_0 = i)$$

  for some $n \ge 0$ if j is accessible from i.

- On the other hand if $i \ne j$ and $p_{ij}^{(n)} = 0$ for all $n \ge 0$, then

$$\begin{aligned} P(\tau_j < \infty \mid X_0 = i) &= \lim_{n\to\infty} P(\tau_j < n \mid X_0 = i) \\ &= \lim_{n\to\infty} P\Big(\bigcup_{k=0}^{n-1} \{X_k = j\} \;\Big|\; X_0 = i\Big) \\ &\le \lim_{n\to\infty} \sum_{k=0}^{n-1} P(X_k = j \mid X_0 = i) = \lim_{n\to\infty} \sum_{k=0}^{n-1} p_{ij}^{(k)} = 0\,. \end{aligned}$$

□

Remarks

- The property of accessibility is
  - *transitive*, i.e., $i \to k$ and $k \to j$ imply that $i \to j$.
  - This is an immediate consequence of the inequality $p_{ij}^{(r+m)} \ge p_{ik}^{(r)} p_{kj}^{(m)}$ (see Corollary 2.2) and of the definition of accessibility.
  - Moreover, in case $i \to j$ *and* $j \to i$ we say that the states i and j *communicate*. (notation: $i \leftrightarrow j$)
- The property of communicating is an *equivalence relation* as
  (a) $i \leftrightarrow i$ (reflexivity),
  (b) $i \leftrightarrow j$ if and only if $j \leftrightarrow i$ (symmetry),
  (c) $i \leftrightarrow k$ and $k \leftrightarrow j$ implies $i \leftrightarrow j$ (transitivity).
- As a consequence,
  - the state space E can be completely divided into disjoint equivalence classes with respect to the equivalence relation $\leftrightarrow$.
  - The Markov chain $\{X_n\}$ with transition matrix $\mathbf{P} = (p_{ij})$ is called *irreducible* if the state space E consists of only one equivalence class, i.e. $i \leftrightarrow j$ for all $i, j \in E$.

Examples

- The definition of irreducibility immediately implies that the 2×2 matrices

$$\mathbf{P}_1 = \begin{pmatrix} 1/2 & 1/2 \\ 1/2 & 1/2 \end{pmatrix} \qquad \text{and} \qquad \mathbf{P}_2 = \begin{pmatrix} 1/2 & 1/2 \\ 1/4 & 3/4 \end{pmatrix}$$

  are irreducible.

- On the other hand the 4×4 block matrix $\mathbf{P}$ consisting of $\mathbf{P}_1$ and $\mathbf{P}_2$

$$\mathbf{P} = \begin{pmatrix} \mathbf{P}_1 & \mathbf{0} \\ \mathbf{0} & \mathbf{P}_2 \end{pmatrix}$$

  is not irreducible.

Besides irreducibility we need a second property of the transition probabilities, namely the so-called *aperiodicity*, in order to characterize the ergodicity of a Markov chain in a simple way.

Definition

- The *period* d_i of the state $i \in E$ is given by $d_i = \gcd\{n \geq 1 : p_{ii}^{(n)} > 0\}$ where „gcd" denotes the greatest common divisor. We define $d_i = \infty$ if $p_{ii}^{(n)} = 0$ for all $n \geq 1$.
- A state $i \in E$ is said to be *aperiodic* if $d_i = 1$.
- The Markov chain $\{X_n\}$ and its transition matrix $\mathbf{P} = (p_{ij})$ are called *aperiodic* if all states of $\{X_n\}$ are aperiodic.

We will now show that the periods d_i and d_j coincide if the states i, j belong to the same equivalence class of communicating states. For this purpose we introduce the notation $i \to j[n]$ if $p_{ij}^{(n)} > 0$.

Theorem 2.8 *If the states $i, j \in E$ communicate, then $d_i = d_j$.*

Proof

- If $j \to j[n]$, $i \to j[k]$ and $j \to i[m]$ for certain $k, m, n \geq 1$, then the inequalities from Corollary 2.2 imply that $i \to i[k+m]$ and $i \to i[k+m+n]$.
- Thus, $k+m$ and $k+m+n$ are divisible by d_i.
- As a consequence the difference $n = (k+m+n) - (k+m)$ is also divisible by d_i.
- This shows that d_i is a common divisor for all natural numbers n having the property that $p_{jj}^{(n)} > 0$, i.e. $d_i \leq d_j$.
- For reasons of symmetry the same argument also proves that $d_j \leq d_i$. □

Corollary 2.5 *Let the Markov chain $\{X_n\}$ be irreducible. Then all states of $\{X_n\}$ have the same period.*

In order to show

- that the characterization of an ergodic Markov chain (see Theorem 2.4) considered in Section 2.2.1 is equivalent to the Markov chain being irreducible and aperiodic,
- we need the following elementary lemma from *number theory*.

Lemma 2.3 *Let $k = 1, 2, \ldots$ an arbitrary but fixed natural number. Then there is a natural number $n_0 \geq 1$ such that*

$$\{n_0, n_0+1, n_0+2, \ldots\} \subset \{n_1 k + n_2(k+1);\ n_1, n_2 \geq 0\}\,.$$

Proof

- If $n \geq k^2$ there are integers $m, d \geq 0$ such that $n - k^2 = mk + d$ and $d < k$.
- Therefore $n = (k - d + m)k + d(k+1)$ and hence

$$n \in \{n_1 k + n_2(k+1);\ n_1, n_2 \geq 0\}\,,$$

  i.e., $n_0 = k^2$ is the desired number. □

Theorem 2.9 *The transition matrix* $\mathbf{P}$ *is quasi-positive if and only if* $\mathbf{P}$ *is irreducible and aperiodic.*

Proof

- Let us first assume the transition matrix $\mathbf{P}$ to be irreducible and aperiodic.
  - For every $i \in E$ we consider the set $J(i) = \{n \geq 1 : p_{ii}^{(n)} > 0\}$ whose greatest common divisor is 1 as $\mathbf{P}$ is aperiodic.
  - The inequalities from Corollary 2.2 yield

$$p_{ii}^{(n+m)} \geq p_{ii}^{(n)} p_{ii}^{(m)}$$

    and hence

$$n + m \in J(i) \qquad \text{if } n, m \in J(i). \tag{50}$$

- We show that $J(i)$ contains two successive numbers.
  - If $J(i)$ did not contain two successive numbers, the elements of $J(i)$ would have a minimal distance $k \geq 2$.
  - The consequence would be that $mk + d \in J(i)$ for some $m = 0, 1, \ldots$ and $d = 1, \ldots, k-1$ as otherwise $n = mk$ for all $n \in J(i)$.
  - But this is a contradiction to our hypothesis $\gcd(J(i)) = 1$.
- Let now $n_1, n_1 + k \in J(i)$. Statement (50) then implies also $a(n_1 + k) \in J(i)$ and $n + bn_1 \in J(i)$ for arbitrary $a, b \in \mathbb{N}$, where

$$n = mk + d \in J(i)\,. \tag{51}$$

- We will show
  - that there are natural numbers $a, b \in \{1, 2, \ldots\}$ such that the difference between $a(n_1 + k) \in J(i)$ and $n + bn_1 \in J(i)$ is less than k.
  - From (51) we obtain

$$a(n_1 + k) - n - bn_1 = (a - b)n_1 + (a - m)k - d$$

    and hence for $a = b = m + 1$

$$a(n_1 + k) - n - bn_1 = k - d < k\,.$$

- Therefore, the set $J(i)$ contains two successive numbers.
- Statement (50) and Lemma 2.3 yield that for every $i \in E$ there is an $n(i) \geq 1$ such that

$$J(i) \supset \{n(i), n(i) + 1, \ldots\}\,. \tag{52}$$

- This result, the irreducibility of $\mathbf{P}$ and the inequality (25) in Corollary 2.2, i.e.

$$p_{ij}^{(r+n+m)} \geq p_{ik}^{(r)} p_{kk}^{(n)} p_{kj}^{(m)}\,,$$

  imply that for each pair $i, j \in E$ of states there is a natural number $n(ij) \geq 1$ such that

$$J(ij) = \{n \geq 0 : p_{ij}^{(n)} > 0\} \supset \{n(ij), n(ij) + 1, \ldots\}\,,$$

  i.e., $\mathbf{P}$ is quasi-positive.
- Conversely, the irreducibility and aperiodicity of quasi-positive transition matrices are immediate consequences of the definitions. □

Remarks

- A simple example for a non–irreducible Markov chain
  - can be given by our well-known model for the *weather forecast* where $E = \{1, 2\}$ and

$$\mathbf{P} = \begin{pmatrix} 1-p & p \\ p' & 1-p' \end{pmatrix} .$$

  - If $p = 0$ or $p' = 0$, then the corresponding Markov chain is clearly not irreducible and therefore by Theorem 2.9 not ergodic.
- It is nevertheless possible that the linear equation system

$$\boldsymbol{\alpha}^\top = \boldsymbol{\alpha}^\top \mathbf{P} \tag{53}$$

has one (or infinitely many) probability solutions $\boldsymbol{\alpha}^\top = (\alpha_1, \alpha_2)$.
  - If for example $p = 0$ and $p' > 0$, then $i = 1$ is a so-called *absorbing state* and $\boldsymbol{\alpha}^\top = (1, 0)$ is the (uniquely determined) solution of the linear equation system (53).
  - If $p = 0$ and $p' = 0$, *every* probability solution $\boldsymbol{\alpha}^\top = (\alpha_1, \alpha_2)$ solves the linear equation system (53).
- Now we give some examples for non-aperiodic Markov chains $X_0, X_1, \ldots : \Omega \to E$.
  - In this context the random variables $X_0, X_1, \ldots : \Omega \to E$ are *not* given by a stochastic recursion formula $X_n = \varphi(X_{n-1}, Z_n)$ of the type (14) where the increments $Z_1, Z_2, \ldots : \Omega \to D$ are independent and identically distributed random variables.
  - We merely assume that the random variables $Z_1, Z_2, \ldots : \Omega \to D$ are conditionally independent in the following sense.
  - Note: As was shown in Section 2.1.3 it is nevertheless possible to construct a Markov chain that is stochastically equivalent to $X_0, X_1, \ldots$ having independent increments, see the construction principle considered in (17)–(19).
- Let E and D be arbitrary finite (or countably finite) sets, let $\varphi : E \times D \to E$ be an arbitrary function and let $X_0, X_1, \ldots : \Omega \to E$ and $Z_1, Z_2, \ldots : \Omega \to D$ be random variables
  - such that

$$X_n = \varphi(X_{n-1}, Z_n) \tag{54}$$

  - and such that for every $n \in \mathbb{N}$ the random variable Z_n is *conditionally independent* of the random variables $Z_1, \ldots, Z_{n-1}, X_0, \ldots, X_{n-2}$ given X_{n-1},
  - i.e., for arbitrary $n \in \mathbb{N}$, $i_0, i_1 \ldots, i_{n-1} \in E$ and $k_1, \ldots, k_n \in D$

$$\begin{aligned} &P(Z_n = k_n, Z_{n-1} = k_{n-1}, \ldots, Z_1 = k_1, X_{n-1} = i_{n-1}, \ldots, X_0 = i_0) \\ &\quad = \quad P(Z_n = k_n \mid X_{n-1} = i_{n-1})\, P(Z_{n-1} = k_{n-1}, \ldots, Z_1 = k_1, X_{n-1} = i_{n-1}, \ldots, X_0 = i_0)\,, \end{aligned}$$

    where we define $P(Z_n = k_n \mid X_{n-1} = i_{n-1}) = 0$ if $P(X_{n-1} = i_{n-1}) = 0$.
  - Moreover, we assume that for arbitrary $i \in E$ and $k \in D$ the probabilities $P(Z_n = k \mid X_{n-1} = i)$ do *not* depend on $n \in \mathbb{N}$.
- One can show that the sequence $X_0, X_1, \ldots : \Omega \to E$ recursively defined by (54) is a Markov chain whose transition matrix $\mathbf{P} = (p_{ij})$ is given by

$$p_{ij} = P(\varphi(i, Z_1) = j \mid X_0 = i)\,,$$

if $P(X_0 = i) > 0$ for all $i \in E$.

Example (*Diffusion Model*)
see P. Brémaud (1999) *Markov Chains, Gibbs Fields, Monte Carlo Simulation, and Queues.* Springer, New York, p. 76

- The following simple model describing a diffusion process through a membrane was suggested in 1907 by the physicists Tatiana and Paul Ehrenfest. It is designed to model the heat exchange between two systems at different temperatures.
  - We consider ℓ particles, which are distributed between two containers A and B that are permeably connected but insulated with respect to their environment.
  - Assume there are $X_{n-1} = i$ particles in A at time $n-1$. Then one of the ℓ particles in the two containers is selected at random and transferred into the other container.
  - The state X_n of the system at time n is hence either $X_n = i-1$ with probability i/ℓ (if the selected particle was in container A) or $X_n = i+1$ with probability $(\ell - i)/\ell$ (if the selected particle was in container B).
- The random variables $X_0, X_1, \ldots : \Omega \to \{0, 1, \ldots, \ell\}$ can thus be defined recursively
  - by the stochastic recursion formula

$$X_n = X_{n-1} + Z_n \,, \tag{55}$$

  - where given X_{n-1} the random variable Z_n is *conditionally independent* of the random variables $Z_1, \ldots, Z_{n-1}, X_0, \ldots, X_{n-1}$ with $P(Z_n = -1) + P(Z_n = 1) = 1$ and

$$P(Z_n = -1 \mid X_{n-1} = i) = \frac{i}{\ell} \qquad \text{if } P(X_{n-1} = i) > 0 \,.$$

  - The entries p_{ij} of the transition matrix $\mathbf{P} = (p_{ij})$ are therefore given by

$$p_{ij} = \begin{cases} \dfrac{\ell - i}{\ell} & \text{if } i < \ell \text{ and } j = i+1, \\ \dfrac{i}{\ell} & \text{if } i > 0 \text{ and } j = i-1, \\ 0 & \text{else} \end{cases}$$

  - In particular this implies $d_i = \gcd\{n \geq 1 : p_{ii}^{(n)} > 0\} = 2$ for all $i \in \{0, 1, \ldots, \ell\}$, i.e. the Markov chain given by (55) is not aperiodic (and thus by Theorem 2.9 not ergodic).
- In spite of this, the linear equation system

$$\boldsymbol{\alpha}^\top = \boldsymbol{\alpha}^\top \mathbf{P} \tag{56}$$

has a (uniquely determined) probability solution $\boldsymbol{\alpha}^\top = (\alpha_0, \ldots, \alpha_\ell)$ where

$$\alpha_i = \frac{1}{2^\ell} \binom{\ell}{i} \,, \qquad \forall\, i \in \{0, 1, \ldots, \ell\} \,. \tag{57}$$

Remarks

- The diffusion model of Ehrenfest is a special case of the following class of Markov chains called *birth and death processes with two reflecting barriers* in literature.

- The state space considered is $E = \{0, 1, \ldots, \ell\}$ whereas the transition matrix $\mathbf{P} = (p_{ij})$ is given by

$$\mathbf{P} = \begin{pmatrix} 0 & 1 & & & & & & \\ q_1 & r_1 & p_1 & & & & & \\ & q_2 & r_2 & p_2 & & & & \\ & & \ddots & \ddots & \ddots & & & \\ & & & q_i & r_i & p_i & & \\ & & & & \ddots & \ddots & \ddots & \\ & & & & & q_{\ell-1} & r_{\ell-1} & p_{\ell-1} \\ & & & & & & 1 & 0 \end{pmatrix}, \tag{58}$$

  where $p_i > 0$, $q_i > 0$ and $p_i + q_i + r_i = 1$ for all $i \in \{1, \ldots, \ell - 1\}$.
- The linear equation system $\boldsymbol{\alpha}^\top = \boldsymbol{\alpha}^\top \mathbf{P}$ is of the form

$$\alpha_i = \begin{cases} p_{i-1}\alpha_{i-1} + r_i\alpha_i + q_{i+1}\alpha_{i+1}\,, & \text{if } 0 < i < \ell, \\ q_1\alpha_1\,, & \text{if } i = 0, \\ p_{\ell-1}\alpha_{\ell-1}\,, & \text{if } i = \ell. \end{cases}$$

  - One can show that
$$\alpha_i = \alpha_0 \, \frac{p_1 p_2 \cdot \ldots \cdot p_{i-1}}{q_1 q_2 \cdot \ldots \cdot q_i}\,,$$
  - where $\alpha_0 > 0$ is defined by the condition $\sum_{i=0}^{\ell} \alpha_i = 1$, i.e.
$$\alpha_0 \left(1 + \frac{1}{q_1} + \frac{p_1}{q_1 q_2} + \ldots + \frac{p_1 p_2 \cdot \ldots \cdot p_{\ell-1}}{q_1 q_2 \cdot \ldots \cdot q_\ell} \right) = 1$$
    and, consequently,
$$\alpha_0 = \left(1 + \frac{1}{q_1} + \frac{p_1}{q_1 q_2} + \ldots + \frac{p_1 p_2 \cdot \ldots \cdot p_{\ell-1}}{q_1 q_2 \cdot \ldots \cdot q_\ell} \right)^{-1}.$$
- As we assume $p_i > 0$ and $q_i > 0$ for all $i \in \{1, \ldots, \ell - 1\}$, birth and death processes with two reflecting barriers are obviously irreducible.
- If the additional condition $r_i > 0$ is satisfied for some $i \in \{1, \ldots, \ell - 1\}$, then birth and death processes with two reflecting barriers are also aperiodic (and hence ergodic by Theorem 2.9).

2.2.4 Stationary Initial Distributions

- Recall
  - If $\{X_n\}$ is an irreducible and aperiodic Markov chain with (finite) state space $E = \{1, \ldots, \ell\}$ and (quasi-positive) transition matrix $\mathbf{P} = (p_{ij})$,
  - then the limit distribution $\boldsymbol{\pi} = \lim_{n\to\infty} \boldsymbol{\alpha}_n$ is the uniquely determined probability solution of the following matrix equation (see Theorem 2.5):
$$\boldsymbol{\alpha}^\top = \boldsymbol{\alpha}^\top \mathbf{P}\,. \tag{59}$$
- If the Markov chain $\{X_n\}$ is not assumed to be irreducible there can be more than one solution for (59).

  - Moreover, if the initial distribution $\boldsymbol{\alpha}_0$ of $\{X_n\}$ is a solution of (59), then Theorem 2.3 and (59) imply

$$\boldsymbol{\alpha}_1^\top = \boldsymbol{\alpha}_0^\top \mathbf{P} = \boldsymbol{\alpha}_0^\top$$

    and thus $\boldsymbol{\alpha}_n = \boldsymbol{\alpha}_0$ for all $n \geq 0$.
  - Due to this invariance property every probability solution $\boldsymbol{\alpha}$ of (59) is called a *stationary initial distribution* of $\{X_n\}$.

- Conversely, it is possible to show that
  - there is a *unique* probability solution $\boldsymbol{\alpha}$ for the matrix equation (59) if $\mathbf{P}$ is irreducible.
  - However, this solution $\boldsymbol{\alpha}$ of (59) is not necessarily the limit distribution $\boldsymbol{\pi} = \lim_{n\to\infty} \boldsymbol{\alpha}_n$ as $\boldsymbol{\pi}$ does not exist if $\mathbf{P}$ is not aperiodic.

Theorem 2.10

- *Let* $\mathbf{P} = (p_{ij})_{i,j\in E}$ *be an irreducible transition matrix, where* $E = \{1, \ldots, \ell\}$.
- *For arbitrary but fixed* $i, j \in E$ *the entries* $q_{ij}^{(n)}$ *of the stochastic* $(\ell \times \ell)$*–dimensional matrices* $\mathbf{Q}_n = (q_{ij}^{(n)})$ *where*

$$\mathbf{Q}_n = \frac{1}{n}\left(\mathbf{P} + \mathbf{P}^2 + \ldots + \mathbf{P}^n\right) \tag{60}$$

  converge to a limit

$$\alpha_j = \lim_{n\to\infty} q_{ij}^{(n)} > 0\,, \tag{61}$$

  which does not depend on i. *The vector* $\boldsymbol{\alpha} = (\alpha_1, \ldots, \alpha_\ell)^\top$ *is a solution of the matrix equation* (59) *and satisfies* $\sum_{j=1}^{\ell} \alpha_j = 1$.
- *The distribution* $\boldsymbol{\alpha}$ *given by* (60)*–*(61) *is the only probability solution of* (59).

A *proof* of Theorem 2.10 can be found in Chapter 7 of E. Behrends (2000) *Introduction to Markov Chains*, Vieweg, Braunschweig.

Remarks

- Besides the invariance property $\boldsymbol{\alpha}_0 = \boldsymbol{\alpha}_1 = \ldots$, the Markov chain $\{X_n\}$ with stationary initial distribution $\boldsymbol{\alpha}_0$ exhibits still another invariance property for *all* finite dimensional distributions that is considerably stronger.
- In this context we consider the following notion of a (strongly) *stationary sequence* of random variables.

Definition

- Let $X_0, X_1, \ldots : \Omega \to E$ be an arbitrary sequence of random variables mapping into $E = \{1, \ldots, \ell\}$ (which is not necessarily a Markov chain).
- The sequence $\{X_n\}$ of E-valued random variables is called *stationary* if for arbitrary $k, n \in \{0, 1, \ldots\}$ and $i_0, \ldots, i_n \in E$

$$P(X_k = i_0, X_{k+1} = i_1, \ldots, X_{k+n} = i_n) = P(X_0 = i_0, X_1 = i_1, \ldots, X_n = i_n)\,. \tag{62}$$

Theorem 2.11

- *Let $X_0, X_1, \ldots : \Omega \to E$ be a Markov chain with state space $E = \{1, \ldots, \ell\}$.*
- *Then $\{X_n\}$ is a stationary sequence of random variables if and only if the Markov chain $\{X_n\}$ has a stationary initial distribution.*

Proof

- The necessity of the condition follows immediately
  - from Theorem 2.3 and from the definitions for a stationary initial distribution and a stationary sequence of random variables, respectively,
  - as (62) in particular implies that $P(X_1 = i) = P(X_0 = i)$ for all $i \in E$
  - and from Theorem 2.3 we thus obtain $\boldsymbol{\alpha}_0^\top = \boldsymbol{\alpha}_1^\top = \boldsymbol{\alpha}_0^\top \mathbf{P}$, i.e., $\boldsymbol{\alpha}_0$ is a stationary initial distribution.
- Conversely, suppose now that $\boldsymbol{\alpha}_0$ is a stationary initial distribution of the Markov chain $\{X_n\}$.
  - Then, by the definition (3) of a Markov chain $\{X_n\}$, we have

$$\begin{aligned}
&P(X_k = i_0, X_{k+1} = i_1, \ldots, X_{k+n} = i_n) \\
&= \sum_{i'_0, \ldots, i'_{k-1} \in E} P(X_0 = i'_0, \ldots, X_{k-1} = i'_{k-1}, X_k = i_0, X_{k+1} = i_1, \ldots, X_{k+n} = i_n) \\
&= \sum_{i'_0, \ldots, i'_{k-1} \in E} \alpha_{i'_0}\, p_{i'_0 i'_1} \,\cdots\, p_{i'_{k-2} i'_{k-1}}\, p_{i'_{k-1} i_0}\, p_{i_0 i_1} \,\cdots\, p_{i_{n-1} i_n} \\
&= \left(\boldsymbol{\alpha}_0^\top \mathbf{P}^k\right)_{i_0} p_{i_0 i_1} \,\cdots\, p_{i_{n-1} i_n} \\
&= \alpha_{0, i_0}\, p_{i_0 i_1} \,\cdots\, p_{i_{n-1} i_n} \\
&= P(X_0 = i_0, X_1 = i_1, \ldots, X_n = i_n)\,,
\end{aligned}$$

  - where the last but one equality is due to the stationarity of the initial distribution $\boldsymbol{\alpha}_0$ and the last equality uses again the definition (3) of the Markov chain $\{X_n\}$. □

Remarks

- For some Markov chains, whose transition matrices exhibit a specific structure, we already calculated their stationary initial distributions in Sections 2.2.2 and 2.2.3.
- Now we will discuss two additional examples of this type.
  - In these examples the state space is *infinite* requiring an additional condition apart from quasi–positivity (or irreducibility and aperiodicity) in order to ensure the ergodicity of the Markov chains.
  - Namely, a so–called *contraction condition* is imposed that prevents the probability mass to „migrate towards infinity".

Examples

1. *Queues*

   see T. Rolski, H. Schmidli, V. Schmidt, J. Teugels (2002) *Stochastic Processes for Insurance and Finance*. J. Wiley & Sons, Chichester, p. 147.

   - We consider the example already discussed in Section 2.1.2
     - of the recursively defined Markov chain $X_0, X_1, \ldots \Omega \to \{0, 1, \ldots\}$ with $X_0 = 0$ and

$$X_n = \max\{0, X_{n-1} + Z_n - 1\}\,, \qquad \forall\, n \geq 1\,, \tag{63}$$

– where the random variables $Z, Z_1, Z_2, \ldots : \Omega \to \{0, 1, \ldots\}$ are independent and identically distributed and the transition matrix $\mathbf{P} = (p_{ij})$ is given by

$$p_{ij} = \begin{cases} P(Z = j + 1 - i) & \text{if } j + 1 \geq i > 0 \text{ or } j > i = 0, \\ P(Z = 0) + P(Z = 1) & \text{if } j = i = 0, \\ 0 & \text{otherwise.} \end{cases} \tag{64}$$

- It is not difficult to show that
  – the Markov chain $\{X_n\}$ defined by the recursion formula (63) with its corresponding transition matrix (64) is irreducible and aperiodic if

$$P(Z = 0) > 0\,, \quad P(Z = 1) > 0 \quad \text{and} \quad P(Z = 2) > 0\,, \tag{65}$$

  – for all $n \geq 1$ the solution of the recursion equation (63) can be written as

$$X_n = \max\Big\{0, \max_{k\in\{1,\ldots,n\}} \sum_{r=k}^{n} (Z_r - 1)\Big\} \stackrel{\mathrm{d}}{=} \max\Big\{0, \max_{k\in\{1,\ldots,n\}} \sum_{r=1}^{k} (Z_r - 1)\Big\}\,, \tag{66}$$

  – the limit probabilities π_i exist for all $i \in \{0, 1, \ldots\}$ where

$$\begin{aligned} \pi_i &= \lim_{n\to\infty} P\Big(\max\Big\{0, \max_{k\in\{1,\ldots,n\}} \sum_{r=1}^{k} (Z_r - 1)\Big\} = i\Big) \\ &= \begin{cases} P\Big(\sup\limits_{k\in\{1,2,\ldots\}} \sum\limits_{r=1}^{k} (Z_r - 1) = i\Big) & \text{for } i > 0, \\ P\Big(\sup\limits_{k\in\{1,2,\ldots\}} \sum\limits_{r=1}^{k} (Z_r - 1) \leq 0\Big) & \text{for } i = 0. \end{cases} \end{aligned}$$

- Furthermore

$$\begin{aligned} &\pi_i = 0 \quad \text{for all } i \in \{0, 1, \ldots\} && \text{if } \mathbb{E}\, Z \geq 1, \\ &\pi_i > 0 \quad \text{for all } i \in \{0, 1, \ldots\} \text{ and } \textstyle\sum_{i\geq 0} \pi_i = 1 && \text{if (65) holds and } \mathbb{E}\, Z < 1. \end{aligned}$$

- Thus, for Markov chains with (countably) infinite state space,
  – irreducibility and aperiodicity do *not always* imply ergodicity,
  – but, additionally, a certain *contraction condition* needs to be satisfied,
  – where in the present example this condition is the requirement of a *negative drift* , i.e., $\mathbb{E}\,(Z - 1) < 0$.
- If the conditions (65) are satisfied and $\mathbb{E}\, Z < 1$, then
  – the equation $\boldsymbol{\alpha}^\top = \boldsymbol{\alpha}^\top \mathbf{P}$ has a uniquely determined probability solution $\boldsymbol{\alpha}^\top = (\alpha_0, \alpha_1, \ldots)$,
  – which coincides with $\boldsymbol{\pi}^\top = (\pi_0, \pi_1, \ldots)$ $(= \lim_{n\to\infty} \boldsymbol{\alpha}_n^\top)$ but which in general cannot be determined explicitly.
  – However, there is a simple formula for the *generating function* $g_{\boldsymbol{\pi}} : (-1, 1) \to [0, 1]$ of $\boldsymbol{\pi} = (\pi_0, \pi_1, \ldots)^\top$, where

$$g_{\boldsymbol{\pi}}(s) = \sum_{i=0}^{\infty} s^i \pi_i \qquad \Big(= \mathbb{E}\, s^{X_\infty}\Big)$$

  and

$$X_\infty = \max\Big\{0, \sup_{k\in\{1,2,\ldots\}} \sum_{r=1}^{k} (Z_r - 1)\Big\}. \tag{67}$$

– Namely, we have

$$g_{\boldsymbol{\pi}}(s) = \frac{(1-\rho)(1-s)}{g_Z(s)-s}\,, \qquad \forall\, s \in (-1,1)\,, \tag{68}$$

where $\rho = \mathbb{E}\, Z$ and $g_Z(s) = \mathbb{E}\, s^Z$ is the generating function of Z.

- *Proof* of (68)
  - By the definition (67) of X_∞, we have $X_\infty \stackrel{\mathrm{d}}{=} \max\{0, X_\infty + (Z-1)\}$.
  - Furthermore, using the notation $x_+ = \max\{0,x\}$, we obtain

$$\begin{aligned} g_{\boldsymbol{\pi}}(s) &= \mathbb{E}\, s^{X_\infty} = \mathbb{E}\, s^{(X_\infty+Z-1)_+} \\ &= \mathbb{E}\left(s^{(X_\infty+Z-1)_+}\, \mathbb{1}(X_\infty+Z-1\geq 0)\right) + \mathbb{E}\left(s^{(X_\infty+Z-1)_+}\, \mathbb{1}(X_\infty+Z-1=-1)\right) \\ &= \frac{1}{s}\sum_{k=1}^{\infty} s^k P(X_\infty+Z=k) + P(X_\infty+Z=0) \\ &= s^{-1} g_{\boldsymbol{\pi}}(s) g_Z(s) + (s^{-1}-1) P(X_\infty+Z=0)\,, \end{aligned}$$

  i.e.

$$g_{\boldsymbol{\pi}}(s) = \frac{(s-1)P(X_\infty+Z=0)}{s-g_Z(s)}\,. \tag{69}$$

  – As

$$\lim_{s\uparrow 1} g_{\boldsymbol{\pi}}(s) = 1 \qquad \text{and} \qquad \lim_{s\uparrow 1} \frac{d}{ds} g_Z(s) = \mathbb{E}\, Z\,,$$

  by l'Hôpital's rule we can conclude that

$$1 = \frac{P(X_\infty+Z=0)}{1-\rho}\,.$$

  – Hence (68) is a consequence of (69).

2. *Birth and death processes with one reflecting barrier*

- We modify the example of the death and birth process discussed in Section 2.2.3 now considering the infinite state space $E = \{0,1,\ldots\}$ and the transition matrix

$$\mathbf{P} = \begin{pmatrix} 0 & 1 & & & & & \\ q_1 & r_1 & p_1 & & & & \\ & q_2 & r_2 & p_2 & & & \\ & & \ddots & \ddots & \ddots & & \\ & & & q_i & r_i & p_i & \\ & & & & \ddots & \ddots & \ddots \end{pmatrix} \tag{70}$$

  where $p_i > 0$, $q_i > 0$ and $p_i + q_i + r_i = 1$ is assumed for all $i \in \{1,2,\ldots\}$.
- The linear equation system $\boldsymbol{\alpha}^\top = \boldsymbol{\alpha}^\top \mathbf{P}$ is of the form

$$\alpha_i = \begin{cases} p_{i-1}\alpha_{i-1} + r_i\alpha_i + q_{i+1}\alpha_{i+1} & \text{if } i > 0, \\ q_1\alpha_1 & \text{if } i = 0. \end{cases} \tag{71}$$

- Similarly to the birth and death processes with two reflecting barriers one can show that

– the equation system (71) has a uniquely determined probability solution $\boldsymbol{\alpha}^\top$ if

$$\sum_{j=1}^{\infty} \frac{p_1 p_2 \cdot \ldots \cdot p_j}{q_1 q_2 \cdot \ldots \cdot q_{j+1}} < \infty \,, \tag{72}$$

– the solution $\boldsymbol{\alpha}^\top = (\alpha_0, \alpha_1, \ldots)$ of (71) is given by

$$\alpha_i = \alpha_0 \, \frac{p_1 p_2 \cdot \ldots \cdot p_{i-1}}{q_1 q_2 \cdot \ldots \cdot q_i} \,, \qquad \forall\, i > 0 \,,$$

– where $\alpha_0 > 0$ is defined by the condition $\sum_{i=0}^{\infty} \alpha_i = 1$, i.e.

$$\alpha_0 \left(1 + \frac{1}{q_1} + \sum_{j=1}^{\infty} \frac{p_1 p_2 \cdot \ldots \cdot p_j}{q_1 q_2 \cdot \ldots \cdot q_{j+1}} \right) = 1$$

and, consequently,

$$\alpha_0 = \left(1 + \frac{1}{q_1} + \sum_{j=1}^{\infty} \frac{p_1 p_2 \cdot \ldots \cdot p_j}{q_1 q_2 \cdot \ldots \cdot q_{j+1}} \right)^{-1} .$$

- As we assume $p_i > 0$ and $q_i > 0$ for all $i \in \{1, 2, \ldots\}$ birth and death processes with one reflecting barrier are obviously irreducible.
- Furthermore, if $r_i > 0$ for some $i \in \{1, 2 \ldots, \}$ then birth and death processes with one reflecting barrier are also aperiodic (as well as ergodic if the contraction condition (72) is satisfied).

2.2.5 Direct and Iterative Computation Methods

First we show how the stationary initial distribution $\boldsymbol{\alpha}_0$ ($= \boldsymbol{\pi} = \lim_{n\to\infty} \boldsymbol{\alpha}_n$) of the Markov chain $\{X_n\}$ can be computed based on methods from linear algebra in case the transition matrix $\mathbf{P}$ does not exhibit a particularly nice structure (but is quasi–positive) and if the number ℓ of states is reasonably small.

Theorem 2.12

- *Let the transition matrix* $\mathbf{P}$ *of the Markov chain* $\{X_n\}$ *be quasi-positive.*
- *Then the matrix* $\mathbf{I} - \mathbf{P} + \mathbf{E}$ *is invertible and the uniquely determined probability solution* $\boldsymbol{\pi} = \lim_{n\to\infty} \boldsymbol{\alpha}_n$ *of the matrix equation* $\boldsymbol{\pi}^\top = \boldsymbol{\pi}^\top \mathbf{P}$ *is given by*

$$\boldsymbol{\pi}^\top = \mathbf{e}^\top \, (\mathbf{I} - \mathbf{P} + \mathbf{E})^{-1} \,, \tag{73}$$

where $\mathbf{e} = (1, \ldots, 1)^\top$ *and all entries of the* $\ell \times \ell$ *matrix* $\mathbf{E}$ *are equal to* 1.

Proof

- In order to prove that the matrix $\mathbf{I} - \mathbf{P} + \mathbf{E}$ is invertible we show that the only solution of the equation

$$(\mathbf{I} - \mathbf{P} + \mathbf{E})\, \mathbf{x} = \mathbf{0} \tag{74}$$

is given by $\mathbf{x} = \mathbf{0}$.

– As $\boldsymbol{\pi}$ satisfies the equation $\boldsymbol{\pi}^\top = \boldsymbol{\pi}^\top \mathbf{P}$ we obtain

$$\boldsymbol{\pi}^\top (\mathbf{I} - \mathbf{P}) = \mathbf{0} \,. \tag{75}$$

– Thus (74) implies

$$0 = \boldsymbol{\pi}^\top (\mathbf{I} - \mathbf{P} + \mathbf{E})\, \mathbf{x} = 0 + \boldsymbol{\pi}^\top \mathbf{E}\mathbf{x}\,,$$

i.e.

$$\boldsymbol{\pi}^\top \mathbf{E}\mathbf{x} = 0\,. \tag{76}$$

- On the other hand, clearly $\boldsymbol{\pi}^\top \mathbf{E} = \mathbf{e}^\top$ and hence as a consequence of (76)

$$\mathbf{e}^\top \mathbf{x} = 0 \qquad \text{and} \qquad \mathbf{E}\mathbf{x} = \mathbf{0}\,. \tag{77}$$

  – Taking into account (74) this implies $(\mathbf{I} - \mathbf{P})\, \mathbf{x} = \mathbf{0}$ and, equivalently, $\mathbf{P}\, \mathbf{x} = \mathbf{x}$.
  – Thus, we also have $\mathbf{x} = \mathbf{P}^n\, \mathbf{x}$ for all $n \geq 1$.
- Furthermore, Theorem 2.4 implies $\mathbf{P}^n \to \boldsymbol{\Pi}$,
  – where $\boldsymbol{\Pi}$ denotes the $\ell \times \ell$ matrix consisting of the ℓ identical (row) vectors $\boldsymbol{\pi}^\top$.
  – In other words: For $n \to \infty$ we have

$$\mathbf{x} = \mathbf{P}^n\, \mathbf{x} \to \boldsymbol{\Pi}\, \mathbf{x}\,,$$

  i.e. $x_i = \sum_{j=1}^{\ell} \pi_j x_j$ for all $i = 1, \ldots, \ell$.
  – As the right hand sides of these equations do not depend on i we can conclude $\mathbf{x} = c\, \mathbf{e}$ for some constant $c \in \mathbb{R}$.
  – Moreover, as a consequence of (77),

$$0 = \mathbf{e}^\top \mathbf{x} = c\, \mathbf{e}^\top \mathbf{e} = c\ell$$

  and hence $c = 0$, i.e. $\mathbf{x} = \mathbf{0}$.
- Thus, the matrix $\mathbf{I} - \mathbf{P} + \mathbf{E}$ is invertible.
- Finally, (75) implies

$$\boldsymbol{\pi}^\top (\mathbf{I} - \mathbf{P} + \mathbf{E}) = \boldsymbol{\pi}^\top \mathbf{E} = \mathbf{e}^\top$$

and, equivalently,

$$\boldsymbol{\pi}^\top = \mathbf{e}^\top\, (\mathbf{I} - \mathbf{P} + \mathbf{E})^{-1}\,. \qquad \square$$

Remarks

- Given a larger number ℓ of states the numerical computation of the inverse matrix $(\mathbf{I} - \mathbf{P} + \mathbf{E})^{-1}$ in (73) can cause difficulties.
- In this case it is often more convenient to solve the matrix equation $\boldsymbol{\pi}^\top = \boldsymbol{\pi}^\top \mathbf{P}$ iteratively.
- If the transition matrix $\mathbf{P}$ is quasi–positive and hence $\pi_\ell > 0$ one can start by setting $\widehat{\pi}_\ell = 1$ and solving the modified equation

$$\widehat{\boldsymbol{\pi}}^\top (\mathbf{I} - \widehat{\mathbf{P}}) = \mathbf{b}^\top \tag{78}$$

  where $\widehat{\mathbf{P}} = (p_{ij})_{i,j=1,\ldots,\ell-1}$ and $\widehat{\boldsymbol{\pi}}^\top = (\widehat{\pi}_1, \ldots, \widehat{\pi}_{\ell-1})$, $\mathbf{b}^\top = (p_{\ell 1}, \ldots, p_{\ell,\ell-1})$.
- The probability function $\boldsymbol{\pi}^\top = (\pi_1, \ldots, \pi_\ell)$ desired originally is given by

$$\pi_i = \widehat{\pi}_i / c \quad \text{with } c = \widehat{\pi}_1 + \ldots + \widehat{\pi}_\ell \qquad \forall\, i = 1, \ldots, \ell\,.$$

- When solving the modified matrix equation (78) we use the facts of $\mathbf{I} - \widehat{\mathbf{P}}$ being invertible and that there is an expansion of $(\mathbf{I} - \widehat{\mathbf{P}})^{-1}$ as a power series, which is a consequence of the following two lemmata.

Lemma 2.4

- *Let* $\mathbf{A}$ *be an* $\ell \times \ell$ *matrix such that* $\mathbf{A}^n \to \mathbf{0}$ *for* $n \to \infty$.
- *Then the matrix* $\mathbf{I} - \mathbf{A}$ *is invertible and for all* $n = 1, 2, \ldots$

$$\mathbf{I} + \mathbf{A} + \ldots + \mathbf{A}^{n-1} = (\mathbf{I} - \mathbf{A})^{-1}(\mathbf{I} - \mathbf{A}^n)\,. \tag{79}$$

Proof

- Obviously for all $n = 1, 2, \ldots$

$$\begin{aligned}(\mathbf{I} - \mathbf{A})(\mathbf{I} + \mathbf{A} + \ldots + \mathbf{A}^{n-1}) &= \mathbf{I} + \mathbf{A} + \ldots + \mathbf{A}^{n-1} - \mathbf{A} - \ldots - \mathbf{A}^n \\ &= \mathbf{I} - \mathbf{A}^n\,. \end{aligned} \tag{80}$$

- Furthermore, the matrix $\mathbf{I} - \mathbf{A}^n$ is invertible for sufficiently large n as by hypothesis $\mathbf{A}^n \to \mathbf{0}$.
- Consequently, for sufficiently large n we have

$$\begin{aligned} 0 &\neq \det(\mathbf{I} - \mathbf{A}^n) \\ &= \det\Big((\mathbf{I} - \mathbf{A})(\mathbf{I} + \mathbf{A} + \ldots + \mathbf{A}^{n-1})\Big) \\ &= \det(\mathbf{I} - \mathbf{A})\det(\mathbf{I} + \mathbf{A} + \ldots + \mathbf{A}^{n-1})\,. \end{aligned}$$

- This implies $\det(\mathbf{I} - \mathbf{A}) \neq 0$ and hence $\mathbf{I} - \mathbf{A}$ is invertible.
- The assertion (79) now follows from (80). □

Lemma 2.5

- *Let the stochastic matrix* $\mathbf{P}$ *be quasi-positive and let* $\widehat{\mathbf{P}}$ *be the* $(\ell - 1) \times (\ell - 1)$ *matrix introduced in* (78).
- *Then,* $\widehat{\mathbf{P}}^n \to \mathbf{0}$ *for* $n \to \infty$, *the matrix* $\mathbf{I} - \widehat{\mathbf{P}}$ *is invertible, and*

$$(\mathbf{I} - \widehat{\mathbf{P}})^{-1} = \sum_{n=0}^{\infty} \widehat{\mathbf{P}}^n\,. \tag{81}$$

Proof

- Because of Lemma 2.4 it suffices to show that $\widehat{\mathbf{P}}^n \to \mathbf{0}$.
- As $\mathbf{P}$ is quasi–positive by hypothesis there is a natural number $n_0 \geq 1$ such that

$$\delta = \max_{i \in \widehat{E}} \sum_{j \in \widehat{E}} p_{ij}^{(n_0)} < 1\,, \qquad \text{where } \widehat{E} = \{1, \ldots, \ell - 1\}.$$

- Furthermore,

$$(\widehat{\mathbf{P}}^n)_{ij} = \sum_{i_1, \ldots, i_{n-1} \in \widehat{E}} p_{ii_1} p_{i_1 i_2} \cdots p_{i_{n-1} j} \leq \sum_{i_1, \ldots, i_{n-1} \in E} p_{ii_1} p_{i_1 i_2} \cdots p_{i_{n-1} j} = (\mathbf{P}^n)_{ij}$$

and thus $0 \leq (\widehat{\mathbf{P}}^n)_{ij} \leq (\mathbf{P}^n)_{ij} = p_{ij}^{(n)} < 1$ for all $n \geq n_0$; $i, j \in \widehat{E}$.

