Mathematics and numerics for data assimilation and state estimation – Lecture 5



Summer semester 2020

Summary of lecture 4

Random walks on \mathbb{Z}^d : described by distribution of X_0 and its iid steps $\{\Delta X_n\}$.



For an RW {X₀, ΔX₀, ΔX₁,...}, on Z^d, a state s ∈ Z^d is recurrent if by setting X₀ = s, we obtain that

 $\mathbb{P}(X_n = s \text{ for infinitely many } n) = 1.$

The last condition is equivalent to (Thm 9, Lecture 4),

$$\mathbb{P}(T < \infty) = 1 \quad \text{for} \quad T = \inf\{n \ge 1 \mid X_n = X_0\}.$$

 Convergence of random variables (Chebychev's inequality, weak law of large numbers, mean-square convergence).

Plan for this lecture

The Markov property – memorylessness

Markov chains

Invariant distributions

Markov chains

We consider the dynamics of a discrete-time stochastic process $\{Z_n\}$ that takes values on a state-space S that is discrete; meaning it is either finite, e.g. $S = \{1, 2, 3\}$, or countable, e.g. $S = \mathbb{Z}^d$.

Definition 1 (Markov chain)

A sequence $\{Z_n\}_{n\geq 0}$ of S-valued rv is a discrete-time (and discrete-space) Markov chain if

- **1** it is equipped with an initial distribution $\pi^0(z) := \mathbb{P}(Z_0 = z)$, and
- 2 satisfies the so-called Markov property ("memorylessness")

$$\mathbb{P}(Z_{n+1} = z_{n+1} \mid Z_n = z_n, \dots, Z_0 = z_0) = \mathbb{P}(Z_{n+1} = z_{n+1} \mid Z_n = z_n) \quad (1)$$

holds for any $n \ge 0$ and $z_0, \ldots, z_n \in \mathbb{S}$ for which

$$\mathbb{P}\left(Z_n=z_n,\ldots,Z_0=z_0\right)>0.$$

Alternative statement of the Markov property

To avoid the provided $\mathbb{P}(Z_n = z_n, ..., Z_0 = z_0) > 0$, one may state the Markov property as follows:

$$\mathbb{P}(Z_{n+1} = z_{n+1}, Z_n = z_n, \dots, Z_0 = z_0) = \mathbb{P}(Z_{n+1} = z_{n+1} \mid Z_n = z_n) \mathbb{P}(Z_n = z_n, \dots, Z_0 = z_0).$$
(2)

Note also that $\sum_{z \in \mathbb{S}} \pi^0(z) = 1$.

Any random walk $\{Z_n\}$ on $\mathbb{S} = \mathbb{Z}^d$ is a Markov chain. Since $Z_{n+1} = Z_n + \Delta Z_n$ with $\{\Delta Z_n\}$ iid, it follows that

$$\mathbb{P}(Z_{n+1} = z_{n+1} | Z_n = z_n, \dots, Z_0 = z_0)$$

= $\mathbb{P}(Z_n + \Delta Z_n = z_{n+1} | Z_n = z_n, \dots, Z_0 = z_0)$
= $\mathbb{P}(\frac{z_n + \Delta Z_n = z_{n+1} | Z_n = z_n, \dots, Z_0 = z_0)$
 $\Delta Z_n \perp \sum_{k=1}^{n} \sum_{k=1}^{n} \mathbb{P}(\frac{z_n + \Delta Z_n = z_{n+1} | Z_n = z_n)$

provided $\mathbb{P}(Z_n = z_n, ..., Z_0 = z_0) > 0.$

Example 3 (Three-state chain)

