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Lecture 14. Markov Chain Monte Carlo Methods. The Exponential Distribution

STK2130 – Modellering av stokastiske prosesser



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Let Z be a discrete random variable with a state space S, and assume that:

$$\mathbb{P}(Z=i)=\pi_i=\frac{b_i}{B}, \quad i\in\mathcal{S}.$$

We assume that b_i is known for all $i \in S$. Since the probabilities must add up to 1, we obviously have:

$$\sum_{i\in\mathcal{S}}\frac{b_i}{B}=B^{-1}\sum_{i\in\mathcal{S}}b_i=1.$$

Hence, it follows that the normalizing constant B is given by:

$$B = \sum_{i \in S} b_i$$
.

Thus, in principle B is known as well. However, if |S| is large, calculating B may be a time-consuming task.

Example

Let T and Z be two discrete random variables with state spaces \mathcal{T} and \mathcal{S} respectively. We assume that the marginal distribution of Z and the conditional distribution of T given Z are known.

The conditional distribution of Z given T is then:

$$\mathbb{P}(Z=i\mid T=t)=\frac{P(Z=i)P(T=t\mid Z=i)}{\sum_{j\in\mathcal{S}}P(Z=j)P(T=t\mid Z=j)}=\frac{b_i(t)}{B(t)},\quad i\in\mathcal{S},t\in\mathcal{T},$$

where we have introduced:

$$b_i(t) = \mathbb{P}(Z=i)\mathbb{P}(T=t\mid Z=i), \quad i\in\mathcal{S}, t\in\mathcal{T},$$
 $B(t) = \sum_{j\in\mathcal{S}} \mathbb{P}(Z=j)\mathbb{P}(T=t\mid Z=j) = \mathbb{P}(T=t), \quad t\in\mathcal{T}.$

If |S| is large, we may want to avoid calculating B(t).

Problem

Construct a Markov chain $\{X_n\}$ with state space S and stationary distribution equal to the distribution of Z.

SOLUTION (Hastings-Metropolis): Let \mathbf{Q} be any given irreducible Markov chain transition probability matrix on \mathcal{S} , and define:

$$lpha_{i,j} = \min\left(rac{b_j Q_{j,i}}{b_i Q_{i,j}}, 1
ight), \quad i,j \in \mathcal{S}.$$

We then let the transition probability matrix of $\{X_n\}$, denoted **P**, be defined as follows:

$$egin{aligned} P_{i,j} &= Q_{i,j} lpha_{i,j}, \quad i
eq j, \ P_{i,i} &= 1 - \sum_{j
eq i} Q_{i,j} lpha_{i,j}, \quad i \in \mathcal{S}. \end{aligned}$$

We then claim that $\{X_n\}$ is **time reversible** and has a stationary distribution equal to the distribution of Z. That is, $\pi_i = b_i/B$, for all $i \in S$, and:

$$\pi_i P_{i,j} = \pi_j P_{j,i}, \quad \text{for all } i, j \in \mathcal{S}.$$
 (1)

Since (1) is trivially satisfied for i = j, we focus on the case where $i \neq j$, where (1) can be expressed as:

$$\frac{b_i}{B}Q_{i,j}\alpha_{i,j} = \frac{b_j}{B}Q_{j,i}\alpha_{j,i}, \quad i \neq j.$$
 (2)

By eliminating B from these equations and inserting the expression for $\alpha_{i,i}$ we get:

$$b_i Q_{i,j} \cdot \min\left(\frac{b_j Q_{j,i}}{b_i Q_{i,j}}, 1\right) = b_j Q_{j,i} \cdot \min\left(\frac{b_i Q_{i,j}}{b_j Q_{j,i}}, 1\right), \quad i \neq j.$$
(3)

CASE 1: $b_i Q_{i,j} \leq b_i Q_{i,j}$.

In this case $\alpha_{i,j} = 1$ while $\alpha_{j,i} = (b_i Q_{i,j})/(b_j Q_{j,i})$, and hence, (3) simplifies to:

$$b_i Q_{i,j} = b_j Q_{j,i} \cdot (b_i Q_{i,j}) / (b_j Q_{j,i}), \quad i \neq j.$$

$$(4)$$

CASE 2: $b_i Q_{i,j} \geq b_j Q_{j,i}$.

In this case $\alpha_{i,j} = (b_j Q_{j,i})/(b_i Q_{i,j})$ while $\alpha_{j,i} = 1$, and hence, (3) simplifies to:

$$b_i Q_{i,j} \cdot (b_j Q_{j,i})/(b_i Q_{i,j}) = b_j Q_{j,i}, \quad i \neq j.$$
 (5)

Since obviously both (4) and (5) hold true, we conclude that (1) holds true as well.