- Writing n as $n = kn_0 + m$ for some $k \geq 1$ and $m \in \{0, \ldots, n_0 - 1\}$ we obtain

$$\begin{aligned}
(\widehat{\mathbf{P}}^n)_{ij} &= \sum_{i_1,\ldots,i_k \in \widehat{E}} (\widehat{\mathbf{P}}^{n_0})_{ii_1} (\widehat{\mathbf{P}}^{n_0})_{i_1 i_2} \ldots (\widehat{\mathbf{P}}^{n_0})_{i_{k-1} i_k} (\widehat{\mathbf{P}}^m)_{i_k j} \\
&\leq \sum_{i_1,\ldots,i_k \in \widehat{E}} p_{ii_1}^{(n_0)} p_{i_1 i_2}^{(n_0)} \ldots p_{i_{k-1} i_k}^{(n_0)} \\
&= \sum_{i_1,\ldots,i_{k-1} \in \widehat{E}} p_{ii_1}^{(n_0)} p_{i_1 i_2}^{(n_0)} \ldots p_{i_{k-2} i_{k-1}}^{(n_0)} \Big(\sum_{i_k \in \widehat{E}} p_{i_{k-1} i_k}^{(n_0)} \Big) \\
&\leq \delta \sum_{i_1,\ldots,i_{k-1} \in \widehat{E}} p_{ii_1}^{(n_0)} p_{i_1 i_2}^{(n_0)} \ldots p_{i_{k-2} i_{k-1}}^{(n_0)} \\
&\vdots \\
&\leq \delta^k .
\end{aligned}$$

- This yields $\lim_{n\to\infty} (\widehat{\mathbf{P}}^n)_{ij} \leq \lim_{k\to\infty} \delta^k = 0$. □

Remarks

- As a consequence of Lemma 2.5 the solution $\widehat{\boldsymbol{\pi}}^\top$ of the equation (78), i.e. $\widehat{\boldsymbol{\pi}}^\top (\mathbf{I} - \widehat{\mathbf{P}}) = \mathbf{b}^\top$, is given by

$$\widehat{\boldsymbol{\pi}}^\top = \mathbf{b}^\top \sum_{n=0}^{\infty} \widehat{\mathbf{P}}^n , \tag{82}$$

  thus allowing an iterative solution of $\widehat{\boldsymbol{\pi}}^\top = (\widehat{\pi}_1, \ldots, \widehat{\pi}_{\ell-1})$.
- Notice that we start the iteration with $\mathbf{b}_0^\top = \mathbf{b}^\top$ as initial value later setting $\mathbf{b}_{n+1}^\top = \mathbf{b}_n^\top \widehat{\mathbf{P}}$ for all $n \geq 0$.
- Thus, (82) can be rewritten as

$$\widehat{\boldsymbol{\pi}}^\top = \sum_{n=0}^{\infty} \mathbf{b}_n^\top , \tag{83}$$

  and $\sum_{n=0}^{n_0} \mathbf{b}_n^\top$ can be used as an approximation for $\widehat{\boldsymbol{\pi}}^\top$ if $n_0 \geq 1$ is sufficiently large.

2.3 Reversibility; Estimates for the Rate of Convergence

2.3.1 Definition and Examples

- A stationary Markov chain $X_0, X_1, \ldots : \Omega \to E$ and its corresponding pair $(\mathbf{P}, \boldsymbol{\alpha})$ consisting of the transition matrix $\mathbf{P}$ and the stationary initial distribution $\boldsymbol{\alpha}$ is called *reversible* if its finite–dimensional distributions do not depend on the orientation of the time axis, i.e., if

$$P(X_0 = i_0, X_1 = i_1, \ldots, X_{n-1} = i_{n-1}, X_n = i_n) = P(X_n = i_0, X_{n-1} = i_1, \ldots, X_1 = i_{n-1}, X_0 = i_n) \tag{84}$$

  for arbitrary $n \geq 0$ and $i_0, \ldots, i_n \in E$.
- The reversibility of Markov chains is a particularly useful property for the construction of dynamic simulation algorithms, see Sections 3.3–3.5.

First of all we will derive a simple characterization for the reversibility of stationary (but not necessarily ergodic) Markov chains.

Theorem 2.13

- *Let $X_0, X_1, \ldots : \Omega \to E$ be a Markov chain with state space E, transition matrix $\mathbf{P} = (p_{ij})$ and stationary initial distribution $\boldsymbol{\alpha} = (\alpha_1, \alpha_2, \ldots)^\top$.*
- *The Markov chain is reversible if and only if*

$$\alpha_i \, p_{ij} = \alpha_j \, p_{ji} \qquad \text{for arbitrary } i, j \in E. \tag{85}$$

Proof

- By definition (84) the condition (85) is clearly necessary as (84) implies in particular

$$P(X_0 = i, X_1 = j) = P(X_1 = i, X_0 = j) \qquad \text{for arbitrary } i, j \in E.$$

- Therefore

$$\begin{aligned} \alpha_i \, p_{ij} &= P(X_0 = i, X_1 = j) \\ &= P(X_1 = i, X_0 = j) \\ &= \alpha_j \, p_{ji} \, . \end{aligned}$$

- Conversely, if (85) holds then the definition (3) of Markov chains yields

$$\begin{aligned} & P(X_0 = i_0, X_1 = i_1, \ldots, X_{n-1} = i_{n-1}, X_n = i_n) \\ \overset{(3)}{=} \;& \alpha_{i_0} p_{i_0 i_1} p_{i_1 i_2} \cdots p_{i_{n-1} i_n} \\ \overset{(85)}{=} \;& p_{i_1 i_0} \alpha_{i_1} p_{i_1 i_2} \cdots p_{i_{n-1} i_n} \\ & \vdots \\ \overset{(85)}{=} \;& p_{i_1 i_0} p_{i_2 i_1} \cdots p_{i_n i_{n-1}} \alpha_{i_n} \\ = \;& \alpha_{i_n} p_{i_n i_{n-1}} \cdots p_{i_2 i_1} p_{i_1 i_0} \\ \overset{(3)}{=} \;& P(X_0 = i_n, X_1 = i_{n-1}, \ldots, X_{n-1} = i_1, X_n = i_0) \\ = \;& P(X_n = i_0, X_{n-1} = i_1, \ldots, X_1 = i_{n-1}, X_0 = i_n) \, . \end{aligned}$$

- i.e., (84) holds. □

Remarks

- The proof of Theorem 2.13 does not require the stationary Markov chain $X_0, X_1, \ldots$ to be ergodic.
- In other words,
  - if the transition matrix $\mathbf{P}$ is not irreducible or not aperiodic and hence the limit distribution $\boldsymbol{\pi}$ does not exist or is not uniquely determined, respectively,
  - then Theorem 2.13 still holds if $\boldsymbol{\alpha}$ is an arbitrary stationary initial distribution.
- As $\mathbf{P} = (p_{ij})$ is a stochastic matrix, (85) implies for arbitrary $i \in E$

$$\alpha_i = \alpha_i \sum_{j \in E} p_{ij} = \sum_{j \in E} \alpha_i \, p_{ij} \overset{(85)}{=} \sum_{j \in E} \alpha_j \, p_{ji} \, .$$

- In other words: *Every* initial distribution $\boldsymbol{\alpha}$ satisfying the so-called *detailed balance condition* (85) is necessarily a stationary initial distribution, i.e. it satisfies the *global balance condition* $\boldsymbol{\alpha}^\top = \boldsymbol{\alpha}^\top \mathbf{P}$.

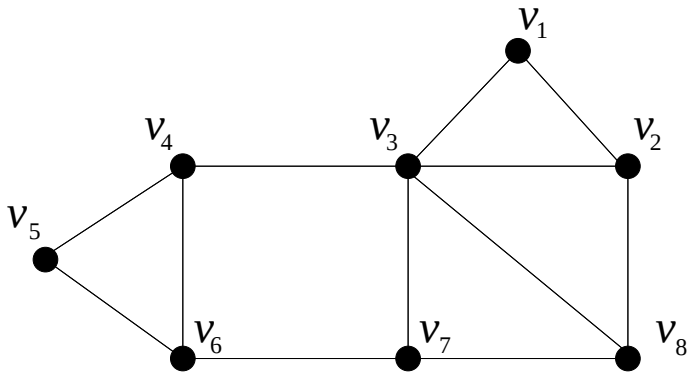


Figure 1: Connected Graph

Examples

1. *Diffusion Model*
   - We return to the diffusion model already discussed in Section 2.2.3 with the finite state space $E = \{0, 1, \ldots, \ell\}$, the irreducible (but aperiodic) transition matrix $\mathbf{P} = (p_{ij})$ where

$$p_{ij} = \begin{cases} \dfrac{\ell - i}{\ell} & \text{if } i < \ell \text{ and } j = i + 1, \\ \dfrac{i}{\ell} & \text{if } i > 0 \text{ and } j = i - 1, \\ 0 & \text{else,} \end{cases} \tag{86}$$

     and the (according to Theorem 2.10 uniquely determined but not ergodic) stationary initial distribution

$$\boldsymbol{\alpha}^\top = (\alpha_0, \ldots, \alpha_\ell)\,, \qquad \text{where} \quad \alpha_i = \frac{1}{2^\ell} \binom{\ell}{i}\,, \qquad \forall\, i \in \{0, 1, \ldots, \ell\}\,. \tag{87}$$

   - One can easily see that

$$\alpha_i\, p_{ij} = \alpha_j\, p_{ji}$$

     for arbitrary $i, j \in E$, i.e., the pair $(\mathbf{P}, \boldsymbol{\alpha})$ given by (86) and (87) is reversible.

2. *Birth and Death Processes*
   - For the birth and death processes with two reflecting barriers considered in Section 2.2.3 let the transition matrix $\mathbf{P} = (p_{ij})$ be of such a form that the equation $\boldsymbol{\alpha}^\top = \boldsymbol{\alpha}^\top \mathbf{P}$ has a uniquely determined probability solution $\boldsymbol{\alpha}^\top = (\alpha_1, \alpha_2, \ldots)$.
   - For this situation one can show that

$$\alpha_i\, p_{ij} = \alpha_j\, p_{ji} \qquad \forall\, i, j \in E\,.$$

3. *Random Walks on Graphs*
   - We consider a connected graph $G = (V, K)$
     - with the set $V = \{v_1, \ldots, v_\ell\}$ of ℓ vertices and the set K of edges, each of them connecting two vertices
     - such that for every pair $v_i, v_j \in V$ of vertices there is a path of edges in K connecting v_i and v_j.
   - We say that two vertices v_i and v_j are *neighbors* if there is an edge connecting them, i.e., an edge having both of them as endpoints, where d_i denotes the number of neighbors of v_i.

- A random walk on the graph $G = (V, K)$ is a Markov chain $X_0, X_1, \ldots : \Omega \to E$ with state space $E = \{1, \ldots, \ell\}$ and transition matrix $\mathbf{P} = (p_{ij})$, where

$$p_{ij} = \begin{cases} \dfrac{1}{d_i} & \text{if the vertices } v_i \text{ and } v_j \text{ are neighbors,} \\ 0 & \text{else.} \end{cases} \tag{88}$$

- Figure 1 shows such a graph $G = (V, K)$ where the set $V = \{v_1, \ldots, v_8\}$ contains 8 vertices and the set K consists of 12 edges. More precisely

$$\begin{aligned} K \;=\; & \big\{(v_1, v_2), (v_1, v_3), (v_2, v_3), (v_2, v_8), (v_3, v_4), (v_3, v_7), (v_3, v_8), (v_4, v_5), (v_4, v_6), (v_5, v_6), \\ & (v_6, v_7), (v_7, v_8)\big\}. \end{aligned}$$

- One can show that
  - the transition matrix given by (88) is irreducible,
  - the (according to Theorem 2.10 uniquely determined) stationary initial distribution $\boldsymbol{\alpha}$ is given by

$$\boldsymbol{\alpha} = \Big(\frac{d_1}{d}, \ldots, \frac{d_\ell}{d}\Big)^\top, \qquad \text{where } d = \sum_{i=1}^{\ell} d_i, \tag{89}$$

  - the pair $(\mathbf{P}, \boldsymbol{\alpha})$ given by (88)–(89) is reversible as for arbitrary $i, j \in \{1, \ldots, \ell\}$

$$\alpha_i\, p_{ij} = \begin{cases} \dfrac{d_i}{d}\dfrac{1}{d_i} = \dfrac{1}{d} = \dfrac{d_j}{d}\dfrac{1}{d_j} = \alpha_j\, p_{ji} & \text{if the vertices } v_i \text{ and } v_j \text{ are neighbors,} \\ 0 = \alpha_j\, p_{ji} & \text{else.} \end{cases}$$

- The transition matrix $\mathbf{P}$ given by (88) for the numerical example defined in Figure 1 is not only irreducible but also aperiodic and the stationary initial distribution $\boldsymbol{\alpha}$ ($= \boldsymbol{\pi} = \lim_{n\to\infty} \boldsymbol{\alpha}_n$) is given by

$$\boldsymbol{\alpha} = \Big(\frac{2}{24}, \frac{3}{24}, \frac{5}{24}, \frac{3}{24}, \frac{2}{24}, \frac{3}{24}, \frac{3}{24}, \frac{3}{24}\Big)^\top.$$

4. *Cyclic Random Walks*

- The following example of a cyclic random walk is *not* reversible.
  - Let $E = \{1, 2, 3, 4\}$ and

$$\mathbf{P} = \begin{pmatrix} 0 & 0.75 & 0 & 0.25 \\ 0.25 & 0 & 0.75 & 0 \\ 0 & 0.25 & 0 & 0.75 \\ 0.75 & 0 & 0.25 & 0 \end{pmatrix} \tag{90}$$

  - i.e., the transition graph is given by Figure 2.
- The transition matrix (90) is obviously irreducible, but not aperiodic, and the initial distribution $\boldsymbol{\alpha}$ (which is uniquely determined by Theorem 2.10) is given by $\boldsymbol{\alpha} = (1/4, 1/4, 1/4, 1/4)^\top$.
- However,

$$\alpha_1 p_{12} = \frac{1}{4}\,\frac{3}{4} = \frac{3}{16} > \frac{1}{16} = \frac{1}{4}\,\frac{1}{4} = \alpha_2 p_{21}\,.$$

- It is intuitively plausible that this cyclic random work is *not* reversible as clockwise steps are much more likely than counterclockwise movements.

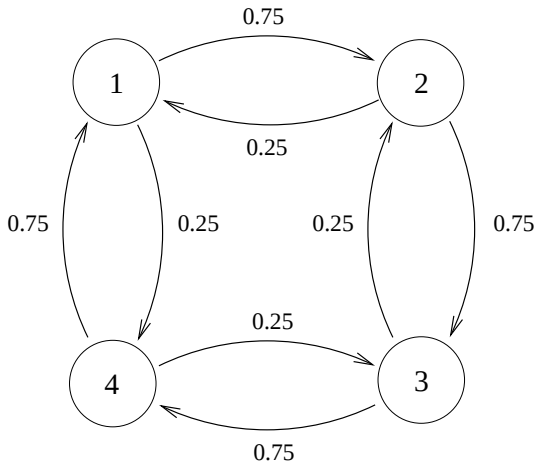


Figure 2: Transition Graph

5. *Doubly–Stochastic Transition Matrix*

   - Finally we consider the following example of a transition matrix $\mathbf{P} = (p_{ij})$ and a stationary initial distribution $\boldsymbol{\alpha} = (\alpha_1, \ldots, \alpha_\ell)^\top$ which are *not* reversible: For $a, b > 0$ such that $b < a$ and $2a+b = 1$ let

$$\mathbf{P} = \begin{pmatrix} a & a-b & 2b \\ a+b & b & a-b \\ 0 & a+b & a \end{pmatrix} . \tag{91}$$

   - This transition matrix $\mathbf{P}$ is *doubly–stochastic*, i.e., the transposed matrix $\mathbf{P}^\top$ is also a stochastic matrix and $\mathbf{P}$ is obviously quasi–positive.
   - The (uniquely determined) stationary initial distribution $\boldsymbol{\pi} = \lim_{n\to\infty} \boldsymbol{\alpha}_n$ is given by

$$\boldsymbol{\pi} = (1/3, 1/3, 1/3)^\top .$$

   - As the transition matrix $\mathbf{P}$ in (91) is not symmetric the pair $(\mathbf{P}, \boldsymbol{\pi})$ is not reversible.

2.3.2 Recursive Construction of the „Past"

- Recall that
  - in Section 2.1.3 we showed that a stationary Markov chain $X_0, X_1, \ldots$ with transition matrix $\mathbf{P} = (p_{ij})$ and stationary initial distribution $\boldsymbol{\alpha} = (\alpha_1, \ldots, \alpha_\ell)^\top$ can be constructed as follows, where
  - we started with a sequence $Z_0, Z_1, \ldots$ of independent and on $[0, 1]$ uniformly distributed random variables and defined

$$X_0 = k \qquad \text{if and only if} \qquad Z_0 \in \Big(\sum_{i=1}^{k-1} \alpha_i, \sum_{i=1}^{k} \alpha_i\Big] ,$$

  for all $k = 1, \ldots, \ell$, i.e.

$$X_0 = \sum_{k=1}^{\ell} k \mathbb{1}\Big(\sum_{i=1}^{k-1} \alpha_i < Z_0 \le \sum_{i=1}^{k} \alpha_i\Big) . \tag{92}$$

– The random variables $X_1, X_2, \ldots$ were defined by the recursion formula

$$X_n = \varphi(X_{n-1}, Z_n) \qquad \text{for } n = 1, 2, \ldots, \tag{93}$$

where the function $\varphi : E \times [0,1] \to E$ was given by

$$\varphi(i,z) = \sum_{k=1}^{\ell} k \mathbb{1}\Big(\sum_{j=1}^{k-1} p_{ij} < z \leq \sum_{j=1}^{k} p_{ij} \Big) . \tag{94}$$

- If the pair $(\mathbf{P}, \boldsymbol{\alpha})$ is reversible, then the stationary Markov chain $X_0, X_1, \ldots$ constructed in (92)–(94) can be tracked back into the past in the following way.
  - First of all we extend the sequence $Z_0, Z_1, \ldots$ of independent and on $[0,1]$ uniformly distributed random variables to a sequence $\ldots, Z_{-1}, Z_0, Z_1, \ldots$ of independent and identically random variables that is unbounded in both directions.
  - Note that due to the assumed independence of $\ldots, Z_{-1}, Z_0, Z_1, \ldots$ this expansion does not pose any problems as the underlying probability space can be constructed via an appropriate product space, product–σ–algebra, and product measure.
  - The random variables $X_{-1}, X_{-2}, \ldots$ are now constructed recursively setting

$$X_{n-1} = \varphi(X_n, Z_{n-1}) \qquad \text{for } n = 0, -1, \ldots, \tag{95}$$

where the function $\varphi : E \times [0,1] \to E$ is defined in (94).

Theorem 2.14

- *Let $X_0, X_1, \ldots : \Omega \to E$ be a reversible Markov chain with state space E, transition matrix $\mathbf{P} = (p_{ij})$ and stationary initial distribution $\boldsymbol{\alpha} = (\alpha_1, \ldots, \alpha_\ell)^\top$.*
- *Then the sequence $\ldots, X_{-1}, X_0, X_1, \ldots : \Omega \to E$ defined by (92)–(95) is*
  - *a stationary Markov chain with transition matrix $\mathbf{P}$ and the one–dimensional marginal distribution $\boldsymbol{\alpha}$,*
  - *i.e., for arbitrary $k \in \mathbb{Z} = \{\ldots, -1, 0, 1, \ldots\}$, $i_k, i_{k+1}, \ldots, i_n \in E$ and $m \geq 1$*

$$\begin{aligned} & P(X_k = i_k, X_{k+1} = i_{k+1}, \ldots, X_{n-1} = i_{n-1}, X_n = i_n) \\ &= P(X_{k+m} = i_k, X_{k+m+1} = i_{k+1}, \ldots, X_{n+m-1} = i_{n-1}, X_{n+m} = i_n) \\ &= \alpha_{i_k} p_{i_k i_{k+1}} \cdots p_{i_{n-1} i_n} . \end{aligned}$$

The *proof* of Theorem 2.14 is quite similar to the ones given for Theorems 2.11 and 2.13 and is therefore omitted.

2.3.3 Determining the Rate of Convergence under Reversibility

- Let $E = \{1, \ldots, \ell\}$ and $\mathbf{P}$ be a quasi-positive (i.e. an irreducible and aperiodic) transition matrix.
  - In case the eigenvalues $\theta_1, \ldots, \theta_\ell$ of $\mathbf{P}$ are pairwise distinct we showed by the Perron–Frobenius–Theorem (see Corollary 2.4) that

$$\max_{j \in E} |\alpha_{nj} - \pi_j| = O(|\theta_2|^n) , \tag{96}$$

where $\boldsymbol{\pi} = (\pi_1, \ldots, \pi_\ell)^\top$ is the (uniquely determined) solution of the equation $\boldsymbol{\pi}^\top = \boldsymbol{\pi}^\top \mathbf{P}$.
  - If $(\mathbf{P}, \boldsymbol{\pi})$ is also reversible one can show that the basis $|\theta_2|$ considered in (96) cannot be improved.

- Let $(\mathbf{P}, \boldsymbol{\pi})$ be reversible, where $\mathbf{P}$ is an irreducible and aperiodic transition matrix.
  - In this case the detailed balance condition (85) implies the symmetry of the matrix $\mathbf{DPD}^{-1}$ where $\mathbf{D} = \operatorname{diag}(\sqrt{\pi_i})$.
  - As the eigenvalues $\theta_1, \dots, \theta_\ell$ of $\mathbf{P}$ coincide with the eigenvalues of $\mathbf{DPD}^{-1}$ we obtain $\theta_i \in \mathbb{R}$ for all $i \in E$,
  - and the right eigenvectors $\boldsymbol{\phi}_1^*, \dots, \boldsymbol{\phi}_\ell^*$ of $\mathbf{DPD}^{-1}$ can be chosen such that all of their components are real,
  - that furthermore $\boldsymbol{\phi}_1^*, \dots, \boldsymbol{\phi}_\ell^*$ are also left eigenvectors of $\mathbf{DPD}^{-1}$ and that the rows as well as the lines of the $\ell \times \ell$ matrix $(\boldsymbol{\phi}_1^*, \dots, \boldsymbol{\phi}_\ell^*)$ are orthonormal vectors.
- The spectral representation (30) of $\mathbf{A} = \mathbf{DPD}^{-1}$ yields for every $n \geq 1$

$$\mathbf{P}^n = \big(\mathbf{D}^{-1}\mathbf{AD}\big)^n = \mathbf{D}^{-1}\mathbf{A}^n\mathbf{D} = \sum_{k=1}^{\ell} \theta_k^n \mathbf{D}^{-1}\boldsymbol{\phi}_k^*(\boldsymbol{\phi}_k^*)^\top \mathbf{D}\,.$$

  - By plugging in $\theta_1 = 1$ and $\boldsymbol{\phi}_1^* = (\sqrt{\pi_1}, \dots, \sqrt{\pi_\ell})^\top$ we obtain for arbitrary $i, j \in E$

$$p_{ij}^{(n)} = \pi_j + \sqrt{\frac{\pi_j}{\pi_i}} \sum_{k=2}^{\ell} \theta_k^n \phi_{ki}^* \phi_{kj}^*\,, \qquad \text{where } \boldsymbol{\phi}_k^* = (\phi_{k1}^*, \dots, \phi_{k\ell}^*)^\top. \tag{97}$$

  - If n is even or all eigenvalues $\theta_2, \dots, \theta_\ell$ are nonnegative, then

$$\sup_{\boldsymbol{\alpha}_0} \max_{j \in E} |\alpha_{nj} - \pi_j| \geq \max_{j \in E} \big| p_{jj}^{(n)} - \pi_j \big| = \max_{j \in E} \Big| \sum_{k=2}^{\ell} \theta_k^n (\phi_{kj}^*)^2 \Big| \geq \theta_2^n \max_{j \in E} (\phi_{2j}^*)^2\,.$$

- This shows that $|\theta_2|$ is the smallest positive number such that the estimate for the rate of convergence considered in (96) holds uniformly for all initial distributions $\boldsymbol{\alpha}_0$.

Remarks

- Notice that (97) yields the following more precise specification of the convergence estimate (96). We have

$$\big| p_{ij}^{(n)} - \pi_j \big| \leq \frac{1}{\sqrt{\min_{i \in E} \pi_i}} \sum_{k=2}^{\ell} |\theta_k|^n |\phi_{ki}^*||\phi_{kj}^*| \leq \frac{\sum_{k=2}^{\ell} |\phi_{ki}^*||\phi_{kj}^*|}{\sqrt{\min_{i \in E} \pi_i}}\, |\theta_2|^n \leq \frac{1}{\sqrt{\min_{i \in E} \pi_i}}\, |\theta_2|^n\,,$$

  as the column vectors $\boldsymbol{\phi}_1^*, \dots, \boldsymbol{\phi}_\ell^*$ and hence also the row vectors $(\phi_{1,j}, \dots, \phi_{\ell,j})$ where $j = 1, \dots, \ell$ form an orthonormal basis in $\mathbb{R}^\ell$ and thus by the Cauchy–Schwarz inequality

$$\sum_{k=2}^{\ell} |\phi_{ki}^*||\phi_{kj}^*| \leq \Big(\sum_{k=1}^{\ell} (\phi_{ki}^*)^2 \Big)^{1/2} \Big(\sum_{k=1}^{\ell} (\phi_{kj}^*)^2 \Big)^{1/2} = 1\,.$$

- Consequently,

$$\max_{j \in E} |\alpha_{nj} - \pi_j| \leq \frac{1}{\sqrt{\min_{i \in E} \pi_i}}\, |\theta_2|^n\,. \tag{98}$$

- However, the practical benefit of the estimate (98) can be limited for several reasons:
  - The factor in front of $|\theta_2|^n$ in (98) does not depend on the choice of the initial distribution $\boldsymbol{\alpha}_0$.

  - The derivation of the estimate (98) requires the Markov chain to be reversible.
  - It can be difficult to determine the eigenvalue θ_2 if the number of states is large.

- Therefore in Section 2.3.5 we consider an *alternative convergence estimate*,
  - which depends on the initial distribution
  - and does not require the reversibility of the Markov chain.
  - Furthermore, in Section 2.3.7 we will derive an upper bound for the second largest absolute value $|\theta_2|$ among the eigenvalues of a reversible transition matrix.

2.3.4 Multiplicative Reversible Version of the Transition Matrix; Spectral Representation

At first we will discuss a method enabling us to transform (ergodic) transition matrices such that the resulting matrix is reversible.

- Let $\mathbf{P} = (p_{ij})$ be an irreducible and aperiodic (but not necessarily reversible) transition matrix and let $\boldsymbol{\pi} = (\pi_1, \ldots, \pi_\ell)^\top$ be the corresponding stationary initial distribution such that $\pi_i > 0$ for all $i \in E$.
- Moreover, we consider the stochastic matrix $\widetilde{\mathbf{P}} = (\widetilde{p}_{ij})$ where

$$\widetilde{p}_{ij} = \frac{\pi_j p_{ji}}{\pi_i} \,, \tag{99}$$

  i.e., $\widetilde{\mathbf{P}} = \mathbf{D}^{-2}\mathbf{P}^\top\mathbf{D}^2$ where $\mathbf{D} = \operatorname{diag}(\sqrt{\pi_i})$ is also an irreducible and aperiodic transition matrix having the same stationary initial distribution $\boldsymbol{\pi} = (\pi_1, \ldots, \pi_\ell)^\top$.
- The pair $(\mathbf{M}, \boldsymbol{\pi})$, where the stochastic matrix $\mathbf{M} = (m_{ij})$ is given by $\mathbf{M} = \mathbf{P}\widetilde{\mathbf{P}}$, is reversible as we observe

$$\pi_i m_{ij} = \pi_i \sum_{k=1}^{\ell} p_{ik} \, \frac{\pi_j p_{jk}}{\pi_k} = \pi_j \sum_{k=1}^{\ell} p_{jk} \, \frac{\pi_i p_{ik}}{\pi_k} = \pi_j m_{ji} \,.$$

Definition The matrix $\mathbf{M} = \mathbf{P}\widetilde{\mathbf{P}}$ is called the *multiplicative reversible* version of the transition matrix $\mathbf{P}$.

Remarks

- All eigenvalues $\theta_{\mathbf{M},1}, \ldots, \theta_{\mathbf{M},\ell}$ of $\mathbf{M}$ are real and in $[0,1]$ because $\mathbf{M}$ has the same eigenvalues as the symmetric and nonnegative definite matrix $\mathbf{M}^* = \mathbf{D}\mathbf{M}\mathbf{D}^{-1}$, where

$$m^*_{ij} = \frac{\sqrt{\pi_i}}{\sqrt{\pi_j}} \, m_{ij} = \frac{\sqrt{\pi_i}}{\sqrt{\pi_j}} \sum_{k=1}^{\ell} p_{ik} \, \frac{\pi_j p_{jk}}{\pi_k} = \sum_{k=1}^{\ell} \Big(\frac{\sqrt{\pi_i}}{\sqrt{\pi_k}} \, p_{ik} \Big) \Big(\frac{\sqrt{\pi_j}}{\sqrt{\pi_k}} \, p_{jk} \Big)$$

  and hence

$$\mathbf{M}^* = \mathbf{D}\mathbf{M}\mathbf{D}^{-1} = \big(\mathbf{D}\mathbf{P}\mathbf{D}^{-1}\big)\big(\mathbf{D}\mathbf{P}\mathbf{D}^{-1}\big)^\top .$$

- As a consequence, the symmetric matrix $\mathbf{M}^*$ is diagonalizable and the right and left eigenvectors $\boldsymbol{\phi}^*_i$ and $\boldsymbol{\psi}^*_i$ can be chosen such that
  - $\boldsymbol{\phi}^*_i = \boldsymbol{\psi}^*_i$ for all $i \in E$
  - the vectors $\boldsymbol{\phi}^*_1, \ldots, \boldsymbol{\phi}^*_\ell$ are an orthonormal basis in $\mathbb{R}^\ell$.

- Then $\boldsymbol{\phi}_1, \ldots, \boldsymbol{\phi}_\ell$ and $\boldsymbol{\psi}_1, \ldots, \boldsymbol{\psi}_\ell$, where

$$\boldsymbol{\phi}_i = \mathbf{D}^{-1}\boldsymbol{\phi}_i^* \qquad \text{and} \qquad \boldsymbol{\psi}_i = \mathbf{D}\boldsymbol{\psi}_i^*\,, \qquad \forall\, i \in E\,, \tag{100}$$

  are right and left eigenvectors of $\mathbf{M}$, respectively, as for every $i \in E$

$$\mathbf{M}\boldsymbol{\phi}_i = \mathbf{M}\mathbf{D}^{-1}\boldsymbol{\phi}_i^* = \mathbf{D}^{-1}\mathbf{D}\mathbf{M}\mathbf{D}^{-1}\boldsymbol{\phi}_i^* = \mathbf{D}^{-1}\theta_{\mathbf{M},i}\boldsymbol{\phi}_i^* = \theta_{\mathbf{M},i}\boldsymbol{\phi}_i$$

  and

$$\boldsymbol{\psi}_i^\top\mathbf{M} = \big(\mathbf{D}\boldsymbol{\psi}_i^*\big)^\top\mathbf{M} = (\boldsymbol{\psi}_i^*)^\top\mathbf{D}\mathbf{M}\mathbf{D}^{-1}\mathbf{D} = \theta_{\mathbf{M},i}(\boldsymbol{\psi}_i^*)^\top\mathbf{D} = \theta_{\mathbf{M},i}\boldsymbol{\psi}_i^\top\,.$$

This yields the following *spectral representation* of the multiplicative reversible version $\mathbf{M}$ obtained from the transition matrix $\mathbf{P}$; see also the spectral representation given by formula (30).

Theorem 2.15 *For arbitrary $n \in \mathbb{N}$ and $\mathbf{x} \in \mathbb{R}^\ell$*

$$\mathbf{M}^n\mathbf{x} = \sum_{i=1}^{\ell} \theta_{\mathbf{M},i}^n \boldsymbol{\phi}_i\boldsymbol{\psi}_i^\top\mathbf{x}\,. \tag{101}$$

where $\boldsymbol{\phi}_i$ and $\boldsymbol{\psi}_i$ are the right and left eigenvectors of $\mathbf{M}$ defined in (100).

Proof

- As the (right) eigenvectors $\boldsymbol{\phi}_1, \ldots, \boldsymbol{\phi}_\ell$ of $\mathbf{M}$ defined in (100) are also a basis in $\mathbb{R}^\ell$, for every $\mathbf{x} \in \mathbb{R}^\ell$ there is a (uniquely determined) vector $\big(x_1^{(\mathrm{r})}, \ldots, x_\ell^{(\mathrm{r})}\big)^\top \in \mathbb{R}^\ell$ such that

$$\mathbf{x} = \sum_{i=1}^{\ell} x_i^{(\mathrm{r})}\boldsymbol{\phi}_i\,.$$

- Furthermore, we have $\mathbf{M}\boldsymbol{\phi}_i = \theta_{\mathbf{M},i}\boldsymbol{\phi}_i$ and hence $\mathbf{M}^n\boldsymbol{\phi}_i = \theta_{\mathbf{M},i}^n\boldsymbol{\phi}_i$ for arbitrary $i \in E$ and $n \in \mathbb{N}$.
- Thus we obtain

$$\mathbf{M}^n\mathbf{x} = \sum_{i=1}^{\ell} x_i^{(\mathrm{r})}\mathbf{M}^n\boldsymbol{\phi}_i = \sum_{i=1}^{\ell} x_i^{(\mathrm{r})}\theta_{\mathbf{M},i}^n\boldsymbol{\phi}_i\,.$$

- On the other hand, (100) implies for arbitrary $i \in E$ and $\mathbf{x} \in \mathbb{R}^\ell$

$$\boldsymbol{\psi}_i^\top\mathbf{x} = \big(\mathbf{D}\boldsymbol{\psi}_i^*\big)^\top\mathbf{x} = \big(\boldsymbol{\psi}_i^*\big)^\top\sum_{j=1}^{\ell} x_j^{(\mathrm{r})}\mathbf{D}\boldsymbol{\phi}_j = \big(\boldsymbol{\psi}_i^*\big)^\top\sum_{j=1}^{\ell} x_j^{(\mathrm{r})}\boldsymbol{\phi}_j^* = \sum_{j=1}^{\ell} x_j^{(\mathrm{r})}\big(\boldsymbol{\psi}_i^*\big)^\top\boldsymbol{\phi}_j^* = x_i^{(\mathrm{r})}\,, \tag{102}$$

  where the last equality takes into account that $\boldsymbol{\psi}_i^* = \boldsymbol{\phi}_i^*$ for all $i \in E$ and that the eigenvectors $\boldsymbol{\phi}_1^*, \ldots, \boldsymbol{\phi}_\ell^*$ von $\mathbf{M}^*$ are an orthonormal basis of $\mathbb{R}^\ell$.
- This proves the spectral representation (101). □

2.3.5 Alternative Estimate for the Rate of Convergence; χ^2-Contrast

Based on the multiplicative reversible version $\mathbf{M} = \mathbf{P}\widetilde{\mathbf{P}}$ of the ergodic (but not necessarily reversible) transition matrix $\mathbf{P}$ we will now deduce an alternative estimate for the rate of convergence $\boldsymbol{\alpha}^\top\mathbf{P}^n \to \boldsymbol{\pi}^\top$ for $n \to \infty$; see Theorem 2.16.

The following abbreviations and lemmata will turn out to be useful in the proof of Theorem 2.16.

- Let $\mathcal{L}(E)$ denote the family of all functions
  - defined on E and mapping into the real line $\mathbb{R}$
  - and let $\boldsymbol{\pi} = (\pi_1, \ldots, \pi_\ell)^\top$ be an arbitrary positive probability function from $\mathcal{L}(E)$, i.e. $\pi_i > 0$ for all $i \in E$ and $\sum_{i=1}^{\ell} \pi_i = 1$.
- For arbitrary vectors $\mathbf{x} = (x_1, \ldots, x_\ell)^\top \in \mathcal{L}(E)$ and $\mathbf{y} = (y_1, \ldots, y_\ell)^\top \in \mathcal{L}(E)$ we denote by $(\mathbf{x}, \mathbf{y})_{\boldsymbol{\pi}}$ the *inner product*

$$(\mathbf{x}, \mathbf{y})_{\boldsymbol{\pi}} = \sum_{i=1}^{\ell} x_i y_i \pi_i \tag{103}$$

and by $\|\mathbf{x}\|_{\boldsymbol{\pi}}$ the induced norm, i.e.,

$$\|\mathbf{x}\|_{\boldsymbol{\pi}} = \sqrt{\sum_{i=1}^{\ell} x_i^2 \pi_i}\,.$$

- The terms ($\boldsymbol{\pi}$–weighted) *mean* $(\mathbf{x})_{\boldsymbol{\pi}}$ and *variance* $\mathrm{Var}_{\,\pi}(\mathbf{x})$ of $\mathbf{x} \in \mathcal{L}(E)$ will be used to denote the quantities

$$(\mathbf{x})_{\boldsymbol{\pi}} = \sum_{i=1}^{\ell} x_i \pi_i \qquad \Big(= (\mathbf{x}, \mathbf{e})_{\boldsymbol{\pi}}\Big) \tag{104}$$

and

$$\mathrm{Var}_{\,\pi}(\mathbf{x}) = \|\mathbf{x}\|_{\boldsymbol{\pi}}^2 - (\mathbf{x})_{\boldsymbol{\pi}}^2\,, \tag{105}$$

respectively.

Lemma 2.6 *For all $\mathbf{x} \in \mathcal{L}(E)$, it holds that*

$$\mathrm{Var}_{\,\boldsymbol{\pi}}(\mathbf{x}) = \mathrm{Var}_{\,\boldsymbol{\pi}}(\widetilde{\mathbf{P}}\mathbf{x}) + \big((\mathbf{I} - \mathbf{M})\mathbf{x}, \mathbf{x}\big)_{\boldsymbol{\pi}}\,. \tag{106}$$

Proof

- Introducing the notation $\widehat{\mathbf{x}} = \mathbf{x} - (\mathbf{x})_{\boldsymbol{\pi}}\mathbf{e}$ we obtain that $(\widehat{\mathbf{x}})_{\boldsymbol{\pi}} = 0$ and

$$(\widetilde{\mathbf{P}}\widehat{\mathbf{x}})_{\boldsymbol{\pi}} = \sum_{i=1}^{\ell}\Big(\sum_{j=1}^{\ell} \widetilde{p}_{ij}\big(x_j - (\mathbf{x})_{\boldsymbol{\pi}}\big)\Big)\pi_i = \sum_{i,j=1}^{\ell} \widetilde{p}_{ij} x_j \pi_i - (\mathbf{x})_{\boldsymbol{\pi}} = \sum_{i,j=1}^{\ell} \pi_j p_{ji} x_j - (\mathbf{x})_{\boldsymbol{\pi}} = 0\,,$$

  where the last but one equality follows from the definition (99) of the matrix $\widetilde{\mathbf{P}}$.
- This implies

$$\|\widehat{\mathbf{x}}\|_{\boldsymbol{\pi}}^2 = \mathrm{Var}_{\,\boldsymbol{\pi}}(\widehat{\mathbf{x}}) = \mathrm{Var}_{\,\boldsymbol{\pi}}(\mathbf{x}) \qquad \text{and} \qquad \|\widetilde{\mathbf{P}}\widehat{\mathbf{x}}\|_{\boldsymbol{\pi}}^2 = \mathrm{Var}_{\,\boldsymbol{\pi}}(\widetilde{\mathbf{P}}\widehat{\mathbf{x}}) = \mathrm{Var}_{\,\boldsymbol{\pi}}(\widetilde{\mathbf{P}}\mathbf{x})\,. \tag{107}$$

- On the other hand

$$\begin{aligned}
\|\widetilde{\mathbf{P}}\widehat{\mathbf{x}}\|_{\boldsymbol{\pi}}^2 &= \big(\widetilde{\mathbf{P}}\widehat{\mathbf{x}}, \widetilde{\mathbf{P}}\widehat{\mathbf{x}}\big)_{\boldsymbol{\pi}} = \sum_{i=1}^{\ell}\Big(\sum_{k=1}^{\ell} \widetilde{p}_{ik}\widehat{\mathbf{x}}_k\Big)^2 \pi_i \\
&= \sum_{i=1}^{\ell}\sum_{j,k=1}^{\ell} \widetilde{p}_{ij} \underbrace{\widetilde{p}_{ik}}_{=\frac{\pi_k p_{ki}}{\pi_i}} \widehat{\mathbf{x}}_j \widehat{\mathbf{x}}_k \pi_i \\
&= \sum_{k=1}^{\ell} \underbrace{\sum_{j=1}^{\ell} (\mathbf{P}\widetilde{\mathbf{P}})_{kj}\widehat{\mathbf{x}}_j}_{=(\mathbf{P}\widetilde{\mathbf{P}}\mathbf{x})_k} \widehat{\mathbf{x}}_k \pi_k \\
&= \big(\mathbf{P}\widetilde{\mathbf{P}}\widehat{\mathbf{x}}, \widehat{\mathbf{x}}\big)_{\boldsymbol{\pi}} = \big(\mathbf{M}\widehat{\mathbf{x}}, \widehat{\mathbf{x}}\big)_{\boldsymbol{\pi}}
\end{aligned}$$

and thus

$$\|\widehat{\mathbf{x}}\|_{\boldsymbol{\pi}}^2 - \|\widetilde{\mathbf{P}}\widehat{\mathbf{x}}\|_{\boldsymbol{\pi}}^2 = \|\widehat{\mathbf{x}}\|_{\boldsymbol{\pi}}^2 - \big(\mathbf{M}\widehat{\mathbf{x}}, \widehat{\mathbf{x}}\big)_{\boldsymbol{\pi}} = \big((\mathbf{I}-\mathbf{M})\widehat{\mathbf{x}}, \widehat{\mathbf{x}}\big)_{\boldsymbol{\pi}} = \big((\mathbf{I}-\mathbf{M})\mathbf{x}, \mathbf{x}\big)_{\boldsymbol{\pi}}\,,$$

as $\mathbf{M}$ is a stochastic matrix such that $\boldsymbol{\pi}^\top\mathbf{M} = \boldsymbol{\pi}^\top$ and therefore $(\mathbf{I}-\mathbf{M})\mathbf{e} = \mathbf{0}$ and

$$\big((\mathbf{I}-\mathbf{M})\mathbf{x},\, \mathbf{e}\big)_{\boldsymbol{\pi}} = \sum_{i,j=1}^{\ell} \big(\delta_j(i) - m_{ij}\big)x_j\pi_i = \sum_{i=1}^{\ell} x_i\pi_i - \sum_{j=1}^{\ell} x_j \underbrace{\sum_{i=1}^{\ell} \pi_i m_{ij}}_{=\pi_j} = 0\,.$$

- Taking into account (107) this shows the validity of (106). □

We introduce the following notions.

- Let $E = \{1, \ldots, \ell\}$, let $\boldsymbol{\alpha} = (\alpha_1, \ldots, \alpha_\ell)^\top$ and $\boldsymbol{\beta} = (\beta_1, \ldots, \beta_\ell)^\top$ be arbitrary probability distributions on E, and let

$$d_{\mathrm{TV}}(\boldsymbol{\alpha}, \boldsymbol{\beta}) = \frac{1}{2}\,\sum_{i\in E} |\alpha_i - \beta_i|\,, \tag{108}$$

  i.e., the distance $d_{\mathrm{TV}}(\boldsymbol{\alpha}, \boldsymbol{\beta})$ between $\boldsymbol{\alpha}$ and $\boldsymbol{\beta}$ is expressed via the *total variation*

$$|\boldsymbol{\alpha} - \boldsymbol{\beta}| = \sum_{i\in E} |\alpha_i - \beta_i| \tag{109}$$

  of the „signed measure" $\boldsymbol{\alpha} - \boldsymbol{\beta}$.

- If $\beta_i > 0$ for all $i \in E$ we also consider the term

$$\chi^2(\boldsymbol{\alpha}; \boldsymbol{\beta}) = \sum_{i\in E} \frac{(\alpha_i - \beta_i)^2}{\beta_i} \tag{110}$$

  which is called the χ^2–*contrast* of $\boldsymbol{\alpha}$ with respect to $\boldsymbol{\beta}$.

The distance $d_{\mathrm{TV}}(\boldsymbol{\alpha}, \boldsymbol{\beta})$ between $\boldsymbol{\alpha}$ and $\boldsymbol{\beta}$ can be estimated via the χ^2–contrast $\chi^2(\boldsymbol{\alpha}; \boldsymbol{\beta})$ of $\boldsymbol{\alpha}$ with respect to $\boldsymbol{\beta}$ as follows.