Consider a Markov chain $\{Z_n\}$ on $\mathbb{S} = \{1, 2, 3\}$. For any $n \ge 0$, let

$$p_{ij} := \mathbb{P}\left(Z_{n+1} = i \mid Z_n = j\right)$$

with dynamics described by the below transition graph



Simplifying notation and terminology

For $0 \le k \le n$ and points $z_k, \ldots, z_n \in \mathbb{S}$ let

$$z_{k:n} := (z_k, \ldots, z_n), (so z_{n:n} = z_n).$$

Similarly, for the Markov chain, let

$$Z_{k:n} := (Z_k, \ldots, Z_n).$$

In the new notation, the Markov property (1) becomes

$$\mathbb{P}(Z_{n+1} = z_{n+1} \mid Z_{0:n} = z_{0:n}) = \mathbb{P}(Z_{n+1} = z_{n+1} \mid Z_n = z_n)$$

whenever $\mathbb{P}(Z_{0:n} = z_{0:n}) > 0.$

Product decomposition of joint Markov-chain distributions

Definition 4

A transition function is a mapping $p:\mathbb{S}\times\mathbb{S}\to[0,1]$ satisfying the constraint

$$\sum_{z\in\mathbb{S}}p(c,z)=1\quad\text{for any}\quad c\in\mathbb{S}.\tag{3}$$

The n + 1-st **transition function** of a Markov chain $\{Z_n\}$ is for all $z, c \in \mathbb{S}$ defined by

$$p_{n+1}(c,z) := egin{cases} \mathbb{P}(Z_{n+1}=z\mid Z_n=c) & ext{if } \mathbb{P}(Z_n=c) > 0 \ \mathbb{1}_{\{c\}}(z) & ext{otherwise.} \end{cases}$$

Note: for all $c \in S$ s.t. $\mathbb{P}(Z_n = c) > 0$, the definition of $p_{n+1}(c, \cdot)$ is unique, but for zero-probability outcomes c, whatever definition satisfying (3) is valid.

Verification of constraint?

Application of the transition function

By the Markov property, we obtain

$$\mathbb{P}(Z_{0:n} = z_{0:n}) = \mathbb{P}(Z_{0:n-1} = z_{0:n-1})\mathbb{P}(Z_n = z_n \mid Z_{n-1} = z_{n-1})$$
$$= \mathbb{P}(Z_{0:n-1} = z_{0:n-1})\rho_n(z_{n-1}, z_n)$$

where two cases must be taken into account:

if P(Z_{n-1} = z_{n-1}) > 0 then this follows from definition, and
 if P(Z_{n-1} = z_{n-1}) = 0 then the euqality still holds as it becomes 0 = 0.

By recursive application,

$$\mathbb{P}(Z_{0:n} = z_{0:n}) = \mathcal{T}^{o}(\mathcal{Z}_{o}) P_{1}(\mathcal{Z}_{o}, \mathcal{Z}_{l}) P_{2}(\mathcal{Z}_{l}, \mathcal{Z}_{2}) \cdots \qquad (4)$$

$$P_{n}(\mathcal{Z}_{n-1}, \mathcal{Z}_{n})$$

Definition 5 (Time-homogeneity)

A Markov chain is time-homogeneous if there exists a transition function p that is independent of time n, such that

$$\mathbb{P}(Z_{n+1}=z\mid Z_n=c)=p(c,z)$$

whenever $\mathbb{P}(Z_n = c) > 0$.

We say that $\{Z_n\}$ is $Markov(\pi^0, p)$.

See for instance, the three-state chain Example , where $p(i,j) = p_{ij}$, and π^0 remains to be specified.

Transition probabilities for time-homogeneous Markov chains

For the rest of this lecture, we consider a chain $\{Z_n\}$ that is $Markov(\pi^0, p)$.