We recall that:

$$P_{i,j} = Q_{i,j} lpha_{i,j}, \quad i
eq j,$$
 $P_{i,i} = 1 - \sum_{j
eq i} Q_{i,j} lpha_{i,j}, \quad i \in \mathcal{S}.$

Assume that $X_n = i$. Then X_{n+1} can be generated using the following two-step Monte Carlo simulation procedure:

STEP 1. Generate a random variable *J* with values in *S* such that $\mathbb{P}(J=j) = Q_{i,j}, j \in S$.

STEP 2. Generate $K \in \{0,1\}$ such that $\mathbb{P}(K=1 \mid J=j) = \alpha_{i,j}$, and let:

$$X_{n+1} = K \cdot j + (1 - K) \cdot i$$

Thus, a transition from state i to state j where $i \neq j$ happens if and only if J = j and K = 1. If not, the process stays in state i.

The Monte Carlo simulation procedure can be used to estimate some unknown parameter in the distribution of Z, e.g.:

$$\theta = \mathbb{E}[h(Z)] = \sum_{i \in S} h(i)\mathbb{P}(Z = i),$$

where h is some function of interest, and the normalizing constant B of the distribution of Z is too time-consuming to calculate.

By simulating the Markov chain $\{X_n\}$, having a stationary distribution which is equal to the distribution of Z, we may estimate θ by:

$$\hat{\theta}_n = \frac{1}{n} \sum_{m=1}^n h(X_m).$$

We know that $\hat{\theta}_n \to \theta$ when $n \to \infty$.

Remark

- X_1, X_2, \ldots are not independent.
- The chain may converge slowly towards its stationary distribution.

Both these issues tend to have a negative effect on the convergence rate of the estimator $\hat{\theta}_n$. If many of the $\alpha_{i,j}$ -s are small, the Markov chain tends to get stuck for a long time before eventually transiting to another state. In such cases the estimator $\hat{\theta}_n$ will converge very slowly.

For optimal performance, i.e., fast convergence, the matrix **Q** should ideally be chosen so that:

$$b_iQ_{i,j}=b_jQ_{j,i}, \quad \text{for all } i,j\in\mathcal{S}.$$

Then it follows that:

$$lpha_{i,j} = \min\left(rac{b_j Q_{j,i}}{b_i Q_{i,j}}, 1
ight) = 1, \quad ext{for all } i,j \in \mathcal{S}.$$

Hence, $\mathbf{Q} = \mathbf{P}$, i.e., \mathbf{Q} is itself the transition probability matrix of $\{X_n\}$.

Finding the optimal matrix \mathbf{Q} implies finding a transition probability matrix with a stationary distribution which is equal to the distribution of \mathbf{Z} . In real-life applications, this can be difficult.

Instead we may think of \mathbf{Q} as our best guess, while the $\alpha_{i,j}$ -s are correction factors which are used to generate a Markov chain with the correct stationary distribution.

Gibbs sampling

Assume that $\mathbf{Z} = (Z_1, ..., Z_r)$ is a discrete random vector with values in S where:

$$\mathbb{P}(\mathbf{Z} = \mathbf{z}) = p(\mathbf{z}) = g(\mathbf{z})/B$$
, for all $z \in \mathcal{S}$,

where the $g(\mathbf{z})$ is known for all $\mathbf{z} \in \mathcal{S}$ and B is an unknown normalizing constant.

Utilization of the Gibbs sampler assumes that for any i and values x_j , $j \neq i$, we can generate a random variable Z having the probability mass function

$$\mathbb{P}(Z=z)=\mathbb{P}(Z_i=z\mid Z_j=z_j,\ j\neq i).$$

We then consider the first step of the Hastings-Metropolis algorithm, and assume that $X_n = \mathbf{z} = (z_1, ..., z_r)$. The candidate for the next state, X_{n+1} , is generated as follows:

- **1** Generate K uniformly from the set $\{1, ..., r\}$.
- ② For K = k, generate $Z_k = z$ conditional on $Z_i = z_i$, i = 1, ..., (k 1), (k + 1), ..., r.