Lemma 2.7 *If $\beta_i > 0$ for all $i \in E$, then*

$$d_{\mathrm{TV}}^2(\boldsymbol{\alpha}, \boldsymbol{\beta}) \le \frac{1}{4}\,\chi^2(\boldsymbol{\alpha}; \boldsymbol{\beta})\,. \tag{111}$$

Proof

- Taking into account that $\sum_{i\in E} \beta_i = 1$, an application of the Cauchy–Schwarz inequality yields

$$\Big(\sum_{i\in E} |\alpha_i - \beta_i|\Big)^2 = \Big(\sum_{i\in E} \frac{1}{\sqrt{\beta_i}}|\alpha_i - \beta_i|\,\sqrt{\beta_i}\Big)^2 \le \sum_{i\in E} \frac{1}{\beta_i}\,(\alpha_i - \beta_i)^2\,.$$

- This implies the assertion of the lemma. □

The rate of convergence $\boldsymbol{\alpha}^\top\mathbf{P}^n \to \boldsymbol{\pi}^\top$ for $n \to \infty$ can now be estimated based on

- the second largest eigenvalue $\theta_{\mathbf{M},2}$ of the multiplicative reversible version $\mathbf{M} = \mathbf{P}\widetilde{\mathbf{P}}$ of the (ergodic) transition matrix $\mathbf{P}$
- and the χ^2 contrast $\chi^2(\boldsymbol{\alpha};\boldsymbol{\pi})$ of the initial distribution $\boldsymbol{\alpha}$ with respect to the stationary limit distribution $\boldsymbol{\pi}$.

Theorem 2.16 *For any initial distribution $\boldsymbol{\alpha}$ and for all $n \in \mathbb{N}$,*

$$d_{\mathrm{TV}}^2\big((\boldsymbol{\alpha}^\top \mathbf{P}^n)^\top, \boldsymbol{\pi}\big) \le \frac{\chi^2(\boldsymbol{\alpha};\boldsymbol{\pi})}{4}\ \theta_{\mathbf{M},2}^n\,. \tag{112}$$

Proof

- Let $\boldsymbol{\rho}_n = (\rho_{n1},\dots,\rho_{n\ell})^\top$ where $\rho_{ni} = (\boldsymbol{\alpha}^\top \mathbf{P}^n)_i/\pi_i$.
  - Then for all $i \in E$
  $$\sum_{k=1}^{\ell} \frac{\pi_k p_{ki}}{\pi_i}\,\frac{(\boldsymbol{\alpha}^\top \mathbf{P}^n)_k}{\pi_k} \;=\; \frac{(\boldsymbol{\alpha}^\top \mathbf{P}^{n+1})_i}{\pi_i}$$
  and thus
  $$\widetilde{\mathbf{P}}\boldsymbol{\rho}_n = \boldsymbol{\rho}_{n+1}\,.$$
  - Moreover, by definition (110) of the χ^2-contrast $\chi_n^2 = \chi^2\big((\boldsymbol{\alpha}^\top \mathbf{P}^n)^\top;\boldsymbol{\pi}\big)$ of $(\boldsymbol{\alpha}^\top \mathbf{P}^n)^\top$ with respect to $\boldsymbol{\pi}$ we obtain
  $$\begin{aligned}\chi_n^2 &= \sum_{i=1}^{\ell} \frac{\big((\boldsymbol{\alpha}^\top \mathbf{P}^n)_i - \pi_i\big)^2}{\pi_i} = \sum_{i=1}^{\ell} \Big(\frac{(\boldsymbol{\alpha}^\top \mathbf{P}^n)_i}{\pi_i} - 1\Big)^2 \pi_i \\ &= \sum_{i=1}^{\ell} \big(\rho_{ni} - (\boldsymbol{\rho}_n)_{\boldsymbol{\pi}}\big)^2 \pi_i = \mathrm{Var}_{\boldsymbol{\pi}}(\boldsymbol{\rho}_n)\,,\end{aligned}$$
  i.e.,
  $$\chi_n^2 = \mathrm{Var}_{\boldsymbol{\pi}}(\boldsymbol{\rho}_n)\,. \tag{113}$$
  - Now the identity (106) derived in Lemma 2.6 yields
  $$\chi_n^2 = \chi_{n+1}^2 + \big((\mathbf{I}-\mathbf{M})\boldsymbol{\rho}_n,\, \boldsymbol{\rho}_n\big)_{\boldsymbol{\pi}}\,. \tag{114}$$
- On the other hand the spectral representation (101) of $\mathbf{M}$ derived in Theorem 2.15 implies
  $$\begin{aligned}\big((\mathbf{I}-\mathbf{M})\boldsymbol{\rho}_n,\, \boldsymbol{\rho}_n\big)_{\boldsymbol{\pi}} &= (\boldsymbol{\rho}_n,\, \boldsymbol{\rho}_n)_{\boldsymbol{\pi}} - (\mathbf{M}\boldsymbol{\rho}_n,\, \boldsymbol{\rho}_n)_{\boldsymbol{\pi}} \\ &= (\boldsymbol{\rho}_n,\, \boldsymbol{\rho}_n)_{\boldsymbol{\pi}} - \sum_{i=1}^{\ell} \theta_{\mathbf{M},i}(\boldsymbol{\phi}_i\boldsymbol{\psi}_i^\top \boldsymbol{\rho}_n,\, \boldsymbol{\rho}_n)_{\boldsymbol{\pi}} \\ &= (\boldsymbol{\rho}_n,\, \boldsymbol{\rho}_n)_{\boldsymbol{\pi}} - 1 - \sum_{i=2}^{\ell} \theta_{\mathbf{M},i}(\boldsymbol{\phi}_i\boldsymbol{\psi}_i^\top \boldsymbol{\rho}_n,\, \boldsymbol{\rho}_n)_{\boldsymbol{\pi}}\,,\end{aligned}$$
  as $\theta_{\mathbf{M},1} = 1$, $\boldsymbol{\phi}_1 = \mathbf{e}$ and $\boldsymbol{\psi}_1^\top = \boldsymbol{\pi}^\top$ and therefore
  $$\big(\boldsymbol{\phi}_1\boldsymbol{\psi}_1^\top \boldsymbol{\rho}_n,\, \boldsymbol{\rho}_n\big)_{\boldsymbol{\pi}} = \big(\boldsymbol{\Pi}\boldsymbol{\rho}_n,\, \boldsymbol{\rho}_n\big)_{\boldsymbol{\pi}} = (\mathbf{e},\, \boldsymbol{\rho}_n)_{\boldsymbol{\pi}} = (\boldsymbol{\rho}_n)_{\boldsymbol{\pi}} = 1 \qquad \Big(= (\boldsymbol{\rho}_n)_{\boldsymbol{\pi}}^2\Big)\,.$$
  - As the eigenvectors $\boldsymbol{\phi}_1,\dots,\boldsymbol{\phi}_\ell$ von $\mathbf{M}$ defined in (100) are a basis of $\mathbb{R}^\ell$ there is a (uniquely determined) vector $\big(\rho_{n1}^{(\mathrm{r})},\dots,\rho_{n\ell}^{(\mathrm{r})}\big)^\top \in \mathbb{R}^\ell$, such that $\boldsymbol{\rho}_n = \sum_{i=1}^{\ell} \rho_{ni}^{(\mathrm{r})}\boldsymbol{\phi}_i$.
  - Moreover, in (102) we have shown that $\boldsymbol{\psi}_i^\top \boldsymbol{\rho}_n = \rho_{ni}^{(\mathrm{r})}$. As $\boldsymbol{\psi}_1^\top = \boldsymbol{\pi}^\top$ we can conclude $\boldsymbol{\psi}_1^\top \boldsymbol{\rho}_n = 1$.

– Furthermore, as $\boldsymbol{\phi}_i = \mathbf{D}^{-1}\boldsymbol{\phi}_i^*$ and $\boldsymbol{\psi}_i = \mathbf{D}\boldsymbol{\phi}_i^*$ for all $i \in E$ we obtain

$$\begin{aligned}
\sum_{i=2}^{\ell} \theta_{\mathbf{M},i}(\boldsymbol{\phi}_i\boldsymbol{\psi}_i^\top \boldsymbol{\rho}_n,\, \boldsymbol{\rho}_n)_{\boldsymbol{\pi}} &= \sum_{i=2}^{\ell}\sum_{j=1}^{\ell} \theta_{\mathbf{M},i}\rho_{ni}^{(\mathrm{r})}\rho_{nj}^{(\mathrm{r})}(\boldsymbol{\phi}_i,\, \boldsymbol{\phi}_j)_{\boldsymbol{\pi}} \\
&= \sum_{i=2}^{\ell}\sum_{j=1}^{\ell} \theta_{\mathbf{M},i}\rho_{ni}^{(\mathrm{r})}\rho_{nj}^{(\mathrm{r})} \underbrace{\big(\mathbf{D}^{-1}\boldsymbol{\phi}_i^*,\, \mathbf{D}^{-1}\boldsymbol{\phi}_j^*\big)_{\boldsymbol{\pi}}}_{=\delta_i(j)} \\
&= \sum_{i=2}^{\ell} \theta_{\mathbf{M},i}\big(\rho_{ni}^{(\mathrm{r})}\big)^2 \\
&\le \theta_{\mathbf{M},2}\sum_{i=2}^{\ell}\big(\rho_{ni}^{(\mathrm{r})}\big)^2 = \theta_{\mathbf{M},2}\Big(\sum_{i=1}^{\ell}\big(\rho_{ni}^{(\mathrm{r})}\big)^2 - \big(\underbrace{\rho_{n1}^{(\mathrm{r})}}_{=\boldsymbol{\psi}_1^\top\boldsymbol{\rho}_n=1}\big)^2\Big) \\
&= \theta_{\mathbf{M},2}\left(\sum_{i=1}^{\ell}\sum_{j=1}^{\ell}\rho_{ni}^{(\mathrm{r})}\rho_{nj}^{(\mathrm{r})}(\boldsymbol{\phi}_i,\, \boldsymbol{\phi}_j)_{\boldsymbol{\pi}} - 1\right) = \theta_{\mathbf{M},2}\,\underbrace{\Big((\boldsymbol{\rho}_n,\, \boldsymbol{\rho}_n)_{\boldsymbol{\pi}} - 1\Big)}_{=\mathrm{Var}_{\boldsymbol{\pi}}(\boldsymbol{\rho}_n)}.
\end{aligned}$$

- Summarizing our results we have seen that

$$\big((\mathbf{I}-\mathbf{M})\boldsymbol{\rho}_n,\, \boldsymbol{\rho}_n\Big)_{\boldsymbol{\pi}} \ge \big(1-\theta_{\mathbf{M},2}\big)\mathrm{Var}_{\boldsymbol{\pi}}(\boldsymbol{\rho}_n)\,.$$

– Because of (113) and (114) this implies

$$\chi_n^2 \ge \chi_{n+1}^2 + \big(1-\theta_{\mathbf{M},2}\big)\chi_n^2 \qquad \text{and} \qquad \chi_{n+1}^2 \le \theta_{\mathbf{M},2}\,\chi_n^2\,.$$

– Thus, we have shown that $\chi_n^2 \le \theta_{\mathbf{M},2}^n\,\chi_0^2$ for all $n \ge 1$ and, consequently, the assertion follows from Lemma 2.7. □

2.3.6 Dirichlet–Forms and Rayleigh–Theorem

- Let $E = \{1, \ldots, \ell\}$ be an arbitrary finite set and let $\mathbf{P}$ be an $(\ell \times \ell)$–dimensional transition matrix, which is irreducible and aperiodic (i.e. quasi–positive) as well as reversible.
- Recall that
  – all eigenvalues of $\mathbf{P}$ are real (see Section 2.3.3), and
  – by the Perron–Frobenius theorem (see Theorem 2.6 and Corollary 2.3) the eigenvalues of $\mathbf{P}$ are in the interval $(-1, 1]$, where
  – the largest eigenvalue is 1 and the absolute values of the other eigenvalues are (strictly) less than 1.

Remarks

- Instead of ordering the eigenvalues according to their absolute values (like above) we will now order them with respect to their *own* size and denote them by $\lambda_1, \ldots, \lambda_\ell$ such that

$$1 = \lambda_1 > \lambda_2 \ge \ldots \ge \lambda_\ell > -1\,.$$

- Moreover, for the multiplicative reversible version $\mathbf{M} = \mathbf{P}\widetilde{\mathbf{P}}$ of the transition matrix $\mathbf{P}$ that was introduced in Section 2.3.4 we have

$$1 = \lambda_1 > \lambda_2 \ge \ldots \ge \lambda_\ell > 0\,,$$

i.e., for the eigenvalues of the matrix $\mathbf{M}$ the notations $\theta_1, \ldots, \theta_\ell$ and $\lambda_1, \ldots, \lambda_\ell$ coincide.

- For large ℓ,
  - the calculation of the second largest absolute value $|\theta_2| = \max\{\lambda_2, |\lambda_\ell|\}$ among the eigenvalues can cause difficulties.
  - Therefore, in Section 2.3.7 we will derive bounds for λ_2 and λ_ℓ, whose calculation is very simple.
- These bounds are particularly useful if
  - the stationary (limit) distribution is at least in principle known,
  - but in spite of this the corresponding Markov chain is started with a non-stationary initial distribution $\boldsymbol{\alpha}$; for example it could be started in a predetermined state $i \in E$, i.e. $\alpha_i = 1$ and $\alpha_j = 0$ for $j \neq i$.

In order to derive an upper bound for λ_2, we need a representation formula for λ_2,

- that is usually called the *Rayleigh–theorem* in literature
- and that is expressed based on the so–called *Dirichlet–form*

$$D_{(\mathbf{P},\boldsymbol{\pi})}(\mathbf{x},\mathbf{x}) = \big((\mathbf{I}-\mathbf{P})\mathbf{x},\mathbf{x}\big)_{\boldsymbol{\pi}} \tag{115}$$

of the reversible pair $(\mathbf{P},\boldsymbol{\pi})$, where $(\mathbf{y},\mathbf{x})_{\boldsymbol{\pi}}$ denotes the inner product of $\mathbf{y}$ and $\mathbf{x}$ with respect to $\boldsymbol{\pi}$; see (103).

First of all we will show the following lemma.

Lemma 2.8 *For all* $\mathbf{x} = (x_1,\ldots,x_\ell)^\top \in \mathbb{R}^\ell$,

$$D_{(\mathbf{P},\boldsymbol{\pi})}(\mathbf{x},\mathbf{x}) = \frac{1}{2}\sum_{i,j\in E}\pi_i p_{ij}(x_j - x_i)^2\,. \tag{116}$$

Proof From the definition (103) of the inner product and the reversibility of the pair $(\mathbf{P},\boldsymbol{\pi})$ we obtain

$$\begin{aligned}
2\big((\mathbf{I}-\mathbf{P})\mathbf{x},\mathbf{x}\big)_{\boldsymbol{\pi}} &= 2\sum_{i,j\in E}\pi_i p_{ij}x_i(x_i - x_j)\\
&\overset{i\to j}{=} \sum_{i,j\in E}\pi_i p_{ij}x_i(x_i - x_j) + \sum_{i,j\in E}\pi_j p_{ji}x_j(x_j - x_i)\\
&\overset{(85)}{=} \sum_{i,j\in E}\pi_i p_{ij}x_i(x_i - x_j) + \sum_{i,j\in E}\pi_i p_{ij}x_j(x_j - x_i)\\
&= \sum_{i,j\in E}\pi_i p_{ij}(x_j - x_i)^2\,.
\end{aligned}$$

□

We will now prove the *Rayleigh–theorem* that yields a representation formula for the second largest eigenvalue λ_2 of the reversible pair $(\mathbf{P},\boldsymbol{\pi})$.

Theorem 2.17

- *Let* $\mathbb{R}^\ell_{\neq} = \big\{\mathbf{x} = (x_1,\ldots,x_\ell)^\top \in \mathbb{R}^\ell : \ x_i \neq x_j \text{ for some pair } i,j \in E\big\}$ *denote the set of all vectors in* $\mathbb{R}^\ell$ *whose components are not all equal.*

- *For the eigenvalue λ_2 of the reversible pair $(\mathbf{P}, \boldsymbol{\pi})$ the following holds*

$$\lambda_2 = 1 - \inf_{\mathbf{x} \in \mathbb{R}^\ell_{\not\perp}} \frac{D_{(\mathbf{P},\boldsymbol{\pi})}(\mathbf{x}, \mathbf{x})}{\mathrm{Var}_{\boldsymbol{\pi}}(\mathbf{x})}\,, \tag{117}$$

where $\mathrm{Var}_{\boldsymbol{\pi}}(\mathbf{x})$ denotes the variance of the components of $\mathbf{x}$ with respect to $\boldsymbol{\pi}$ defined in (105).

Proof

- Lemma 2.8 implies for arbitrary $c \in \mathbb{R}$ and $\mathbf{x} \in \mathbb{R}^\ell$

$$D_{(\mathbf{P},\boldsymbol{\pi})}(\mathbf{x}, \mathbf{x}) = D_{(\mathbf{P},\boldsymbol{\pi})}(\mathbf{x} - c\,\mathbf{e}, \mathbf{x} - c\,\mathbf{e})\,.$$

  - Thus, the assertion (117) is equivalent to

$$1 - \lambda_2 = \inf_{\mathbf{x} \in \mathbb{R}^\ell_0} \frac{D_{(\mathbf{P},\boldsymbol{\pi})}(\mathbf{x}, \mathbf{x})}{\mathrm{Var}_{\boldsymbol{\pi}}(\mathbf{x})}\,, \tag{118}$$

    where $\mathbb{R}^\ell_0 = \big\{\mathbf{x} = (x_1, \ldots, x_\ell)^\top \in \mathbb{R}^\ell : \ (\mathbf{x})_{\boldsymbol{\pi}} = 0,\, \mathbf{x} \neq \mathbf{0}\big\}$.
  - Let now the left eigenvectors $\boldsymbol{\phi}_1, \ldots, \boldsymbol{\phi}_\ell$ of $\mathbf{P}$ be chosen such that they are an orthonormal basis of $\mathbb{R}^\ell$ with respect to the inner product $(\cdot\,,\cdot)_{\boldsymbol{\pi}}$, i.e. $(\boldsymbol{\phi}_i, \boldsymbol{\phi}_j)_{\boldsymbol{\pi}} = 1$ if $i = j$ and $(\boldsymbol{\phi}_i, \boldsymbol{\phi}_j)_{\boldsymbol{\pi}} = 0$ if $i \neq j$ where $\boldsymbol{\phi}_1 = \mathbf{e}$.
  - First of all, the eigenvectors $\boldsymbol{\phi}^*_1, \ldots, \boldsymbol{\phi}^*_\ell$ of the symmetric vectors $\mathbf{DPD}^{-1}$ are chosen such that they are orthonormal with respect to the ordinary Euclidian inner product. Then we can define $\boldsymbol{\phi}_i = \mathbf{D}^{-1}\boldsymbol{\phi}^*_i$ for all $i \in E$ (see also Section 2.3.3).
  - For every $\mathbf{x} \in \mathbb{R}^\ell$ there is now a uniquely determined vector $\big(x^{(\mathrm{r})}_1, \ldots, x^{(\mathrm{r})}_\ell\big)^\top \in \mathbb{R}^\ell$ such that

$$\mathbf{x} = \sum_{i=1}^{\ell} x^{(\mathrm{r})}_i \boldsymbol{\phi}_i\,.$$

  - As $\lambda_1 = 1$ we obtain

$$(\mathbf{I} - \mathbf{P})\mathbf{x} = \sum_{i=2}^{\ell} (1 - \lambda_i) x^{(\mathrm{r})}_i \boldsymbol{\phi}_i \qquad \text{and hence} \qquad D_{(\mathbf{P},\boldsymbol{\pi})}(\mathbf{x}, \mathbf{x}) = \sum_{i=2}^{\ell} (1 - \lambda_i)\big(x^{(\mathrm{r})}_i\big)^2\,.$$

- On the other hand as $\boldsymbol{\phi}_1 = \mathbf{e}$ and the eigenvectors $\boldsymbol{\phi}_1, \ldots, \boldsymbol{\phi}_\ell$ are orthonormal with respect to the inner product $(\cdot\,,\cdot)_{\boldsymbol{\pi}}$ we can conclude that

$$(\mathbf{x})_{\boldsymbol{\pi}} = (\mathbf{x},\, \mathbf{e})_{\boldsymbol{\pi}} = x^{(\mathrm{r})}_1 \qquad \text{and} \qquad \mathrm{Var}_{\boldsymbol{\pi}}(\mathbf{x}) = \sum_{i=2}^{\ell} \big(x^{(\mathrm{r})}_i\big)^2\,, \quad \text{if } (\mathbf{x})_{\boldsymbol{\pi}} = 0\,.$$

  - Thus for every $\mathbf{x} \in \mathbb{R}^\ell_0$

$$\begin{aligned}
\frac{D_{(\mathbf{P},\boldsymbol{\pi})}(\mathbf{x}, \mathbf{x})}{\mathrm{Var}_{\boldsymbol{\pi}}(\mathbf{x})} &= \frac{\sum_{i=2}^{\ell} (1 - \lambda_i)\big(x^{(\mathrm{r})}_i\big)^2}{\sum_{i=2}^{\ell} \big(x^{(\mathrm{r})}_i\big)^2} \\
&= (1 - \lambda_2) + \frac{\sum_{i=2}^{\ell} (1 - \lambda_i)\big(x^{(\mathrm{r})}_i\big)^2 - (1 - \lambda_2) \sum_{i=2}^{\ell} \big(x^{(\mathrm{r})}_i\big)^2}{\sum_{i=2}^{\ell} \big(x^{(\mathrm{r})}_i\big)^2} \\
&= (1 - \lambda_2) + \frac{\sum_{i=3}^{\ell} (\lambda_2 - \lambda_i)\big(x^{(\mathrm{r})}_i\big)^2}{\sum_{i=2}^{\ell} \big(x^{(\mathrm{r})}_i\big)^2} \ \geq\ 1 - \lambda_2\,.
\end{aligned}$$

– This shows that (118) holds as the last expression for the quotient $D_{(\mathbf{P},\boldsymbol{\pi})}(\mathbf{x},\mathbf{x})/\mathrm{Var}_{\boldsymbol{\pi}}(\mathbf{x})$ implies

$$\frac{D_{(\mathbf{P},\boldsymbol{\pi})}(\mathbf{x},\mathbf{x})}{\mathrm{Var}_{\boldsymbol{\pi}}(\mathbf{x})} = 1-\lambda_2\,,$$

for $\mathbf{x}=\boldsymbol{\phi}_2$ where $\boldsymbol{\phi}_2\in\mathbb{R}_0^\ell$ as $\boldsymbol{\phi}_1=\mathbf{e}$ and $\boldsymbol{\phi}_2$ are linearly independent. □

2.3.7 Bounds for the Eigenvalues λ_2 and λ_ℓ

In order to derive bounds for the eigenvalues λ_2 and λ_ℓ the following notions and notations are necessary.

- For each pair $i,j\in E$ such that $i\neq j$ and $p_{ij}>0$ we denote
  - by $e=e_{ij}$ the corresponding directed *edge* of the transition graph
  - by $e^-=i$ and $e^+=j$ the *starting* and *target* vertices of e, respectively.
  - Let $\mathcal{E}$ be the set of all directed edges $e=e_{ij}$ such that $i\neq j$ and $p_{ij}>0$.

- Furthermore, for each $i,j\in E$ such that $i\neq j$ we consider exactly one *path* γ_{ij} from i to j,
  - which is given by a vector $\gamma_{ij}=(i_0,i_1,\ldots,i_{m-1},i_m)$ of states such that $i=i_0$, $j=i_m$ and

    $$p_{ii_1}p_{i_1i_2}\,\ldots\,p_{i_{m-1}j}>0\,,$$

    such that none of the edges $e_{i_{k-1}i_k}$ is contained more than once (and m is the smallest possible number).
  - Let Γ be the set of all these paths and for each path $\gamma_{ij}\in\Gamma$ define

    $$|\gamma_{ij}| = \sum_{e\in\gamma_{ij}}\frac{1}{Q(e)} = \frac{1}{\pi_i p_{ii_1}} + \frac{1}{\pi_{i_1}p_{i_1i_2}} + \ldots + \frac{1}{\pi_{i_{m-1}}p_{i_{m-1}j}}\,, \tag{119}$$

    where $Q(e_{i_{k-1}i_k})=\pi_{i_{k-1}}p_{i_{k-1}i_k}$.
  - The so–called *Poincaré–coefficient* κ of the set of paths Γ is then defined as

    $$\kappa=\kappa(\Gamma)=\max_{e\in\mathcal{E}}\sum_{\gamma_{ij}\ni e}|\gamma_{ij}|\pi_i\pi_j\,. \tag{120}$$

- Finally we consider
  - the extended set of edges $\mathcal{E}'\supset\mathcal{E}$ also containing the edges of the type $i\to i$ in case $p_{ii}>0$.
  - for all $i\in E$ exactly one path γ_i from i to i which contains an odd number of edges in $\mathcal{E}'$ such that no edge occurs more than once.
  - Let Γ' be the set of all these paths and for every path $\gamma_i\in\Gamma'$ let

    $$|\gamma_i| = \sum_{e\in\gamma_i}\frac{1}{Q(e)}\,. \tag{121}$$

  - The coefficient ζ of the path set Γ' is then defined as

    $$\zeta=\zeta(\Gamma')=\max_{e\in\mathcal{E}'}\sum_{\gamma_i\ni e}|\gamma_i|\pi_i\,. \tag{122}$$

Theorem 2.18 *For the eigenvalues λ_2 and λ_ℓ of $\mathbf{P}$ the following inequalities hold*

$$1 - \frac{1}{\kappa} \geq \lambda_2 \geq \lambda_\ell \geq -1 + \frac{2}{\zeta} \tag{123}$$

and hence

$$\max\{\lambda_2, |\lambda_\ell|\} \leq 1 - \min\Big\{ \frac{1}{\kappa} \,,\, \frac{2}{\zeta} \Big\} . \tag{124}$$

Proof

- First we will show that $\lambda_2 \leq 1 - \kappa^{-1}$.
  - Because of Theorem 2.17 it suffices to show that

$$\mathrm{Var}_{\boldsymbol{\pi}}(\mathbf{x}) \leq \kappa \, D_{(\mathbf{P},\boldsymbol{\pi})}(\mathbf{x},\mathbf{x}) \,, \qquad \forall\, \mathbf{x} \in \mathbb{R}^\ell \,. \tag{125}$$

  - Using the notation introduced in (119) we obtain

$$\begin{aligned}
\mathrm{Var}_{\boldsymbol{\pi}}(\mathbf{x}) &= \frac{1}{2}\Big(2\|\mathbf{x}\|_{\boldsymbol{\pi}}^2 - 2(\mathbf{x})_{\boldsymbol{\pi}}^2\Big) \\
&= \frac{1}{2}\Big(\sum_{i\in E} x_i^2\pi_i + \sum_{j\in E} x_j^2\pi_j - 2\sum_{i,j\in E} x_i x_j \pi_i \pi_j\Big) \\
&= \frac{1}{2}\sum_{i,j\in E} (x_i - x_j)^2 \pi_i \pi_j \\
&= \frac{1}{2}\sum_{i,j\in E}\Big(\sum_{e\in\gamma_{ij}} \frac{1}{\sqrt{Q(e)}}\,\sqrt{Q(e)}(x_{e^-} - x_{e^+})\Big)^2 \pi_i\pi_j \,.
\end{aligned}$$

  - An application of the Cauchy–Schwarz inequality yields

$$\begin{aligned}
\mathrm{Var}_{\boldsymbol{\pi}}(\mathbf{x}) &\leq \frac{1}{2}\sum_{i,j\in E}\Big(|\gamma_{ij}| \sum_{e\in\gamma_{ij}} Q(e)(x_{e^-} - x_{e^+})^2\Big)\pi_i\pi_j \\
&= \frac{1}{2}\sum_{e\in\mathcal{E}}\left(Q(e)(x_{e^-} - x_{e^+})^2\Big(\sum_{\gamma_{ij}\ni e} |\gamma_{ij}|\,\pi_i\pi_j\Big)\right) \\
&\leq \kappa \, D_{(\mathbf{P},\boldsymbol{\pi})}(\mathbf{x},\mathbf{x}) \,,
\end{aligned}$$

    where the last inequality follows from Lemma 2.8 and by definition of the Poincaré–coefficient; see (120). This shows (125).

- In order to finish the proof it is left to show that $\lambda_\ell \geq -1 + 2\zeta^{-1}$.
  - For this purpose we exploit the following equation: For all $\mathbf{x} = (x_1, \ldots, x_\ell)^\top \in \mathbb{R}^\ell$

$$\frac{1}{2}\sum_{i,j\in E} (x_i + x_j)^2 \pi_i p_{ij} = (\mathbf{P}\mathbf{x},\mathbf{x})_{\boldsymbol{\pi}} + \|x\|_{\boldsymbol{\pi}}^2 \,, \tag{126}$$

    as the reversibility of $(\mathbf{P},\boldsymbol{\pi})$ implies

$$\begin{aligned}
\frac{1}{2}\sum_{i,j\in E} (x_i + x_j)^2 \pi_i p_{ij} &= \frac{1}{2}\underbrace{\sum_{i,j\in E} x_i^2 \pi_i p_{ij}}_{=\sum_{i\in E} x_i^2\pi_i} + \sum_{i,j\in E} x_i x_j \pi_i p_{ij} + \frac{1}{2}\underbrace{\sum_{i,j\in E} x_j^2 \underbrace{\pi_i p_{ij}}_{\overset{(85)}{=}\pi_j p_{ji}}}_{=\sum_{j\in E} x_j^2\pi_j} \\
&= \|x\|_{\boldsymbol{\pi}}^2 + (\mathbf{P}\mathbf{x},\mathbf{x})_{\boldsymbol{\pi}} \,.
\end{aligned}$$

– Let now $\gamma_i = (i_0, i_1, \ldots, i_{2m}, i_{2m+1})$ where $i = i_0 = i_{2m+1}$ is a path from i to i, containing an odd number of edges such that every edge does not occur more than once.

– Then

$$\begin{aligned} x_i &= \frac{1}{2}\Big((x_i + x_{i_1}) - (x_{i_1} + x_{i_2}) + \ldots + (x_{i_{2m}} + x_i)\Big) \\ &= \frac{1}{2}\sum_{e\in\gamma_i}(-1)^{n(e)}(x_{e^+} + x_{e^-})\,, \end{aligned}$$

where $n(e) = k$ if $e = (i_k, i_{k+1}) \in \gamma_i$.

– Similarly to the first part of the proof, the Cauchy–Schwarz inequality implies that for all $\mathbf{x} = (x_1, \ldots, x_\ell)^\top \in \mathbb{R}^\ell$

$$\begin{aligned} \|\mathbf{x}\|_{\boldsymbol{\pi}}^2 &= \sum_{i\in E}\frac{\pi_i}{4}\Big(\sum_{e\in\gamma_i}\frac{1}{\sqrt{Q(e)}}\sqrt{Q(e)}(-1)^{n(e)}(x_{e^+} + x_{e^-})\Big)^2 \\ &\le \sum_{i\in E}\Big(\frac{\pi_i}{4}\,|\gamma_i|\sum_{e\in\gamma_i}(x_{e^+} + x_{e^-})^2 Q(e)\Big) \\ &= \frac{1}{4}\sum_{e\in\mathcal{E}'}\Big((x_{e^+} + x_{e^-})^2 Q(e)\sum_{\gamma_i \ni e}|\gamma_i|\pi_i\Big) \\ &\le \frac{\zeta}{4}\sum_{e\in\mathcal{E}'}(x_{e^+} + x_{e^-})^2 Q(e)\,. \end{aligned}$$

– From (126) we can now conclude that

$$\|\mathbf{x}\|_{\boldsymbol{\pi}}^2 \le \frac{\zeta}{2}\Big((\mathbf{P}\mathbf{x}, \mathbf{x})_{\boldsymbol{\pi}} + \|\mathbf{x}\|_{\boldsymbol{\pi}}^2\Big)\,.$$

– For $\mathbf{x} = \boldsymbol{\phi}_\ell$ we obtain in particular that

$$1 \le \frac{\zeta}{2}\,(\lambda_\ell + 1) \qquad \text{and} \qquad \lambda_\ell \ge -1 + \frac{2}{\zeta}\,. \qquad \square$$

Example *Random Walk on a Graph*

- We return to the example of a random walk on a graph that has been already discussed in Section 2.3.1.
  – Let $G = (V, K)$ be a connected graph with vertices $V = \{v_1, \ldots, v_\ell\}$ and edges K where each edge connects two vertices,
  – such that for each pair $v_i, v_j \in V$ of vertices there is a „path" of edges in K connecting v_i and v_j.
- A random walk on the graph $G = (V, K)$ is a Markov chain $X_0, X_1, \ldots : \Omega \to E$
  – with state space $E = \{1, \ldots, \ell\}$ and transition matrix $\mathbf{P} = (p_{ij})$ where

$$p_{ij} = \begin{cases} \dfrac{1}{d_i} & \text{if the vertices } v_i \text{ and } v_j \text{ are neighbors,} \\ 0 & \text{else.} \end{cases} \tag{127}$$

  – Recall that two vertices v_i and v_j are called neighbors if they are endpoints of the same edge where, for each vertex v_i, d_i denotes its number of neighbors.
- We already showed that
  – the transition matrix $\mathbf{P}$ given in (127) is always irreducible (where we now additionally assume $\mathbf{P}$ to be aperiodic),

– the uniquely determined initial distribution $\boldsymbol{\pi}$ is given by

$$\boldsymbol{\pi} = \Big(\frac{d_1}{d}\,,\ldots,\,\frac{d_\ell}{d}\Big)^\top, \qquad \text{where } d = \sum_{i=1}^{\ell} d_i, \tag{128}$$

– the pair $(\mathbf{P}, \boldsymbol{\pi})$ given by (127)–(128) is reversible.

- For the Poincaré–coefficient κ introduced in (120) we obtain

$$\kappa = \kappa(\Gamma) = \max_{e\in\mathcal{E}} \sum_{\gamma_{ij}\ni e} |\gamma_{ij}|\pi_i\pi_j\,,$$

where

$$|\gamma_{ij}| = \sum_{e\in\gamma_{ij}} \frac{1}{Q(e)} = d\,\Delta(\gamma_{ij})$$

and $\Delta(\gamma_{ij}) = \#\{e : e \in \gamma_{ij}\}$ denotes the number of edges (i.e. the length) of the path γ_{ij}.

- Taking into account (127)–(128), this implies

$$\kappa(\Gamma) \;\le\; \frac{\delta^2\Delta\beta}{d}\,, \tag{129}$$

where $d/2$ denotes the total number of edges,

– $\delta = \max_{i\in E} d_i$ is the maximum number of edges originating at a vertex,
– $\Delta = \max_{\gamma\in\Gamma} \Delta(\gamma)$ denotes the maximal path length and
– $\beta = \max_{e\in\mathcal{E}} \#\{\gamma \in \Gamma : \gamma \ni e\}$ is the so–called *Bottleneck–coefficient*, i.e. the maximal number of paths containing a single edge.

- From (123) and (129) we obtain the following estimate

$$\lambda_2 \;\le 1 - \;\frac{1}{\kappa} \;\le\; 1 - \;\frac{d}{\delta^2\Delta\beta} \tag{130}$$

for the second largest eigenvalue λ_2 of $\mathbf{P}$.

- In a similar way one obtains the upper bound

$$\zeta = \zeta(\Gamma') = \max_{e\in\mathcal{E}'} \sum_{\gamma_i\ni e} |\gamma_i|\pi_i \le \delta\,\Delta'\,\beta'\,,$$

where

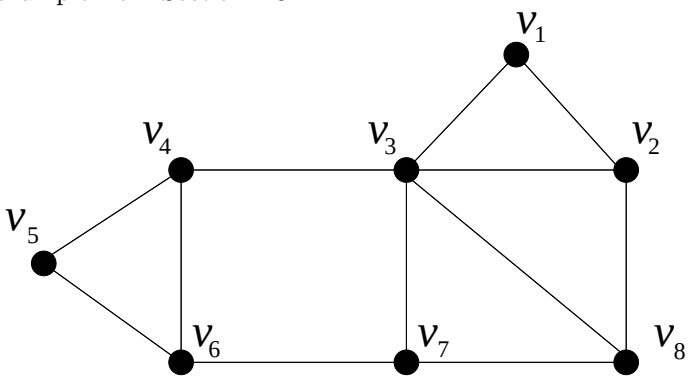
$$|\gamma_i| = \sum_{e\in\gamma_i} \frac{1}{Q(e)} = d\,\Delta(\gamma_i)\,, \qquad \Delta' = \max_{\gamma\in\Gamma'} \Delta(\gamma)\,, \qquad \beta' = \max_{e\in\mathcal{E}'} \#\{\gamma \in \Gamma' : \gamma \ni e\}$$

and hence

$$\lambda_\ell \;\ge\; -1 + \;\frac{2}{\zeta} \;\ge\; -1 + \;\frac{2}{\delta\,\Delta'\,\beta'}\,. \tag{131}$$

- Remarks.

– For the numerical example from Section 2.3.1



the following holds:

$$d = 24,\ \delta = 5,\ \Delta = 3,\ \beta = 7 \qquad \text{and} \qquad \Delta' = 3,\ \beta' = 3.$$

– The inequalities (130) and (131) thus imply

$$\lambda_2 \ \leq\ 1 - \frac{24}{25 \cdot 3 \cdot 7} \ <\ \frac{24}{25} \qquad \text{and} \qquad \lambda_8 \ >\ -1 + \frac{2}{5 \cdot 3 \cdot 3} \ =\ -\frac{43}{45}\,,$$

and hence

$$\max\{\lambda_2, |\lambda_8|\} \ <\ \frac{24}{25}\,.$$

3 Monte–Carlo Simulation

- Besides the traditional ways of data acquisition in laboratory experiments and field tests the generation of so-called *synthetic data* via computer simulation has gained increasing importance.
- There is a variety of reasons for the increased benefit drawn from computer simulation used to investigate a wide range of issues, objects and processes:
  - The most prominent reason is the rapidly growing performance of modern computer systems which has extended our computational capabilities in a way that would not have been imaginable even a short time ago.
  - Consequently, computer-based data generation is often considerably *cheaper* and *less time-consuming* than traditional data acquisition in laboratory experiments and field tests.
  - Moreover, computer experiments can be repeated under constant conditions as frequently as necessary whereas in traditional scientific experiments the investigated object is often damaged or even destroyed.
- A further reason for the value of computer simulations is the fact
  - that volume and structure of the analyzed data is often very complex
  - and that in this case data processing and evaluation is typically based on mathematical models whose characteristics cannot be (completely) described by analytical formulae.
  - Thus, computer simulations of the considered models present a valuable alternative tool for analysis.
- Computer experiments for the investigation of the issues, objects and processes of scientific interest are based on *stochastic simulation algorithms*. In this context one also uses the term *Monte–Carlo simulation* summarizing a huge variety of simulation algorithms.
  1. *Random number generators* are the basis for Monte–Carlo simulation of single features, quantities and variables.
     - By these algorithms realizations of random variables can be generated via the computer. Those are called *pseudo–random numbers*.
     - The simulation of random variables is based on so–called *standard random number generators* providing realizations of random variables that are uniformly distributed on the unit interval $(0, 1]$.
     - Certain *transformation and rejection methods* can be applied to these standard pseudo–random numbers in order to generate pseudo–random numbers for other (more complex) random variables having e.g. binomial, Poisson or normal distributions.
  2. Computer experiments designed to investigate *high–dimensional random vectors* or the evolution of certain objects in time are based on more sophisticated algorithms from so–called dynamic Monte–Carlo simulation.
     - In this context *Markov–Chain–Monte–Carlo–Simulation* (MCMC simulation) is a construction principle for algorithms that are particularly appropriate to simulate time stationary equilibria of objects or processes.
     - Another example for the application of MCMC simulation is *statistical image analysis*.
     - An active field of research that resulted in numerous publications during the last years are so-called *coupling algorithms for perfect MCMC simulation*.
     - These coupling algorithms enable us to simulate time–stationary equilibria of objects and processes in a way that does not only allow approximations but simulations that are „perfect” in a certain sense.

3.1 Generation of Pseudo-Random Numbers

3.1.1 Simple Applications; Monte–Carlo Estimators

First we recall two simple problems that can be solved by means of Monte–Carlo simulation and have already been discussed in the course „Elementare Wahrscheinlichkeitsrechnung und Statistik".

1. *Algorithm to determine the number π*

   - A simple computer algorithm for the Monte–Carlo simulation of π is the following improved version of Buffon's needle experiment; see Sections 2.5 and 5.2.3 of the course „Elementare Wahrscheinlichkeitsrechnung und Statistik".
   - This algorithm is based on the following geometrical facts.
     - We consider the square
       $$B = (-1, 1] \times (-1, 1] \subset \mathbb{R}^2 \,,$$
     - the circle C inscribed into B, where
       $$C = \{(x, y) : (x, y) \in B,\, x^2 + y^2 < 1\} \,,$$
     - and *arbitrarily* toss a point into the set B.
   - Translated into the language of stochastics this means:
     - We consider two independent random variables S and T that are uniformly distributed on the interval $(-1, 1]$ and
     - determine the probability of the event
       $$A = \{(S, T) \in C\} = \{S^2 + T^2 < 1\} \,,$$
       i.e. that the „random point" (S, T) is in $C \subset B$.
     - Then
       $$P(A) = P(S^2 + T^2 < 1) = \frac{|C|}{|B|} = \frac{\pi}{4} \,,$$
       where $|B|$ and $|C|$ denote the area of B and C, respectively.
   - Similarly to Buffon's needle experiment the equation $P(A) = \pi/4$ yields a
     - method for the *statistical estimation* of π,
     - which is based on the *strong law of large numbers* (SLLN) and can be easily implemented.
   - Let $(S_1, T_1), \ldots, (S_n, T_n)$ be independent and identically distributed random vectors,
     - whose distribution coincides with the one of (S, T)
     - and which are regarded as a stochastic model for n (independent) experiments.
     - Then $X_1, X_2, \ldots, X_n$ where
       $$X_i = \begin{cases} 1 & \text{if } S_i^2 + T_i^2 < 1, \\ 0 & \text{else} \end{cases}$$
       are independent and identically distributed random variables with expectation $\mathbb{E}\, X_i = \pi/4$.
   - Furthermore, the SLLN (see Theorem WR-5.15) implies
     - that the arithmetic mean
       $$Y_n = n^{-1} \sum_{i=1}^{n} X_i$$
       converges to $\pi/4$ almost surely.

  - Thus, Y_n is an *unbiased* and (strongly) *consistent estimator* for $\pi/4$,
  - i.e., the probability of $4Y_n$ to be a good approximation for π is very high if n is large.

- For the implementation of this simulation algorithm one can proceed as follows
  - Use a random number generator to generate $2n$ pseudo–random numbers $u_1, \ldots, u_{2n}$ that are realizations of random variables being uniformly distributed on $(0, 1]$.
  - Put $s_i = 2u_i - 1$ and $t_i = 2u_{n+i} - 1$ for $i = 1, \ldots, n$.
  - Define
$$x_i = \begin{cases} 1 & \text{if } s_i^2 + t_i^2 < 1, \\ 0 & \text{else} \end{cases}$$
  - Compute $4(x_1 + \ldots + x_n)/n$.

2. *Monte Carlo Integration*

- Let $\varphi : [0, 1] \to [0, 1]$ be a continuous function.
  - Our goal is to find an estimator for the value of the integral $\int_0^1 \varphi(x)\, dx$ that can be determined by Monte–Carlo simulation.
  - We consider the following stochastic model.
- Let the random variables $X_1, X_2, \ldots : \Omega \to \mathbb{R}$ be independent and uniformly distributed on $(0, 1]$, with probability density f_X given by
$$f_X(x) = \begin{cases} 1 & \text{if } x \in [0, 1], \\ 0 & \text{else.} \end{cases}$$
  - Let $Z_k = \varphi(X_k)$ for all $k = 1, 2, \ldots$.
  - By the transformation theorem for independent and identically distributed random variables (see Theorem WR-3.18) the random variables $Z_1, Z_2, \ldots$ are independent and identically distributed
  - with
$$\mathbb{E}\, Z_1 = \int_0^1 \varphi(x) f_X(x)\, dx = \int_0^1 \varphi(x)\, dx\,.$$
- Furthermore the SSLN (see Theorem WR-5.15) implies that for $n \to \infty$
$$\frac{1}{n} \sum_{k=1}^{n} Z_k \xrightarrow{\text{a.s.}} \int_0^1 \varphi(x)\, dx\,.$$
  - Hence $\frac{1}{n} \sum_{k=1}^{n} Z_k$ is an *unbiased* and (strongly) *consistent estimator* for $\int_0^1 \varphi(x)\, dx$,
  - i.e., the probability for $\frac{1}{n} \sum_{k=1}^{n} Z_k$ to be a good approximation of the integral $\int_0^1 \varphi(x)\, dx$ is high for sufficiently large n.