Applying (4) in the time-homogeneous setting yields

$$\mathbb{P}(Z_{0:n} = z_{0:n}) = \pi^{0}(z_{0}) \prod_{i=0}^{n-1} p(z_{i}, z_{i+1})$$
(5)

As an extension of the initial state distribution, we introduce for *n*-th state distribution

$$\pi^n(z_n):=\mathbb{P}(Z_n=z_n)$$

Observation: By marginalization,

$$\pi^{n}(z_{n}) = \sum_{z_{0:n-1} \in S^{n}} \mathbb{P}(Z_{0:n} = z_{0:n})$$

Theorem 6

Let $\{Z_n\}$ be Markov (π^0, p) and for any $k \ge 2$, define

$$p^{*k}(z_0, z_k) = \sum_{z_{1:k-1} \in \mathbb{S}^{k-1}} p(z_0, z_1) p(z_1, z_2) \dots p(z_{k-1}, z_k).$$

Then p^{*k} is a transition function for $\{Z_{kn}\}_n$ and, in particular,

$$p^{*k}(z_0, z_k) = \mathbb{P}(Z_k = z_k \mid Z_0 = z_0)$$
 (\checkmark

whenever $\mathbb{P}(Z_0 = z_0) > 0$.

Verification: $|P(2_{k}=2_{k}(Z_{0}=2_{0})) = \sum_{\substack{z_{1:k-1} \\ z_{1:k-1} \\ z$

Transition functions and *n*-th state distributions Note that

$$\pi^{1}(z_{1}) = \sum_{z_{0} \in \mathbb{S}} \pi^{0}(z_{0}) p(z_{0}, z_{1})$$

and,

$$\pi^{n}(z_{n}) = \sum_{z_{n-1} \in \mathbb{S}} \pi^{n-1}(z_{n-1})p(z_{n-1}, z_{n})$$



For finite state-spaces this can be associated to vector-matrix products.

Corollary 7

Let $\{Z_n\}$ be Markov (π^0, p) on a finite state-space $\mathbb{S} = \{1, 2, ..., d\}$ and introduce the notation

$$\pi^n_i:=\pi^n(i),\quad p_{ij}:=p(i,j) \quad ext{and} \quad p^k_{ij}:=p^{*k}(i,j).$$

Then

$$p^k = pp^{k-1} = p^{k-1}p \quad k \ge 2$$

and, with π^n representing a row-vector in \mathbb{R}^d ,

$$\pi^n = \pi^{n-1} p = \pi^0 p^n \quad n \ge 1.$$

Theorem 8 (Transition probabilities for time-homogeneous Markov chains)

Let $\{Z_n\}$ be Markov (π^0, p) . Then for any $m > n \ge 0$ and $z_n, \ldots, z_m \in S$, it holds that

$$\mathbb{P}\left(Z_{n:m}=z_{n:m}\right)=\pi^n(z_n)\prod_{i=n}^{m-1}p(z_i,z_{i+1})$$

Let $\mathbb{S}=\{1,2,3,4\}$ and

$$\pi^{0}= egin{pmatrix} 1 & 1 & 1 \end{pmatrix}/4$$

and

$$p = egin{pmatrix} 1/2 & 1/2 & 0 & 0 \ 1/2 & 0 & 1/2 & 0 \ 0 & 1/2 & 0 & 1/2 \ 0 & 0 & 1/2 & 1/2 \end{pmatrix}$$



Invariant distributions

Definition 10

Let π be a probability distribution on S. We call π an **invariant/stationary/equilibrium** distribution for the transition function p if it holds that

$$\pi(z) = \sum_{c \in \mathbb{S}} \pi(c) p(c, z) \quad \forall z \in \mathbb{S},$$

or, in matrix notation, if

$$\pi = \pi p.$$

Note that for $\{Z_n\}$ that is $Markov(\pi^0, p)$ where π^0 is invariant, it holds that

$$Z_0 \stackrel{D}{=} Z_1 \stackrel{D}{=} Z_2 \stackrel{D}{=} \dots$$

How many invariant distributions?

For a finite state-space $\mathbb{S} = \{1, 2, \dots, d\}$ there is either 1 or infinitely many invariant distributions.