The resulting candidate for the next state, denoted **y**, is then:

$$\mathbf{y} = (z_1, ..., z_{k-1}, z, z_{k+1}, ..., z_r).$$

Gibbs sampling

This implies that we have the following transition probabilities:

$$Q_{\mathbf{z},\mathbf{y}} = \frac{1}{r} \mathbb{P}(Z_k = z \mid Z_i = z_i, i \neq k)$$

$$= \frac{g(\mathbf{y})/B}{r \cdot \sum_{z_k} g(z_1, ..., z_k, ...z_r)/B} = \frac{g(\mathbf{y})}{r \cdot \sum_{z_k} g(z_1, ..., z_k, ...z_r)}$$

By the same type of argument, we also have:

$$Q_{\mathbf{y},\mathbf{z}} = rac{g(\mathbf{z})}{r \cdot \sum_{z_k} g(\mathbf{z})}.$$

This implies that:

$$g(\mathbf{z})Q_{\mathbf{z},\mathbf{y}} = g(\mathbf{y})Q_{\mathbf{y},\mathbf{z}}, \quad \text{for all } \mathbf{z},\mathbf{y} \in \mathcal{S}.$$

Hence, $\alpha_{z,y} = 1$ for all $z, y \in \mathcal{S}$, and thus, Q is an optimal transition probability matrix.

Definition

A continuous random variable X is said to have an **exponential distribution** with parameter $\lambda > 0$, denoted as $X \sim exp(\lambda)$, if its probability density function is given by:

$$f(x) = \begin{cases} \lambda e^{-\lambda x}, & x \ge 0, \\ 0, & x < 0. \end{cases}$$

If $X \sim exp(\lambda)$, then the **cumulative distribution function** of X is given by:

$$F(x) = \mathbb{P}(X \le x) = \int_0^x f(t)dt = \begin{cases} 1 - e^{-\lambda x}, & x \ge 0, \\ 0, & x < 0. \end{cases}$$

Moreover, the **survival function** of *X* is given by:

$$ar{F}(x) = \mathbb{P}(X > x) = 1 - F(x) = egin{cases} e^{-\lambda x}, & x \geq 0, \\ 1, & x < 0. \end{cases}$$

The exponential distribution is a special case of the **gamma distribution** with parameters $\alpha > 0$ and $\lambda > 0$, denoted as $X \sim \text{Gamma}(\alpha, \lambda)$ with probability density function:

$$f(x) = \begin{cases} \frac{\lambda^{\alpha}}{\Gamma(\alpha)} x^{\alpha-1} e^{-\lambda x}, & x \geq 0, \\ 0, & x < 0, \end{cases}$$

where $\Gamma(\alpha)$, defined for all $\alpha > 0$, is the gamma function given by:

$$\Gamma(\alpha) = \int_0^\infty x^{\alpha-1} e^{-x} dx, \quad \Gamma(n) = (n-1)!, \quad n = 1, 2, ...$$

By substituting $u = \lambda x$ and $du = \lambda dx$, we find that:

$$\int_0^\infty f(x)dx = \frac{1}{\Gamma(\alpha)} \int_0^\infty u^{\alpha-1} e^{-u} du = 1.$$

Thus, f(x) is indeed a proper probability density.

Assume that $X \sim exp(\lambda)$, and let p > -1. We then have:

$$\mathbb{E}[X^{p}] = \int_{0}^{\infty} x^{p} f(x) dx = \int_{0}^{\infty} \lambda x^{p} e^{-\lambda x} dx$$
$$= \frac{\Gamma(p+1)}{\lambda^{p}} \int_{0}^{\infty} \frac{\lambda^{p+1}}{\Gamma(p+1)} x^{(p+1)-1} e^{-\lambda x} dx$$
$$= \frac{Gamma(p+1)}{\lambda^{p}}.$$

In particular:

$$\mathbb{E}[X] = \frac{\Gamma(2)}{\lambda^{1}} = \frac{(2-1)!}{\lambda} = \frac{1}{\lambda}, \quad \mathbb{E}[X^{2}] = \frac{\Gamma(3)}{\lambda^{2}} = \frac{(3-1)!}{\lambda^{2}} = \frac{2}{\lambda^{2}},$$

$$Var[X] = \mathbb{E}[X^{2}] - (\mathbb{E}[X])^{2} = \frac{2}{\lambda^{2}} - \frac{1}{\lambda^{2}} = \frac{1}{\lambda^{2}}.$$

Assume that $X \sim Gamma(\alpha, \lambda)$. Then the moment generating function of X is given by:

$$M_X(t) = \mathbb{E}[e^{tX}] = \int_0^\infty e^{tx} \frac{\lambda^\alpha}{\Gamma(\alpha)} x^{\alpha-1} e^{-\lambda x} dx$$

$$= \int_0^\infty \frac{\lambda^\alpha}{\Gamma(\alpha)} x^{\alpha-1} e^{-(\lambda-t)x} dx$$

$$= \frac{\lambda^\alpha}{(\lambda-t)^\alpha} \int_0^\infty \frac{(\lambda-t)^\alpha}{\Gamma(\alpha)} x^{\alpha-1} e^{-(\lambda-t)x} dx$$

$$= \frac{\lambda^\alpha}{(\lambda-t)^\alpha},$$

for all $t < \lambda$.