- For the implementation of this simulation algorithm one can proceed similarly to Example 1:
  - Use a random number generator to generate n pseudo-random numbers $x_1, \ldots, x_n$ that are realizations of random variables being uniformly distributed in $(0, 1]$.
  - Define $z_k = \varphi(x_k)$ for $k = 1, \ldots, n$.
  - Compute $\frac{1}{n} \sum_{k=1}^{n} z_k$.

3.1.2 Linear Congruential Generators

- Most simulation algorithms are based on *standard random number generators*,
  - whose goal is to generate sequences $u_1, \ldots, u_n$ of numbers in the unit interval $(0, 1]$. These are the so-called *standard pseudo–random numbers*,
  - which can be regarded as realizations of independent and on $(0, 1]$ uniformly distributed random variables $U_1, \ldots, U_n$.
- A commonly established procedure to generate standard pseudo-random numbers is the following *linear congruential method*,
  - where first of all the numbers $z_1, \ldots, z_n$ are generated according to a recursion formula

$$z_k = (az_{k-1} + c) \mod (m), \qquad \forall\, k = 1, \ldots, n \tag{1}$$

    .
  - The initial value $z_0 \in \{0, 1, \ldots, m-1\}$ the algorithm is starting from is called *germ* of the linear congruential generator.
  - $m \in \mathbb{N}$, $a \in \{0, 1, \ldots, m-1\}$ and $c \in \{0, 1, \ldots, m-1\}$ are further parameters called *modulus*, *factor* and *increment* of the congruential generator.
  - The scaling

$$u_k = \frac{z_k}{m} \tag{2}$$

    yields the standard pseudo–random numbers $u_1, \ldots, u_n$.

As a next step we will solve the recursion equation (1), i.e., we will show how the number z_k that has been recursively defined in (1) can be expressed *directly* by the initial value z_0 and the parameters m, a and c.

Theorem 3.1 *For all* $k \in \{1, \ldots, n\}$

$$z_k = \left(a^k z_0 + c\,\frac{a^k - 1}{a - 1}\right) \mod (m). \tag{3}$$

Proof

- We show the assertion by mathematical induction. For $k = 1$ the claim (3) coincides with the recursion equation (1).
- Let (3) be true for a certain $k \geq 1$, i.e., there is an integer $j \geq 0$ such that

$$z_k = a^k z_0 + c\,\frac{a^k - 1}{a - 1} - jm. \tag{4}$$

- We show that this implies that (3) also holds for $k + 1$.
- By the recursion equation (1) and by induction hypothesis (4) we get that

$$\begin{aligned} z_{k+1} &= (az_k + c) \mod (m) \\ &= \left(a\left(a^k z_0 + c\,\frac{a^k - 1}{a - 1} - jm\right) + c\right) \mod (m) \\ &= \left(a^{k+1} z_0 + c\,\frac{a(a^k - 1) + a - 1}{a - 1} - ajm\right) \mod (m) \\ &= \left(a^{k+1} z_0 + c\,\frac{a^{k+1} - 1}{a - 1}\right) \mod (m), \end{aligned}$$

  i.e., (3) also holds for $k + 1$. □

Remarks

- Obviously, the linear congruential generator defined in (1) can generate no more than m different numbers $z_1, \ldots, z_n$.
  - As soon as a number z_k is repeated for the first time, i.e., there is some $m_0 > 0$ such that $z_k = z_{k-m_0}$,
  - the same period of length m_0, which has already been completely generated, is started again, i.e.

$$z_{k+j} = z_{k-m_0+j} \qquad \text{for all } j \geq 1.$$

- An unfavorable choice of the parameters m, a, c and z_0, respectively, may result in a very short length m_0 of the period.
  - For example we have

$$m_0 = 2 \qquad \text{for } a = c = z_0 = 5 \text{ and } m = 10,$$

    where the sequence $5, 0, 5, 0, \ldots$ is generated.
  - A desirable feature for the period length m_0 of linear congruence generators is to be as close as possible to the maximum length m.

We will now mention some (sufficient and necessary) conditions for the parameters m, a, c and z_0, respectively, ensuring that the maximal possible period m is obtained.

Theorem 3.2

1. *If $c > 0$, then for every initial value $z_0 \in \{0, 1, \ldots, m-1\}$ the linear congruential generator defined in (1) generates a sequence $z_1, \ldots, z_n$ of numbers with maximal possible period m if and only if the following conditions are satisfied:*

   (a_1) *The parameters c and m are relatively prime.*

   (a_2) *For every prime number r dividing m, $a - 1$ is a multiple of r.*

   (a_3) *If m is a multiple of 4 then also $a - 1$ is multiple of 4.*

2. *If $c = 0$ then $m_0 = m - 1$ for all $z_0 \in \{1, \ldots, m-1\}$ if and only if*

   (b_1) *m is prime and*

   (b_2) *for any prime r dividing $m - 1$ the number $a^{(m-1)/r} - 1$ is not divisible by m.*

3. *If $c = 0$ and if there is $k \in \mathbb{N}$ such that $m = 2^k \geq 16$ then $m_0 = m/4$ if and only if z_0 is an odd number and $a \mod (8) = 5$ or $= 3$.*

A *proof* of Theorem 3.2 using results from number theory (one of them being Fermat's little theorem) can be found e.g.

- in Section 2.7 of B.D. Ripley *Stochastic Simulation*, J. Wiley & Sons, New York (1987) or
- in Section 3.2 of D.E. Knuth (1997) *The Art of Computer Programming*, Vol. II, Addison-Wesley, Reading MA.

- We also refer to these two texts for the discussion
  - of other generators for standard pseudo–random numbers like nonlinear congruential generators, shift–register generators and lagged Fibonacci generators as well as their combinations,
  - alternative conditions for the parameters m, a, c and z_0 of the linear congruential generator defined in (1),

  - ensuring the generation of sequences $z_1, \ldots, z_n$ whose period m_0 is as large as possible and also exhibiting other desirable properties.

- One of those properties is
  - that the points $(u_1, u_2), \ldots, (u_{n-1}, u_n)$ formed by pairs of consecutive pseudo–random numbers u_{i-1}, u_i are uniformly spread over the unit square $[0, 1]^2$.
  - The following numerical examples illustrate that relatively small changes of the parameters a and c can result in completely different *point patterns* $(u_1, u_2), \ldots (u_{n-1}, u_n)$.

- Further details can be found in the text by Ripley (1987) that has been already mentioned and in the lecture notes by H. Künsch (ftp://stat.ethz.ch/U/Kuensch/skript-sim.ps) that also contains the following figures.

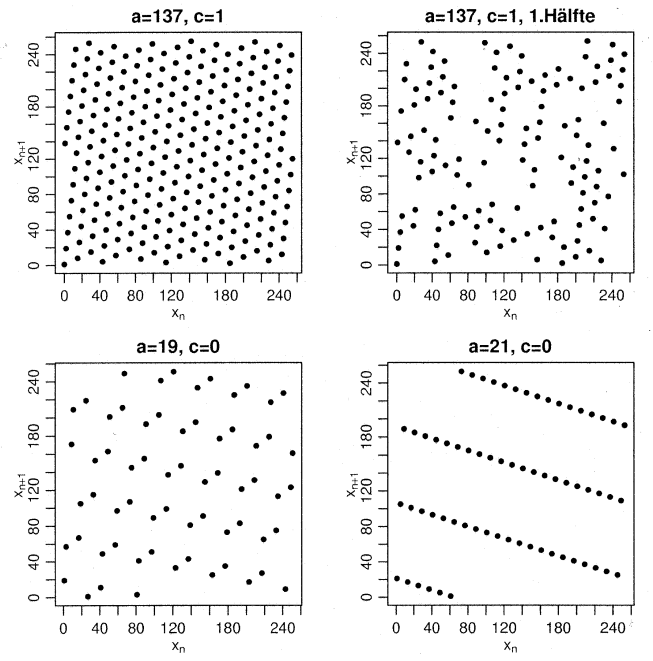


Figure 3: Point patterns for pairs (u_{i-1}, u_i) of consecutive pseudo-random numbers for $m = 256$

3.1.3 Statistical Tests

- In literature numerous *statistical significance tests* are discussed in order to investigate characteristics of random number generators; see e.g. G.S. Fishman (1996) *Monte Carlo: Concepts, Algorithms and Applications*, Springer, New York.

- We only recall two such tests which are important for investigating characteristics of linear congruential generators (and other random number generators).

- Pearson's χ^2–goodness of fit test is used to check
  - if the generated pseudo–random numbers can be regarded as realizations of uniformly distributed random variables
  - and if we may assume the independence of these random variables.

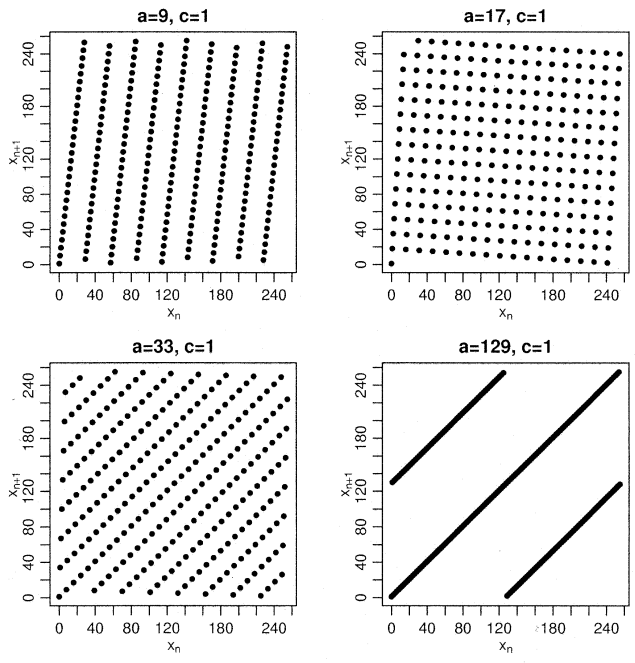


Figure 4: Point patterns for pairs (u_{i-1}, u_i) of consecutive pseudo–random numbers for $m = 256$

- Another method for the generation of sequences $u_1, u_2, \ldots$ of numbers having desirable characteristics
  - is based on minimizing the *Kolmogorov distance*

$$D_n(u_1, \ldots, u_n) = \sup_{x \in (0,1]} \left| \frac{1}{n} \#\{i : 1 \le i \le n,\, 0 < u_i \le x\} - x \right|$$

    between the empirical distribution function of the „sample" $u_1, \ldots, u_n$ and the distribution function of the uniform distribution on $(0, 1]$ for *every* natural number n.
  - In literature this procedure is referred to as *Quasi-Monte-Carlo-Method*; see e.g. H. Niederreiter (1992) *Random Number Generation and Quasi-Monte-Carlo Methods*, SIAM, Philadelphia.

1. χ^2*–goodness of fit test of uniform distribution*

   The following test is considered in order to check if the pseudo-random numbers $u_1, \ldots, u_n$
   - can be regarded as realizations of independent sampling variables $U_1, \ldots, U_n$ that are uniformly distributed on the interval $(0, 1]$.
   - The interval $(0, 1]$ is divided in r subintervals of equal length $(0, 1/r], \ldots, ((r-1)/r, 1]$ and
     - we consider the $(r-1)$–dimensional (hypothetical) vector of parameters $\mathbf{p}_0 = (1/r, \ldots, 1/r)$ and
     - the test statistic $T_n : \mathbb{R}^n \to [0, \infty)$ where

$$T_n(u_1, \ldots, u_n) = \sum_{j=1}^{r} \frac{(Z_j(u_1, \ldots, u_n) - n/r)^2}{n/r} ,$$

       and $Z_j(u_1, \ldots, u_n) = \#\{i : 1 \le i \le n,\, j - 1 < r u_i \le j\}$ denotes the number of pseudo–random numbers $u_1, \ldots, u_n$ in the interval $((j-1)/r, j/r]$.

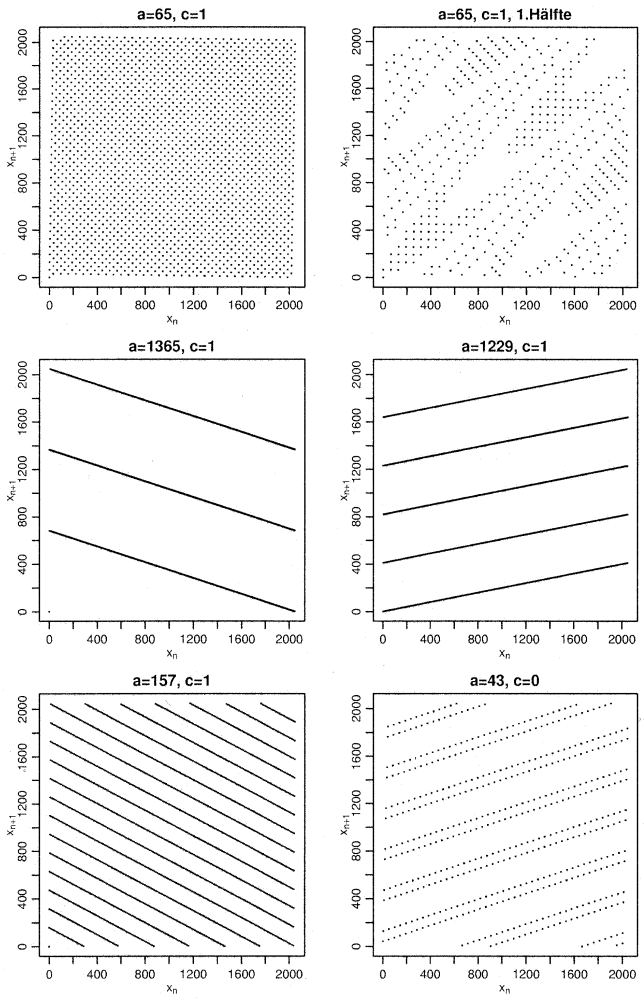


Figure 5: Point patterns for pairs (u_{i-1}, u_i) of consecutive pseudo–random numbers for $m = 2048$

- If the sampling variables $U_1, \ldots, U_n$ are independent and uniformly distributed on the interval $(0, 1]$, the test statistic T_n is asymptotically χ^2_{r-1} distributed.
- Thus, for sufficiently large n the hypothesis $H_0 : \mathbf{p} = \mathbf{p}_0$ is rejected if

$$T_n(u_1, \ldots, u_n) > \chi^2_{r-1,1-\alpha}\,,$$

  where $\chi^2_{r-1,1-\alpha}$ denotes the $(1-\alpha)$-quantile of the χ^2 distribution with $r-1$ degrees of freedom.
- We will illustrate this test by the following numerical example. For $\alpha = 0.05$, $n = 100\,000$ and $r = 10$ we want to check if
  - the hypothesis that the sampling variables are uniformly distributed is conformable with a sample $(u_1, \ldots, u_{100\,000})$ of pseudo–random numbers. The sample has the following vector $(z_1, \ldots, z_{10})$ of class frequencies:

z_1	z_2	z_3	z_4	z_5	z_6	z_7	z_8	z_9	z_{10}
9 995	10 045	10 127	9 816	10 130	10 040	9 890	9 858	10 083	10 016

– In this case we obtain $T_{100\,000}(u_1, \ldots, u_{100\,000}) = 10.99$ and hence

$$T_{100\,000}(u_1, \ldots, u_{100\,000}) = 10.99 < \chi^2_{9,0.95} = 16.92\,.$$

– Thus, the hypothesis of a uniform distribution on $(0, 1]$ is not rejected.

Remarks

- As a generalization of the χ^2–goodness of fit test for checking the uniform distribution of some sample variables one can also check
  – if for a given natural number $d \geq 1$ (e.g. $d = 2$ or $d = 3$) the pseudo–random vectors $(u_1, \ldots, u_d), \ldots, (u_{(n-1)d+1}, \ldots, u_{nd})$ can be regarded
  – as realizations of independent random vectors $(U_1, \ldots, U_d), \ldots, (U_{(n-1)d+1}, \ldots, U_{nd})$ that are uniformly distributed on $(0, 1]^d$.
- For this purpose the unit cube $(0, 1]^d$ is divided into r^d smaller cubes B_j of equal size,
  – which are of the form $((i_1 - 1)/r, i_1/r] \times \ldots \times ((i_d - 1)/r, i_d/r]$.
  – Furthermore, we consider the $(r^d - 1)$–dimensional (hypothetical) vector $\mathbf{p}_0 = (1/r^d, \ldots, 1/r^d)$ of parameters and
  – the test statistic $T_n : \mathbb{R}^{nd} \to [0, \infty)$ where

$$T_n(\mathbf{u}_1, \ldots, \mathbf{u}_n) = \sum_{j=1}^{r^d} \frac{(Z_j(\mathbf{u}_1, \ldots, \mathbf{u}_n) - n/r^d)^2}{n/r^d}\,,$$

$\mathbf{u}_i = (u_{(i-1)d+1}, \ldots, u_{id})$ and $Z_j(\mathbf{u}_1, \ldots, \mathbf{u}_n) = \#\{i : 1 \leq i \leq n, \mathbf{u}_i \in B_j\}$. Notice that $Z_j(\mathbf{u}_1, \ldots, \mathbf{u}_n)$ denotes the number of pseudo-random vectors in W_j.

2. *Run Test*

There are a number of other significance tests allowing to evaluate the quality of random number generators. In particular it can be verified

- if the generated pseudo-random numbers $u_1, \ldots, u_n$ can be regarded as realizations of independent random variables $U_1, \ldots, U_n$ having a certain distribution. In our case we consider the hypothesis of a uniform distribution on $(0, 1]$.
- The following *run test* checks in particular
  – if the *independence* assumption for the sampling variables $U_1, \ldots, U_n$ is reflected sufficiently well by the pseudo–random numbers $u_1, \ldots, u_n$.
  – This is done by analyzing the lengths of monotonically increasing subsequences, also called *runs*, within the sequence $u_1, u_2, \ldots$ of pseudo-random numbers.
- For this purpose we define the random variables $V_1, V_2, \ldots$ by the recursion formula

$$V_{j+1} = \min\{i : i > V_j + 1, U_i > U_{i+1}\}\,, \qquad \forall\, j = 1, 2, \ldots\,, \tag{5}$$

where $V_1 = \min\{i : i \geq 1, U_i > U_{i+1}\}$.

- The random variables $W_1, W_2, \ldots$ where

$$W_1 = V_1 \qquad \text{and} \qquad W_{j+1} = V_{j+1} - (V_j + 1) \quad \text{for } j = 1, 2, \ldots \tag{6}$$

are called the runs of the sequence $U_1, U_2, \ldots$.

The significance test that will be constructed is based on the following property of the runs $W_1, W_2, \ldots$.

Theorem 3.3 *The random variables $W_1, W_2, \ldots$ introduced in* (6) *are independent and identically distributed such that*

$$P(W_j = k) = \frac{k}{(k+1)!}\,, \qquad \forall\, k = 1, 2, \ldots\,, \tag{7}$$

if the random variables $U_1, U_2, \ldots$ are independent and uniformly distributed on $(0, 1]$.

Proof

- Let $U_1, U_2, \ldots$ be independent and uniformly distributed on $(0, 1]$.
  - Then for all $n \geq 1$ and for arbitrary natural numbers $k_1, \ldots, k_n \geq 1$, we get that

$$\begin{aligned}
P(W_1 = k_1, \ldots, W_n = k_n) &= P(V_1 = k_1, V_2 - V_1 - 1 = k_2, \ldots, V_n - V_{n-1} - 1 = k_n) \\
&= P\big(V_1 = k_1, V_2 = k_2 + k_1 + 1, \ldots, V_n = k_n + \ldots + k_1 + n - 1\big) \\
&= P\big(U_i \leq U_{i+1},\, \forall\, i = 1, \ldots, k_1 - 1,\, U_{k_1} > U_{k_1+1}, \\
&\quad U_i \leq U_{i+1},\, \forall\, i = k_1 + 2, \ldots, k_1 + 1 + k_2 - 1,\, U_{k_1+1+k_2} > U_{k_1+1+k_2+1}, \ldots, \\
&\quad U_i \leq U_{i+1},\, \forall\, i = k_1 + 1 + \ldots + k_{n-1} + 2, \ldots, k_1 + 1 + \ldots + k_{n-1} + 1 + k_n - 1, \\
&\qquad\qquad U_{k_1+1+\ldots+k_{n-1}+1+k_n} > U_{k_1+1+\ldots+k_{n-1}+1+k_n+1}\big) \\
&= P\big(U_i \leq U_{i+1},\, \forall\, i = 1, \ldots, k_1 - 1,\, U_{k_1} > U_{k_1+1}\big) \\
&\quad P\big(U_i \leq U_{i+1},\, \forall\, i = k_1 + 2, \ldots, k_1 + 1 + k_2 - 1,\, U_{k_1+1+k_2} > U_{k_1+1+k_2+1}\big) \\
&\quad \ldots P\big(U_i \leq U_{i+1},\, \forall\, i = k_1 + 1 + \ldots + k_{n-1} + 2, \ldots, k_1 + 1 + \ldots + k_{n-1} + 1 + k_n - 1, \\
&\qquad\qquad U_{k_1+1+\ldots+k_{n-1}+1+k_n} > U_{k_1+1+\ldots+k_{n-1}+1+k_n+1}\big) \\
&= P\big(U_i \leq U_{i+1},\, \forall\, i = 1, \ldots, k_1 - 1,\, U_{k_1} > U_{k_1+1}\big) \\
&\quad \ldots P\big(U_i \leq U_{i+1},\, \forall\, i = 1, \ldots, k_n - 1,\, U_{k_n} > U_{k_n+1}\big)\,.
\end{aligned}$$

  - This implies that the runs $W_1, W_2, \ldots$ are independent and identically distributed.
- Furthermore, an induction argument shows that for arbitrary $k \in \mathbb{R}$ and $t \in (0, 1]$

$$P(U_1 \leq \ldots \leq U_k \leq t) = \frac{t^k}{k!}\,. \tag{8}$$

  - For $k = 1$, equation (8) obviously holds. By the formula of total probability we obtain

$$\begin{aligned}
P(U_1 \leq \ldots \leq U_{k+1} \leq t) &= \int_0^1 P(U_1 \leq \ldots \leq U_k \leq U_{k+1} \leq t \mid U_{k+1} = x)\, P(U_{k+1} \in dx) \\
&= \int_0^1 P(U_1 \leq \ldots \leq U_k \leq x \leq t \mid U_{k+1} = x)\, P(U_{k+1} \in dx) \\
&= \int_0^1 P(U_1 \leq \ldots \leq U_k \leq x \leq t)\, dx\,,
\end{aligned}$$

    where the last equality is a consequence of the independence and $(0, 1]$-uniform distribution of $U_1, U_2, \ldots$.
  - Assume now that (8) is true for some $k \geq 1$. Then

$$\begin{aligned}
P(U_1 \leq \ldots \leq U_{k+1} \leq t) &= \int_0^t P(U_1 \leq \ldots \leq U_k \leq x)\, dx \\
&= \int_0^t \frac{x^k}{k!}\, dx = \frac{t^{k+1}}{(k+1)!}\,,
\end{aligned}$$

    where the second but one equality uses the induction hypothesis.

– This shows (8) for any $k \geq 1$.

- Moreover, by (8) we can conclude that for any $k \in \mathbb{N}$

$$\begin{aligned} P(U_1 \leq \ldots \leq U_k,\, U_k > U_{k+1}) &= \int_0^1 P(U_1 \leq \ldots \leq U_k,\, U_k > x)\, dx \\ &= \int_0^1 \Big(P(U_1 \leq \ldots \leq U_k \leq 1) - P(U_1 \leq \ldots \leq U_k \leq x) \Big)\, dx \\ &= \int_0^1 \Big(\frac{1}{k!} - \frac{x^k}{k!} \Big)\, dx \\ &= \frac{1}{k!} - \frac{1}{(k+1)!} = \frac{k}{(k+1)!}\,. \end{aligned}$$

□

Remarks

- Let us assume that sufficiently many pseudo-random numbers $u_1, u_2 \ldots$ have been generated that are resulting in the n runs $w_1, \ldots, w_n$ according to (5) and (6).
- We choose r pairwise disjoint intervals $(a_1, b_1], \ldots, (a_r, b_r]$ on the positive real axis such that
  – the probabilities
  $$p_{0,j} = \sum_{k \in \mathbb{N} \cap (a_j, b_j]} \frac{k}{(k+1)!}\,, \qquad j = 1, \ldots, r$$
  are almost equal.
  – For these probabilities we consider the $(r-1)$–dimensional (hypothetical) vector $\mathbf{p}_0 = (p_{0,1}, \ldots, p_{0,r-1})$ and
  – the test statistic $T_n : \mathbb{R}^n \to [0, \infty)$ where
  $$T_n(w_1, \ldots, w_n) = \sum_{j=1}^{r} \frac{(Y_j(w_1, \ldots, w_n) - np_{0,j})^2}{np_{0,j}}\,,$$
  and $Y_j(w_1, \ldots, w_n) = \#\{i : 1 \leq i \leq n,\, a_j < w_i \leq b_j\}$ denotes the number of run lengths $w_1, \ldots, w_n$ belonging to class j.
- According to Theorem 3.3 for large n the hypothesis $H_0 : \mathbf{p} = \mathbf{p}_0$ will be rejected if $T(w_1, \ldots, w_n) > \chi^2_{r-1,1-\alpha}$. Note that this requires the generation of a sufficiently large number of pseudo–random numbers $u_1, u_2, \ldots$.

3.2 Transformation of Uniformly Distributed Random Numbers

- Based on standard pseudo–random numbers $u_1, u_2 \ldots$ that can be generated by methods like the linear congruential generator
  – it is possible to generate pseudo–random numbers $x_1, x_2 \ldots$ that can be regarded as realizations of random variables $X_1, X_2 \ldots$ having other than uniform distributions.
  – Examples are realizations $x_1, x_2, \ldots$ of exponentially, Poisson, binomially or normally distributed random variables $X_1, X_2, \ldots$.
- For this purpose one can apply algorithms like the so-called *inversion method* and *rejection–sampling*, whose basic ideas will be explained by some examples.
- A much more comprehensive discussion of these algorithms can be found e.g. in
  – L. Devroye (1986) *Nonuniform Random Variate Generation.* Springer, New York,
  – G.S. Fishman (1996) *Monte Carlo: Concepts, Algorithms and Applications.* Springer, New York,
  – C.P. Robert and G. Casella (1999) *Monte Carlo Statistical Methods.* Springer, New York.

3.2.1 Inversion Method

- The following property of the generalized inverse can be used as a basis for the generation of pseudo–random numbers $x_1, x_2 \ldots$ that can be regarded as realizations of random variables $X_1, X_2 \ldots$ whose distribution function $F : \mathbb{R} \to [0,1]$ is an arbitrary monotonically nondecreasing and right–continuous function such that $\lim_{x \to -\infty} F(x) = 0$ and $\lim_{x \to \infty} F(x) = 1$.
- Recall the following auxiliary result.
  - Let $F : \mathbb{R} \to [0,1]$ be an arbitrary distribution function. Then the function $F^{-1} : (0,1] \to \mathbb{R} \cup \{\infty\}$ where
  $$F^{-1}(y) = \inf\{x : F(x) \geq y\} \tag{9}$$
  is called the *generalized inverse* of the distribution function F.
  - For arbitrary $x \in \mathbb{R}$ and $y \in (0,1)$
  $$y \leq F(x) \qquad \text{if and only if} \qquad F^{-1}(y) \leq x\,, \tag{10}$$
  see Lemma WR-4.1.

Theorem 3.4

- *Let $U_1, U_2, \ldots$ be a sequence of independent and uniformly distributed random variables on $(0,1]$ and let $F : \mathbb{R} \to [0,1]$ be a distribution function.*
- *Then the random variables $X_1, X_2, \ldots$ where $X_i = F^{-1}(U_i)$ for $i = 1, 2, \ldots$ are independent and their distribution function is given by F.*

Proof

- The independence of $X_1, X_2, \ldots$ is an immediate consequence of the transformation theorem for independent random variables; see Theorem WR-3.18.
- Furthermore, (10) implies for arbitrary $x \in \mathbb{R}$ and $i \in \mathbb{N}$
$$P(X_i \leq x) = P\big(F^{-1}(U_i) \leq x\big) \overset{(10)}{=} P\big(U_i \leq F(x)\big) = F(x)\,.$$
□

Examples

- In the following we discuss some examples illustrating
  - how Theorem 3.4 can be used in order to generate pseudo-random numbers $x_1, x_2 \ldots$
  - that can be regarded as realizations of independent random variables $X_1, X_2 \ldots$ with a given distribution function $F : \mathbb{R} \to [0,1]$.
- These numbers are also referred to as F–distributed pseudo–random numbers $x_1, x_2 \ldots$,
  - in spite of the fact that the empirical distribution function $\widehat{F}_n$ of the sample $x_1, \ldots, x_n$
  - is only an approximation of F for large n.
- Note that Theorem 3.4 can only be applied *directly* if
  - the generalized inverse F^{-1} of F is given explicitly (i.e. by an analytical formula).

– Unfortunately, this situation is merely an exception.

1. *Exponential distribution*

- Let $\lambda > 0$ and $F : \mathbb{R} \to [0,1]$ be the distribution function of the Exp(λ)–distribution, i.e.

$$F(x) = \begin{cases} 1 - e^{-\lambda x} & \text{if } x \geq 0, \\ 0 & \text{if } x < 0. \end{cases}$$

- Then $F^{-1}(u) = -\lambda^{-1} \log(1-u)$ for all $u \in (0,1]$.

- By Theorem 3.4,
  - we have $X = -\lambda^{-1} \log U \sim \text{Exp}(\lambda)$ if U and hence also $1 - U$ are uniformly distributed on $(0,1]$
  - and the pseudo-random numbers $x_1, \ldots, x_n$ where

$$x_i = -\frac{\log u_i}{\lambda} \qquad \text{for } i = 1, \ldots, n$$

    can be regarded as realizations of Exp(λ)–distributed random variables
  - if $u_1, \ldots, u_n$ are realizations of independent and uniformly on $(0,1]$ distributed random variables $U_1, \ldots, U_n$.

2. *Erlang distribution*

- Let $\lambda > 0$, $r \in \mathbb{N}$ and let $F : \mathbb{R} \to [0,1]$ be the distribution function of the Erlang distribution, i.e., of the $\Gamma(\lambda, r)$–distribution where

$$F(x) = \begin{cases} \displaystyle\int_0^x \frac{\lambda e^{-\lambda v} (\lambda v)^{r-1}}{(r-1)!}\, dv & \text{if } x \geq 0, \\ 0 & \text{if } x < 0. \end{cases} \tag{11}$$

- Then the generalized inverse F^{-1} of F cannot be determined explicitly and therefore Theorem 3.4 cannot be applied *directly*.

- However, one can show that $X_1 + \ldots + X_r \sim \Gamma(\lambda, r)$ if the random variables $X_1, \ldots, X_r$ are independent and Exp(λ)–distributed.

- By Theorem 3.4
  - the pseudo–random numbers $y_1, \ldots, y_n$ where

$$y_i = x_{r(i-1)+1} + \ldots + x_{ri} = -\frac{\log\bigl(u_{r(i-1)+1} \cdot \ldots \cdot u_{ri}\bigr)}{\lambda} \qquad \text{for } i = 1, \ldots, n$$

    can be regarded as realizations of independent $\Gamma(\lambda, r)$–distributed random variables,
  - if $u_1, \ldots, u_{rn}$ are realizations of independent and uniformly distributed random variables on $(0,1]$.
  - In particular, for $\lambda = 1/2$ the pseudo–random numbers $y_1, \ldots, y_n$ can be regarded as realizations of a χ^2_{2r}–distributed random variable.

3. *Normal distribution*

- In order to generate normally distributed pseudo–random numbers one can apply the so–called *Box–Muller algorithm*, which also requires exponentially distributed pseudo–random numbers.
- Assume the random numbers U_1, U_2 to be independent and uniformly distributed on $(0, 1]$.
  - By Theorem 3.4, we get that $X = -2 \log U_1$ is an Exp(1/2)–distributed random variable and
  - the random vector (Y_1, Y_2) where

$$Y_1 = \sqrt{X} \cos(2\pi U_2)\,, \qquad Y_2 = \sqrt{X} \sin(2\pi U_2)$$

    turns out to be $\mathrm{N}(\mathbf{o}, \mathbf{I})$–distributed, i.e., Y_1, Y_2 are independent and $\mathrm{N}(0, 1)$–distributed random variables
  - as for arbitrary $y_1, y_2 \in \mathbb{R}$

$$\begin{aligned} P(Y_1 \le y_1,\, Y_2 \le y_2) &= P\Big(\sqrt{-2\log U_1}\cos(2\pi U_2) \le y_1,\, \sqrt{-2\log U_1}\sin(2\pi U_2) \le y_2\Big) \\ &= \frac{1}{2}\int_0^1 \int_0^\infty \mathbb{1}\Big(\sqrt{x}\cos(2\pi u) \le y_1,\, \sqrt{x}\sin(2\pi u) \le y_2\Big) e^{-x/2}\,dx\,du \\ &= \frac{1}{2\pi}\int_{-\infty}^{y_2}\int_{-\infty}^{y_1} e^{-(v^2+w^2)/2}\,dv\,dw \\ &= \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{y_1} e^{-v^2/2}\,dv\;\frac{1}{\sqrt{2\pi}}\int_{-\infty}^{y_2} e^{-w^2/2}\,dw\,, \end{aligned}$$

    where the last but one equality follows from the substitution

$$v = \sqrt{x}\cos(2\pi u)\,, \qquad w = \sqrt{x}\sin(2\pi u)$$

    whose functional determinant is π.
- The pseudo–random numbers $y_1, \ldots, y_{2n}$ where

$$y_{2k-1} = \sqrt{-2\log u_{2k-1}}\cos(2\pi u_{2k})\,, \qquad y_{2k} = \sqrt{-2\log u_{2k-1}}\sin(2\pi u_{2k}) \tag{12}$$

  - can thus be regarded as realizations of independent and $\mathrm{N}(0, 1)$–distributed random variables ,
  - if $u_1, \ldots, u_{2n}$ are realizations of independent and uniformly on $(0, 1]$ distributed random variables $U_1, \ldots, U_{2n}$.
- For arbitrary $\mu \in \mathbb{R}$ and $\sigma^2 > 0$ the pseudo-random numbers $y'_1, \ldots, y'_{2n}$ where $y'_i = \sigma(y_i + \mu)$ can be regarded as realizations of independent and $\mathrm{N}(\mu, \sigma^2)$–distributed random variables.

- Remarks
  - A faster algorithm for the generation of normally distributed pseudo-random numbers is obtained if additionally a method of rejection sampling is applied that will be introduced in Section 3.2.3.
  - This method avoids the relatively time-consuming computation of the trigonometric functions in (12).

3.2.2 Transformation Algorithms for Discrete Distributions

- If pseudo–random numbers $x_1, x_2 \ldots$ need to be generated
  - that can be regarded as realizations of discrete random variables $X_1, X_2 \ldots$
  - taking the values $a_0, a_1 \ldots \in \mathbb{R}$ with probabilities $p_j = P(X_i = a_j) \ge 0$ for $j = 0, 1, \ldots,$

- then it is sometimes advisable to proceed as follows:
  - Let U be a $(0,1]$–uniformly distributed random variable and let the random variable X be given by

$$X = \begin{cases} a_0 & \text{if } U < p_0, \\ a_1 & \text{if } p_0 \le U < p_0 + p_1, \\ \vdots & \\ a_j & \text{if } p_0 + \ldots + p_{j-1} \le U < p_0 + \ldots + p_j, \\ \vdots & \end{cases} \tag{13}$$

  - Then $P(X = a_j) = p_j$ for all $j = 0, 1, \ldots$.
- The pseudo–random numbers $x_1, \ldots, x_n$ where

$$x_i = \begin{cases} a_0 & \text{if } u_i < p_0, \\ a_1 & \text{if } p_0 \le u_i < p_0 + p_1, \\ \vdots & \\ a_j & \text{if } p_0 + \ldots + p_{j-1} \le u_i < p_0 + \ldots + p_j, \\ \vdots & \end{cases}$$

  - can thus be regarded as realizations of independent and $\mathbf{p}$-distributed random variables where $\mathbf{p} = (p_0, p_1, \ldots)^\top$,
  - if $u_1, \ldots, u_n$ are realizations of independent and uniformly distributed random variables on $(0,1]$.

Example *(Geometric distribution)*

- We consider the following values for a_j and the corresponding probabilities p_j.
  - Let $a_j = j$ for $j = 0, 1, \ldots$, and for $0 < p < 1$, $q = 1 - p$ let

$$p_j = \begin{cases} 0 & \text{if } j = 0, \\ p\, q^{j-1} & \text{if } j \ge 1. \end{cases}$$

  - Then, for all $j \ge 1$,

$$1 - (p_1 + \ldots + p_j) = p_{j+1} + p_{j+2} + \ldots = p \sum_{i=j}^{\infty} q^i = q^j \tag{14}$$

    and $p_j = q^{j-1} - q^j$.

- Furthermore, we consider the random variable

$$X = \left\lfloor \frac{\log U}{\log q} \right\rfloor + 1\,, \tag{15}$$

  where U is a $(0,1]$–uniformly distributed random variable and $\lfloor z \rfloor$ denotes the integer part of z.

- Then $P(X = j) = p\, q^{j-1}$ for all $j = 1, 2, \ldots$, i.e. $X \sim \mathrm{Geo}(p)$,

– as (14) and (15) imply

$$\begin{aligned} X &\overset{(15)}{=} \min\Big\{ j \geq 1 :\ j > \frac{\log U}{\log q} \Big\} \\ &= \min\Big\{ j \geq 1 :\ j \log q < \log U \Big\} \\ &= \min\Big\{ j \geq 1 :\ q^j < U \Big\} \\ &= \sum_{j=1}^{\infty} j\ \mathbb{1}\big(q^j < U \leq q^{j-1}\big) \\ &\overset{(14)}{=} \sum_{j=1}^{\infty} j\ \mathbb{1}\big(p_1 + \ldots + p_{j-1} \leq 1 - U < p_1 + \ldots + p_j\big)\,, \end{aligned}$$

– where the random variable $1 - U$ is also uniformly distributed on $(0, 1]$.

- The pseudo–random numbers $x_1, \ldots, x_n$ where

$$x_i = \left\lfloor \frac{\log u_i}{\log q} \right\rfloor + 1$$

– can thus be regarded as realizations of independent and geometrically distributed random variables $X_1, \ldots, X_n \sim \mathrm{Geo}(p)$
– if $u_1, \ldots, u_n$ are realizations of independent random variables $U_1, \ldots, U_n$ that are uniformly distributed on the interval $(0, 1]$.

For some discrete distributions there are *specific* transformation algorithms allowing the generation of pseudo–random numbers having this distribution.

Examples

1. *Poisson distribution* (with small expectation λ)
   - If $\lambda > 0$ is a small number, then the following procedure is appropriate to generate Poisson–distributed pseudo–random numbers
     – by transformation of exponentially distributed pseudo–random numbers (as in Section 3.2.1)
     – or directly based on $(0, 1]$–uniformly distributed pseudo–random numbers.
   - Let the random variables $X_1, X_2, \ldots$ be independent and $\mathrm{Exp}(\lambda)$–distributed.
     – If we consider the random variable $Y = \max\{k \geq 0 :\ X_1 + \ldots + X_k \leq 1\}$, formula (11) for the distribution function of the Erlang–distribution yields for all $j \geq 0$

$$\begin{aligned} P(Y = j) &= P(Y \geq j) - P(Y \geq j + 1) \\ &= P(X_1 + \ldots + X_j \leq 1) - P(X_1 + \ldots + X_{j+1} \leq 1) \\ &= \int_0^1 \frac{\lambda e^{-\lambda v} (\lambda v)^{j-1}}{(j-1)!}\, dv \ - \ \int_0^1 \frac{\lambda e^{-\lambda v} (\lambda v)^{j}}{j!}\, dv \\ &= \int_0^1 \frac{d}{dv} \Big(\frac{e^{-\lambda v} (\lambda v)^j}{j!} \Big)\, dv \\ &= \frac{e^{-\lambda} \lambda^j}{j!}\,. \end{aligned}$$

     – In other words we obtained $Y \sim \mathrm{Poi}(\lambda)$.

- The pseudo–random numbers $y_1, \ldots, y_n$ where

$$y_i = \max\{k \geq 0 : x_1 + \ldots + x_k \leq i\} - y_{i-1}\,, \qquad \forall\, i = 1, \ldots, n\,, \tag{16}$$

and

$$y_i = \max\{k \geq 0 : u_1 \cdot \ldots \cdot u_k \geq e^{-i\lambda}\} - y_{i-1}\,, \qquad \forall\, i = 1, \ldots, n\,, \tag{17}$$

where $y_0 = 0$ and $x_j = -\lambda^{-1} \log u_j$ for $j = 1, 2, \ldots$,
  - can thus be regarded as realizations of independent and Poi(λ)–distributed random variables,
  - if $x_1, x_2 \ldots$ are realizations of Exp(λ)–distributed random variables $X_1, X_2 \ldots$ and
  - if $u_1, \ldots, u_n$ are realizations of independent random variables $U_1, \ldots, U_n$ that are uniformly distributed on the interval $(0, 1]$, respectively.
- Remarks
  - As the expectation of the Poi(λ)–distribution is given by λ, the mean number of uniformly distributed pseudo–random numbers necessary in order to generate a new Poi(λ)–distributed pseudo-random number is also λ.
  - For large λ this effort can be reduced if one proceeds as follows.

2. *Poisson distribution* (with large expectation λ)
- If $\lambda > 0$ is large, $a_j = j$ and $p_j = e^{-\lambda}\lambda^j/j!$ for $j = 0, 1, \ldots$,
  - then the procedure based directly on the transformation formula (13) is more appropriate to generate Poi(λ)–distributed pseudo–random numbers,
  - The validity of the inequalities

$$U < p_0\,, \quad p_0 \leq U < p_0 + p_1,\ \ldots,\ p_0 + \ldots + p_{j-1} \leq U < p_0 + \ldots + p_j\,,\ \ldots \tag{18}$$

needs to be checked in the order defined below.
  - Note that the recursion formula

$$p_{j+1} = \frac{\lambda}{j+1}\, p_j\,, \qquad \forall\, j \geq 0\,,$$

is applied to calculate the sums $P_j = \sum_{k=0}^{j} p_k$ for $j \geq 0$.
- Let $\lfloor\lambda\rfloor > 0$ be the integer part of λ. Then it is firstly checked if $U < P_{\lfloor\lambda\rfloor}$.
  - If this inequality holds it is checked if $U < P_{\lfloor\lambda\rfloor-1}, U < P_{\lfloor\lambda\rfloor-2}, \ldots$ where we define $X = \min\{k : U < P_k\}$.
  - If the inequality $U < P_{\lfloor\lambda\rfloor}$ does not hold then it is checked if $U < P_{\lfloor\lambda\rfloor+1}, U < P_{\lfloor\lambda\rfloor+2}, \ldots$ and we also define $X = \min\{k : U < P_k\}$.
- For the expectation $\mathbb{E}\,V$ of the necessary number V of checking steps we obtain the approximation

$$\begin{aligned} \mathbb{E}\,V &\approx 1 + \mathbb{E}\,|X - \lambda| \\ &= 1 + \sqrt{\lambda}\mathbb{E}\left(\frac{|X-\lambda|}{\sqrt{\lambda}}\right) \\ &\approx 1 + 0.798\,\sqrt{\lambda}\,, \end{aligned}$$

  - where the last approximation uses the fact that the random variable $(X - \lambda)/\sqrt{\lambda}$ is approximately N(0, 1)-distributed for large λ for the following reasons.
  - As the Poisson distribution is stable under convolutions, i.e.,

$$\mathrm{Poi}(\lambda_1) * \ldots * \mathrm{Poi}(\lambda_n) = \mathrm{Poi}\Big(\sum_{k=1}^{n} \lambda_i\Big)\,,$$

the random variable $X \sim \mathrm{Poi}(\lambda)$ can be viewed as the sum $\sum_{i=1}^{n} X_i$ of n independent and Poi(λ/n)–distributed random variables X_i. The last approximation then follows from the central limit theorem for sums of independent and identically distributed random variables; see Theorem WR-5.16.