Theorem 12 (FJK 2.2.33)

Consider $S = \{1, 2, ..., d\}$ and a transition function p. If there exists an $m \ge 1$ such that p^m is strictly positive, then there exists a unique invariant distribution $\pi = (\pi_1, ..., \pi_d)$ and

$$\lim_{n \to \infty} \pi_j^n = \pi_j \quad \forall j \in \mathbb{S}$$

and

$$\lim_{n\to\infty}p_{ij}^n=\pi_j\quad\forall i,j\in\mathbb{S}.$$

Meaning any initial distribution π^0 converges to the invariant distribution.

Observation: If
$$\lim_{n\to\infty} p_{ij}^n = \pi_j$$
, then

$$\lim_{n\to\infty} p_{ij}^n = \lim_{n\to\infty} p_{ij}^{n+1} = \underbrace{\mathcal{I}}_{\mathcal{K}} \cdot \lim_{k \in I} \frac{p_{ik} \cdot p_{kj}}{p_{ik} \cdot p_{kj}} \int_{\mathcal{K}} \cdot \frac{p_{ik} \cdot p_{kj}}{p_{ik} \cdot p_{kj}} = \underbrace{(\Pi P)_j}_{j}$$

Matrix-eigenvalue interpretation of invariant distributions

• π invariant distribution implies that $(\pi, 1)$ is an eigenpair of p since

$$\pi p = \pi 1$$

- Since every row of p sums to 1, (p − I)[1, 1, ..., 1]^T = 0 meaning 1 is an eigenvalue of p.
- Need to verify that corresponding row-eigenvector π is non-negative (at least one such is (FJK 2.2.39)).
- If (π, λ) is unique eigenpair of p with $\pi \ge 0$ and $\lambda = 1$, then the invariant distribution is unique.
- Otherwise, convex combinations invariant distributions will also be invariant.

Example 13 Z Let $\mathbb{S} = \{1, 2\}$ and $p = \begin{pmatrix} 1/2 & 1/2 \\ 1/4 & 3/4 \end{pmatrix}$ Eigenvalues $\lambda_1 = 1, \quad \lambda_2 = 1/4,$ with ℓ^1 -normalized right-eigenvectors $\pi_1 = [1, 2]/3, \quad \pi_2 = [1, -1]/2.$ And, $\lim_{n \to \infty} p^n = \begin{pmatrix} 1/3 & 2/3 \\ 1/3 & 2/3 \end{pmatrix}.$

Relation to irreducibility

What are sufficient conditions to ensure that for some $m \ge 1$, p^m is strictly positive?

Definition 14

Consider a transition matrix p associated to Markov chains on $\mathbb{S} = \{1, 2, \dots, d\}$. p is said to be

irreducible if for any $i, j \in \mathbb{S}$ there exists an $m \ge 1$ such that $p_{ij}^m > 0$, and

the *i*-th state is said to be aperiodic if pⁿ_{ii} > 0 for any sufficiently large n. Meaning for any n 2N for some

Lemma 15 (1.8.2, Norris, Markov Chains)

If p is irreducible and has an aperiodic state, then p^m is strictly positive for some $m \ge 1$.

Pij > 0 for some m means that i=; there is an m-path from i to;, for some in Pji>0 for some in means that iej: there is an m-path from itoi, for some m Irreducibility is equivalent to it for all states i, jes



$$ho = egin{pmatrix} 0 & 1 & 0 \ 1 & 0 & 0 \ 0 & 0.1 & 0.9 \end{pmatrix}$$



Irreducible? No

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Aperiodic states?

Tes, all states is are a periodic

Reducible chain $\mathbb{S} = \{1,2,3\}$



Aperiodic states?

Yes, all states.

Recall the result:

Lemma 19 (1.8.2, Norris, Markov Chains)

If p is irreducible and has an aperiodic state, then p^m is strictly positive for some $m \ge 1$.