In particular, if $X \sim exp(\lambda)$, we have:

$$M_X(t) = \frac{\lambda}{\lambda - t},$$

for all $t < \lambda$.

Proposition 5.1

Assume that $X_1,...,X_n$ are independent and $X_i \sim exp(\lambda)$, i = 1,...,n, and let:

$$Y = X_1 + \cdots + X_n$$

Then $Y \sim Gamma(n, \lambda)$.

PROOF: Using moment generating functions we get:

$$M_{Y}(t) = \mathbb{E}[e^{tY}] = \mathbb{E}[e^{tX_{1} + \dots + tX_{n}}] = M_{X_{1}}(t) \cdot \dots \cdot M_{X_{n}}(t)$$

$$= \frac{\lambda}{\lambda - t} \cdot \dots \cdot \frac{\lambda}{\lambda - t} = \frac{\lambda^{n}}{(\lambda - t)^{n}}.$$

Hence, $Y \sim Gamma(n, \lambda)$.

Proposition 5.1 is a special case of the following more general result:

Proposition 5.1b

Assume that X_1, \ldots, X_n are independent and $X_i \sim Gamma(\alpha_i, \lambda)$, i = 1, ..., n, and let:

$$Y = X_1 + \cdots + X_n$$
.

Then $Y \sim Gamma(\alpha, \lambda)$, where $\alpha = \sum_{i=1}^{n} \alpha_i$.

PROOF: Using moment generating functions we get:

$$M_{Y}(t) = \mathbb{E}[e^{tY}] = \mathbb{E}[e^{tX_{1} + \cdots + tX_{n}}] = M_{X_{1}}(t) \cdots M_{X_{n}}(t)$$

$$= \frac{\lambda^{\alpha_{1}}}{(\lambda - t)^{\alpha_{1}}} \cdots \frac{\lambda^{\alpha_{n}}}{(\lambda - t)^{\alpha_{n}}} = \frac{\lambda^{\alpha}}{(\lambda - t)^{\alpha}}.$$

Hence, $Y \sim Gamma(\alpha, \lambda)$.

A random variable *X* is said to be memoryless if:

$$\mathbb{P}(X > s + t \mid X > t) = \mathbb{P}(X - t > s \mid X > t) = \mathbb{P}(X > s), \text{ for all } s, t \ge 0.$$

Thus, X is memoryless if $(X - t) \mid (X > t)$ has the same distribution as X.

Note that if X is the lifetime of some unit, (X - t) is the remaining lifetime given that the unit has survived up to the time t.

If $X \sim exp(\lambda)$, we have:

$$\mathbb{P}(X > s + t \mid X > t) = \frac{\mathbb{P}(\{X > s + t\} \cap \{X > t\})}{\mathbb{P}(X > t)} = \frac{\mathbb{P}(X > s + t)}{\mathbb{P}(X > t)}$$
$$= \frac{e^{-\lambda(s+t)}}{e^{-\lambda t}} = e^{-\lambda s} = \mathbb{P}(X > s).$$

Hence, we conclude that X is memoryless.

The memoryless property:

$$\mathbb{P}(X > s + t \mid X > t) = \mathbb{P}(X > s)$$
, for all $s, t \ge 0$.

is equivalent to the following:

$$\mathbb{P}(X > s + t) = \mathbb{P}(X > s)\mathbb{P}(X > t)$$
, for all $s, t \ge 0$.

Since $\bar{F}(x) = \mathbb{P}(X > x)$, this property can also be written as:

$$\bar{F}(s+t) = \bar{F}(s)\bar{F}(t)$$
, for all $s, t \ge 0$.

We now show that the exponential distribution is essentially the only distribution with this property.

Proposition

Let X be a random variable and let $\overline{F}(x) = \mathbb{P}(X > x)$ be such that:

$$\bar{F}(x+y) = \bar{F}(x) \cdot \bar{F}(y), \quad \text{for all } x, y \ge 0.$$
 (6)

Denote

$$\lambda := -\log(\bar{F}(1)) > 0. \tag{7}$$

Then $X \sim exp(\lambda)$.