- We observe that
  - for increasing λ the mean number of checking steps only grows with rate $\sqrt{\lambda}$ if this simulation procedure is applied,
  - whereas for the formerly discussed method generating $\mathrm{Poi}(\lambda)$–distributed pseudo–random numbers the necessary number of standard pseudo–random numbers grows linearly in λ.

3. *Binomial distribution*
   - For the generation of binomially distributed pseudo–random numbers one can proceed similarly to the Poisson case.
     - For arbitrary but fixed numbers $n \in \mathbb{N}$ and $p \in (0,1)$ where $q = 1-p$ let

$$a_j = j \qquad \text{and} \qquad p_j = \frac{n!}{j!\,(n-j)!}\, p^j\, q^{n-j}\,, \qquad \forall\, j = 0, 1, \ldots, n\,.$$

     - For $j = 0, 1, \ldots, n$ the sums $P_j = \sum_{k=0}^{j} p_k$ are calculated via the recursion formula

$$p_{j+1} = \frac{n-j}{j+1}\,\frac{p}{q}\,p_j\,, \qquad \forall\, j = 0, 1, \ldots, n-1$$

   - If $np > 0$ is small, then
     - the validity of the inequalities (18) is checked in the natural order
     - starting at $U < p_0$ and defining $X = \min\{k : U < P_k\}$.
   - If np is large,
     - then it is more efficient to check the validity of the inequalities (18) in the following order. It is firstly checked if $U < P_{\lfloor np \rfloor}$.
     - If this inequality holds it is checked if $U < P_{\lfloor np \rfloor - 1}, U < P_{\lfloor np \rfloor - 2}, \ldots$ where we also define $X = \min\{k : U < P_k\}$.
     - If the inequality $U < P_{\lfloor np \rfloor}$ does not hold it is checked if $U < P_{\lfloor np \rfloor + 1}, U < P_{\lfloor np \rfloor + 2}, \ldots$ where we again define $X = \min\{k : U < P_k\}$.

3.2.3 Acceptance-Rejection Method

- In this section we discuss another method for the generation of pseudo–random numbers $y_1, y_2, \ldots$
  - that can be regarded as realizations of independent and identically distributed random variables $Y_1, Y_2 \ldots$. Their distribution function is assumed to be given; it is denoted by G.
  - This method also requires a sequence of independent and identically distributed pseudo–random numbers $x_1, x_2, \ldots$, but we abandon the condition that they need to be uniformly distributed on $(0,1]$.
  - The only condition we impose on their distribution function F is that G needs to be *absolutely continuous* with respect to F with bounded density $g(x) = dG(x)/dF(x)$,
  - i.e., for some constant $c > 0$, we have

$$g(x) \le c \qquad \text{and} \qquad G(y) = \int_{-\infty}^{y} g(x)\, dF(x)\,, \qquad \forall\, x, y \in \mathbb{R}\,. \tag{19}$$

- First of all we consider the discrete case.
  - Let $a_j = j$ for all $j = 0, 1, \ldots$, and let $\mathbf{p} = (p_0, p_1, \ldots)^\top$ and $\mathbf{q} = (q_0, q_1, \ldots)^\top$ be two arbitrary probability functions such that for all $j = 0, 1, \ldots$ $p_j = 0$ implies $q_j = 0$.
  - Let $X : \Omega \to \{0, 1, \ldots\}$ be a random variable $P(X = j) = p_j$ for all $j = 0, 1, \ldots$,

– and let $c > 0$ be a positive number

$$\Big(g(j) = \Big) \qquad \frac{q_j}{p_j} \le c \qquad \text{for all } j \ge 0 \text{ such that } p_j > 0. \tag{20}$$

Theorem 3.5

- *Let $(U_1, X_1), (U_2, X_2), \ldots$ be a sequence of independent and identically distributed random vectors whose components are independent. Furthermore, let U_i be a $(0,1]$–uniformly distributed random variable and X_i be distributed according to $\mathbf{p}$.*
- *Then*
  - *the random variable*
$$I = \min\Big\{ k \ge 1 : U_k < \frac{q_{X_k}}{c\, p_{X_k}} \Big\} \tag{21}$$
  is geometrically distributed with expectation c, i.e., $I \sim \mathrm{Geo}(c^{-1})$,
  - *and the random variable $Y = X_I$ is distributed according to $\mathbf{q}$.*

Proof

- By the definition of I given in (21), we obtain for all $j \ge 1$

$$\begin{aligned} P(I = j) &= P\Big(U_1 \ge \frac{q_{X_1}}{c\, p_{X_1}}, \ldots, U_{j-1} \ge \frac{q_{X_{j-1}}}{c\, p_{X_{j-1}}}, U_j < \frac{q_{X_j}}{c\, p_{X_j}}\Big) \\ &= P\Big(U_1 \ge \frac{q_{X_1}}{c\, p_{X_1}}\Big) \ldots P\Big(U_{j-1} \ge \frac{q_{X_{j-1}}}{c\, p_{X_{j-1}}}\Big)\, P\Big(U_j < \frac{q_{X_j}}{c\, p_{X_j}}\Big) \\ &= p\, q^{j-1}, \end{aligned}$$

  – where $q = 1 - p$ and

$$\begin{aligned} p &= P\Big(U_1 < \frac{q_{X_1}}{c\, p_{X_1}}\Big) \\ &= \sum_{k:\, p_k > 0} P\Big(U_1 < \frac{q_{X_1}}{c\, p_{X_1}} \mid X_1 = k\Big)\, P(X_1 = k) \\ &= \sum_{k:\, p_k > 0} P\Big(U_1 < \frac{q_k}{c\, p_k}\Big)\, p_k \\ &= \sum_{k:\, p_k > 0} \frac{q_k}{c\, p_k}\, p_k = \frac{1}{c}. \end{aligned}$$

  – This shows $I \sim \mathrm{Geo}(c^{-1})$.
- Furthermore, for any $j \ge 1$ such that $p_j > 0$, we get that

$$\begin{aligned} P(Y = j) &= P(X_I = j) = \sum_{k=1}^{\infty} P(X_I = j,\, I = k) \\ &= \sum_{k=1}^{\infty} P(X_k = j,\, I = k) = \sum_{k=1}^{\infty} P(X_k = j)\, q^{k-1}\, P\Big(U_k \le \frac{q_j}{c p_j}\Big) \\ &= \sum_{k=1}^{\infty} p_j\, q^{k-1}\, \frac{q_j}{c p_j} = \frac{q_j}{c} \sum_{k=1}^{\infty} q^{k-1} \\ &= \frac{q_j}{c}\, \frac{1}{1-q} = q_j, \end{aligned}$$

and for all $j \geq 1$ such that $p_j = 0$

$$P(Y = j) \;=\; \sum_{k=1}^{\infty} P(X_k = j,\, I = k) \;\leq\; \sum_{k=1}^{\infty} P(X_k = j) \;=\; 0\,. \qquad \square$$

Remarks

- Theorem 3.5 implies that the mean number of F–distributed pseudo-random numbers necessary to obtain a G–distributed random number is c.
- In case there are several alternatives for the choice of the the distribution function F,
  - possessing equally nice properties with respect to the generation of F–distributed pseudo–random numbers,
  - then one should choose the distribution function with the smallest c.
- Furthermore, as a consequence of Theorem 3.5,
  - the values $g(x)$ and $g(j)$ of the density in (19) and (20), respectively need only be known up to a constant factor.

In the general (i.e. not necessarily discrete) case one can proceed in a similar way. The following result will serve as foundation for constructing acceptance–rejection algorithms.

Theorem 3.6

- *Let $F, G : \mathbb{R} \to [0,1]$ be two arbitrary distribution functions such that* (19) *holds.*
- *Let $(U_1, X_1), (U_2, X_2), \ldots$ be a sequence of independent and identically distributed random vectors whose components are independent. Furthermore, let U_i be a $(0,1]$–uniformly distributed random variable and X_i be distributed according to F.*
- *Then the random variable*

$$I = \min\Big\{k \geq 1 : U_k < \frac{g(X_k)}{c}\Big\} \tag{22}$$

is geometrically distributed with expectation c, i.e., $I \sim \mathrm{Geo}(c^{-1})$ and the random variable $Y = X_I$ is distributed according to G.

Proof

- Similarly to the proof of Theorem 3.5 we obtain $P(I = j) = p\,q^{j-1}$ for any $j \geq 1$ where

$$\begin{aligned} p &= P\Big(U_1 < \frac{g(X_1)}{c}\Big) = \int_{\mathbb{R}} P\Big(U_1 < \frac{g(X_1)}{c} \mid X_1 = x\Big)\, dF(x) \\ &= \int_{\mathbb{R}} P\Big(U_1 < \frac{g(x)}{c}\Big)\, dF(x) = \int_{\mathbb{R}} \frac{g(x)}{c}\, dF(x) = \frac{1}{c}\,. \end{aligned}$$

- Furthermore, for all $y \in \mathbb{R}$ we have

$$\begin{aligned} P(Y \leq y) &= P(X_I \leq y) \;=\; \sum_{k=1}^{\infty} P(X_I \leq y,\, I = k) = \sum_{k=1}^{\infty} P(X_k \leq y,\, I = k) \\ &= \sum_{k=1}^{\infty} \int_{-\infty}^{y} P(I = k \mid X_k = v)\, dF(v) = \sum_{k=1}^{\infty} q^{k-1} \int_{-\infty}^{y} P\Big(U_k < \frac{g(v)}{c}\Big)\, dF(v) \\ &= \frac{1}{1-q} \int_{-\infty}^{y} \frac{g(v)}{c}\, dF(v) = \int_{-\infty}^{y} g(v) dF(v) \;=\; G(y)\,, \end{aligned}$$

  where $1 - q = p = c^{-1}$. $\square$

In the same way we obtain the following vectorial version of Theorem 3.6.

Theorem 3.7

- *Let $m \geq 1$ be an arbitrary but fixed natural number and let $F, G : \mathbb{R}^m \to [0,1]$ be two arbitrary distribution functions (of m–dimensional random vectors) and let $c > 0$ be a constant such that*

$$g(\mathbf{x}) \leq c \qquad \text{and} \qquad G(\mathbf{y}) = \int_{(-\infty,\mathbf{y}]} g(\mathbf{x})\, dF(\mathbf{x})\,, \qquad \forall\, \mathbf{x}, \mathbf{y} \in \mathbb{R}^m\,. \tag{23}$$

- *Let $(U_1, \mathbf{X}_1), (U_2, \mathbf{X}_2), \ldots$ be a sequence of independent and identically distributed random vectors whose components are also independent. Furthermore, let U_i be a $(0,1]$–uniformly distributed random variable and $\mathbf{X}_i$ be distributed according to F.*

- *Then the random variable*

$$I = \min\Big\{k \geq 1 : U_k < \frac{g(\mathbf{X}_k)}{c}\Big\} \tag{24}$$

is geometrically distributed with expectation c, i.e., $I \sim \text{Geo}(c^{-1})$ and the random vector $\mathbf{Y} = \mathbf{X}_I$ is distributed according to G.

Examples

1. *Uniform distribution on bounded Borel sets*
   - Let the random vector $\mathbf{X} : \Omega \to \mathbb{R}^m$ (with distribution function F) be uniformly distributed on the square $(-1,1]^m$ and let $B \in \mathcal{B}((-1,1]^m$ be an arbitrary Borel subset of $(-1,1]^m$ of positive Lebesgue measure $|B|$.
   - Then the distribution function $G : \mathbb{R}^m \to [0,1]$ given by

$$G(\mathbf{y}) = \int_{(-\infty,\mathbf{y}]} \frac{\mathbb{1}(\mathbf{x} \in B)}{|B|}\, dF(\mathbf{x})\,, \qquad \forall\, \mathbf{y} \in \mathbb{R}^m$$

     is absolutely continuous with respect to F and we obtain for the (Radon–Nikodym) density $g : \mathbb{R}^m \to [0,\infty)$ that

$$g(\mathbf{x}) = \frac{\mathbb{1}(\mathbf{x} \in B)}{|B|} \leq c = |B|^{-1} \qquad \text{and} \qquad \frac{g(\mathbf{x})}{c} = \mathbb{1}(\mathbf{x} \in B)\,, \qquad \forall\, \mathbf{x} \in \mathbb{R}^m\,.$$

   - By Theorem 3.7 we can now in the following way generate pseudo–random vectors $\mathbf{y}_1, \mathbf{y}_2, \ldots$ that are uniformly distributed on B.
     1. Generate m pseudo–random numbers $u_1, \ldots, u_m$ that are uniformly distributed on the interval $(0,1]$.
     2. If $(2u_1 - 1, \ldots, 2u_m - 1)^\top \notin B$, then return to step 1.
     3. Otherwise put $\mathbf{y} = (2u_1 - 1, \ldots, 2u_m - 1)^\top$.

2. *Normal distribution*
   - As an alternative to the Box-Muller algorithm discussed in Section 3.2.1 we will now introduce another method to generate normally distributed pseudo–random numbers,
     - which is often called the *polar method*.
     - Notice that the polar method avoids calculating the trigonometric functions in (12).
   - Let the random vector (V_1, V_2) be uniformly distributed on the unit circle B, where $B = \{(x_1, x_2) \in \mathbb{R}^2 : x_1^2 + x_2^2 \leq 1\}$.

- Then, the random vector (Y_1, Y_2) where

$$Y_1 = \sqrt{-2\log(V_1^2+V_2^2)}\;\frac{V_1}{\sqrt{V_1^2+V_2^2}}\,, \qquad Y_2 = \sqrt{-2\log(V_1^2+V_2^2)}\;\frac{V_2}{\sqrt{V_1^2+V_2^2}}$$

  is $\mathrm{N}(\mathbf{o}, \mathbf{I})$-distributed, i.e., Y_1, Y_2 are independent and $\mathrm{N}(0,1)$-distributed random variables. This can be seen as follows.
  - By the substitution

$$v_1 = r\cos\theta\,, \qquad v_2 = r\sin\theta\,,$$

  - i.e. by a transformation into polar coordinates we obtain for arbitrary $y_1, y_2 \in \mathbb{R}$

$$\begin{aligned} & P(Y_1 \le y_1,\, Y_2 \le y_2) \\ &= \frac{1}{\pi}\int_B \mathbb{1}\Big(\frac{v_1\sqrt{-2\log(v_1^2+v_2^2)}}{\sqrt{v_1^2+v_2^2}} \le y_1\,,\; \frac{v_2\sqrt{-2\log(v_1^2+v_2^2)}}{\sqrt{v_1^2+v_2^2}} \le y_2\Big)\, d(v_1,v_2) \\ &= \frac{1}{\pi}\int_0^{2\pi}\int_0^1 r\,\mathbb{1}\Big(\sqrt{-2\log(r^2)}\,\cos\theta \le y_1\,,\; \sqrt{-2\log(r^2)}\,\sin\theta \le y_2\Big)\, dr\, d\theta \\ &= \frac{1}{2}\,\frac{1}{2\pi}\int_0^{2\pi}\int_0^{\infty} \mathbb{1}\Big(\sqrt{x}\cos\theta \le y_1,\, \sqrt{x}\sin\theta \le y_2\Big)\, e^{-x/2}\, dx\, d\theta\,, \end{aligned}$$

  - where the last equality results from the following substitution:

$$x = -2\log(r^2) \qquad \text{bzw.} \qquad -\,\frac{1}{2}\,e^{-x/2}\,dx = 2r\,dr\,.$$

  - By the same argument that was used to verify formula (12) in Section 3.2.1 one can check that the last term can be written as the product $F(y_1)F(y_2)$ of two $\mathrm{N}(0,1)$–distribution functions.
- The pseudo–random numbers $y_1, \ldots, y_{2n}$ with

$$y_{2k-1} = \sqrt{-2\log(v_{2k-1}^2+v_{2k}^2)}\;\frac{v_{2k-1}}{\sqrt{v_{2k-1}^2+v_{2k}^2}}\,, \qquad y_{2k} = \sqrt{-2\log(v_{2k-1}^2+v_{2k}^2)}\;\frac{v_{2k}}{\sqrt{v_{2k-1}^2+v_{2k}^2}}$$

  - can thus be regarded as realizations of independent and $\mathrm{N}(0,1)$–distributed random variables,
  - if $(v_1, v_2), \ldots, (v_{2n-1}, v_{2n})$ are realizations of the random variables $(V_1, V_2), \ldots, (V_{2n-1}, V_{2n})$ that are independent and uniformly distributed on the unit circle

$$B = \{(x_1, x_2) \in \mathbb{R}^2 : x_1^2 + x_2^2 \le 1\}\,.$$

  - Those can be generated via acceptance–rejection sampling as explained in the last example.

3.2.4 Quotients of Uniformly Distributed Random Variables

In many cases random variables having absolutely continuous distributions can be represented as quotients of uniformly distributed random variables.

- Combined with acceptance–rejection sampling (see Section 3.2.3) this yields another type of simulation algorithm.
- The mathematical foundation for this type of algorithm is the following transformation theorem for the density of absolutely continuous random vectors.

Theorem 3.8

- *Let* $\mathbf{X} = (X_1, \dots, X_n)^\top : \Omega \to \mathbb{R}^n$ *be an absolutely continuous random vector with joint density* $f_{\mathbf{X}} : \mathbb{R}^n \to [0, \infty)$ *and let* $\boldsymbol{\varphi} = (\varphi_1, \dots, \varphi_n) : \mathbb{R}^n \to \mathbb{R}^n$ *be a Borel-measurable function with continuous partial derivatives* $\partial\varphi_i/\partial x_j(x_1, \dots, x_n)$.
- *Let now the Borel-set* $C \in \mathcal{B}(\mathbb{R}^n)$ *be picked in a way such that*

$$\{\mathbf{x} \in \mathbb{R}^n : f_{\mathbf{X}}(\mathbf{x}) \neq 0\} \subset C$$

and

$$\det\Big(\frac{\partial\varphi_i}{\partial x_j}(x_1, \dots, x_n)\Big) \neq 0\,, \qquad \forall \mathbf{x} = (x_1, \dots, x_n) \in C\,,$$

which ensures that the restriction $\boldsymbol{\varphi} : C \to D$ *of* $\boldsymbol{\varphi}$ *to the set* C *is a bijection where* $D = \{\boldsymbol{\varphi}(\mathbf{x}) : \mathbf{x} \in C\}$ *denotes the image of* φ.

- *Let* $\boldsymbol{\varphi}^{-1} = (\varphi_1^{-1}, \dots, \varphi_n^{-1}) : D \to C$ *be the inverse of* $\boldsymbol{\varphi} : C \to D$.
- *Then the random vector* $\mathbf{Y} = \boldsymbol{\varphi}(\mathbf{X})$ *is also absolutely continuous and the density* $f_{\mathbf{Y}}(\mathbf{y})$ *of* $\mathbf{Y}$ *is given by*

$$f_{\mathbf{Y}}(\mathbf{y}) = \begin{cases} f_{\mathbf{X}}(\varphi_1^{-1}(\mathbf{y}), \dots, \varphi_n^{-1}(\mathbf{y})) \,\Big|\det\Big(\dfrac{\partial\varphi_i^{-1}}{\partial y_j}(y_1, \dots, y_n)\Big)\Big| & \text{if } \mathbf{y} = (y_1, \dots, y_n) \in D, \\ 0 & \text{if } \mathbf{y} \notin D. \end{cases} \tag{25}$$

which is the same as

$$f_{\mathbf{Y}}(\mathbf{y}) = \begin{cases} f_{\mathbf{X}}(\varphi_1^{-1}(\mathbf{y}), \dots, \varphi_n^{-1}(\mathbf{y})) \,\Big|\det\Big(\dfrac{\partial\varphi_i}{\partial x_j}(\boldsymbol{\varphi}^{-1}(y_1, \dots, y_n))\Big)\Big|^{-1} & \text{if } \mathbf{y} = (y_1, \dots, y_n) \in D, \\ 0 & \text{if } \mathbf{y} \notin D. \end{cases} \tag{26}$$

From Theorem 3.8 we obtain the following result concerning the representation of absolutely continuous random variables as quotients of uniformly distributed random variables.

Theorem 3.9

- *Let* $f' : \mathbb{R} \to [0, \infty)$ *be Borel measurable and bounded such that*

$$0 < \int_{\mathbb{R}} f'(x)\,dx < \infty \qquad \text{and} \qquad \sup_{x \in \mathbb{R}} |x| \sqrt{f'(x)} < \infty\,. \tag{27}$$

- *Let the random vector* (V_1, V_2) *be uniformly distributed on the (bounded) Borel set*

$$B = \{(x_1, x_2) \in \mathbb{R}^2 : 0 < x_1 < \sqrt{f'(x_2/x_1)}\}\,. \tag{28}$$

- *Then the quotient* V_2/V_1 *is an absolutely continuous random variable with density* $f : \mathbb{R} \to [0, \infty)$ *where*

$$f(x) \;=\; \frac{f'(x)}{\int_{\mathbb{R}} f'(y)\,dy}\,, \qquad \forall\, x \in \mathbb{R}\,.$$

Proof

- Notice that (27) implies that the Borel set B defined in (28) is bounded, i.e. $0 < |B| < \infty$. This is due to the following reasons.
  - For $x_2 > 0$ the inequality $x_1 < \sqrt{f'(x_2/x_1)}$ is equivalent to $x_2 < x_2/x_1\sqrt{f'(x_2/x_1)}$.

– If on the other hand $x_2 < 0$ it is equivalent to $x_2 > x_2/x_1\sqrt{f'(x_2/x_1)}$.
– Therefore

$$B \subset [0, \sup_{x\in\mathbb{R}} \sqrt{f'(x)}] \times [\inf_{x<0} x\sqrt{f'(x)}, \sup_{x>0} x\sqrt{f'(x)}] \tag{29}$$

and

$$B \subset [0, \sup_{x\in\mathbb{R}} \sqrt{f'(x)}] \times [-\sup_{x\in\mathbb{R}} |x|\sqrt{f'(x)}, \sup_{x\in\mathbb{R}} |x|\sqrt{f'(x)}] .$$

- The following joint density $f_{(V_1,V_2)}(v_1, v_2)$ of the random vector (V_1, V_2) is thus well defined

$$f_{(V_1,V_2)}(v_1, v_2) = |B|^{-1} \mathbb{1}\big(0 < v_1 < \sqrt{f'(v_2/v_1)}\big) .$$

- The function $\boldsymbol{\varphi} : C \to C$ where $C = (0, \infty) \times \mathbb{R}$ and $\varphi(x_1, x_2) = (x_1, x_2/x_1)$
  – is a bijection of C onto itself
  – and its functional determinant is given by

$$\det\Big(\frac{\partial\varphi_i}{\partial x_j}(x_1, x_2)\Big) \;=\; \det\begin{pmatrix} 1 & 0 \\ -\dfrac{x_2}{x_1^2} & \dfrac{1}{x_1} \end{pmatrix} \;=\; \frac{1}{x_1} , \qquad \forall\, (x_1, x_2) \in C .$$

- Theorem 3.8 therefore implies
  – that the density $f_{(V_1,V_2/V_1)}(y_1, y_2)$ of the random vector $(V_1, V_2/V_1)^\top$ has the following form:

$$f_{(V_1,V_2/V_1)}(y_1, y_2) = |B|^{-1} y_1 \mathbb{1}\big(0 < y_1 < \sqrt{f'(y_2)}\big)$$

  – Moreover, the marginal density $f_{V_2/V_1}(y_2)$ of the second component V_2/V_1 of $(V_1, V_2/V_1)^\top$ is given by

$$f_{V_2/V_1}(y_2) \;=\; |B|^{-1} \int_0^{\sqrt{f'(y_2)}} y_1\, dy_1 \;=\; \frac{f'(y_2)}{2\,|B|} .$$ □

Example *(Normal distribution)*

- Theorem 3.9 yields a third method to generate $\mathrm{N}(0, 1)$–distributed pseudo-random numbers (as an alternative to the Box–Muller algorithm from Section 3.2.1 and the polar method explained in Section 3.2.3).
- Consider the function $f' : \mathbb{R} \to [0, \infty)$ where $f'(x) = \exp(-x^2/2)$ for all $x \in \mathbb{R}$. For the bounds in (29) we obtain:

$$\sup_{x\in\mathbb{R}} \sqrt{f'(x)} = 1 , \qquad \inf_{x<0} x\sqrt{f'(x)} = -\sqrt{2/e} , \qquad \sup_{x>0} x\sqrt{f'(x)} = \sqrt{2/e} .$$

- According to Theorem 3.9 a sequence $x_1, x_2, \ldots$ of $\mathrm{N}(0, 1)$–distributed pseudo–random numbers can now be generated as follows.
  1. Generate a $(0, 1]$–uniformly distributed pseudo-random number u and a $(-\sqrt{2/e},\ \sqrt{2/e}]$–uniformly distributed pseudo–random number v.
  2. If $u \geq \sqrt{\exp(-v^2/(2u^2))}$, i.e., if $\log u \geq -v^2/(4u^2) \Leftrightarrow v^2 \geq -4u^2 \log u$, then return to step 1.
  3. Otherwise put $x = v/u$.

3.3 Simulation Methods Based on Markov Chains

- Let E be an arbitrary finite set, e.g. a family of possible digital binary or greyscale images $\mathbf{x} = (x(v),\, v \in V)$,
  - where V is a finite set of pixels
  - and every pixel $v \in V$ in the observation window V gets mapped to a greyscale value $x(v) \geq 0$,
  - resulting in a „matrix" $(x(v),\, v \in V)$ that has certain properties.
- Let $\boldsymbol{\pi} : E \to (0, 1)$ be an arbitrary probability function, i.e.

$$\sum_{\mathbf{x} \in E} \pi_{\mathbf{x}} = 1 \qquad \text{and} \qquad \pi_{\mathbf{x}} > 0\,, \quad \forall\, \mathbf{x} \in E\,.$$

- If the number $|E|$ of elements in E is large,
  - the inversion method discussed in Section 3.2 as well as acceptance-rejection sampling are *inefficient* algorithms
  - for the generation of pseudo–random numbers $\mathbf{x}_1, \mathbf{x}_2, \ldots$ in E that are distributed according to $\boldsymbol{\pi}$.

Remarks

- An alternative simulation method is based on
  - constructing a Markov chain $\mathbf{X}_0, \mathbf{X}_1, \ldots$ with state space E
  - and an (appropriately chosen) irreducible and aperiodic transition matrix $\mathbf{P}$,
  - such that $\boldsymbol{\pi}$ is the ergodic limit distribution of the Markov chain.
- For sufficiently large n
  - $\mathbf{X}_n$ is approximately $\boldsymbol{\pi}$–distributed
  - and can thus serve as an efficient tool for the generation of (approximately) $\boldsymbol{\pi}$–distributed pseudo–random elements in E.
- Therefore one also uses the term *Markov–Chain–Monte–Carlo Simulation* (MCMC).

3.3.1 Example: Hard–Core Model

(see O. Häggström (2002) *Finite Markov Chains and Algorithmic Applications.* CU Press, Cambridge)

- We consider a connected graph $G = (V, K)$
  - with finitely many vertices $V = \{v_1, \ldots, v_{|V|}\}$
  - and a certain set $K \subset V^2$ of edges, each of them connecting two vertices.
- Each vertex in V gets either mapped to 0 or 1,
  - where we consider the following set $E \subset \{0, 1\}^{|V|}$ of *admissible configurations*,
  - characterized by the property that pairs of connected vertices are not allowed to obtain the value 1 on both vertices; see also Figure 6.
- As we want to pick one of the admissible configurations $\mathbf{x} \in E$ „at random" we consider the (discrete) uniform distribution $\boldsymbol{\pi}$ on E, i.e.

$$\pi_{\mathbf{x}} = \frac{1}{\ell}\,, \qquad \forall\, \mathbf{x} \in E\,, \tag{30}$$

  where $\ell = |E|$ denotes the number of all admissible configurations.

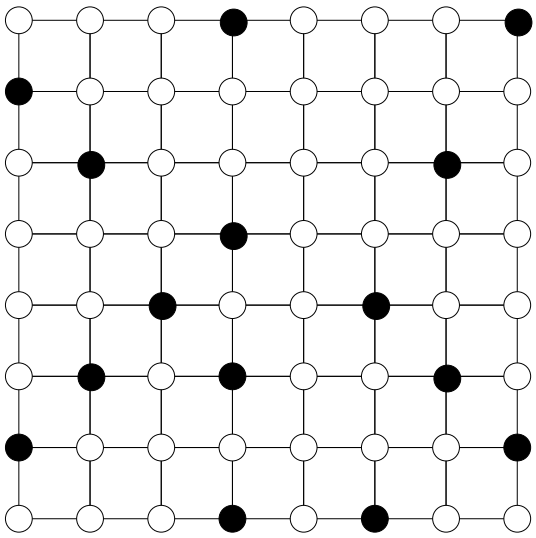


Figure 6: Lattice G of size 8×8, black pixels are corresponding to value 1

- If the numbers $|V|$ and $|K|$ of vertices and edges, respectively, of the connected graph $G = (V, K)$ are large,
  - the explicit description of the admissible configurations E will cause difficulties.
  - Therefore, the number ℓ of all admissible configurations is typically unknown.
  - Consequently, formula (30) cannot be applied directly for the simulation of „randomly" picked admissible configurations.

MCMC Simulation Algorithm

- Alternatively, a Markov chain $\mathbf{X}_0, \mathbf{X}_1, \ldots$ can be constructed
  - that has the state space E and an (appropriately chosen) irreducible and aperiodic transition matrix $\mathbf{P}$,
  - such that the ergodic limit distribution $\boldsymbol{\pi}$ is given by (30).
- Then we generate a path $\mathbf{x}_0, \mathbf{x}_1, \ldots$ of the Markov chain using the recursive construction of Markov chains that has been discussed in Section 2.1.3:
  1. Pick an admissible initial configuration $\mathbf{x}_0 \in E$.
  2. Pick an arbitrary vertex $v \in V$ „at random" and toss a fair coin.
  3. If the event „head" occurs and if $x_n(w) = 0$ for all vertices $w \in V$ connected to $v \in V$, then set $x_{n+1}(v) = 1$; else set $x_{n+1}(v) = 0$.
  4. The values of all edges $w \neq v$ are not changed, i.e., $x_{n+1}(w) = x_n(w)$ for all $w \neq v$.

Remarks

- In order to implement steps 2 – 4 of this algorithm, the update function $\varphi : E \times [0, 1] \to E$ considered in (2.19) needs to be specified.
- For this purpose the unit interval $(0, 1]$ is divided into $2|V|$ parts of equal length $1/2|V|$
  - that correspond to the events (v_1, head), (v_1, tail), …, ($v_{|V|}$, head), ($v_{|V|}$, tail).

– Then $\mathbf{x}' = \varphi(\mathbf{x}, z)$ where

$$x'(v_i) = \begin{cases} 1 & \text{if } z \in \Big(\frac{2i-2}{2|V|}\,,\,\frac{2i-1}{2|V|}\Big] \text{ and } x(w) = 0 \text{ for all vertices } w \in V \\ & \text{connected to } v \in V, \\ 0 & \text{if } z \in \Big(\frac{2i-1}{2|V|}\,,\,\frac{2i}{2|V|}\Big] \text{ or } z \in \Big(\frac{2i-2}{2|V|}\,,\,\frac{2i-1}{2|V|}\Big] \text{ and } x(w) = 0 \\ & \textit{not} \text{ for all vertices } w \in V \text{ connected to } v \in V, \\ x(v_i) & \text{if } z \notin \Big(\frac{2i-2}{2|V|}\,,\,\frac{2i}{2|V|}\Big]. \end{cases} \tag{31}$$

- The following theorem implies that for sufficiently large n the return $\mathbf{x}_n = (x_n(v),\, v \in V)$ of the algorithm can be regarded as a configuration that has been approximately picked according to the distribution $\boldsymbol{\pi}$.

Theorem 3.10

- *Let* $\mathbf{P} = (p_{\mathbf{x}\mathbf{x}'})$ *be the transition matrix of the MCMC algorithm simulating the hard core model in* (31) *and let* $\boldsymbol{\pi}$ *be the probability function given in* (30).
- *Then* $\mathbf{P}$ *is irreducible and aperiodic and the pair* $(\mathbf{P}, \boldsymbol{\pi})$ *is reversible.*

Proof

- In order to show that $\mathbf{P} = (p_{\mathbf{x}\mathbf{x}'})$ is aperiodic it suffices to note that all diagonal elements $p_{\mathbf{x}\mathbf{x}}$ of $\mathbf{P}$ are positive.
- The following considerations show that $\mathbf{P}$ is also irreducible.
  - Let $\mathbf{x}, \mathbf{x}' \in E$ be two admissible configurations and let $m(\mathbf{x})$ and $m(\mathbf{x}')$ denote the number of vertices set to 1 in $\mathbf{x}$ and $\mathbf{x}'$, respectively.
  - First we observe that the transition $\mathbf{x} \longrightarrow \mathbf{x}_0$ to the „zero configuration" $\mathbf{x}_0 \in E$ is possible in $m(\mathbf{x})$ steps with positive probability, where $\mathbf{x}_0(v) = 0$ for all $v \in V$.
  - For this transition all vertices that were originally set to 1 are subsequently set to 0. Each of these steps happens with positive probability.
  - Afterwards, in a similar way the chain can transfer from the „zero state" $\mathbf{x}_0$ to state $\mathbf{x}'$ taking $m(\mathbf{x}')$ steps where each of them happens again with positive probability.
  - Thus the transition $\mathbf{x} \longrightarrow \mathbf{x}'$ in a finite number of steps is possible with positive probability.
- It is left to check that the detailed balance equation (2.85) holds, i.e.

$$\pi_{\mathbf{x}}\, p_{\mathbf{x}\mathbf{x}'} = \pi_{\mathbf{x}'}\, p_{\mathbf{x}'\mathbf{x}}\,, \qquad \forall\, \mathbf{x}, \mathbf{x}' \in E\,. \tag{32}$$

  - If the configurations $\mathbf{x}, \mathbf{x}' \in E$ coincide then (32) obviously holds.
  - If $x(v) \neq x'(v)$ for more than one vertex $v \in V$ then $p_{\mathbf{x}\mathbf{x}'} = p_{\mathbf{x}'\mathbf{x}} = 0$ and thus (32) also holds for this case.
  - Let now $x(v) \neq x'(v)$ for exactly one $v \in V$ (and hence $x(w) = x'(w)$ for all $w \neq v$).
  - Then $x(w) = x'(w) = 0$ for all vertices $w \neq v$ connected to v and consequently

$$\pi_{\mathbf{x}}\, p_{\mathbf{x}\mathbf{x}'} \;=\; \frac{1}{\ell}\,\frac{1}{2|V|} \;=\; \pi_{\mathbf{x}'}\, p_{\mathbf{x}'\mathbf{x}}\,. \qquad \square$$

Remarks

- For all $\mathbf{x} \in E$ let $m(\mathbf{x})$ be the number of vertices set to 1 of the admissible configuration $\mathbf{x}$.
- If the admissible configuration is picked „at random" then the expectation $\mathbb{E}\,Y$ of the random number Y of vertices set to 1 is given as
$$\mathbb{E}\,Y = \frac{1}{\ell} \sum_{\mathbf{x} \in E} m(\mathbf{x})\,. \tag{33}$$
- If ℓ is large the direct calculation of the expectation $\mathbb{E}\,Y$ via formula (33) is in general not possible because it is difficult to determine the numbers $m(\mathbf{x})$ analytically.
- A method to approximate the expectation $\mathbb{E}\,Y$ is based on generating k „randomly picked" admissible configurations $\mathbf{x}_n^{(1)}, \mathbf{x}_n^{(2)}, \ldots, \mathbf{x}_n^{(k)} \in E$ by k runs of the MCMC simulation algorithm described above.
- As a consequence of the strong law of large numbers the arithmetic mean $\big(m(\mathbf{x}_n^{(1)}) + m(\mathbf{x}_n^{(2)}) + \ldots + m(\mathbf{x}_n^{(k)})\big)/k$ is close to $\mathbb{E}\,Y$ with high probability if the run length n and the sample size k are sufficiently large.

3.3.2 Gibbs Sampler

The MCMC algorithm for the generation of „randomly picked" admissible configurations of the hard core model (see Section 3.3.1) is a special case of a so–called *Gibbs sampler* for the simulation of discrete (high–dimensional) random vectors.

- Let V be a finite (nonempty) index set and let $\mathbf{X} = (X(v),\, v \in V)$ be a discrete random vector
  - taking values in the finite state space $E \subset \mathbb{R}^{|V|}$ with probability 1 where we assume
  - that for every pair $\mathbf{x}, \mathbf{x}' \in E$ there is a finite sequence of states $\mathbf{y}_0, \mathbf{y}_1, \ldots, \mathbf{y}_n \in E$ such that
$$\mathbf{y}_0 = \mathbf{x}\,, \quad \mathbf{y}_n = \mathbf{x}' \qquad \text{and} \qquad \#\{v \in V :\, y_i(v) \neq y_{i+1}(v)\} = 1\,, \quad \forall\, i = 0, \ldots, n-1\,. \tag{34}$$
- Let $\boldsymbol{\pi} = (\pi_{\mathbf{x}},\, \mathbf{x} \in E)$ be the probability function of the random vector $\mathbf{X}$ with $\pi_{\mathbf{x}} > 0$ for all $\mathbf{x} \in E$, and for all $v \in V$ let
$$\pi_{x(v)\,|\,\mathbf{x}(-v)} = P\big(X(v) = x(v) \mid \mathbf{X}(-v) = \mathbf{x}(-v)\big) \tag{35}$$
  - denote the conditional probability that the component $X(v)$ of $\mathbf{X}$ has the value $x(v)$
  - given that the vector $\mathbf{X}(-v) = (X(w),\, w \in V \setminus \{v\})$ of the other components equals $\mathbf{x}(-v)$ where we assume $(x(v), \mathbf{x}(-v)) \in E$.

MCMC Simulation Algorithm

- Similar to Section 3.3.1 we construct a Markov chain $\mathbf{X}_0, \mathbf{X}_1, \ldots$
  - with state space E and an (appropriately chosen) irreducible and aperiodic transition matrix $\mathbf{P}$,
  - such that $\boldsymbol{\pi}$ is the ergodic limit distribution of $\mathbf{X}_0, \mathbf{X}_1, \ldots$.
- Then we generate a „path" $\mathbf{x}_0, \mathbf{x}_1, \ldots$ of the Markov chain by the recursive construction discussed in Section 2.1.3:

  1. Pick an initial state $\mathbf{x}_0 \in E$.
  2. Pick a component $v \in V$ according to a given probability function $\mathbf{q} = (q_v,\, v \in V)$ such that $q_v > 0$ for all $v \in V$.

3. Generate the update $x_{n+1}(v)$ of the vth component according to the (conditional) probability function
$$\boldsymbol{\pi}_{\cdot\,|\,\mathbf{x}_n(-v)} = \big(\pi_{x(v)|\,\mathbf{x}_n(-v)},\, \forall\, x(v) \text{ such that } (x(v), \mathbf{x}_n(-v)) \in E\big)\,.$$
4. The values of all components $w \neq v$ are not changed, i.e. $x_{n+1}(w) = x_n(w)$ for all $w \neq v$.

Theorem 3.11 *Let the transition matrix $\mathbf{P} = (p_{\mathbf{x}\mathbf{x}'})$ be given as*
$$p_{\mathbf{x}\mathbf{x}'} = \sum_{v\in V} q_v \pi_{x'(v)|\,\mathbf{x}(-v)}\, \mathbb{1}\big(\mathbf{x}(-v) = \mathbf{x}'(-v)\big)\,, \qquad \forall\, \mathbf{x}, \mathbf{x}' \in E\,, \tag{36}$$
where the conditional probabilities $\pi_{x'(v)|\,\mathbf{x}(-v)}$ are defined in (35)*. Then $\mathbf{P}$ is irreducible and aperiodic and the pair $(\mathbf{P}, \boldsymbol{\pi})$ is reversible.*

Proof The assertion can be proved similarly to the proof of Theorem 3.10.

- In order to see that $\mathbf{P} = (p_{\mathbf{x}\mathbf{x}'})$ is aperiodic it suffices to notice
  - that for all $\mathbf{x} \in E$
$$p_{\mathbf{x},\mathbf{x}} = \sum_{v\in V} q_v \pi_{x(v)|\,\mathbf{x}(-v)} = \sum_{v\in V} q_v\, \frac{\boldsymbol{\pi}_{\mathbf{x}}}{\sum\limits_{\mathbf{z}\in E:\,\mathbf{z}(-v)=\mathbf{x}(-v)} \pi_{\mathbf{z}}} > 0$$
  - and hence all diagonal elements $p_{\mathbf{x},\mathbf{x}}$ of $\mathbf{P}$ are positive.
- The following considerations show that $\mathbf{P}$ is irreducible.
  - For arbitrary but fixed $\mathbf{x}, \mathbf{x}' \in E$ let $k \leq |V|$ be the number of components $v \in V$ such that $x(v) \neq x'(v)$.
  - For $k = 0$, i.e. $\mathbf{x} = \mathbf{x}'$, we already showed while proving the aperiodicity that $p_{\mathbf{x}\mathbf{x}} > 0$.
  - Let now $k > 0$. Without loss of generality we may assume that the components are linearly ordered and that the first k components of $\mathbf{x}$ and $\mathbf{x}'$ differ.
  - By hypothesis (34) the state space E contains a sequence $\mathbf{y}_0, \ldots, \mathbf{y}_k \in E$ such that $\mathbf{y}_0 = \mathbf{x}$ and
$$\mathbf{y}_1 = \big(x'(v_1), x(v_2), \ldots, x(v_{|V|})\big)\,,\ \ldots\ ,\ \mathbf{y}_k = \big(x'(v_1), \ldots, x'(v_k), x(v_{k+1}), \ldots, x(v_{|V|})\big) = \mathbf{x}'\,.$$
  - Moreover, for each $i = 0, \ldots, k-1$
$$p_{\mathbf{y}_i\mathbf{y}_{i+1}} = q_{v_i} \pi_{y_{i+1}(v_i)|\,\mathbf{y}_i(-v_i)} = q_{v_i}\, \frac{\pi_{\mathbf{y}_{i+1}}}{\sum\limits_{\mathbf{z}\in E:\,\mathbf{z}(-v_i)=\mathbf{y}_i(-v_i)} \pi_{\mathbf{z}}} > 0 \tag{37}$$
    and thus $p^{(k)}_{\mathbf{x}\mathbf{x}'} \geq \prod_{i=0}^{k-1} p_{\mathbf{y}_i\mathbf{y}_{i+1}} > 0$.
- It is left to show that the detailed balance equation (2.85) holds, i.e.
$$\pi_{\mathbf{x}}\, p_{\mathbf{x}\mathbf{x}'} = \pi_{\mathbf{x}'}\, p_{\mathbf{x}'\mathbf{x}}\,, \qquad \forall\, \mathbf{x}, \mathbf{x}' \in E\,. \tag{38}$$
  - If $\mathbf{x} = \mathbf{x}'$, then (38) obviously holds.
  - If $x(v) \neq x'(v)$ for more than one component $v \in V$, then $p_{\mathbf{x}\mathbf{x}'} = p_{\mathbf{x}'\mathbf{x}} = 0$ and hence (38) holds.
  - Let now $x(v) \neq x'(v)$ for exactly one $v \in V$ (and hence $x(w) = x'(w)$ for all $w \neq v$). Then (37) implies
$$\pi_{\mathbf{x}}\, p_{\mathbf{x}\mathbf{x}'} = \pi_{\mathbf{x}}\, \frac{q_v \pi_{\mathbf{x}'}}{\sum\limits_{\mathbf{z}\in E:\,\mathbf{z}(-v)=\mathbf{x}(-v)} \pi_{\mathbf{z}}} = \pi_{\mathbf{x}'}\, \frac{q_v \pi_{\mathbf{x}}}{\sum\limits_{\mathbf{z}\in E:\,\mathbf{z}(-v)=\mathbf{x}'(-v)} \pi_{\mathbf{z}}} = \pi_{\mathbf{x}'}\, p_{\mathbf{x}'\mathbf{x}}\,.$$

□

Let $\mathbf{X}_0, \mathbf{X}_1, \ldots$ be a Markov chain with state space E and the transition matrix $\mathbf{P} = (p_{\mathbf{x}\mathbf{x}'})$ given by (36). As a consequence of Theorem 3.11 we get that in this case

$$\lim_{n\to\infty} d_{\mathrm{TV}}(\boldsymbol{\alpha}_n, \boldsymbol{\pi}) = 0 \tag{39}$$

for any initial concentration $\boldsymbol{\alpha}_0$ where $\boldsymbol{\alpha}_n$ denotes the distribution of $\mathbf{X}_n$. Furthermore, the Gibbs sampler shows the following *monotonic behavior*.