Proof: Assume the index $i \in S$ is aperiodic, i.e., $p_{ii}^n > 0$ for all $n \ge N$. For indices $j, k \in S$, let us show that there exist an m_{jk} such that

$$p_{jk}^{ar{m}} > 0 \quad orall ar{m} \geq m_{jk}.$$

Since p is irreducible, there exists n_{ji} , $n_{ik} \ge 1$ such that

$$p_{ji}^{n_{ji}} > 0$$
 and $p_{ik}^{n_{ik}} > 0$.

Consequently, for any $\bar{m} \ge n_{ji} + n_{ik} + N$

$$p_{jk}^{ar{m}}=p_{jk}^{n_{ji}+n_{ik}+ar{m}-(n_{ji}+n_{ik})}\geq p_{ji}^{n_{ji}}p_{ik}^{n_{ik}}p_{ii}^{ar{m}-(n_{ji}+n_{ik})}>0.$$

Recurrence and construction of invariant distributions

Definition 20

Consider an **irreducible** transition function p associated to a state-space \mathbb{S} . Then we say that p is recurrent if it for any state $i \in \mathbb{S}$ and Markov chain $\{Z_n^i\} \sim Markov(\mathbb{1}_{\{i\}}, p)$ holds that

$$\mathbb{P}(Z_n^i = i \quad \text{for infinitely many } n) = 1, \tag{6}$$

which for the hitting time $T_i := \inf\{n \ge 1 \mid Z_n^i = i\}$ is equivalent to

$$\mathbb{P}(T_i < \infty) = 1.$$

Lemma 21

If p is irreducible and the state-space is finite, then p is recurrent.

Proof: Let us write $\mathbb{S} = \{1, 2, \dots, d\}$. Since \mathbb{S} is finite, there must be at least one pair of states $i, j \in \mathbb{S}$ satisfying

$$\mathbb{P}(Z_n^i = j \quad \text{for infinitely many } n) > 0 \tag{7}$$

since otherwise we reach the contradiction

$$egin{aligned} 0 &= bP(Z_n^i
ot\in \mathbb{S} \quad ext{for infinitely many } n) \ &\geq 1 - \sum_{j\in \mathbb{S}} bP(Z_n^i = j \quad ext{for infinitely many } n) = 1. \end{aligned}$$

And

$$\mathbb{P}(Z_n^j = j \text{ for infinitely many } n)$$

= $\mathbb{P}(Z_n^i = j \text{ for infinitely many } n \cap \{Z_n^i = j \text{ for some } n\})$ (8)
= $\mathbb{P}(Z_n^i = j \text{ for infinitely many } n) > 0.$

Theorem 9, Lecture 4 extends to the current setting, so by defining

$$N^j := \sum_{n \in \mathbb{N}} \mathbb{1}_{Z_n^j = j}$$
 (total visits at state j),

we obtain for $\lambda_j := \mathbb{P}(T^j < \infty)$ that

$$\mathbb{P}(N^j=k)=egin{cases} (1-\lambda_j)\lambda_j^{k-1} & ext{if }\lambda_j<1\ \mathbb{1}_{k=\infty} & ext{if }\lambda_j=1 \end{cases}$$

Consequently,

$$0 < \mathbb{P}(Z_n^j = j \text{ for infinitely many } n) = \mathbb{P}(N^j = \infty) = \begin{cases} 0 & \text{if } \lambda_j < 1 \\ 1 & \text{if } \lambda_j = 1. \end{cases}$$

Conclusion: λ_j must equal 1 and j is a recurrent state.