Theorem 3.12 *For all $n = 0, 1, \ldots$,*

$$d_{\mathrm{TV}}(\boldsymbol{\alpha}_n, \boldsymbol{\pi}) \geq d_{\mathrm{TV}}(\boldsymbol{\alpha}_{n+1}, \boldsymbol{\pi})\,. \tag{40}$$

Proof

- For arbitrary $v \in V$ and $\mathbf{x}' \in E$, formula (35) implies

$$\begin{aligned}\sum_{\mathbf{x}\in E:\,\mathbf{x}(-v)=\mathbf{x}'(-v)} \pi_{x'(v)|\,\mathbf{x}(-v)}\ \pi_{\mathbf{x}} &\overset{(35)}{=} \sum_{\mathbf{x}\in E:\,\mathbf{x}(-v)=\mathbf{x}'(-v)} \pi_{\mathbf{x}'}\pi_{x(v)|\,\mathbf{x}'(-v)} \\ &= \pi_{\mathbf{x}'} \underbrace{\sum_{\mathbf{x}\in E:\,\mathbf{x}(-v)=\mathbf{x}'(-v)} \pi_{x(v)|\,\mathbf{x}'(-v)}}_{=1} = \pi_{\mathbf{x}'}\,.\end{aligned} \tag{41}$$

- Using this and the definition (36) of the transition matrix $\mathbf{P} = (p_{\mathbf{x}\mathbf{x}'})$ we obtain

$$\begin{aligned}2\,d_{\mathrm{TV}}(\boldsymbol{\alpha}_{n+1}, \boldsymbol{\pi}) &= \sum_{\mathbf{x}'\in E} \bigl|\,\alpha_{n+1,\,\mathbf{x}'} - \pi_{\mathbf{x}'}\bigr| \\ &= \sum_{\mathbf{x}'\in E} \Bigl|\sum_{\mathbf{x}\in E} \alpha_{n,\,\mathbf{x}}\, p_{\mathbf{x}\mathbf{x}'} - \pi_{\mathbf{x}'}\Bigr| \\ &\overset{(36)}{=} \sum_{\mathbf{x}'\in E} \Bigl|\sum_{\mathbf{x}\in E} \alpha_{n,\,\mathbf{x}} \sum_{v\in V} q_v \pi_{x'(v)|\,\mathbf{x}(-v)}\, \mathbb{1}\bigl(\mathbf{x}(-v) = \mathbf{x}'(-v)\bigr) - \pi_{\mathbf{x}'}\Bigr| \\ &= \sum_{\mathbf{x}'\in E} \Bigl|\sum_{v\in V} q_v \sum_{\mathbf{x}\in E:\,\mathbf{x}(-v)=\mathbf{x}'(-v)} \pi_{x'(v)|\,\mathbf{x}(-v)}\alpha_{n,\,\mathbf{x}} - \pi_{\mathbf{x}'}\Bigr| \\ &\overset{(41)}{=} \sum_{\mathbf{x}'\in E} \Bigl|\sum_{v\in V} q_v \sum_{\mathbf{x}\in E:\,\mathbf{x}(-v)=\mathbf{x}'(-v)} \pi_{x'(v)|\,\mathbf{x}(-v)}\bigl(\alpha_{n,\,\mathbf{x}} - \pi_{\mathbf{x}}\bigr)\Bigr| \\ &\leq \sum_{\mathbf{x}'\in E} \sum_{v\in V} q_v \sum_{\mathbf{x}\in E:\,\mathbf{x}(-v)=\mathbf{x}'(-v)} \pi_{x'(v)|\,\mathbf{x}(-v)}\bigl|\,\alpha_{n,\,\mathbf{x}} - \pi_{\mathbf{x}}\bigr| \\ &= \sum_{\mathbf{x}\in E} \underbrace{\sum_{v\in V} q_v \sum_{\mathbf{x}'\in E:\,\mathbf{x}'(-v)=\mathbf{x}(-v)} \pi_{x'(v)|\,\mathbf{x}(-v)}}_{\overset{(36)}{=}\sum_{\mathbf{x}'\in E} p_{\mathbf{x}\mathbf{x}'}=1} \bigl|\,\alpha_{n,\,\mathbf{x}} - \pi_{\mathbf{x}}\bigr| \\ &= \sum_{\mathbf{x}\in E} \bigl|\,\alpha_{n,\,\mathbf{x}} - \pi_{\mathbf{x}}\bigr| \;=\; 2\,d_{\mathrm{TV}}(\boldsymbol{\alpha}_n, \boldsymbol{\pi})\,.\end{aligned}$$

□

Remarks

- A modified version of the Gibbs sampler that was considered in this section is the so-called *cyclic Gibbs sampler*, which uses a different procedure for picking the component $v \in V$ that will be updated.

  - Namely, it is *not* chosen according to a (given) probability function $\mathbf{q} = (q_v,\, v \in V)$, where $q_v > 0$ for all $v \in V$,
  - but the components $v \in V$ are sorted linearly and chosen one after another according to this order. The selection of the update candidates thus becomes a deterministic procedure.
- If $k = n|V| + i$ for some numbers $n = 0, 1, \ldots$ and $i = 1, \ldots, |V|$, then the matrix $\mathbf{P}(k) = \big(p_{\mathbf{x}\mathbf{x}'}(k)\big)$ of the transition probabilities $p_{\mathbf{x}\mathbf{x}'}(k)$ in step k is given as

$$p_{\mathbf{x}\mathbf{x}'}(k) = \pi_{x'(v_i)|\,\mathbf{x}(-v_i)}\, \mathbb{1}\big(\mathbf{x}(-v_i) = \mathbf{x}'(-v_i)\big)\,, \qquad \forall\, \mathbf{x}, \mathbf{x}' \in E\,. \tag{42}$$

- For an entire (scan) cycle, updating each component exactly once, one obtains the following transition matrix

$$\mathbf{P} = \mathbf{P}(1) \cdot \ldots \cdot \mathbf{P}(|V|)\,. \tag{43}$$

- It is easy to show that the matrix $\mathbf{P} = (p_{\mathbf{x}\mathbf{x}'})$ given by (42) and (43)
  - is irreducible and aperiodic
  - and that $\boldsymbol{\pi}$ is the stationary (limit) distribution of $\mathbf{P}$ as
  - for all $i = 1, \ldots, |V|$ and for all $\mathbf{x}' \in E$ formulae (41) and (42) imply that

$$\sum_{\mathbf{x}\in E} \pi_{\mathbf{x}} p_{\mathbf{x}\mathbf{x}'}(i) \overset{(42)}{=} \sum_{\mathbf{x}\in E} \pi_{\mathbf{x}} \pi_{x'(v_i)|\,\mathbf{x}(-v_i)}\, \mathbb{1}\big(\mathbf{x}(-v_i) = \mathbf{x}'(-v_i)\big) \overset{(41)}{=} \pi_{\mathbf{x}'}$$

  - and hence also

$$\sum_{\mathbf{x}\in E} \pi_{\mathbf{x}} p_{\mathbf{x}\mathbf{x}'} = \pi_{\mathbf{x}'}\,.$$

- The pair $(\mathbf{P}, \boldsymbol{\pi})$ is in general not reversible. However, in Section 2.3.4 we showed that the pair $(\mathbf{M}, \boldsymbol{\pi})$ is reversible where

$$\mathbf{M} = \mathbf{P}\widetilde{\mathbf{P}} \qquad \text{for} \qquad \widetilde{\mathbf{P}} = \operatorname{diag}(\pi_{\mathbf{x}}^{-1})\mathbf{P}^{\top} \operatorname{diag}(\pi_{\mathbf{x}}) \tag{44}$$

  denotes the multiplicative reversible version of $\mathbf{P}$.

Theorem 3.13 *The matrix* $\mathbf{M}$ *has the following representation*

$$\mathbf{M} = \mathbf{P}(1) \cdot \ldots \cdot \mathbf{P}(|V|) \cdot \mathbf{P}(|V|) \cdot \ldots \cdot \mathbf{P}(1)\,, \tag{45}$$

i.e., the multiplicative reversible version $\mathbf{M}$ *of the „forward–scan matrix"* $\mathbf{P}$ *coincides with the „forward–backward scan matrix".*

Proof

- It suffices to show that $\widetilde{\mathbf{P}} = \mathbf{P}(|V|) \cdot \ldots \cdot \mathbf{P}(1)$ for the matrix $\widetilde{\mathbf{P}} = (\widetilde{p}_{\mathbf{x}\mathbf{x}'})$ defined by (44).
- Formulae (42)–(44) imply for arbitrary $\mathbf{x}, \mathbf{x}' \in E$

$$\begin{aligned}
\widetilde{\mathbf{p}}_{\mathbf{x}\mathbf{x}'} &= \Big(\operatorname{diag}(\pi_{\mathbf{x}}^{-1})\mathbf{P}^{\top} \operatorname{diag}(\pi_{\mathbf{x}}) \Big)_{\mathbf{x}\mathbf{x}'} \\
&= \Big(\operatorname{diag}(\pi_{\mathbf{x}}^{-1})\mathbf{P}^{\top}(|V|) \cdot \ldots \cdot \mathbf{P}^{\top}(1) \operatorname{diag}(\pi_{\mathbf{x}}) \Big)_{\mathbf{x}\mathbf{x}'} \\
&= \sum_{\mathbf{y}_1, \ldots, \mathbf{y}_{|V|-1} \in E} \frac{1}{\pi_{\mathbf{x}}}\, \pi_{x(v_{|V|})|\,\mathbf{y}_1(-v_{|V|})}\, \mathbb{1}\big(\mathbf{x}(-v_{|V|}) = \mathbf{y}_1(-v_{|V|})\big) \pi_{y_1(v_{|V|-1})|\,\mathbf{y}_2(-v_{|V|-1})} \\
&\qquad \times \mathbb{1}\big(\mathbf{y}_1(-v_{|V|-1}) = \mathbf{y}_2(-v_{|V|-1})\big) \ldots \pi_{y_{|V|-1}(v_1)|\,\mathbf{x}'(-v_1)}\, \mathbb{1}\big(\mathbf{y}_{|V|-1}(-v_1) = \mathbf{x}'(-v_1)\big) \pi_{\mathbf{x}'}\,.
\end{aligned}$$

- This and (35) yield (similar to the proof of (38))

$$\begin{aligned}\widetilde{\mathbf{p}}_{\mathbf{x}\mathbf{x}'} &= \sum_{\mathbf{y}_1,\ldots,\mathbf{y}_{|V|-1}\in E} \pi_{y_1(v_{|V|})|\,\mathbf{x}(-v_{|V|})}\,\mathbb{1}\big(\mathbf{x}(-v_{|V|})=\mathbf{y}_1(-v_{|V|})\big)\pi_{y_2(v_{|V|-1})|\,\mathbf{y}_1(-v_{|V|-1})} \\ &\qquad \times \mathbb{1}\big(\mathbf{y}_1(-v_{|V|-1})=\mathbf{y}_2(-v_{|V|-1})\big)\ldots\pi_{x'(v_1)|\,\mathbf{y}_{|V|-1}(-v_1)}\,\mathbb{1}\big(\mathbf{y}_{|V|-1}(-v_1)=\mathbf{x}'(-v_1)\big) \\ &= \Big(\mathbf{P}(|V|)\cdot\ldots\cdot\mathbf{P}(1)\Big)_{\mathbf{x}\mathbf{x}'}\,. \end{aligned}$$

□

Remarks

- If Gibbs samplers are used in practice it is always assumed
  - that the conditional probabilities considered in (36) and (42)

$$\pi_{x(v)|\,\mathbf{x}(-v)} = P\big(X(v)=x(v)\mid \mathbf{X}(-v)=\mathbf{x}(-v)\big)$$

    only depend on the vector $\big(x(w),\, w\in\mathcal{N}(v)\big)$ of the values
  - obtained by the random vector $\mathbf{X}=(X(w),\, w\in V)$ in a certain small neighborhood $\mathcal{N}(v)\subset V$ of $v\in V$.
- The family $\mathcal{N}=\{\mathcal{N}(v),\, v\in V\}$ of subsets of V is called a *system of neighborhoods* if for arbitrary $v,w\in V$
  (a) $v\notin\mathcal{N}(v)$,
  (b) $w\in\mathcal{N}(v)$ implies $v\in\mathcal{N}(w)$.
- For the hard–core model from Section 3.3.1, $\mathcal{N}(v)$ is the set of those vertices $w\neq v$ that are directly connected to v by an edge.

3.3.3 Metropolis–Hastings Algorithm

- We will now show that the Gibbs sampler discussed in Section 3.3.2 is a special case of a class of MCMC algorithms that are of the so–called *Metropolis–Hastings type*. This class generalizes two aspects of the Gibbs sampler.

  1. The transition matrix $\mathbf{P}=(p_{\mathbf{x}\mathbf{x}'})$ can be of a more general form than the one defined by

$$p_{\mathbf{x}\mathbf{x}'} = \sum_{v\in V} q_v\pi_{x'(v)|\,\mathbf{x}(-v)}\,\mathbb{1}\big(\mathbf{x}(-v)=\mathbf{x}'(-v)\big)\,,\qquad \forall\,\mathbf{x},\mathbf{x}'\in E. \tag{46}$$

  2. Besides this, a *procedure for acceptance or rejection* of the updates $\mathbf{x}\longrightarrow\mathbf{x}'$ is integrated into the algorithm. It is based on a similar idea as the acceptance-rejection sampling discussed in Section 3.2.3; see in particular Theorem 3.5.

- Let V be a finite nonempty index set and let $\mathbf{X}=(X(v),\, v\in V)$ be a discrete random vector,
  - taking values in the finite state space $E\subset\mathbb{R}^{|V|}$ with probability 1.
  - As usual we assume $\pi_{\mathbf{x}}>0$ for all $\mathbf{x}\in E$ where $\boldsymbol{\pi}=(\pi_{\mathbf{x}},\,\mathbf{x}\in E)$ is the probability function of the random vector $\mathbf{X}$.
- We construct a Markov chain $\mathbf{X}_0,\mathbf{X}_1,\ldots$ with ergodic limit distribution $\boldsymbol{\pi}$ whose transition matrix $\mathbf{P}=\big(p_{\mathbf{x}\mathbf{x}'}\big)$ is given by

$$p_{\mathbf{x}\mathbf{x}'} = q_{\mathbf{x}\mathbf{x}'}a_{\mathbf{x}\mathbf{x}'}\,,\qquad \forall\,\mathbf{x},\mathbf{x}'\in E \text{ with } \mathbf{x}\neq\mathbf{x}', \tag{47}$$

– where $\mathbf{Q} = \left(q_{\mathbf{x}\mathbf{x}'}\right)$ is an arbitrary stochastic matrix that is irreducible and aperiodic, i.e. in particular $q_{\mathbf{x}\mathbf{x}'} = 0$ if and only if $q_{\mathbf{x}'\mathbf{x}} = 0$.

– Moreover, the matrix $\mathbf{A} = \left(a_{\mathbf{x}\mathbf{x}'}\right)$ is defined as

$$a_{\mathbf{x}\mathbf{x}'} = \frac{s_{\mathbf{x}\mathbf{x}'}}{1 + t_{\mathbf{x}\mathbf{x}'}}\,, \tag{48}$$

where

$$t_{\mathbf{x}\mathbf{x}'} = \begin{cases} \dfrac{\pi_{\mathbf{x}} q_{\mathbf{x}\mathbf{x}'}}{\pi_{\mathbf{x}'} q_{\mathbf{x}'\mathbf{x}}} & \text{if } q_{\mathbf{x}\mathbf{x}'} > 0, \\ 0 & \text{if } q_{\mathbf{x}\mathbf{x}'} = 0, \end{cases} \tag{49}$$

– and $\mathbf{S} = \left(s_{\mathbf{x}\mathbf{x}'}\right)$ is an arbitrary symmetric matrix such that

$$0 < s_{\mathbf{x}\mathbf{x}'} \leq 1 + \min\left\{t_{\mathbf{x}\mathbf{x}'}\,, t_{\mathbf{x}'\mathbf{x}}\right\}. \tag{50}$$

Remarks

- The structure given by (47) of the transition matrix $\mathbf{P} = \left(p_{\mathbf{x}\mathbf{x}'}\right)$ can be interpreted as follows.
  – At first a candidate $\mathbf{x}' \in E$ for the update $\mathbf{x} \longrightarrow \mathbf{x}'$ is selected according to $\mathbf{Q} = \left(q_{\mathbf{x}\mathbf{x}'}\right)$.
  – If $\mathbf{x}' \neq \mathbf{x}$, then $\mathbf{x}'$ is accepted with probability $a_{\mathbf{x}\mathbf{x}'}$,
  – i.e., with probability $1 - a_{\mathbf{x}\mathbf{x}'}$ the update $\mathbf{x} \longrightarrow \mathbf{x}'$ is rejected (and the current state is thus not changed).
- In order to apply the Metropolis–Hastings algorithm defined by (47)–(50), for a given „potential" transition matrix $\mathbf{Q} = \left(q_{\mathbf{x}\mathbf{x}'}\right)$ only the quotients $\pi_{\mathbf{x}}/\pi_{\mathbf{x}'}$ need to be known for all pairs $\mathbf{x}, \mathbf{x}' \in E$ of states such that $q_{\mathbf{x}\mathbf{x}'} > 0$.
- The special case of the Gibbs sampler (see Section 3.3.2) is obtained
  – if the „potential" transition probabilities $q_{\mathbf{x}\mathbf{x}'}$ are defined by (46).
  – Then for arbitrary $\mathbf{x}, \mathbf{x}' \in E$ such that $\#\{v \in V : x(v) \neq x'(v)\} \leq 1$

$$\pi_{\mathbf{x}} q_{\mathbf{x}\mathbf{x}'} = \pi_{\mathbf{x}'} q_{\mathbf{x}'\mathbf{x}} \qquad \text{and thus} \qquad t_{\mathbf{x}\mathbf{x}'} = 1\,.$$

  – By defining $s_{\mathbf{x}\mathbf{x}'} = 1 + \min\left\{t_{\mathbf{x}\mathbf{x}'}\,, t_{\mathbf{x}'\mathbf{x}}\right\}$ we obtain $a_{\mathbf{x}\mathbf{x}'} = 1$ for arbitrary $\mathbf{x}, \mathbf{x}' \in E$ such that $\#\{v \in V : x(v) \neq x'(v)\} \leq 1$.

Theorem 3.14 *The transition matrix* $\mathbf{P} = (p_{\mathbf{x}\mathbf{x}'})$ *defined by* (47)–(50) *is irreducible and aperiodic and the pair* $(\mathbf{P}, \boldsymbol{\pi})$ *is reversible.*

Proof

- As the acceptance probabilities $a_{\mathbf{x}\mathbf{x}'}$ given by (48)–(50) are positive for arbitrary $\mathbf{x}\,, \mathbf{x}' \in E$ the irreducibility and aperiodicity of $\mathbf{P} = (p_{\mathbf{x}\mathbf{x}'})$ are inherited from the corresponding properties of $\mathbf{Q} = (q_{\mathbf{x}\mathbf{x}'})$.
- In order to check the detailed balance equation (2.85), i.e.

$$\pi_{\mathbf{x}}\, p_{\mathbf{x}\mathbf{x}'} = \pi_{\mathbf{x}'}\, p_{\mathbf{x}'\mathbf{x}}\,, \qquad \forall\, \mathbf{x}, \mathbf{x}' \in E\,, \tag{51}$$

we consider two cases.

– If $q_{\mathbf{x}\mathbf{x}'} = q_{\mathbf{x}'\mathbf{x}} = 0$, then $p_{\mathbf{x}\mathbf{x}'} = p_{\mathbf{x}'\mathbf{x}} = 0$ and (51) holds.

– If $q_{\mathbf{x}\mathbf{x}'} > 0$, then also $q_{\mathbf{x}'\mathbf{x}} > 0$ and (47)–(50) imply

$$\begin{aligned} \pi_{\mathbf{x}} p_{\mathbf{x}\mathbf{x}'} &= \pi_{\mathbf{x}} q_{\mathbf{x}\mathbf{x}'} a_{\mathbf{x}\mathbf{x}'} \\ &= \pi_{\mathbf{x}} q_{\mathbf{x}\mathbf{x}'} \, \frac{s_{\mathbf{x}\mathbf{x}'} \pi_{\mathbf{x}'} q_{\mathbf{x}'\mathbf{x}}}{\pi_{\mathbf{x}'} q_{\mathbf{x}'\mathbf{x}} + \pi_{\mathbf{x}} q_{\mathbf{x}\mathbf{x}'}} \\ &= \pi_{\mathbf{x}'} p_{\mathbf{x}'\mathbf{x}} \,, \end{aligned}$$

where the last equality follows by the symmetry of the matrix $\mathbf{S} = \big(s_{\mathbf{x}\mathbf{x}'}\big)$. □

Examples

1. *Metropolis Algorithm*
   - The classic Metropolis algorithm is obtained if we consider equality in (50), i.e. if
   $$s_{\mathbf{x}\mathbf{x}'} = 1 + \min\left\{t_{\mathbf{x}\mathbf{x}'} \,, t_{\mathbf{x}'\mathbf{x}}\right\}, \qquad \forall\, \mathbf{x},\, \mathbf{x}' \in E \,.$$
   - In this case the acceptance probabilities $a_{\mathbf{x}\mathbf{x}'}$ for arbitrary $\mathbf{x},\, \mathbf{x}' \in E$ such that $q_{\mathbf{x}\mathbf{x}'} > 0$ are of the following form:
   $$\begin{aligned} a_{\mathbf{x}\mathbf{x}'} &= \frac{1 + \min\left\{t_{\mathbf{x}\mathbf{x}'} \,, t_{\mathbf{x}'\mathbf{x}}\right\}}{1 + t_{\mathbf{x}'\mathbf{x}}} \\ &= \frac{\min\left\{1 + t_{\mathbf{x}\mathbf{x}'} \,,\, 1 + t_{\mathbf{x}'\mathbf{x}}\right\}}{1 + t_{\mathbf{x}\mathbf{x}'}} = \min\left\{1,\ \frac{1 + t_{\mathbf{x}'\mathbf{x}}}{1 + t_{\mathbf{x}\mathbf{x}'}}\right\} \\ &= \min\left\{1,\ \frac{\pi_{\mathbf{x}'} q_{\mathbf{x}'\mathbf{x}}}{\pi_{\mathbf{x}} q_{\mathbf{x}\mathbf{x}'}}\right\}, \end{aligned}$$
   i.e.
   $$a_{\mathbf{x}\mathbf{x}'} = \min\left\{1,\ \frac{\pi_{\mathbf{x}'} q_{\mathbf{x}'\mathbf{x}}}{\pi_{\mathbf{x}} q_{\mathbf{x}\mathbf{x}'}}\right\}, \qquad \forall\, \mathbf{x},\, \mathbf{x}' \in E \text{ such that } q_{\mathbf{x}\mathbf{x}'} > 0. \tag{52}$$
   - If the matrix $\mathbf{Q} = (q_{\mathbf{x}\mathbf{x}'})$ of the „potential" transition probabilities is symmetric, then (52) implies
   $$a_{\mathbf{x}\mathbf{x}'} = \min\left\{1,\ \frac{\pi_{\mathbf{x}'}}{\pi_{\mathbf{x}}}\right\}, \qquad \forall\, \mathbf{x},\, \mathbf{x}' \in E \text{ such that } q_{\mathbf{x}\mathbf{x}'} > 0. \tag{53}$$
   - In particular, if the „potential" updates $\mathbf{x} \longrightarrow \mathbf{x}'$ are chosen „randomly", i.e. if
   $$q_{\mathbf{x}\mathbf{x}'} = \frac{1}{|E|} \,, \qquad \forall\, \mathbf{x},\, \mathbf{x}' \in E \,,$$
   then the acceptance probabilities $a_{\mathbf{x}\mathbf{x}'}$ are also given by (53).

2. *Barker Algorithm*
   - The so–called Barker algorithm is obtained if we consider the matrix $\mathbf{S} = \big(s_{\mathbf{x}\mathbf{x}'}\big)$ where $s_{\mathbf{x}\mathbf{x}'} = 1$ for arbitrary $\mathbf{x},\, \mathbf{x}' \in E$.
   - The acceptance probabilities $a_{\mathbf{x}\mathbf{x}'}$ are then given by
   $$a_{\mathbf{x}\mathbf{x}'} = \frac{\pi_{\mathbf{x}'} q_{\mathbf{x}'\mathbf{x}}}{\pi_{\mathbf{x}'} q_{\mathbf{x}'\mathbf{x}} + \pi_{\mathbf{x}} q_{\mathbf{x}\mathbf{x}'}} \,, \qquad \forall\, \mathbf{x},\, \mathbf{x}' \in E \text{ such that } q_{\mathbf{x}\mathbf{x}'} > 0. \tag{54}$$
   - If the matrix $\mathbf{Q} = (q_{\mathbf{x}\mathbf{x}'})$ of „potential" transition probabilities is symmetric, then
   $$a_{\mathbf{x}\mathbf{x}'} = \frac{\pi_{\mathbf{x}'}}{\pi_{\mathbf{x}'} + \pi_{\mathbf{x}}} \,, \qquad \forall\, \mathbf{x},\, \mathbf{x}' \in E \text{ such that } q_{\mathbf{x}\mathbf{x}'} > 0. \tag{55}$$

MCMC Simulation Algorithm

- As it was done for the Gibbs sampler (see Section 3.3.2) we construct a Markov chain $\mathbf{X}_0, \mathbf{X}_1, \ldots$
  - with state space E and with the (irreducible and aperiodic) transition matrix $\mathbf{P} = (p_{\mathbf{x}\mathbf{x}'})$ defined by (47)–(50)
  - such that $\boldsymbol{\pi}$ is the ergodic limit distribution of $\mathbf{X}_0, \mathbf{X}_1, \ldots$.
- For sufficiently large n the distribution $\boldsymbol{\alpha}_n$ on $\mathbf{X}_n$ coincides approximately with $\boldsymbol{\pi}$.
- In estimating the approximation error for MCMC simulation algorithms it is useful
  - to know the *variational distance* $d_{\mathrm{TV}}(\boldsymbol{\alpha}_n, \boldsymbol{\pi})$ between the distributions $\boldsymbol{\alpha}_n$ and $\boldsymbol{\pi}$
  - as well as its *upper bounds*; see Section 3.4.1.

3.4 Error Analysis for MCMC Simulation

3.4.1 Estimate for the Rate of Convergence

- We will now show how the upper bounds for the variational distance $d_{\mathrm{TV}}(\boldsymbol{\alpha}_n, \boldsymbol{\pi})$ and the second largest absolute value $|\theta_2| = \max\{\lambda_2, |\lambda_\ell|\}$ of the eigenvalues $\lambda_1, \ldots, \lambda_\ell$ of the transition matrix $\mathbf{P}$ derived in Section 2.3 can be used
  - in order to determine upper bounds for the distance $d_{\mathrm{TV}}(\boldsymbol{\alpha}_n, \boldsymbol{\pi})$ occurring in the nth step of the MCMC simulation via the Metropolis algorithm,
  - if the simulated distribution $\boldsymbol{\pi}$ satisfies the following conditions.
- Namely we assume
  - that $\pi_{\mathbf{x}} \neq \pi_{\mathbf{x}'}$ for arbitrary $\mathbf{x}$, $\mathbf{x}' \in E$ such that $\mathbf{x} \neq \mathbf{x}'$,
  - and that the states $\mathbf{x}_1, \ldots, \mathbf{x}_\ell \in E$ are ordered such that $\pi_{\mathbf{x}_1} > \ldots > \pi_{\mathbf{x}_\ell}$.
- We may thus (w.l.o.g.) return to the notation used in Section 2.3 and identify the states $\mathbf{x}_1, \ldots, \mathbf{x}_\ell \in E$ and the first ℓ natural numbers, i.e. $E = \{1, \ldots, \ell\}$.
- The probabilities π_i $(= \pi_{\mathbf{x}_i})$ can thus be written in the following way:

$$\pi_i = \frac{b^{h(i)}}{z(b)}\,, \qquad \forall\, i = 1, \ldots, \ell\,, \tag{56}$$

  - where $h : \{1, \ldots, \ell\} \to (1, \infty)$ is a monotonically increasing function,
  - and $b \in (0, 1)$ is chosen such that for a certain constant $c \geq 1$

$$h(i+1) - h(i) \geq c\,, \qquad \forall\, i = 1, \ldots, \ell - 1 \tag{57}$$

  - and $z(b) = \sum_{i=1}^{\ell} b^{h(i)}$ is an (in general unknown) factor.
- Furthermore, the definition of a Metropolis algorithm for the MCMC simulation of $\boldsymbol{\pi} = (\pi_1, \ldots, \pi_\ell)^\top$ requires
  - that the basis b and the differences $h(i+1) - h(i)$ are known for all $i = 1, \ldots, \ell - 1$,
  - i.e. in particular that the quotients π_{i+1}/π_i are known for all $i = 1, \ldots, \ell - 1$.

- Let the matrix $\mathbf{Q} = (q_{ij})$ of the „potential" transitions $i \to j$ be given by

$$q_{ij} = \begin{cases} \frac{1}{2} & \text{if } i = 1,\ j = 1, 2 \text{ or } i = \ell,\ j = \ell, \ell - 1, \\ \frac{1}{2} & \text{if } i = 2, \ldots, \ell - 1 \text{ and } j = i - 1,\ i + 1, \\ 0\,, & \text{else.} \end{cases} \tag{58}$$

  - Let the acceptance probability a_{ij} be defined as in (53), i.e.

$$a_{ij} = \min\Big\{1,\ \frac{\pi_j\, q_{ji}}{\pi_i q_{ij}}\Big\} = \min\big\{1,\ b^{h(j)-h(i)}\big\}\,, \qquad \forall\, i, j \in \{1, \ldots, \ell\} \text{ where } q_{ij} = q_{ji} > 0.$$

  - By (56) and (58) the entries $p_{ij} = q_{ij} a_{ij}$ of the transition matrix $\mathbf{P} = (p_{ij})$ for the MCMC simulation are thus be given as

$$p_{11} = 1 - \frac{b^{h(2)-h(1)}}{2}\,, \qquad p_{12} = \frac{b^{h(2)-h(1)}}{2}\,, \qquad p_{\ell,\ell-1} = p_{\ell\ell} = \frac{1}{2} \tag{59}$$

  and for $i = 2, \ldots, \ell - 1$

$$p_{i,i-1} = \frac{1}{2}\,, \qquad p_{i,i+1} = \frac{b^{h(i+1)-h(i)}}{2}\,, \qquad p_{ii} = 1 - p_{i,i-1} - p_{i,i+1}\,. \tag{60}$$

Theorem 3.15 *The second largest eigenvalue λ_2 of the transition matrix $\mathbf{P} = (p_{ij})$ defined by* (59)–(60) *has the following upper bound*

$$\lambda_2 \le 1 - \frac{(1 - b^{c/2})^2}{2}\,. \tag{61}$$

Proof

- By Theorem 3.14 the pair $(\mathbf{P}, \boldsymbol{\pi})$ is reversible.
- Hence, *Rayleigh's theorem* (see Theorem 2.17) yields the following representation formula

$$\lambda_2 = 1 - \inf_{\mathbf{x} \in \mathbb{R}^\ell_{\neq}} \frac{D_{(\mathbf{P},\boldsymbol{\pi})}(\mathbf{x}, \mathbf{x})}{\mathrm{Var}_{\boldsymbol{\pi}}(\mathbf{x})}\,, \tag{62}$$

  - where $\mathbb{R}^\ell_{\neq} = \big\{\mathbf{x} = (x_1, \ldots, x_\ell)^\top \in \mathbb{R}^\ell :\ x_i \neq x_j \text{ for somer } i, j \in E\big\}$ denotes the subset of vectors in $\mathbb{R}^\ell$ whose components are not all equal,
  - $\mathrm{Var}_{\boldsymbol{\pi}}(\mathbf{x}) = \|\mathbf{x}\|^2_{\boldsymbol{\pi}} - (\mathbf{x})^2_{\boldsymbol{\pi}}$ is the variance of the components of $\mathbf{x}$ with respect to $\boldsymbol{\pi}$
  - and $D_{(\mathbf{P},\boldsymbol{\pi})}(\mathbf{x}, \mathbf{x}) = \big((\mathbf{I} - \mathbf{P})\mathbf{x}, \mathbf{x}\big)_{\boldsymbol{\pi}}$ denotes the Dirichlet form of the reversible pair $(\mathbf{P}, \boldsymbol{\pi})$.
- Due to (62) it is sufficient to show that

$$\mathrm{Var}_{\boldsymbol{\pi}}(\mathbf{x}) \le a D_{(\mathbf{P},\boldsymbol{\pi})}(\mathbf{x}, \mathbf{x})\,, \qquad \forall\, \mathbf{x} \in \mathbb{R}^\ell \tag{63}$$

  for some constant a such that

$$0 < a \le \frac{2}{(1 - b^{c/2})^2}\,. \tag{64}$$

  - Similar to the proof of Theorem 2.18 we obtain by copying the notation that for all $\theta \in (0, 1)$

$$\begin{aligned} 2\,\mathrm{Var}_{\boldsymbol{\pi}}(\mathbf{x}) &= \sum_{i,j \in E} (x_i - x_j)^2 \pi_i \pi_j \\ &= \sum_{i,j \in E} \Big(\sum_{e \in \gamma_{ij}} \frac{1}{Q(e)^\theta}\, Q(e)^\theta (x_{e^-} - x_{e^+}) \Big)^2 \pi_i \pi_j \\ &\le \sum_{i,j \in E} \Big(\sum_{e \in \gamma_{ij}} Q(e)^{2\theta} (x_{e^-} - x_{e^+})^2 \Big) \Big(\sum_{e \in \gamma_{ij}} \frac{1}{Q(e)^{2\theta}} \Big)\, \pi_i \pi_j\,, \end{aligned}$$

where the „edge probability" $Q(e) = \pi_{e^-}\, p_{e^-e^+}$ is assigned to the „directed" edge $e = (e^-, e^+)$ and γ_{ij} denotes the „path" from i to j.

– Using the notation $|\gamma_{ij}|_\theta = \sum_{e\in\gamma_{ij}} Q(e)^{-2\theta}$ we thus obtain

$$\begin{aligned} 2\mathrm{Var}_{\boldsymbol{\pi}}(\mathbf{x}) &\le \sum_{i,j\in E} |\gamma_{ij}|_\theta \sum_{e\in\gamma_{ij}} Q(e)^{2\theta}(x_{e^-} - x_{e^+})^2\, \pi_i\pi_j \\ &= \sum_{e\in\mathcal{E}} (x_{e^-} - x_{e^+})^2 Q(e) Q(e)^{2\theta-1} \sum_{\gamma_{ij}\ni e} \pi_i\pi_j |\gamma_{ij}|_\theta\,. \end{aligned}$$

– This shows (63) for

$$a = \max_{e\in\mathcal{E}} \Big\{ Q(e)^{2\theta-1} \sum_{\gamma_{ij}\ni e} \pi_i\pi_j |\gamma_{ij}|_\theta \Big\}, \tag{65}$$

as we showed in Lemma 2.8 that

$$2\, D_{(\mathbf{P},\boldsymbol{\pi})}(\mathbf{x},\mathbf{x}) = \sum_{e\in\mathcal{E}} (x_{e^-} - x_{e^+})^2 Q(e)\,.$$

- It is left to show that the constant a considered in (65) satisfies the inequality (64).
  – For this purpose we choose the path $\gamma_{ij} = (i, i+1, \ldots, j-1, j)$ for each pair $i, j \in E$ such that $i < j$.
  – Then (56) and (59)–(60) imply

$$Q(i,i+1) = \pi_i p_{i,i+1} = \frac{b^{h(i)}}{z(b)}\, \frac{b^{h(i+1)-h(i)}}{2} = \frac{\pi_{i+1}}{2}\,.$$

  – Thus, the reversibility of the pair $(\mathbf{P}, \boldsymbol{\pi})$ shown in Theorem 3.14 yields

$$Q(i+1,i) = Q(i,i+1) = \frac{\pi_{i+1}}{2}\,.$$

  – Because of (56) and (57) we obtain for arbitrary $i, j \in E$ such that $i < j$

$$\begin{aligned} |\gamma_{ij}|_\theta &= \left(\Big(\frac{\pi_{i+1}}{\pi_j}\Big)^{-2\theta} + \ldots + \Big(\frac{\pi_j}{\pi_j}\Big)^{-2\theta} \right) \Big(\frac{\pi_j}{2}\Big)^{-2\theta} \le \Big(b^{2(j-i-1)c\theta} + \ldots + b^{2c\theta} + 1 \Big) \Big(\frac{\pi_j}{2}\Big)^{-2\theta} \\ &\le \frac{2^{2\theta}\pi_j^{-2\theta}}{1 - b^{2c\theta}}\,. \end{aligned}$$

  – Moreover, all edges $e \in \mathcal{E}$ are of the form $e = (i, i+1)$ or $e = (i, i-1)$, as for the entries p_{ij} of the transition matrix $\mathbf{P} = (p_{ij})$ defined by (58)–(60) we have $p_{ij} = 0$ if $|i - j| > 1$.

- Thus, for $\theta < 1/2$,

$$\begin{aligned} a &= \max_{e\in\mathcal{E}} \Big\{ Q(e)^{2\theta-1} \sum_{\gamma_{ij}\ni e} \pi_i\pi_j |\gamma_{ij}|_\theta \Big\} \\ &\le \max_{k=1,\ldots,\ell-1} \left\{ Q(k,k+1)^{2\theta-1} \sum_{1\le i\le k, k+1\le j\le \ell} 2^{2\theta}\, \frac{\pi_i \pi_j^{1-2\theta}}{1 - b^{2c\theta}} \right\} \\ &\le \frac{2}{(1 - b^{2c\theta})(1 - b^{c(1-2\theta)})}\,, \end{aligned}$$

as $Q(k,k+1)^{2\theta-1} = \big(\pi_{k+1}/2\big)^{2\theta-1}$ and $\sum_{1\le i\le k} \pi_i \le 1$ and hence

$$\sum_{k+1\le j\le \ell} \pi_j^{1-2\theta} = \left(\Big(\frac{\pi_{k+1}}{\pi_{k+1}}\Big)^{1-2\theta} + \ldots + \Big(\frac{\pi_\ell}{\pi_{k+1}}\Big)^{1-2\theta} \right) \pi_{k+1}^{1-2\theta} \le \frac{\pi_{k+1}^{1-2\theta}}{1 - b^{c(1-2\theta)}}\,.$$

- For $\theta = 1/4$ we obtain the estimate (64). □

The following lemma will turn out to be useful in order to derive a lower bound for the smallest eigenvalue λ_ℓ of the transition matrix $\mathbf{P} = (p_{ij})$ defined by (59)–(60).

Lemma 3.1

- *Let $\mathbf{A} = (a_{ij})$ be an arbitrary $\ell \times \ell$–matrix and for all $i = 1, \ldots, \ell$ let $r_i = \sum_{j:\, 1 \le j \le \ell,\, j \ne i} |a_{ij}|$.*
- *Let λ be an arbitrary eigenvalue of $\mathbf{A}$, let $\boldsymbol{\phi} = (\phi_1, \ldots, \phi_\ell)^\top \ne \mathbf{o}$ be a left eigenvector corresponding to λ and let k be the number of the component ϕ_k where*

$$|\phi_k| = \max_{i=1,\ldots,\ell} |\phi_i| > 0\,.$$

- *Then,*

$$|\lambda - a_{kk}| \le r_k\,. \tag{66}$$

Proof

- By definition of λ and $\boldsymbol{\phi}$ we have $\mathbf{A}\boldsymbol{\phi} = \lambda\boldsymbol{\phi}$. In particular

$$\sum_{j=1}^{\ell} a_{kj}\phi_j = \lambda\,\phi_k \qquad \text{and} \qquad (\lambda - a_{kk})\phi_k = \sum_{j:\, 1 \le j \le \ell,\, j \ne k} a_{kj}\phi_j\,.$$

- This implies

$$|\lambda - a_{kk}||\phi_k| \le \sum_{j:\, 1 \le j \le \ell,\, j \ne k} |a_{kj}||\phi_j| \le r_k|\phi_k| \qquad \text{and} \qquad |\lambda - a_{kk}| \le r_k\,.$$ □

Theorem 3.16 *The smallest eigenvalue λ_ℓ of the transition matrix $\mathbf{P} = (p_{ij})$ defined by (59)–(60) has the following lower bound*

$$\lambda_\ell \ge -b^c\,. \tag{67}$$

Proof

- By Lemma 3.1 applied to $\mathbf{A} = \mathbf{P}$ (and to the index k determined for λ_ℓ)

$$|\lambda_\ell - p_{kk}| \le \sum_{j:\, 1 \le j \le \ell,\, j \ne k} p_{kj} = 1 - p_{kk} \qquad \Rightarrow \qquad \lambda_\ell \ge -1 + 2p_{kk}\,.$$

- Thus, taking into account (59)–(60) we derive

$$\lambda_\ell \ge -1 + 2 \min_{i=1,\ldots,\ell} p_{ii} \ge -1 + 2\Big(1 - \frac{1}{2} - \frac{b^c}{2}\Big) = -b^c\,.$$ □

Remark Summarizing the results of Theorems 3.15 and 3.16 we have shown that

$$|\theta_2| = \max\{\lambda_2, |\lambda_\ell|\} \le \max\Big\{1 - \frac{(1 - b^{c/2})^2}{2}\,,\, b^c\Big\} = 1 - \frac{(1 - b^{c/2})^2}{2}\,. \tag{68}$$

3.4.2 MCMC Estimators; Bias and Fundamental Matrix

In this section we will investigate the characteristics of Monte–Carlo estimators for expectations.

- Examples for similar problems were already discussed in Section 3.1.1,
  - when we estimated π by statistical means
  - and the value of integrals via Monte–Carlo simulation.
- However, for these purposes we assumed
  - that the pseudo–random numbers can be regarded as realizations of independent and identically distributed sampling variables.
  - In the present section we assume that the sample variables form an (appropriately chosen) Markov chain.
- This is the reason why these estimators are called *Markov–Chain–Monte–Carlo estimators* (MCMC estimators).

Statistical Model

- Let V be a finite (nonempty) index set and let $\mathbf{X} = (X(v),\, v \in V)$ be a discrete random vector,
  - taking values in the finite state space $E \subset \mathbb{R}^{|V|}$ with probability 1,
  - where E is identified with the set $E = \{1, \ldots, \ell\}$ of the first $\ell = |E|$ natural numbers.
  - Furthermore, we assume $\pi_i > 0$ for all $i \in E$ where $\boldsymbol{\pi} = (\pi_i,\, i \in E)$ denotes the probability function of the random vector $\mathbf{X}$.
- Our goal
  - is to estimate the expectation $\theta = \mathbb{E}\,\varphi(\mathbf{X})$ via MCMC simulation where
$$\theta = \boldsymbol{\pi}^\top \boldsymbol{\varphi} \tag{69}$$
  - and $\boldsymbol{\varphi} = (\varphi_1, \ldots, \varphi_\ell)^\top : E \to \mathbb{R}$ is an arbitrary but fixed function.
- As an estimator for θ we consider the random variable
$$\widehat{\theta}_n = \frac{1}{n} \sum_{k=0}^{n-1} \varphi(\mathbf{X}_k)\,, \qquad \forall\, n \geq 1\,, \tag{70}$$
  - where $\mathbf{X}_0, \mathbf{X}_1, \ldots$ is a Markov chain with state space E, arbitrary but fixed initial distribution $\boldsymbol{\alpha}$ and
  - an irreducible and aperiodic transition matrix $\mathbf{P} = \big(p_{ij}\big)$, such that $\boldsymbol{\pi}$ is the ergodic limit distribution with respect to $\mathbf{P}$.

Remarks

- Typically, the initial distribution $\boldsymbol{\alpha}$ does *not* coincide with the simulated distribution $\boldsymbol{\pi}$.
  - Consequently, the MCMC estimator $\widehat{\theta}_n$ defined by (70) is not unbiased for fixed (finite) sample size,
  - i.e. in general $\mathbb{E}\,\widehat{\theta}_n \neq \theta$ for all $n \geq 1$.
- For determining the *bias* $\mathbb{E}\,\widehat{\theta}_n - \theta$ the following representation formula will be helpful.

Theorem 3.17 *For all $n \geq 1$,*
$$\mathbb{E}\,\widehat{\theta}_n = \frac{1}{n}\, \boldsymbol{\alpha}^\top \sum_{k=0}^{n-1} \mathbf{P}^k \boldsymbol{\varphi}\,. \tag{71}$$

Proof

- In Theorem 2.3 we proved that for all $k \geq 1$ the distribution $\boldsymbol{\alpha}_k$ of $\mathbf{X}_k$ is given by $\boldsymbol{\alpha}_k^\top = \boldsymbol{\alpha}^\top \mathbf{P}^k$.
- Thus, by definition (70) of the MCMC estimator $\widehat{\theta}_n$, we get that

$$\mathbb{E}\,\widehat{\theta}_n = \frac{1}{n}\,\sum_{k=0}^{n-1} \mathbb{E}\,\varphi(\mathbf{X}_k) = \frac{1}{n}\,\sum_{k=0}^{n-1} \boldsymbol{\alpha}_k^\top \boldsymbol{\varphi} = \frac{1}{n}\,\sum_{k=0}^{n-1} \boldsymbol{\alpha}^\top \mathbf{P}^k \boldsymbol{\varphi} = \frac{1}{n}\,\boldsymbol{\alpha}^\top \sum_{k=0}^{n-1} \mathbf{P}^k \boldsymbol{\varphi}\,. \qquad \square$$

Remarks

- As an immediate consequence of Theorem 3.17, the ergodicity of the transition matrix $\mathbf{P}$, and (69), one obtains

$$\lim_{n\to\infty} \mathbb{E}\,\widehat{\theta}_n = \theta\,,$$

- i.e., the MCMC estimator $\widehat{\theta}_n$ for θ defined in (70) is asymptotically unbiased.

Apart from this, the asymptotic behavior of $n\big(\mathbb{E}\,\widehat{\theta}_n - \theta\big)$ for $n \to \infty$ can be determined. For this purpose we need the following two lemmata.

Lemma 3.2 *Let $\boldsymbol{\Pi}$ be the $\ell \times \ell$ matrix consisting of the ℓ identical row vectors $\boldsymbol{\pi}^\top$. Then*

$$(\mathbf{P} - \boldsymbol{\Pi})^n = \mathbf{P}^n - \boldsymbol{\Pi} \tag{72}$$

for all $n \geq 1$ and in particular

$$\lim_{n\to\infty} (\mathbf{P} - \boldsymbol{\Pi})^n = \mathbf{0}\,. \tag{73}$$

Proof

- Evidently, (72) holds for $n = 1$.
  - If we assume that (72) holds for some $n - 1 \geq 1$, then

$$\begin{aligned} (\mathbf{P} - \boldsymbol{\Pi})^n &= (\mathbf{P} - \boldsymbol{\Pi})^{n-1}(\mathbf{P} - \boldsymbol{\Pi}) = (\mathbf{P}^{n-1} - \boldsymbol{\Pi})(\mathbf{P} - \boldsymbol{\Pi}) \\ &= \mathbf{P}^n - \boldsymbol{\Pi}\mathbf{P} - \mathbf{P}^{n-1}\boldsymbol{\Pi} + \boldsymbol{\Pi}^2 = \mathbf{P}^n - \boldsymbol{\Pi}\,, \end{aligned}$$

    where the last equality follows from the fact that

$$\boldsymbol{\pi}^\top \mathbf{P} = \boldsymbol{\pi}^\top \qquad \text{and thus} \qquad \boldsymbol{\Pi}\mathbf{P} = \mathbf{P}\boldsymbol{\Pi} = \boldsymbol{\Pi} = \boldsymbol{\Pi}^2\,.$$

  - This proves (72) for all $n \geq 1$.
- As $\mathbf{P}$ is assumed to be irreducible and aperiodic,
  - by Theorems 2.4 and 2.9 we get that $\mathbf{P}^n - \boldsymbol{\Pi} \to \mathbf{0}$ if $n \to \infty$.
  - Thus, by (72), also $(\mathbf{P} - \boldsymbol{\Pi})^n \to \mathbf{0}$ if $n \to \infty$. $\square$

Remarks

- By the zero convergence $(\mathbf{P}-\boldsymbol{\Pi})^n \to \mathbf{0}$ for $n \to \infty$ in Lemma 3.2 and Lemma 2.4, the matrix $\mathbf{I}-(\mathbf{P}-\boldsymbol{\Pi})$ is invertible.
- In order to show this it suffices to consider the matrix $\mathbf{A} = \mathbf{P} - \boldsymbol{\Pi}$ in Lemma 2.4.
- The inverse matrix

$$\mathbf{Z} = (\mathbf{I} - (\mathbf{P} - \boldsymbol{\Pi}))^{-1} \tag{74}$$

  is hence well defined. It is called the *fundamental matrix* of $\mathbf{P}$.

Lemma 3.3 *The fundamental matrix* $\mathbf{Z} = (\mathbf{I} - (\mathbf{P} - \mathbf{\Pi}))^{-1}$ *of the irreducible and aperiodic transition matrix* $\mathbf{P}$ *has the representation formulae*

$$\mathbf{Z} = \mathbf{I} + \sum_{k=1}^{\infty} (\mathbf{P}^k - \mathbf{\Pi}) \tag{75}$$

and

$$\mathbf{Z} = \mathbf{I} + \lim_{n\to\infty} \sum_{k=1}^{n-1} \frac{n-k}{n} (\mathbf{P}^k - \mathbf{\Pi}) . \tag{76}$$

Proof

- Formula (75) follows from Lemmas 2.4 and 3.2 as for $\mathbf{A} = \mathbf{P} - \mathbf{\Pi}$

$$\begin{aligned}
\mathbf{Z} &= (\mathbf{I} - \mathbf{A})^{-1} \\
&= (\mathbf{I} - \mathbf{A})^{-1} \lim_{n\to\infty} (\mathbf{I} - \mathbf{A}^n) \\
&= \lim_{n\to\infty} \Big((\mathbf{I} - \mathbf{A})^{-1} (\mathbf{I} - \mathbf{A}^n) \Big) \\
&\overset{(2.79)}{=} \lim_{n\to\infty} \Big(\mathbf{I} + \mathbf{A} + \ldots + \mathbf{A}^{n-1} \Big) \\
&= \mathbf{I} + \sum_{k=1}^{\infty} \mathbf{A}^k \qquad \left(= \mathbf{I} + \sum_{k=1}^{\infty} (\mathbf{P} - \mathbf{\Pi})^k \right) \\
&\overset{(72)}{=} \mathbf{I} + \sum_{k=1}^{\infty} (\mathbf{P}^k - \mathbf{\Pi}) .
\end{aligned}$$

- In order to show (76) it suffices to notice that

$$\sum_{k=1}^{n} (\mathbf{P}^k - \mathbf{\Pi}) - \sum_{k=1}^{n-1} \frac{n-k}{n} (\mathbf{P}^k - \mathbf{\Pi}) = \sum_{k=1}^{n} \frac{k}{n} (\mathbf{P}^k - \mathbf{\Pi}) = \frac{1}{n} \sum_{k=1}^{n} k (\mathbf{P} - \mathbf{\Pi})^k$$

  and that the last expression converges to $\mathbf{0}$ for $n \to \infty$.

- The zero convergence is due to the fact that for every $\ell \times \ell$ matrix $\mathbf{A}$

$$(\mathbf{I} - \mathbf{A}) \sum_{k=1}^{n} k \mathbf{A}^k = \sum_{k=1}^{n} \mathbf{A}^k - n \mathbf{A}^{n+1}$$

  and thus for $\mathbf{A} = \mathbf{P} - \mathbf{\Pi}$

$$\begin{aligned}
\lim_{n\to\infty} \frac{1}{n} \sum_{k=1}^{n} k (\mathbf{P} - \mathbf{\Pi})^k &= \lim_{n\to\infty} \left(\frac{1}{n} \mathbf{Z} \sum_{k=1}^{n} (\mathbf{P} - \mathbf{\Pi})^k - \mathbf{Z} (\mathbf{P} - \mathbf{\Pi})^{n+1} \right) \\
&\overset{(72)}{=} \mathbf{Z} \left(\lim_{n\to\infty} \frac{1}{n} \underbrace{\sum_{k=1}^{n} (\mathbf{P}^k - \mathbf{\Pi})}_{\overset{(75)}{\longrightarrow} \mathbf{Z} - \mathbf{I}} - \underbrace{\lim_{n\to\infty} (\mathbf{P} - \mathbf{\Pi})^{n+1}}_{\overset{(73)}{\longrightarrow} \mathbf{0}} \right) \\
&= \mathbf{0} .
\end{aligned}$$

□

Theorem 3.17 and Lemma 3.3 enable us to give a more detailed description of the asymptotic behavior of the bias $\mathbb{E}\, \widehat{\theta}_n - \theta$.

Theorem 3.18

- *Let* $a = \big(\boldsymbol{\alpha}^\top \mathbf{Z} - \boldsymbol{\pi}^\top\big)\boldsymbol{\varphi}$ *where* $\mathbf{Z}$ *denotes the fundamental matrix of* $\mathbf{P}$ *that was introduced by* (74).
- *Then, for all* $n \geq 1$,
$$n\big(\mathbb{E}\,\widehat{\theta}_n - \theta\big) = a + e_n\,, \tag{77}$$
where e_n *is a remainder such that* $e_n \to 0$ *for* $n \to \infty$.

Proof

- The representation formula (75) in Lemma 3.3 yields
$$\begin{aligned}
\boldsymbol{\alpha}^\top \mathbf{Z}\boldsymbol{\varphi} &= \boldsymbol{\alpha}^\top\boldsymbol{\varphi} + \boldsymbol{\alpha}^\top \lim_{n\to\infty} \sum_{k=1}^{n-1} (\mathbf{P}^k - \boldsymbol{\Pi})\boldsymbol{\varphi} \\
&= \boldsymbol{\alpha}^\top\boldsymbol{\varphi} + \lim_{n\to\infty} \Big(\boldsymbol{\alpha}^\top \Big(\sum_{k=1}^{n-1} \mathbf{P}^k\Big)\boldsymbol{\varphi} - (n-1)\underbrace{\boldsymbol{\alpha}^\top\boldsymbol{\Pi}}_{=\boldsymbol{\pi}^\top}\boldsymbol{\varphi}\Big) \\
&= \lim_{n\to\infty} \Big(\boldsymbol{\alpha}^\top \Big(\sum_{k=0}^{n-1} \mathbf{P}^k\Big)\boldsymbol{\varphi} - (n-1)\boldsymbol{\pi}^\top\boldsymbol{\varphi}\Big)\,.
\end{aligned}$$
- Hence by taking into account Theorem 3.17 we obtain the following for a certain sequence $\{e_n\}$ such that $e_n \to 0$:
$$\begin{aligned}
a &= \big(\boldsymbol{\alpha}^\top \mathbf{Z} - \boldsymbol{\pi}^\top\big)\boldsymbol{\varphi} \\
&= \boldsymbol{\alpha}^\top \Big(\sum_{k=0}^{n-1} \mathbf{P}^k\Big)\boldsymbol{\varphi} - n\boldsymbol{\pi}^\top\boldsymbol{\varphi} - e_n \\
&\overset{(71)}{=} n\,\mathbb{E}\,\widehat{\theta}_n - n\boldsymbol{\pi}^\top\boldsymbol{\varphi} - e_n \\
&\overset{(69)}{=} n\big(\mathbb{E}\,\widehat{\theta}_n - \theta\big) - e_n\,.
\end{aligned}$$
□

3.4.3 Asymptotic Variance of Estimation; Mean Squared Error

For the statistical model introduced in Section 3.4.2 we now investigate the asymptotic behavior of the variance $\operatorname{Var}\widehat{\theta}_n$ if $n \to \infty$.

Theorem 3.19 *Define* $\sigma^2 = \sum_{i=1}^{\ell} \pi_i(\varphi_i - \theta)^2$ *and let* $\mathbf{Z} = (\mathbf{I} - (\mathbf{P} - \boldsymbol{\Pi}))^{-1}$ *be the fundamental matrix of* $\mathbf{P}$ *defined by* (74). *Then*
$$\lim_{n\to\infty}\; n \operatorname{Var}\widehat{\theta}_n = \sigma^2 + 2\boldsymbol{\pi}^\top \operatorname{diag}(\boldsymbol{\varphi})(\mathbf{Z} - \mathbf{I})\boldsymbol{\varphi}\,. \tag{78}$$

Proof

- Clearly,
$$n^2 \operatorname{Var}\widehat{\theta}_n = \mathbb{E}\,\Big(\sum_{k=0}^{n-1} \varphi(\mathbf{X}_k)\Big)^2 - \Big(\sum_{k=0}^{n-1} \mathbb{E}\,\varphi(\mathbf{X}_k)\Big)^2 \tag{79}$$
and thus
$$n^2 \operatorname{Var}\widehat{\theta}_n = \sum_{k=0}^{n-1} \mathbb{E}\,\varphi^2(\mathbf{X}_k) + 2 \sum_{0\leq k<k'\leq n-1} \mathbb{E}\,\Big(\varphi(\mathbf{X}_k)\varphi(\mathbf{X}_{k'})\Big) - \Big(\sum_{k=0}^{n-1} \mathbb{E}\,\varphi(\mathbf{X}_k)\Big)^2\,.$$

- This representation will now be used to show (78) for the case $\boldsymbol{\alpha}_0 = \boldsymbol{\pi}$.
  - In this case we observe
$$\Big(\sum_{k=0}^{n-1} \mathbb{E}\,\varphi(\mathbf{X}_k)\Big)^2 = (n\theta)^2 \qquad \text{and} \qquad \sum_{k=0}^{n-1} \mathbb{E}\,\varphi^2(\mathbf{X}_k) = n\sum_{i=1}^{\ell} \pi_i \varphi_i^2\,.$$
  - Furthermore, by the stationarity of the Markov chain $\{\mathbf{X}_n\}$,
$$\sum_{0\le k<k'\le n-1} \mathbb{E}\left(\varphi(\mathbf{X}_k)\varphi(\mathbf{X}_{k'})\right) = \sum_{k=1}^{n-1}(n-k)\mathbb{E}\left(\varphi(\mathbf{X}_0)\varphi(\mathbf{X}_k)\right),$$
    where
$$\mathbb{E}\left(\varphi(\mathbf{X}_0)\varphi(\mathbf{X}_k)\right) = \sum_{i=1}^{\ell}\sum_{j=1}^{\ell} \pi_i\varphi_i p_{ij}^{(k)} \varphi_j = \boldsymbol{\pi}^\top \operatorname{diag}(\boldsymbol{\varphi})\mathbf{P}^k\boldsymbol{\varphi}$$
    and $\mathbf{P}^k = \mathbf{P}^{(k)} = (p_{ij}^{(k)})$ denotes the matrix of the k-step transition probabilities.
  - A combination of the results above yields
$$\begin{aligned}\frac{1}{n}\operatorname{Var}\Big(\sum_{k=0}^{n-1}\varphi(\mathbf{X}_k)\Big) &= \sum_{i=1}^{\ell}\pi_i\varphi_i^2 + 2\boldsymbol{\pi}^\top\operatorname{diag}(\boldsymbol{\varphi})\sum_{k=1}^{n-1}\frac{n-k}{n}\,\mathbf{P}^k\boldsymbol{\varphi} - n\theta^2\\ &= \sigma^2 + 2\boldsymbol{\pi}^\top\operatorname{diag}(\boldsymbol{\varphi})\left(\sum_{k=1}^{n-1}\frac{n-k}{n}\,\mathbf{P}^k\boldsymbol{\varphi} - \frac{n-1}{2}\,\boldsymbol{\Pi}\boldsymbol{\varphi}\right)\\ &= \sigma^2 + 2\boldsymbol{\pi}^\top\operatorname{diag}(\boldsymbol{\varphi})\left(\sum_{k=1}^{n-1}\frac{n-k}{n}\,\left(\mathbf{P}^k - \boldsymbol{\Pi}\right)\right)\boldsymbol{\varphi}\,,\end{aligned}$$
  - where the second equality is due to the identity
$$\theta^2 = \boldsymbol{\pi}^\top\,\operatorname{diag}(\boldsymbol{\varphi})\boldsymbol{\Pi}\boldsymbol{\varphi}\,.$$
  - Taking into account the representation formula (76) for $\mathbf{Z} - \mathbf{I}$ this implies (78).
- It is left to show that (78) is also true for an arbitrary initial distribution $\boldsymbol{\alpha}$.
  - At this point we will use a more precise notation: We will write $\mathbf{X}_0^{(\boldsymbol{\alpha})}, \mathbf{X}_1^{(\boldsymbol{\alpha})}, \ldots$ instead of $\mathbf{X}_0, \mathbf{X}_1, \ldots$ and $\widehat{\theta}_n^{(\boldsymbol{\alpha})}$ instead of $\widehat{\theta}_n$.
  - It suffices to show that
$$\lim_{n\to\infty}\; n\left(\operatorname{Var}\,\widehat{\theta}_n^{(\boldsymbol{\pi})} - \operatorname{Var}\,\widehat{\theta}_n^{(\boldsymbol{\alpha})}\right) = 0\,. \tag{80}$$
  - For this purpose we introduce the following notation: For $0 < r < n-1$ let
$$Y_r^{(\cdot)} = \sum_{k=0}^{r-1}\varphi(\mathbf{X}_k^{(\cdot)}) \qquad \text{und} \qquad Z_{rn}^{(\cdot)} = \sum_{k=r}^{n-1}\varphi(\mathbf{X}_k^{(\cdot)})\,.$$
  - Then, by (79),
$$\begin{aligned}&n^2\left(\operatorname{Var}\,\widehat{\theta}_n^{(\boldsymbol{\pi})} - \operatorname{Var}\,\widehat{\theta}_n^{(\boldsymbol{\alpha})}\right)\\ &= \left(\mathbb{E}\left(Y_r^{(\boldsymbol{\pi})} + Z_{rn}^{(\boldsymbol{\pi})}\right)^2 - \mathbb{E}\left(Y_r^{(\boldsymbol{\alpha})} + Z_{rn}^{(\boldsymbol{\alpha})}\right)^2\right) - \left(\left(\mathbb{E}\,Y_r^{(\boldsymbol{\pi})} + \mathbb{E}\,Z_{rn}^{(\boldsymbol{\pi})}\right)^2 - \left(\mathbb{E}\,Y_r^{(\boldsymbol{\alpha})} + \mathbb{E}\,Z_{rn}^{(\boldsymbol{\alpha})}\right)^2\right)\\ &= \left(\mathbb{E}\left(Y_r^{(\boldsymbol{\pi})}\right)^2 - \left(\mathbb{E}\,Y_r^{(\boldsymbol{\pi})}\right)^2 - \mathbb{E}\left(Y_r^{(\boldsymbol{\alpha})}\right)^2 + \left(\mathbb{E}\,Y_r^{(\boldsymbol{\alpha})}\right)^2\right)\\ &\quad +2\mathbb{E}\left(\left(Y_r^{(\boldsymbol{\pi})} - \mathbb{E}\left(Y_r^{(\boldsymbol{\pi})}\right)\right)\left(Z_{rn}^{(\boldsymbol{\pi})} - \mathbb{E}\left(Z_{rn}^{(\boldsymbol{\pi})}\right)\right)\right) - 2\mathbb{E}\left(\left(Y_r^{(\boldsymbol{\alpha})} - \mathbb{E}\left(Y_r^{(\boldsymbol{\alpha})}\right)\right)\left(Z_{rn}^{(\boldsymbol{\alpha})} - \mathbb{E}\left(Z_{rn}^{(\boldsymbol{\alpha})}\right)\right)\right)\\ &\quad +\left(\mathbb{E}\left(Z_{rn}^{(\boldsymbol{\pi})}\right)^2 - \left(\mathbb{E}\,Z_{rn}^{(\boldsymbol{\pi})}\right)^2\right) - \left(\mathbb{E}\left(Z_{rn}^{(\boldsymbol{\alpha})}\right)^2 - \left(\mathbb{E}\,Z_{rn}^{(\boldsymbol{\alpha})}\right)^2\right),\end{aligned}$$
    where we denote the three summands in the last expression by I_r, II_{rn} and III_{rn}, respectively.

– I_r does not depend on n and hence $\lim_{n\to\infty} n^{-1} I_r = 0$.
– As the state space E is finite we obtain for $c = \max_{i\in E} |\varphi(i)| < \infty$ that

$$\frac{1}{n}\, II_{rn} \le 4rc\,\mathbb{E}\Big(\frac{1}{n}\,\big|Z_{rn}^{(\boldsymbol{\pi})} - \mathbb{E}\,(Z_{rn}^{(\boldsymbol{\pi})})\big|\Big) + 4rc\,\mathbb{E}\Big(\frac{1}{n}\,\big|Z_{rn}^{(\boldsymbol{\alpha})} - \mathbb{E}\,(Z_{rn}^{(\boldsymbol{\alpha})})\big|\Big)\,.$$

– This implies $\lim_{n\to\infty} n^{-1} II_{rn} = 0$ for any $r > 0$, as

$$\frac{1}{n}\,\big|Z_{rn}^{(\cdot)} - \mathbb{E}\,(Z_{rn}^{(\cdot)})\big| \le 2c$$

with probability 1 for all $n > r$ and

$$\lim_{n\to\infty} \frac{1}{n}\,\big|Z_{rn}^{(\boldsymbol{\pi})} - \mathbb{E}\,(Z_{rn}^{(\boldsymbol{\pi})})\big| = \lim_{n\to\infty} \frac{1}{n}\,\big|Z_{rn}^{(\boldsymbol{\alpha})} - \mathbb{E}\,(Z_{rn}^{(\boldsymbol{\alpha})})\big| = 0\,.$$

– Furthermore, for $n > r > 0$ we have the following estimate

$$\begin{aligned}\frac{1}{n}\, III_{rn} &\le \frac{1}{n}\sum_{i=1}^{\ell}\Big(\mathbb{E}\,(Z_{0,n-r}^{(\delta_i)})^2 - (\mathbb{E}\,Z_{0,n-r}^{(\delta_i)})^2\Big)|\pi_i - \alpha_{ri}| \\ &\le \underbrace{\sup_{n>0}\max_{j\in\{1,\dots,\ell\}} \frac{1}{n+r}\,\mathbb{E}\,\Big(Z_{0n}^{(\delta_j)} - \mathbb{E}\,Z_{0n}^{(\delta_j)}\Big)^2}_{<\infty} \sum_{i=1}^{\ell} |\pi_i - \alpha_{ri}|\,,\end{aligned}$$

where it is easy to see that the supremum is finite.
– Due to the ergodicity of the Markov chain $\mathbf{X}_0^{(\boldsymbol{\alpha})}, \mathbf{X}_1^{(\boldsymbol{\alpha})}, \dots$, the last summand will become arbitrarily small for sufficiently large r. This completes the proof of (80). □

Remarks

- Note that
  – for the *mean squared error* $\mathbb{E}\,((\widehat{\theta}_n - \theta)^2)$ of the MCMC estimator $\widehat{\theta}_n = \widehat{\theta}(\mathbf{X}_1, \dots, \mathbf{X}_n)$ for θ defined in (70) it holds that

$$\mathbb{E}\,((\widehat{\theta}_n - \theta)^2) = (\mathbb{E}\,\widehat{\theta}_n - \theta)^2 + \mathrm{Var}\,\widehat{\theta}_n\,, \tag{81}$$

  – i.e., the mean squared error of the MCMC estimator $\widehat{\theta}_n$ is equal to the sum of the squared bias $(\mathbb{E}\,\widehat{\theta}_n - \theta)^2$ and the variance $\mathrm{Var}\,\widehat{\theta}_n$ of the estimator $\widehat{\theta}_n$.
- Both summands on the right hand side of (81) converge to 0 if $n \to \infty$ but with different rates of convergence.
  – In Theorem 3.19 we showed that $\mathrm{Var}\,\widehat{\theta}_n = O(n^{-1})$.
  – On the other hand, by Theorem 3.18 we get that $(\mathbb{E}\,\widehat{\theta}_n - \theta)^2 = O(n^{-2})$.
- Consequently, the asymptotic behavior of the mean squared error $\mathbb{E}\,((\widehat{\theta}_n - \theta)^2)$ of $\widehat{\theta}_n$ is crucially influenced by the *asymptotic variance* $\mathrm{Var}\,\widehat{\theta}_n$ of the estimator, whereas the *bias* plays a minor role.
- In other words: It can make sense to choose the simulation matrix $\mathbf{P}$ such that
  – the asymptotic variance $\lim_{n\to\infty} n\mathrm{Var}\,\widehat{\theta}_n$ is as small as possible,
  – even if this results in a certain increase of the asymptotic bias $\lim_{n\to\infty} n(\mathbb{E}\,\widehat{\theta}_n - \theta)$.

In order to investigate this problem more deeply we introduce the following notation: Let

$$V(\varphi, \mathbf{P}, \boldsymbol{\pi}) = \lim_{n\to\infty} n\mathrm{Var}\,\widehat{\theta}_n\,,$$

where $\varphi : E \to \mathbb{R}$ is an arbitrary function and $(\mathbf{P}, \boldsymbol{\pi})$ is an arbitrary reversible pair.

Theorem 3.20

- *Let* $\mathbf{P}_1 = (p_{1,ij})$ *and* $\mathbf{P}_2 = (p_{2,ij})$ *be two transition matrices on* E *such that* $(\mathbf{P}_1, \boldsymbol{\pi})$ *and* $(\mathbf{P}_2, \boldsymbol{\pi})$ *are reversible.*
  - *For arbitrary* $i, j \in E$ *such that* $i \neq j$ *let* $p_{1,ij} \geq p_{2,ij}$,
  - *i.e., outside the diagonal all entries of the transition matrix* $\mathbf{P}_1$ *are greater or equal than the corresponding entries of the transition matrix* $\mathbf{P}_2$.
- *Then, for any function* $\varphi : E \to \mathbb{R}$,

$$V(\varphi, \mathbf{P}_1, \boldsymbol{\pi}) \leq V(\varphi, \mathbf{P}_2, \boldsymbol{\pi})\,. \tag{82}$$

Proof

- Let $\mathbf{P} = (p_{ij})$ be a transition matrix such that the pair $(\mathbf{P}, \boldsymbol{\pi})$ is reversible. It suffices to show that

$$\frac{\partial}{\partial p_{ij}}\, V(\varphi, \mathbf{P}, \boldsymbol{\pi}) \leq 0\,, \qquad \forall\, i, j \in E \text{ with } i \neq j. \tag{83}$$

- By Theorem 3.19,

$$\frac{\partial}{\partial p_{ij}}\, V(\varphi, \mathbf{P}, \boldsymbol{\pi}) = 2\boldsymbol{\pi}^\top\, \mathrm{diag}(\boldsymbol{\varphi})\, \frac{\partial \mathbf{Z}}{\partial p_{ij}}\, \boldsymbol{\varphi}\,, \tag{84}$$

  where $\mathbf{Z}$ denotes the fundamental matrix of $\mathbf{P}$ introduced by (74).
  - On the other hand, as $\mathbf{Z}\mathbf{Z}^{-1} = \mathbf{I}$, we get that

$$\Big(\frac{\partial \mathbf{Z}}{\partial p_{ij}}\Big)\mathbf{Z}^{-1} + \mathbf{Z}\Big(\frac{\partial \mathbf{Z}^{-1}}{\partial p_{ij}}\Big) = \mathbf{0}$$

    and thus

$$\frac{\partial \mathbf{Z}}{\partial p_{ij}} = -\mathbf{Z}\, \frac{\partial \mathbf{Z}^{-1}}{\partial p_{ij}}\, \mathbf{Z}\,.$$

  - Taking into account (84) this implies

$$\frac{\partial}{\partial p_{ij}}\, V(\varphi, \mathbf{P}, \boldsymbol{\pi}) = -2\boldsymbol{\pi}^\top\, \mathrm{diag}(\boldsymbol{\varphi})\mathbf{Z}\, \frac{\partial \mathbf{Z}^{-1}}{\partial p_{ij}}\, \mathbf{Z}\boldsymbol{\varphi}\,. \tag{85}$$

- As the pair $(\mathbf{P}, \boldsymbol{\pi})$ is reversible, by the representation formula (75) for the fundamental matrix $\mathbf{Z} = (z_{ij})$ that was derived in Lemma 3.3 we obtain for arbitrary $i, j \in E$

$$\pi_i z_{ij} = \pi_i \delta_{ij} + \sum_{k=1}^{\infty}\Big(\pi_i p_{ij}^{(k)} - \pi_i \pi_j\Big) = \pi_j \delta_{ji} + \sum_{k=1}^{\infty}\Big(\pi_j p_{ji}^{(k)} - \pi_j \pi_i\Big) = \pi_j z_{ji}\,.$$

  - This implies

$$\begin{aligned}
\boldsymbol{\pi}^\top\, \mathrm{diag}(\boldsymbol{\varphi})\mathbf{Z} &= \Big(\sum_{i=1}^{\ell} \pi_i \varphi_i z_{i1}, \ldots, \sum_{i=1}^{\ell} \pi_i \varphi_i z_{i\ell}\Big) \\
&= \Big(\pi_1 \sum_{i=1}^{\ell} z_{1i}\varphi_i, \ldots, \pi_\ell \sum_{i=1}^{\ell} z_{\ell i}\varphi_i\Big) \\
&= \big(\mathbf{Z}\boldsymbol{\varphi}\big)^\top\, \mathrm{diag}(\boldsymbol{\pi})\,.
\end{aligned}$$

– Thus, by (85),

$$\frac{\partial}{\partial p_{ij}} V(\varphi, \mathbf{P}, \boldsymbol{\pi}) = -2\big(\mathbf{Z}\boldsymbol{\varphi}\big)^\top \operatorname{diag}(\boldsymbol{\pi}) \frac{\partial \mathbf{Z}^{-1}}{\partial p_{ij}} \mathbf{Z}\boldsymbol{\varphi} = 2\big(\mathbf{Z}\boldsymbol{\varphi}\big)^\top \operatorname{diag}(\boldsymbol{\pi}) \frac{\partial \mathbf{P}}{\partial p_{ij}} \mathbf{Z}\boldsymbol{\varphi}\,, \tag{86}$$

where the last equality is due to the fact that

$$\frac{\partial \mathbf{Z}^{-1}}{\partial p_{ij}} = -\frac{\partial \mathbf{P}}{\partial p_{ij}}$$

which is an immediate consequence of the definition (74) of $\mathbf{Z}$.

- As $\mathbf{P} = (p_{ij})$ is a stochastic matrix and $(\mathbf{P}, \boldsymbol{\pi})$ is reversible
  - only the entries p_{ij} where $i < j$ (or alternatively the entries p_{ij} where $i > j$) can be chosen arbitrarily. This can be seen as follows.
  - For every pair $i, j \in E$ such that $i \neq j$ the entries p_{ji}, p_{ii} and p_{jj} can be expressed via p_{ij} in the following way:

$$p_{ji} = \frac{\pi_i}{\pi_j}\, p_{ij}\,, \qquad p_{ii} = c - p_{ij}\,, \qquad p_{jj} = c' - \frac{\pi_i}{\pi_j}\, p_{ij}\,,$$

where c and c' are constants that do not depend on p_{ij}.

  - For arbitrary $i', j' \in E$ the entry $\big(\operatorname{diag}(\boldsymbol{\pi})(\partial \mathbf{P}/\partial p_{ij})\big)_{i',j'}$ of the matrix product $\operatorname{diag}(\boldsymbol{\pi})(\partial \mathbf{P}/\partial p_{ij})$ is given by

$$\Big(\operatorname{diag}(\boldsymbol{\pi})\, \frac{\partial \mathbf{P}}{\partial p_{ij}}\Big)_{i',j'} = \begin{cases} -\pi_i & \text{if } (i',j') = (i,i) \text{ or } (i',j') = (j,j), \\ \pi_i & \text{if } (i',j') = (i,j) \text{ or } (i',j') = (j,i), \\ 0\,, & \text{else} \end{cases}$$

  - This implies that the matrix $\operatorname{diag}(\boldsymbol{\pi})(\partial \mathbf{P}/\partial p_{ij})$ is non-negative definite, i.e., for all $\mathbf{x} \in \mathbb{R}^\ell$

$$\mathbf{x}^\top \operatorname{diag}(\boldsymbol{\pi})\, \frac{\partial \mathbf{P}}{\partial p_{ij}}\, \mathbf{x} \leq 0\,.$$

  - By (86) this yields for arbitrary $i, j \in E$ such that $i \neq j$

$$\frac{\partial}{\partial p_{ij}} V(\varphi, \mathbf{P}, \boldsymbol{\pi}) = 2\big(\mathbf{Z}\boldsymbol{\varphi}\big)^\top \operatorname{diag}(\boldsymbol{\pi})\, \frac{\partial \mathbf{P}}{\partial p_{ij}}\, \mathbf{Z}\boldsymbol{\varphi} \leq 0\,.$$

- This completes the proof of (83). □

Remarks As a particular consequence of Theorem 3.20 we get that

- the simulation matrix $\mathbf{P}$ of the Metropolis algorithm (i.e. if we consider equality in (50)) minimizes the asymptotic variance $V(\varphi, \mathbf{P}, \boldsymbol{\pi})$
- within the class of all Metropolis–Hastings algorithms having an arbitrary but fixed „potential transition matrix" $\mathbf{Q} = \big(q_{ij}\big)$.

3.5 Coupling Algorithms; Perfect MCMC Simulation

- In this section we will discuss algorithms
  - that are also based on Markov chains,
  - but this new class of algorithms simulates a given discrete distribution $\boldsymbol{\pi}$ not only approximately but in a certain sense exactly.
- Therefore, these techniques are referred to as methods of „perfect" MCMC simulation.

3.5.1 Coupling to the Future; Counterexample

- First of all we consider a method for „coupling" the paths of Markov chains where the „time"
  - is running forward, i.e. in a way that is perceived as natural.
  - Therefore, one also refers to this method as *coupling to the future*.
- For all $i \in \{1,\dots,\ell\}$ let $\mathbf{X}^{(i)} = \big(\mathbf{X}_0^{(i)}, \mathbf{X}_1^{(i)}, \dots\big)$ be a homogenous Markov chain with finite state space $E = \{\mathbf{x}_1, \dots, \mathbf{x}_\ell\}$
  - with deterministic initial state $\mathbf{X}_0^{(i)} = \mathbf{x}_i$ and with an irreducible and aperiodic transition matrix $\mathbf{P} = (p_{\mathbf{x}\mathbf{x}'})$,
  - such that $\boldsymbol{\pi} = (\pi_{\mathbf{x}},\, \mathbf{x} \in E)$ is the ergodic limit distribution of the Markov chain $\mathbf{X}^{(i)}$.

Definitions

- For all $k \in \{1,\dots,\ell\}$ we consider
  - a sequence $\mathbf{U}^{(k)} = \big(U_1^{(k)}, U_2^{(k)}, \dots\big)$ of independent and $(0,1]$–uniformly distributed random variables $U_n^{(k)}$,
  - called *innovations* in step n for the current state $\mathbf{x}_k \in E$.
- We consider two different cases:
  - Either we assume the sequences $\mathbf{U}^{(1)}, \dots, \mathbf{U}^{(\ell)}$ to be independent
  - or we merely consider a *single* sequence $\mathbf{U} = \big(U_1, U_2, \dots\big)$ and define $\mathbf{U}^{(1)} = \dots = \mathbf{U}^{(\ell)} = \mathbf{U}$.
- Let the Markov chain $\mathbf{X}^{(i)}$ be defined recursively by

$$\mathbf{X}_n^{(i)} = \varphi\big(\mathbf{x}_k, U_n^{(k)}\big) \qquad \text{if } X_{n-1}^{(i)} = \mathbf{x}_k, \tag{87}$$

  where $\varphi : E \times (0,1] \to E$ is a so–called *valid update function*, i.e.
  - $\varphi(\mathbf{x}, \cdot) : (0,1] \to E$ is piecewise constant for all $\mathbf{x} \in E$
  - and for arbitrary $\mathbf{x}, \mathbf{x}' \in E$ such that $p_{\mathbf{x}\mathbf{x}'} > 0$ the total length of the set $\{u \in (0,1] :\, \varphi(\mathbf{x}, u) = \mathbf{x}'\}$ equals $p_{\mathbf{x}\mathbf{x}'}$.
- The random variable $\tau = \min\big\{n \geq 1 :\, \mathbf{X}_n^{(1)} = \dots = \mathbf{X}_n^{(\ell)}\big\}$ is called *coupling time* where we define $\tau = \infty$ if there is no natural number n such that $\mathbf{X}_n^{(1)} = \dots = \mathbf{X}_n^{(\ell)}$.

Theorem 3.21 *If the sequences of innovations $\mathbf{U}^{(1)}, \dots, \mathbf{U}^{(\ell)}$ are independent, then $\tau < \infty$ with probability 1 and $\mathbf{X}_n^{(1)} = \dots = \mathbf{X}_n^{(\ell)}$ for all $n > \tau$.*

Proof

- The recursive definition (87) of the Markov chains $\mathbf{X}^{(1)}, \dots, \mathbf{X}^{(\ell)}$ immediately implies $\mathbf{X}_n^{(1)} = \dots = \mathbf{X}_n^{(\ell)}$ for all $n > \tau$.
- It is left to show that $P(\tau < \infty) = 1$. We notice that it suffices to show that for arbitrary $i \neq i'$

$$\lim_{r\to\infty} P\Big(\max\big\{n : \mathbf{X}_n^{(i)} \neq \mathbf{X}_n^{(i')}\big\} \leq r\Big) = 1\,.$$

  - As

$$\begin{aligned} P\Big(\max\big\{n : \mathbf{X}_n^{(i)} \neq \mathbf{X}_n^{(i')}\big\} \leq r\Big) &= 1 - P\Big(\max\big\{n : \mathbf{X}_n^{(i)} \neq \mathbf{X}_n^{(i')}\big\} > r\Big) \\ &= 1 - P\Big(\mathbf{X}_r^{(i)} \neq \mathbf{X}_r^{(i')}\Big) \end{aligned}$$

    this is equivalent to

$$\lim_{r\to\infty} P\Big(\mathbf{X}_r^{(i)} \neq \mathbf{X}_r^{(i')}\Big) = 0\,.$$

– Let now $n_0 \geq 1$ be a natural number such that

$$\min_{\mathbf{x},\mathbf{x}' \in E} p_{\mathbf{x}\mathbf{x}'}^{(n_0)} = c > 0\,,$$

and consider the decomposition $r = m(r)n_0 + k$ for some $m(r) \in \{0, 1, \ldots\}$ and $k \in \{0, 1, \ldots, n_0 - 1\}$.

– The independence of the innovation sequences $\mathbf{U}^{(1)}, \ldots, \mathbf{U}^{(\ell)}$ yields for $r \to \infty$

$$\begin{aligned}
P\Big(\mathbf{X}_r^{(i)} \neq \mathbf{X}_r^{(i')}\Big) &= P\Big(\mathbf{X}_{n_0}^{(i)} \neq \mathbf{X}_{n_0}^{(i')},\, \mathbf{X}_r^{(i)} \neq \mathbf{X}_r^{(i')}\Big) \\
&= \sum_{j=1}^{\ell} \sum_{j' \neq j} P\Big(\mathbf{X}_{n_0}^{(i)} = \mathbf{x}_j,\, \mathbf{X}_{n_0}^{(i')} = \mathbf{x}_{j'}\Big)\; P\Big(\mathbf{X}_r^{(i)} \neq \mathbf{X}_r^{(i')} \mid \mathbf{X}_{n_0}^{(i)} = \mathbf{x}_j,\, \mathbf{X}_{n_0}^{(i')} = \mathbf{x}_{j'}\Big) \\
&= \sum_{j=1}^{\ell} \sum_{j' \neq j} P\Big(\mathbf{X}_{n_0}^{(i)} = \mathbf{x}_j\Big)\; P\Big(\mathbf{X}_{n_0}^{(i')} = \mathbf{x}_{j'}\Big)\; P\Big(\mathbf{X}_{r-n_0}^{(j)} \neq \mathbf{X}_{r-n_0}^{(j')}\Big) \\
&= \underbrace{\sum_{j=1}^{\ell} p_{\mathbf{x}_i\mathbf{x}_j}^{(n_0)} \sum_{j' \neq j} p_{\mathbf{x}_{i'}\mathbf{x}_{j'}}^{(n_0)}}_{\leq 1-c}\; P\Big(\mathbf{X}_{r-n_0}^{(j)} \neq \mathbf{X}_{r-n_0}^{(j')}\Big) \\
&\leq (1-c) \max_{j \neq j} P\Big(\mathbf{X}_{r-n_0}^{(j)} \neq \mathbf{X}_{r-n_0}^{(j')}\Big) \\
&\;\;\vdots \\
&\leq (1-c)^{m(r)} \longrightarrow 0\,.
\end{aligned}$$

□

Remarks

- Under additional assumptions about the irreducible and periodic transition matrix $\mathbf{P} = (p_{\mathbf{x}\mathbf{x}'})$ it can be shown that the coupling time τ is finite even if
  - only a *single* sequence $\mathbf{U} = \big(U_1, U_2, \ldots\big)$ innovations is considered, i.e. $\mathbf{U} = \mathbf{U}^{(1)} = \ldots = \mathbf{U}^{(\ell)}$,
  - and if for all $\mathbf{x} \in E$ the update function $\varphi : E \times (0, 1] \to E$ is given by

$$\varphi(\mathbf{x},\, u) = \mathbf{x}_j\,, \qquad \text{if } \sum_{r=1}^{j-1} p_{\mathbf{x}\mathbf{x}_r} < u \leq \sum_{r=1}^{j} p_{\mathbf{x}\mathbf{x}_r}. \tag{88}$$

- Such an additional condition imposed on $\mathbf{P}$ will be discussed in the following theorem, see also the monotonicity condition in Section 3.5.3.

Theorem 3.22

- *Let* $\mathbf{U}^{(1)} = \ldots = \mathbf{U}^{(\ell)} = \mathbf{U}$ *and let the update function* $\varphi : E \times (0, 1] \to E$ *be given by* (88). *Furthermore, for some* $\mathbf{x}_{i_0} \in E$, *let*

$$\max_{\mathbf{x} \in E} \sum_{r=1}^{i_0 - 1} p_{\mathbf{x}\mathbf{x}_r} < \min_{\mathbf{x} \in E} \sum_{r=1}^{i_0} p_{\mathbf{x}\mathbf{x}_r}\,. \tag{89}$$

- *Then* $\tau < \infty$ *with probability* 1 *and for all* $n > \tau$ $\mathbf{X}_n^{(1)} = \ldots = \mathbf{X}_n^{(\ell)}$.