It remains to verify that $N^k = \infty$ a.s. for all $k \in \mathbb{S} \setminus \{j\}$. Observe first that

$$\mathbb{P}(N^{k} = \infty) = 1 \iff \mathbb{P}(N^{k} = \infty) > 0$$
$$\iff \mathbb{E}\left[N^{k}\right] = \infty \iff \sum_{n \in \mathbb{N}} p_{kk}^{n} = \infty$$

where the last \iff follows from

$$\mathbb{E}\left[N^{k}\right] = \sum_{n \in \mathbb{N}} \mathbb{E}\left[\mathbbm{1}_{Z_{n}^{k}=k}\right] = \sum_{n \in \mathbb{N}} \mathbb{P}(\mathbbm{1}_{Z_{n}^{k}=k}) = \sum_{n \in \mathbb{N}} p_{kk}^{n}.$$

Since $\mathbb{P}(N^j = \infty) = 1$, we know that $\sum_{n \in \mathbb{N}} p_{jj}^n = \infty$. And by the irreducibility of p, there exist $m_1, m_2 \ge 1$ such that $p_{kj}^{m_1} p_{jk}^{m_2} > 0$. So for any $n \ge m_1 + m_2$,

$$p_{kk}^n \ge p_{kj}^{m_1} p_{jj}^{n-(m_1+m_2)} p_{jk}^{m_2}$$

and

$$\sum_{n\in\mathbb{N}}p_{kk}^n\geq p_{kj}^{m_1}p_{jk}^{m_2}\sum_{n\in\mathbb{N}}p_{jj}^n=\infty.$$

Q.E.D.

Construction of invariant measures

For an irreducible transition function p associated to $\mathbb{S} = \{1, 2, ..., d\}$, we fix a state $k \in \mathbb{S}$, the chain $\{Z_n^k\} \sim Markov(\mathbb{1}_{\{k\}}, p)$ and introduce

$$\gamma_j^k := \mathbb{E}\left[egin{array}{c} T^{k-1} \ \sum_{n=0} \mathbbm{1}_{Z_n^k = j} \end{array}
ight] \quad ext{for} \quad j \in \mathbb{S}.$$

(the expected number of visits spent at state j in between vists to k).

Theorem 22 (Theorem 1.7.5, Norris, Markov Chains) For every $k \in S$, $\gamma^k = \gamma^k p$,

which makes

$$\pi := \frac{\gamma^k}{\sum_{j \in \mathbb{S}} \gamma_j^k}$$

is an invariant distribution.

$$p = \begin{pmatrix} 0 & 1 & 0 \\ 0 & 0 & 1 \\ 1 & 0 & 0 \end{pmatrix}$$

Irreducible but periodic chain. $p_{ii}^n > 0$ only for $n = 3, 6, 9, \ldots$ So Lemma 19 does not apply. But $\gamma^1 = \gamma^2 = \gamma^3 = [1, 1, 1]$, giving rise to $\pi = \gamma^1/3$.

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



Irreducible chain with aperiodic state 3. So Lemma 19 does apply. But theorem 22 also:

$$\gamma^1 = [1, 0.5, 1], \quad \gamma^2 = [2, 1, 2], \quad \gamma^3 = [1, 0.5, 1]$$

Simulation of a time-homogeneous Markov chain

For $\{Z_n\} \sim Markov(\pi^0, p)$ on $\mathbb{S} = \{1, 2, ..., d\}$ the main challenges for simulation are to draw the initial state and the transitions:

1 Draw
$$Z_0 \sim \pi^0$$

2 ...
3 given $Z_n = i$, draw $Z_{n+1} \sim [p_{i1}, p_{i,2}, \dots, p_{id}]$

Same challenge for every step: draw a sample/new state from a distribution $f = [f_1, \ldots, f_d]$.

Sampling method:

1 construct a vector

$$\bar{f} = \begin{pmatrix} f_1 \\ f_1 + f_2 \\ \vdots \\ \sum_{j=1}^{d-1} f_j \\ 1 \end{pmatrix}$$

2 Draw a uniformly distributed rv $U \sim U[0,1]$ and determine new state by:

$$j(U) := \min\{k \in \{1, 2, \dots, d\} \mid \overline{f}_k > U\}.$$

Exercise: verify that $\mathbb{P}(j(U) = \ell) = f_{\ell}$.

Next time

Filtering of discrete time and space Markov Chains