Proof

- Similar to the proof of Theorem 3.21 it suffices to show that for arbitrary $i \neq i'$

$$\lim_{r\to\infty} P\Big(\mathbf{X}_r^{(i)} \neq \mathbf{X}_r^{(i')}\Big) = 0\,.$$

Observe that

- $$\begin{aligned}
P\Big(\mathbf{X}_r^{(i)} \neq \mathbf{X}_r^{(i')}\Big) &= P\Big(\mathbf{X}_1^{(i)} \neq \mathbf{X}_1^{(i')},\, \mathbf{X}_r^{(i)} \neq \mathbf{X}_r^{(i')}\Big) \\
&= \sum_{j=1}^{\ell} \sum_{j'\neq j} P\Big(\mathbf{X}_1^{(i)} = \mathbf{x}_j,\, \mathbf{X}_1^{(i')} = \mathbf{x}_{j'}\Big)\; P\Big(\mathbf{X}_r^{(i)} \neq \mathbf{X}_r^{(i')} \mid \mathbf{X}_1^{(i)} = \mathbf{x}_j,\, \mathbf{X}_1^{(i')} = \mathbf{x}_{j'}\Big) \\
&= \sum_{j=1}^{\ell} \sum_{j'\neq j} P\Big(\mathbf{X}_1^{(i)} = \mathbf{x}_j,\, \mathbf{X}_1^{(i')} = \mathbf{x}_{j'}\Big)\; P\Big(\mathbf{X}_{r-1}^{(j)} \neq \mathbf{X}_{r-1}^{(j')}\Big) \\
&\leq \Big(1 - \underbrace{P\Big(\mathbf{X}_1^{(i)} = \mathbf{X}_1^{(i')}\Big)}_{\geq d>0}\Big) \max_{j'\neq j} P\Big(\mathbf{X}_{r-1}^{(j)} \neq \mathbf{X}_{r-1}^{(j')}\Big) \\
&\;\;\vdots \\
&\leq (1-d)^r \longrightarrow 0\,,
\end{aligned}$$

where we use that (87) – (89) imply

$$0 < d = \max_{\mathbf{x}\in E} \sum_{r=1}^{i_0-1} p_{\mathbf{x}\mathbf{x}_r} - \min_{\mathbf{x}\in E} \sum_{r=1}^{i_0} p_{\mathbf{x}\mathbf{x}_r} \leq P\Big(\mathbf{X}_1^{(i)} = \mathbf{X}_1^{(i')} = \mathbf{x}_{i_0}\Big) \leq P\Big(\mathbf{X}_1^{(i)} = \mathbf{X}_1^{(i')}\Big)\,. \qquad \square$$

Remarks

- In general $P(\tau < \infty) = 1$ does *not* imply $\mathbf{X}_\tau^{(i)} \sim \boldsymbol{\pi}$,
  - i.e., at the coupling time τ the distribution of the Markov chain $\mathbf{X}^{(i)}$ does in general not coincide with the stationary limit distribution $\boldsymbol{\pi}$ although this could be a conjecture.
- The following *counterexample* illustrates this paradox.
  - Consider the state space $E = \{1, 2\}$ and the irreducible and aperiodic transition matrix

$$\mathbf{P} = \begin{pmatrix} 0.5 & 0.5 \\ 1 & 0 \end{pmatrix}$$

whose stationary limit distribution is $\boldsymbol{\pi} = (2/3,\, 1/3)^\top$.
  - If $\mathbf{X}_{\tau-1}^{(1)} \neq \mathbf{X}_{\tau-1}^{(2)}$ we necessarily obtain $\mathbf{X}_{\tau-1}^{(1)} = 2$ or $\mathbf{X}_{\tau-1}^{(2)} = 2$ and therefore $\mathbf{X}_\tau^{(1)} = \mathbf{X}_\tau^{(2)} = 1$.

3.5.2 Propp–Wilson Algorithm; Coupling from the Past

- Recall that
  - the procedure of coupling to the future discussed in Section 3.5.1 starts at a deterministic time 0 whereas the final state, i.e. the coupling time τ of the simulation is *random*.
  - Moreover, the state distribution of the Markov chain $\mathbf{X}^{(i)}$ at the coupling time τ is in general *not* equal to the stationary limit distribution $\boldsymbol{\pi}$.

- Therefore, we will now consider a different coupling method,
  - which is called *Coupling from the Past* (CFTP).
  - It was developed in the mid 90s by Propp and Wilson at the *Massachusetts Institute of Technology* (MIT).
- The procedure is similar to coupling to the future (see Section 3.5.1) but now the initial „time" of the simulation will be chosen *randomly* whereas the final „time" is *deterministic*.
  - In other words, the Markov chains $\mathbf{X}^{(1)}, \ldots, \mathbf{X}^{(\ell)}$ are *not* started at „time" 0,
  - but sufficiently far away in the „past" such that by time 0 at the latest all paths will have merged.

For the precise mathematical modelling of this procedure we need the following notation.

- For each potential „initial time" $m \in \{-1, -2, \ldots\}$ and for all $i \in \{1, \ldots, \ell\}$ let
$$\mathbf{X}^{(m,i)} = \big(\mathbf{X}_m^{(m,i)}, \mathbf{X}_{m+1}^{(m,i)}, \ldots\big)$$
  - be a homogenous Markov chain with finite state space $E = \{\mathbf{x}_1, \ldots, \mathbf{x}_\ell\}$,
  - with the (deterministic) initial state $\mathbf{X}_m^{(m,i)} = \mathbf{x}_i$ and with the irreducible and aperiodic transition matrix $\mathbf{P} = (p_{\mathbf{x}\mathbf{x}'})$,
  - such that $\boldsymbol{\pi} = (\pi_{\mathbf{x}},\, \mathbf{x} \in E)$ is the ergodic limit distribution of $\mathbf{X}^{(m,i)}$.
- For every $k \in \{1, \ldots, \ell\}$ we consider
  - a sequence $\mathbf{U}^{(k)} = \big(U_0^{(k)}, U_{-1}^{(k)}, \ldots\big)$ of independent and $(0,1]$–uniformly distributed random variables.
  - Like in Section 3.5.1 we call $U_{-n}^{(k)}$ an *innovation* in step $-n$ if the current state is $\mathbf{x}_k \in E$.
- We consider two cases:
  - The innovation sequences $\mathbf{U}^{(1)}, \ldots, \mathbf{U}^{(\ell)}$ are either independent
  - or $\mathbf{U}^{(1)} = \ldots = \mathbf{U}^{(\ell)} = \mathbf{U}$.
- Let the Markov chain $\mathbf{X}^{(m,i)}$ be defined recursively via the update function $\varphi : E \times (0,1] \to E$, i.e.
$$\mathbf{X}_n^{(m,i)} = \varphi\big(\mathbf{x}_k, U_n^{(k)}\big) \qquad \text{if } X_{n-1}^{(m,i)} = \mathbf{x}_k. \tag{90}$$

Definition The random variable $\zeta = \min\big\{-m \geq 1 : \mathbf{X}_0^{(m,1)} = \ldots = \mathbf{X}_0^{(m,\ell)}\big\}$ is called *CFTP coupling time* where we define $\zeta = \infty$ if there is no integer $-m$ such that $\mathbf{X}_0^{(m,1)} = \ldots = \mathbf{X}_0^{(m,\ell)}$.

Theorem 3.23 *Let $P(\zeta < \infty) = 1$. Then, for all $m \leq -\zeta$,*
$$\mathbf{X}_0^{(m,1)} = \ldots = \mathbf{X}_0^{(m,\ell)}\,.$$
Moreover, for arbitrary $m \leq -\zeta$ and $i, j \in \{1, \ldots, \ell\}$,
$$\mathbf{X}_0^{(m,i)} = \mathbf{X}_0^{(-\zeta,j)} \sim \boldsymbol{\pi}\,.$$

Proof

- Directly by the recursive definition (90) of the Markov chains $\mathbf{X}^{(m,1)}, \ldots, \mathbf{X}^{(m,\ell)}$, we get that $\mathbf{X}_0^{(m,1)} = \ldots = \mathbf{X}_0^{(m,\ell)}$ and $\mathbf{X}_0^{(m,i)} = \mathbf{X}_0^{(-\zeta,j)}$ for arbitrary $m \le -\zeta$ and $i, j \in \{1, \ldots, \ell\}$.
- As by hypothesis $P(\zeta < \infty) = 1$, we obtain for arbitrary $k \in \{1, \ldots, \ell\}$ that

$$\begin{aligned} P\Big(\mathbf{X}_0^{(-\zeta,i)} = \mathbf{x}_k\Big) &= \lim_{m \to -\infty} P\Big(\mathbf{X}_0^{(-\zeta,i)} = \mathbf{x}_k,\, \zeta \le -m\Big) \\ &= \lim_{m \to -\infty} P\Big(\mathbf{X}_0^{(m,i)} = \mathbf{x}_k,\, \zeta \le -m\Big) \\ &= \lim_{m \to -\infty} P\Big(\mathbf{X}_0^{(m,i)} = \mathbf{x}_k\Big) - \underbrace{\lim_{m \to -\infty} P\Big(\mathbf{X}_0^{(m,i)} = \mathbf{x}_k,\, \zeta > -m\Big)}_{=0} \\ &= \lim_{m \to -\infty} P\Big(\mathbf{X}_0^{(m,i)} = \mathbf{x}_k\Big) \\ &= \lim_{m \to -\infty} P\Big(\mathbf{X}_{-m}^{(0,i)} = \mathbf{x}_k\Big) = \boldsymbol{\pi}_{\mathbf{x}_k}\,, \end{aligned}$$

  where the last but one equality is a consequence of the homogeneity of the Markov chain $\mathbf{X}^{(m,i)}$. □

Remarks

- If the number ℓ of elements in the state space $E = \{\mathbf{x}_1, \ldots, \mathbf{x}_\ell\}$ is large,
  - the MCMC simulation of $\boldsymbol{\pi}$ based on the CFTP algorithm by Propp and Wilson can be computationally inefficient
  - as for every initial state $\mathbf{x}_1, \ldots, \mathbf{x}_\ell$ a complete path needs to be generated.
- However, in some cases the computational complexity can be reduced. Examples will be discussed in Sections 3.5.3 and 3.5.4.
  - In these special situations the state space $E = \{\mathbf{x}_1, \ldots, \mathbf{x}_\ell\}$ and the update function $\varphi : E \times (0,1] \to E$ possess certain monotonicity properties.
  - As a consequence it suffices to consider a *single* sequence $\mathbf{U} = \big(U_0, U_{-1}, \ldots\big)$ of independent and $(0,1]$–uniformly distributed innovations.
  - Moreover, only *two* different paths need to be generated.

3.5.3 Monotone Coupling Algorithms

- We additionally assume that the state space $E = \{\mathbf{x}_1, \ldots, \mathbf{x}_\ell\}$ is partially ordered and has a maximal element $\mathbf{1} \in E$ and a minimal element $\mathbf{0} \in E$, i.e., there is a relation $\preceq$ on E such that
  (a) $\mathbf{x} \preceq \mathbf{x}\,, \qquad \forall\, \mathbf{x} \in E\,,$
  (b) $\mathbf{x} \preceq \mathbf{y}$ and $\mathbf{y} \preceq \mathbf{z} \Rightarrow \mathbf{x} \preceq \mathbf{z}\,, \qquad \forall\, \mathbf{x}, \mathbf{y}, \mathbf{z} \in E\,,$
  (c) $\mathbf{x} \preceq \mathbf{y}$ and $\mathbf{y} \preceq \mathbf{x} \Rightarrow \mathbf{x} = \mathbf{y}\,, \qquad \forall\, \mathbf{x}, \mathbf{y} \in E\,,$
  (d) $\mathbf{0} \preceq \mathbf{x} \preceq \mathbf{1}\,, \qquad \forall\, \mathbf{x} \in E\,.$
- Furthermore, we impose the condition
  - that the update function $\varphi : E \times (0,1] \to E$ is *monotonously nondecreasing* with respect to the partial order $\preceq$, i.e., for arbitrary $\mathbf{x}, \mathbf{y} \in E$ such that $\mathbf{x} \preceq \mathbf{y}$ we have

$$\varphi(\mathbf{x}, u) \preceq \varphi(\mathbf{y}, u)\,, \qquad \forall\, u \in (0,1]\,. \tag{91}$$

- Let the innovations $\mathbf{U}^{(1)}, \ldots, \mathbf{U}^{(\ell)}$ be identical with probability 1,
  - i.e., we merely consider a *single* sequence $\mathbf{U} = \big(U_0, U_{-1}, \ldots\big)$ of independent and $(0,1]$–uniformly distributed random variables and define $\mathbf{U}^{(1)} = \ldots = \mathbf{U}^{(\ell)} = \mathbf{U}$.
  - For arbitrary $m \in \{-1, -2, \ldots\}$ and $i \in \{1, \ldots, \ell\}$ the Markov chain $\mathbf{X}^{(m,i)}$ is recursively defined by

$$\mathbf{X}_n^{(m,i)} = \varphi\big(\mathbf{X}_{n-1}^{(m,i)}, U_n\big)\,, \qquad \forall\, n = m+1, m+2, \ldots\,. \tag{92}$$

Remarks

- If $\mathbf{x}_i \preceq \mathbf{x}_j$, then by (91) and (92) we get that for all $n \geq m$

$$\mathbf{X}_n^{(m,i)} \preceq \mathbf{X}_n^{(m,j)}\,. \tag{93}$$

- In particular, for arbitrary $n \geq m$ and $i \in \{1, \ldots, \ell\}$,

$$\mathbf{X}_n^{(m,\min)} \preceq \mathbf{X}_n^{(m,i)} \preceq \mathbf{X}_n^{(m,\max)}\,, \tag{94}$$

  - where $\mathbf{X}^{(m,\min)}$ and $\mathbf{X}^{(m,\max)}$ denote the Markov chains

$$\mathbf{X}^{(m,\min)} = (\mathbf{X}_m^{(m,\min)}, \mathbf{X}_{m+1}^{(m,\min)}, \ldots) \qquad \text{and} \qquad \mathbf{X}^{(m,\max)} = (\mathbf{X}_m^{(m,\max)}, \mathbf{X}_{m+1}^{(m,\max)}, \ldots)$$

  - that are recursively defined by (92) with $\mathbf{X}_m^{(m,\min)} = \mathbf{0}$ and $\mathbf{X}_m^{(m,\max)} = \mathbf{1}$.
- Due to (94) it suffices to choose an initial „time" that lies far enough in the past
  - such that the paths of $\mathbf{X}^{(m,\min)}$ and $\mathbf{X}^{(m,\max)}$ will have merged by „time" 0,
  - i.e., we consider the *CFTP coupling time*

$$\zeta = \min\big\{-m \geq 1 :\, \mathbf{X}_0^{(m,\min)} = \mathbf{X}_0^{(m,\max)}\big\}\,. \tag{95}$$

Theorem 3.24 *Let the update function $\varphi : E \times (0,1] \to E$ satisfy the monotonicity condition* (91)*.*

- *Then, for the CFTP coupling time defined by* (95)*, it holds that $\zeta < \infty$ with probability* 1*.*
- *Moreover, for arbitrary $m \leq -\zeta$ and $i, j \in \{1, \ldots, \ell\}$, $\mathbf{X}_0^{(m,i)} = \mathbf{X}_0^{(-\zeta,j)} \sim \boldsymbol{\pi}$.*

Proof

- As the argument showing that $\mathbf{X}_0^{(m,i)} = \mathbf{X}_0^{(-\zeta,j)} \sim \boldsymbol{\pi}$ for arbitrary $m \leq -\zeta$ and $i, j \in \{1, \ldots, \ell\}$ if $P(\zeta < \infty) = 1$, is similar to the proof of Theorem 3.23 this part of the proof is omitted.
- We merely show that $P(\zeta < \infty) = 1$.
  - First of all, we observe that for all $r \geq 1$

$$\{\zeta > r\} \subset \Big\{\mathbf{X}_{-r+1}^{(-r,\min)} \neq \mathbf{1},\, \ldots,\, \mathbf{X}_0^{(-r,\min)} \neq \mathbf{1}\Big\}\,, \tag{96}$$

    as (94) implies

$$\begin{aligned}
\{\zeta > r\} &= \Big\{\mathbf{X}_0^{(-r,\min)} \neq \mathbf{X}_0^{(-r,\max)}\Big\} \\
&= \Big\{\mathbf{X}_{-r+1}^{(-r,\min)} \neq \mathbf{X}_{-r+1}^{(-r,\max)},\, \ldots,\, \mathbf{X}_0^{(-r,\min)} \neq \mathbf{X}_0^{(-r,\max)}\Big\} \\
&\overset{(94)}{\subset} \Big\{\mathbf{X}_{-r+1}^{(-r,\min)} \neq \mathbf{1},\, \ldots,\, \mathbf{X}_0^{(-r,\min)} \neq \mathbf{1}\Big\}\,.
\end{aligned}$$

– As in the proof of Theorem 3.21 let $n_0 \geq 1$ be a natural number such that

$$\min_{\mathbf{x},\mathbf{x}' \in E} p_{\mathbf{x}\mathbf{x}'}^{(n_0)} = c > 0\,, \tag{97}$$

and decompose r such that $r = m(r)n_0 + k$ for some $m(r) \in \{0, 1, \ldots\}$ and $k \in \{0, 1, \ldots, n_0 - 1\}$.

– By (96) and (97) we obtain

$$\begin{aligned} P\big(\zeta = \infty\big) &= \lim_{r\to\infty} P\big(\zeta > r\big) \\ &\overset{(96)}{\leq} \lim_{r\to\infty} P\Big(\mathbf{X}_{-r+1}^{(-r,\min)} \neq \mathbf{1},\, \ldots,\, \mathbf{X}_0^{(-r,\min)} \neq \mathbf{1}\Big) \\ &\leq \lim_{r\to\infty} \sum_{\mathbf{x}_1,\ldots,\mathbf{x}_{m(r)} \neq \mathbf{1}} p_{\mathbf{0}\mathbf{x}_1}^{(n_0)} p_{\mathbf{x}_1\mathbf{x}_2}^{(n_0)} \cdot \ldots \cdot p_{\mathbf{x}_{m(r)-1}\mathbf{x}_{m(r)}}^{(n_0)} \\ &\overset{(97)}{\leq} \lim_{r\to\infty} (1-c)^{m(r)} = 0\,. \end{aligned}$$

□

Remarks

- Sometimes the update function $\varphi : E \times (0,1] \to E$ is not monotonously nondecreasing but nonincreasing with respect to the partial order $\preceq$, i.e., for arbitrary $\mathbf{x}, \mathbf{y} \in E$ such that $\mathbf{x} \preceq \mathbf{y}$ we have

$$\varphi(\mathbf{x}, u) \succeq \varphi(\mathbf{y}, u)\,, \qquad \forall\, u \in (0,1]\,. \tag{98}$$

- In this case the following *cross-over technique* turns out to be useful.
  - Based on the update function $\varphi : E \times (0,1] \to E$ we construct a new nondecreasing update function $\varphi' : E \times (0,1]^2 \to E$ which is given as

$$\varphi'(\mathbf{x}; u_1, u_2) = \varphi(\varphi(\mathbf{x}, u_1), u_2)\,, \qquad \forall\, \mathbf{x} \in E;\, u_1, u_2 \in (0,1]\,. \tag{99}$$

  - This function has the desired property as by (98) and (99) we obtain for arbitrary $\mathbf{x}, \mathbf{y} \in E$ such that $\mathbf{x} \preceq \mathbf{y}$

$$\varphi'(\mathbf{x}; u_1, u_2) = \varphi(\varphi(\mathbf{x}, u_1), u_2) \preceq \varphi(\varphi(\mathbf{y}, u_1), u_2) = \varphi'(\mathbf{y}; u_1, u_2)\,, \qquad \forall\, u_1, u_2 \in (0,1]\,,$$

    i.e., $\varphi' : E \times (0,1]^2 \to E$ is nondecreasing if $\varphi : E \times (0,1] \to E$ is nonincreasing.
- Let now $\varphi : E \times (0,1] \to E$ be an update function with respect to the irreducible and aperiodic transition matrix $\mathbf{P} = (p_{\mathbf{x}\mathbf{x}'})$ with ergodic limit distribution $\boldsymbol{\pi} = (\pi_{\mathbf{x}},\, \mathbf{x} \in E)$.
  - Then the map $\varphi' : E \times (0,1]^2 \to E$ defined by (99) is a valid update function with respect to the irreducible and aperiodic two–step transition matrix $\mathbf{P}^{(2)} = (p_{\mathbf{x}\mathbf{x}'}^{(2)})$ and it has the same ergodic limit distribution $\boldsymbol{\pi} = (\pi_{\mathbf{x}},\, \mathbf{x} \in E)$.
  - In the same way that was used to prove Theorem 3.24 one can show that the coupling time $\zeta' = \min\big\{-m \geq 1 : \mathbf{X}_0^{(2m,\min)} = \mathbf{X}_0^{(2m,\max)}\big\}$ is finite with probability 1, i.e., $\zeta' < \infty$ and $\mathbf{X}_0^{(-2\zeta',i)} \sim \boldsymbol{\pi}$ for all $i \in \{1, \ldots, \ell\}$ if $\varphi : E \times (0,1] \to E$ is nonincreasing.

3.5.4 Examples: Birth–and–Death Processes; Ising Model

1. *Birth–and–Death Processes*

- The update function $\varphi : E \times (0,1] \to E$ defined in (88) satisfies the monotonicity condition (91)

– if the state space can identified with the set $E = \{1, \ldots, \ell\}$ equipped with the natural order $\leq$ of the numbers $1, \ldots, \ell$
– and if the simulation matrix $\mathbf{P} = (p_{ij})$ is *monotonously nondecreasing* with respect to the order $\leq$, i.e., for arbitrary $i, j \in E$ such that $i \leq j$ we have

$$\sum_{r=k}^{\ell} p_{ir} \leq \sum_{r=k}^{\ell} p_{jr}\,, \qquad \forall\, k = 1, \ldots, \ell\,. \tag{100}$$

- A whole class of transition matrices $\mathbf{P} = (p_{ij})$ satisfying the monotonicity condition (100) is given by the tridiagonal matrices of *birth–and–death processes* which are of the type

$$\mathbf{P} = \begin{pmatrix} 1-p_{12} & p_{12} & 0 & \ldots & 0 \\ p_{21} & 1-p_{21}-p_{23} & p_{23} & \ldots & 0 \\ 0 & p_{32} & 1-p_{32}-p_{34} & \ldots & 0 \\ \vdots & \vdots & \vdots & & \vdots \\ 0 & 0 & 0 & \ldots & p_{\ell-1,\ell} \\ 0 & 0 & 0 & \ldots & 1-p_{\ell,\ell-1} \end{pmatrix},$$

where $0 < p_{i,i+1} \leq 1/2$ for all $i = 1, \ldots, \ell-1$ and $0 < p_{i,i-1} \leq 1/2$ for all $i = 2, \ldots, \ell$.

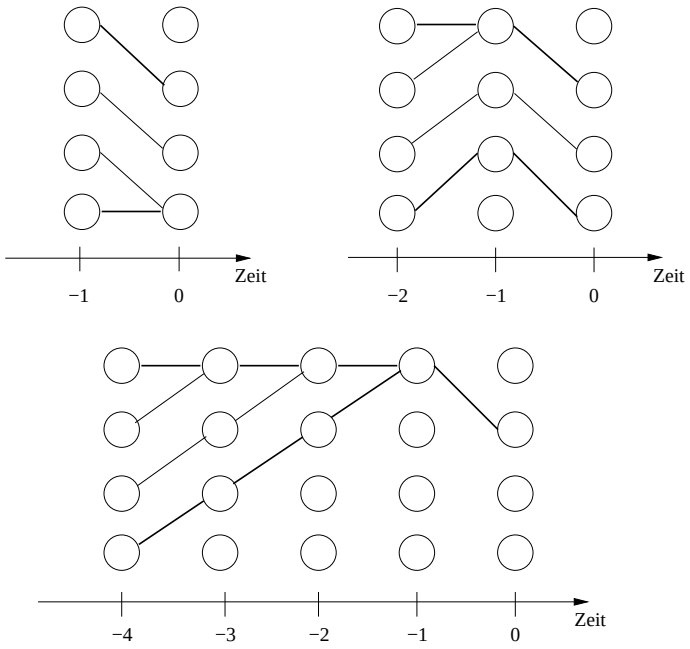


Figure 7: Monotonic coupling to the past for monotonously nondecreasing death–and–birth processes

- On the other hand, the update function $\varphi : E \times (0,1] \to E$ defined in (88) is monotonously nonincreasing, see (98),
  – if $\mathbf{P} = (p_{ij})$ is *monotonously nonincreasing* with respect to $\leq$,
  – i.e., if for arbitrary $i, j \in E$ such that $i \leq j$ we have

$$\sum_{r=k}^{\ell} p_{ir} \geq \sum_{r=k}^{\ell} p_{jr}\,, \qquad \forall\, k = 1, \ldots, \ell\,. \tag{101}$$

- It is easy to show that there is no tridiagonal transition matrix $\mathbf{P} = (p_{ij})$ satisfying the condition (101), i.e., birth–and–death processes are never monotonously nonincreasing.

- However, condition (101) holds for example for the following matrix:

$$\mathbf{P} = \begin{pmatrix} 0 & \dots & 0 & 0 & 1 \\ 0 & \dots & 0 & 1/2 & 1/2 \\ 0 & \dots & 1/3 & 1/3 & 1/3 \\ \vdots & & \vdots & \vdots & \vdots \\ 0 & \dots & 1/(\ell-1) & 1/(\ell-1) & 1/(\ell-1) \\ 1/\ell & \dots & 1/\ell & 1/\ell & 1/\ell \end{pmatrix}$$

2. *Ising Model*

- Like for the hard–core model discussed in Section 3.3.1
  - we consider a connected graph $G = (V, K)$ with finitely many vertices $V = \{v_1, \dots, v_{|V|}\}$
  - and a certain set $K \subset V^2$ of edges $e = (v_i, v_j)$, each of them connecting two vertices v_i, v_j.

- One of the values -1 and 1 is assigned to each vertex,
  - and we consider the state space $E = \{-1, 1\}^{|V|}$ of all configurations $\mathbf{x} = (x(v),\, v \in V)$, i.e. for each $v \in V$ either $x(v) = -1$ or $x(v) = 1$.
  - If this is interpreted as an image, $x(v) = -1$ is regarded as a white pixel and $x(v) = 1$ as a black pixel.

- For each $\mathbf{x} \in E$ let the probability $\pi_{\mathbf{x}}$ of the configuration $\mathbf{x}$ be given by

$$\pi_{\mathbf{x}} = \frac{1}{z_{G,J}} \exp\left(J \sum_{e=(v_i,v_j)\in K} x(v_i)x(v_j) \right) \tag{102}$$

  for a certain parameter $J \geq 0$, which is interpreted as „inverse temperature" in physics:

  - For $J = 0$ (infinite temperature) the distribution $\boldsymbol{\pi} = (\pi_{\mathbf{x}},\, \mathbf{x} \in E)$ given by (102) is the discrete uniform distribution.
  - For $J \gg 0$ (low temperature) those configurations possess a large probability that have a small number of connected pairs of vertices being differently colored.
  - For $J \to \infty$ (zero temperature) the distribution $\boldsymbol{\pi} = (\pi_{\mathbf{x}},\, \mathbf{x} \in E)$ given by (102) converges to the „two point uniform distribution" $\big(\delta_{\mathbf{0}} + \delta_{\mathbf{1}}\big)/2$,
  - where $\mathbf{0}$ and $\mathbf{1}$ denote the (extreme) configurations consisting either only of white or only of black pixels, i.e. either $0(v) = -1$ or $1(v) = 1$ for all $v \in V$.

- Notice that $z_{G,J} > 0$ is an (in general unknown) normalizing constant where

$$z_{G,J} = \sum_{\mathbf{x}\in E} \exp\left(-J \sum_{e=(v_i,v_j)\in K} x(v_i)x(v_j) \right).$$

- The following figure was taken from O. Häggström (2002) *Finite Markov Chains and Algorithmic Applications*, CU Press, Cambridge.

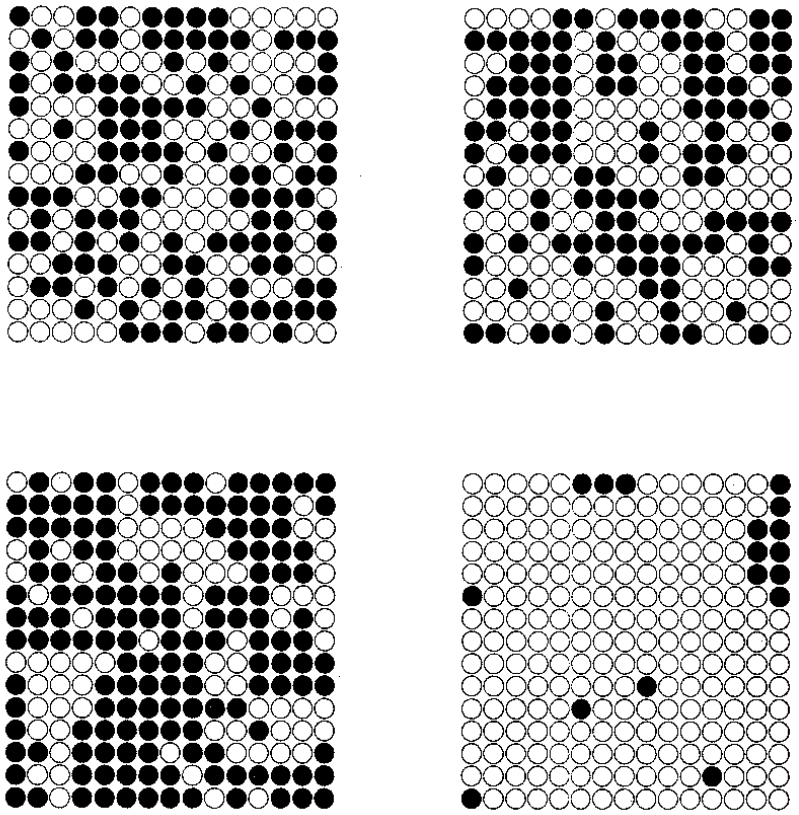


Figure 8: Typical configuration of the Ising model for $J = 0$ (upper left corner), $J = 0.15$ (upper right corner), $J = 0.3$ (lower left corner) and $J = 0.5$ (lower right corner)

- It illustrates the role of the parameter J,
- i.e., an increase of J results in a more pronounced clumping tendency of identically colored pixels.

- Let the simulation matrix $\mathbf{P} = (p_{\mathbf{x}\mathbf{x}'})$ be given by the Gibbs sampler, i.e., assume that (36) holds, namely

$$p_{\mathbf{x}\mathbf{x}'} = \sum_{v \in V} q_v \pi_{x'(v)|\,\mathbf{x}(-v)}\, \mathbb{1}\big(\mathbf{x}(-v) = \mathbf{x}'(-v)\big)\,, \qquad \forall\, \mathbf{x}, \mathbf{x}' \in E\,.$$

  - where for arbitrary $\mathbf{x}, \mathbf{x}' \in E$ such that $\mathbf{x}(-v) = \mathbf{x}'(-v)$

$$\pi_{x'(v)|\,\mathbf{x}(-v)} = \begin{cases} \dfrac{\pi_{\mathbf{x}_+}}{\pi_{\mathbf{x}_+} + \pi_{\mathbf{x}_-}} & \text{if } x'(v) = 1, \\ \dfrac{\pi_{\mathbf{x}_-}}{\pi_{\mathbf{x}_+} + \pi_{\mathbf{x}_-}} & \text{if } x'(v) = -1, \end{cases}$$

    using the notation $x_-(v) = -1$ and $\mathbf{x}_-(-v) = \mathbf{x}(-v)$ and similarly $x_+(v) = 1$ and $\mathbf{x}_+(-v) = \mathbf{x}(-v)$.
  - By (102) we obtain for $x'(v) = 1$ that

$$\pi_{x'(v)|\,\mathbf{x}(-v)} = \frac{\exp\Big(J\big(k_+(\mathbf{x}(-v)) - k_-(\mathbf{x}(-v))\big)\Big)}{\exp\Big(J\big(k_-(\mathbf{x}(-v)) - k_+(\mathbf{x}(-v))\big)\Big) + \exp\Big(J\big(k_+(\mathbf{x}(-v)) - k_-(\mathbf{x}(-v))\big)\Big)}$$

and in the same way for $x'(v) = -1$ that

$$\pi_{x'(v)|\,\mathbf{x}(-v)} = \frac{\exp\Big(J\big(k_-(\mathbf{x}(-v)) - k_+(\mathbf{x}(-v))\big)\Big)}{\exp\Big(J\big(k_+(\mathbf{x}(-v)) - k_-(\mathbf{x}(-v))\big)\Big) + \exp\Big(J\big(k_-(\mathbf{x}(-v)) - k_+(\mathbf{x}(-v))\big)\Big)}$$

Thus, we can summarize

$$\pi_{x'(v)|\,\mathbf{x}(-v)} = \begin{cases} \dfrac{1}{1+\exp\Big(-2\,J\big(k_+(\mathbf{x}(-v)) - k_-(\mathbf{x}(-v))\big)\Big)} & \text{if } x'(v) = 1, \\ \dfrac{1}{1+\exp\Big(-2\,J\big(k_-(\mathbf{x}(-v)) - k_+(\mathbf{x}(-v))\big)\Big)} & \text{if } x'(v) = -1, \end{cases} \tag{103}$$

where $k_+(\mathbf{x}(-v))$ and $k_-(\mathbf{x}(-v))$ denote the number of vertices connected to v having the values 1 and -1, respectively.

- For the state space $E = \{-1, 1\}^{|V|}$ we define the partial order $\preceq$
  - by $\mathbf{x} \preceq \mathbf{y}$ if $x(v) \le y(v)$ for all $v \in V$ such that $\mathbf{0} \preceq \mathbf{x} \preceq \mathbf{1}$ for all $\mathbf{x} \in E$,
  - where we assume the elements of the state space $E = \{\mathbf{x}_1, \ldots, \mathbf{x}_\ell\}$ to be indexed in a way ensuring $i \le j$ if $\mathbf{x}_i \preceq \mathbf{x}_j$ (this is e.g. the case if E is ordered *lexicographically*).
- Then (103) implies for arbitrary $\mathbf{x}, \mathbf{y} \in E$ such that $\mathbf{x} \preceq \mathbf{y}$

$$\pi_{1|\,\mathbf{x}(-v)} \le \pi_{1|\,\mathbf{y}(-v)} \qquad \text{and} \qquad \pi_{-1|\,\mathbf{x}(-v)} \ge \pi_{-1|\,\mathbf{y}(-v)}\,, \tag{104}$$

because $1/(1+e^{-a}) \le 1/(1+e^{-b})$ for arbitrary $a, b \in \mathbb{R}$ such that $a \le b$.

- Let the update function $\varphi : E \times (0,1]^2 \to E$ be given by $\varphi(\mathbf{x}; u_1, u_2) = \mathbf{x}'$, where $\mathbf{x}' = \big(\mathbf{x}'(v),\, v \in V\big)$ and for all $i = 1, \ldots, |V|$

$$\mathbf{x}'(v_i) = \begin{cases} 1 & \text{if } \sum_{j=1}^{i-1} q(v_j) < u_1 \le \sum_{j=1}^{i} q(v_j) \text{ and } u_2 < \pi_{1|\,\mathbf{x}(-v_i)}, \\ -1 & \text{if } \sum_{j=1}^{i-1} q(v_j) < u_1 \le \sum_{j=1}^{i} q(v_j) \text{ and } u_2 \ge \pi_{1|\,\mathbf{x}(-v_i)}, \\ \mathbf{x}(v_i)\,, & \text{else.} \end{cases}$$

  - By (104), for arbitrary $\mathbf{x}, \mathbf{y} \in E$ such that $\mathbf{x} \preceq \mathbf{y}$ we have

$$\varphi(\mathbf{x}; u_1, u_2) \preceq \varphi(\mathbf{y}; u_1, u_2)\,, \qquad \forall\, u_1, u_2 \in (0,1]\,,$$

  - i.e., condition (91) with respect to $\preceq$ is satisfied.

3.5.5 Read–Once Modification of the CFTP Algorithm

- A problem of the „monotone" CFTP algorithm discussed in Sections 3.5.3 and 3.5.4 is
  - the necessity to save *all* innovations $U_0, U_{-1}, \ldots, U_{-\zeta}$ where ζ denotes the coupling time defined in (95), i.e.

$$\zeta = \min\big\{-m \ge 1 :\, \mathbf{X}_0^{(m,\min)} = \mathbf{X}_0^{(m,\max)}\big\}\,.$$

  - Therefore, in the year 2000, David Wilson suggested the following modifications of the CFTP algorithm aiming at a reduction of the necessary memory allocation.
- The main idea of the modification is to realize coupling to the past (see Sections 3.5.2 – 3.5.4)

– based on a sequence of independent and identically distributed blocks of „forward simulation", where

– the (potential) „initial times" $m \in \{-1, -2, \ldots\}$ of the Markov chain $\mathbf{X}^{(m,i)} = \big(\mathbf{X}_m^{(m,i)}, \mathbf{X}_{m+1}^{(m,i)}, \ldots\big)$ can be picked *at random*.

- The innovation sequences $\mathbf{U}^{(1)}, \ldots, \mathbf{U}^{(\ell)}$ are chosen identical with probability 1,

  – i.e., we merely consider a *single* sequence $\mathbf{U} = \big(\ldots, U_{-1}, U_0, U_1, \ldots\big)$ of independent and uniformly distributed random variables and define $\mathbf{U}^{(1)} = \ldots = \mathbf{U}^{(\ell)} = \mathbf{U}$.

  – Furthermore, we assume that the Markov chains $\mathbf{X}^{(1)}, \ldots, \mathbf{X}^{(\ell)}$ and $\mathbf{X}^{(m,1)}, \ldots, \mathbf{X}^{(m,\ell)}$ defined by (87) and (90) have finite forward and backward coupling times

$$\tau = \min\big\{n \geq 1 : \mathbf{X}_n^{(1)} = \ldots = \mathbf{X}_n^{(\ell)}\big\} \quad \text{bzw.} \quad \zeta = \min\big\{-m \geq 1 : \mathbf{X}_0^{(m,1)} = \ldots = \mathbf{X}_0^{(m,\ell)}\big\}$$

  with probability 1.

- Now we consider blocks of forward simulation of (at first deterministic) length T for some $T \geq 1$.

  – For arbitrary $k \geq 0$ and $i = 1, ..., \ell$, let $\mathbf{X}_{kT}^{(kT,i)} = \mathbf{x}_i$ and

$$\mathbf{X}_n^{(kT,i)} = \varphi(\mathbf{X}_{n-1}^{(kT,i)}, U_n)\,, \qquad \forall\, n = kT+1, kT+2, \ldots\,.$$

  – Furthermore, for each $k \geq 0$ we consider the event

$$C_{kT} = \Big\{\mathbf{X}_{(k+1)T}^{(kT,i)} = \mathbf{X}_{(k+1)T}^{(kT,j)}\,, \qquad \forall\, i \neq j \in \{1, ..., l\}\Big\}\,,$$

  where the length T of the blocks is chosen such that

$$0 < P(C_T) \qquad \Big(= P(C_{kT})\,, \quad \forall\, k \geq 0\Big)\,. \tag{105}$$

- Starting at $k = 0$ the read–once modification of the CFTP algorithm is given as follows.

  1. Simulate $\mathbf{X}_n^{(kT,i)}$ via φ and $\mathbf{U}$ for $n = kT+1, ..., (k+1)T$.
  2. Set $m = k$ and $k = k+1$. If the event C_{mT} has occurred proceed with step 3, otherwise return to step 1.
  3. Repeat steps 1 and 2 until the event $C_{m'T}$ occurs for some $m' > m$ and return the value of $\mathbf{X}_{m'T}^{(mT,i)}$ for an arbitrary $i \in \{1, ..., l\}$ as a realization of $\boldsymbol{\pi}$.

Example

- For $\ell = 3$ states we consider the irreducible and aperiodic transition matrix

$$\mathbf{P} = \begin{pmatrix} 1/2 & 0 & 1/2 \\ 1/3 & 1/3 & 1/3 \\ 0 & 1 & 0 \end{pmatrix}\,.$$

- For block length $T = 2$ and the $(0, 1]$–uniformly distributes pseudo–random numbers

$$\mathbf{u} = (0.01, 0.60, 0.82, 0.47, 0.36, 0.59, 0.34, 0.89, ...)$$

  we obtain the simulation run shown in Fig. 9.

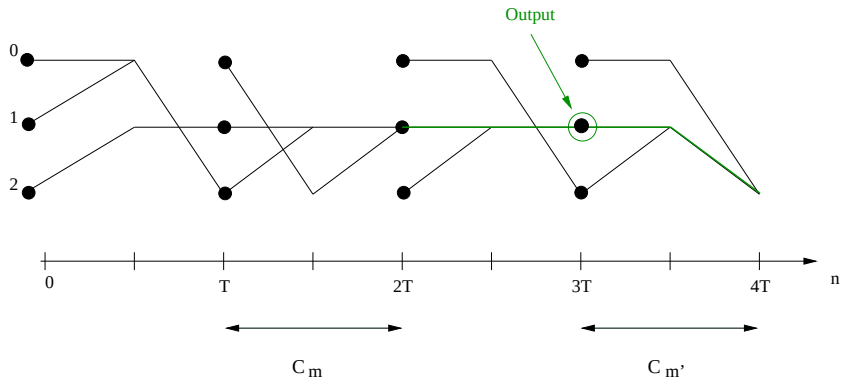


Figure 9: Read once algorithm

Remarks

- As the simulation blocks and hence the events C_T, C_{2T}, ... are independent and as $P(C_T) = P(C_{2T}) = \ldots$,
  - the first m' blocks of forward simulation of the algorithm described above in particular yield the coupling from the past discussed in Section 3.5.2 if they are considered in reversed order.
  - Therefore, $\mathbf{X}_{m'T}^{(mT,i)} \sim \boldsymbol{\pi}$ for all $i \in \{1, ..., l\}$.
  - The last, i.e. the $(m'+1)$st block of forward simulation serves only to define a stopping rule.

- The read–once modification of the CFTP algorithm terminates with probability 1
  - if condition (105) is satisfied, i.e. if $P(C_T) > 0$.
  - For monotonously nondecreasing update functions this holds if $T \geq n_0$ where $n_0 \geq 1$ is a natural number such that
$$\min_{\mathbf{x},\mathbf{x}' \in E} p_{\mathbf{x}\mathbf{x}'}^{(n_0)} = c > 0\,,$$
see the proof of Theorem 3.24.

- If T is a random variable
  - having the same distribution as the forward coupling time τ and which is independent of the innovation sequence $\mathbf{U} = \big(U_0, U_{-1}, \ldots\big)$,
  - then by the following elementary but useful properties of the coupling times τ and ζ we obtain $P(C_T) \geq 1/2$.

Theorem 3.25 *The random variables τ and ζ have the same distribution, i.e. $\tau \stackrel{\mathrm{d}}{=} \zeta$. Moreover, if the coupling times τ and ζ are independent and almost surely finite, then*

$$P(\zeta \leq \tau) \;\geq\; \frac{1}{2}\,. \tag{106}$$

Proof

- By the homogeneity of the Markov chains $\mathbf{X}^{(1)}, \ldots, \mathbf{X}^{(\ell)}$ and $\mathbf{X}^{(m,1)}, \ldots, \mathbf{X}^{(m,\ell)}$, for any natural number $k \geq 1$ we have

$$\begin{aligned} P(\tau = k) &= P\Big(\min\big\{n \geq 1 :\, \mathbf{X}_n^{(1)} = \ldots = \mathbf{X}_n^{(\ell)}\big\} = k\Big) \\ &= P\Big(\min\big\{-m \geq 1 :\, \mathbf{X}_0^{(m,1)} = \ldots = \mathbf{X}_0^{(m,\ell)}\big\} = k\Big) \\ &= P(\zeta = k)\,. \end{aligned}$$

- Let now the coupling times τ and ζ be independent and finite with probability 1.
  - This implies

$$\begin{aligned} P(\zeta \le \tau) &= \sum_{k=1}^{\infty} P(\zeta \le \tau \mid \tau = k) P(\tau = k) = \sum_{k=1}^{\infty} P(\zeta \le k \mid \tau = k) P(\tau = k) \\ &= \sum_{k=1}^{\infty} P(\zeta \le k) P(\tau = k) = \sum_{k=1}^{\infty} P(\tau \le k) P(\zeta = k) \\ &\vdots \\ &= P(\zeta \ge \tau)\,, \end{aligned}$$

  - where the last equality follows from $\tau \stackrel{\mathrm{d}}{=} \zeta$ which has been shown in the first part of the proof.
- Thus,

$$\begin{aligned} 2\,P(\zeta \le \tau) &= P(\zeta \le \tau) + P(\zeta \ge \tau) \\ &= 1 - P(\zeta > \tau) + 1 - P(\zeta < \tau) \\ &= 2 - P(\zeta \ne \tau) \\ &\ge 2 - 1 = 1\,. \end{aligned}$$

□