PROOF: We first note that by (7), it follows that:

$$0 < \bar{F}(1) = e^{-\lambda} < 1. \tag{8}$$

Secondly we note that since cumulative distribution functions always are right-continuous, it follows that $\bar{F} = 1 - F$ is right-continuous as well.

By repeated use of (6) it follows that for $n, m \in \mathbb{N}^+$, we have:

$$\bar{F}\left(\frac{m}{n}\right) = \bar{F}\left(\frac{1}{n} + \dots + \frac{1}{n}\right) = \bar{F}^m\left(\frac{1}{n}\right),$$
 (9)

where the sum contains m terms. In particular, by letting m = n, we get:

$$\bar{F}(1) = \bar{F}\left(\frac{n}{n}\right) = \bar{F}^n\left(\frac{1}{n}\right).$$
 (10)

Alternatively, (10) can be written as:

$$\bar{F}\left(\frac{1}{n}\right) = (\bar{F}(1))^{1/n}.\tag{11}$$

By (8) and that \bar{F} is right-continuous, (11) implies that:

$$\bar{F}(0) = \lim_{n \to \infty} \bar{F}\left(\frac{1}{n}\right) = \lim_{n \to \infty} (\bar{F}(1))^{1/n} = 1.$$

Hence, since \bar{F} must be non-increasing, $\bar{F}(x) = 1$ for all $x \leq 0$.

We now combine (9) and (11), and get:

$$\bar{F}\left(\frac{m}{n}\right) = \bar{F}^m\left(\frac{1}{n}\right) = \bar{F}(1)^{m/n}, \text{ for all } m, n \in \mathbb{N}^+.$$

Thus, since $\bar{F}(1) = e^{-\lambda}$, we have proved that:

$$ar{F}(q) = ar{F}(1)^q = e^{-\lambda q}, \quad ext{for all } q \in \mathbb{Q}^+.$$

Now, let $x \in \mathbb{R}^+$. Since the set \mathbb{Q}^+ is dense in \mathbb{R}^+ , there exists a decreasing sequence $\{q_r\} \subset \mathbb{Q}^+$ such that:

$$\lim_{r\to\infty}q_r=x.$$

Since \bar{F} is right-continuous, this implies that:

$$\bar{F}(x) = \lim_{r \to \infty} \bar{F}(q_r) = \lim_{r \to \infty} e^{-\lambda q_r} = e^{-\lambda x}.$$

Hence, we conclude that $X \sim exp(\lambda)$.

Example 5.2

Problem

The amount of time one spends in a bank, denoted X, is exponentially distributed with mean ten minutes. That is, $X \sim exp(\lambda) = exp(\frac{1}{10})$.

- What is the probability that a customer will spend more than fifteen minutes in the bank?
- 2 What is the probability that a customer will spend more than fifteen minutes in the bank given that she is still in the bank after ten minutes?

SOLUTION:

0

$$\mathbb{P}(X > 15) = e^{-15\lambda} = e^{-15/10} \approx 0.223.$$

2

$$\mathbb{P}(X > 15 \mid X > 10) = e^{-(15-10)\lambda} = e^{-5/10} \approx 0.607.$$

Assume that X_1 , X_2 are independent and that $X_i \sim exp(\lambda_i)$, i = 1, 2. We want to calculate the probability of the event that $X_1 < X_2$.

The 2-dimensional random variable (X_1, X_2) has distribution with density

$$f(x_1,x_2) = \lambda_1 \lambda_2 e^{-(\lambda_1 x_1 + \lambda_2 x_2)} \mathbb{1}_{\{x_1 > 0, x_2 > 0\}},$$

therefore

$$\begin{split} \mathbb{P}(X_1 < X_2) &= \int \int_{x_1 < x_2} f(x_1, x_2) dx_1 dx_2 = \lambda_1 \lambda_2 \int_0^\infty \int_0^{x_2} e^{-(\lambda_1 x_1 + \lambda_2 x_2)} dx_1 dx_2 \\ &= \lambda_1 \lambda_2 \int_0^\infty e^{-\lambda_2 x_2} \left(\int_0^{x_2} e^{-\lambda_1 x_1} dx_1 \right) dx_2 = \lambda_1 \lambda_2 \int_0^\infty e^{-\lambda_2 x_2} \frac{1}{\lambda_1} \left(1 - e^{-\lambda_1 x_2} \right) dx_2 \\ &= \lambda_2 \int_0^\infty e^{-\lambda_2 x_2} dx_2 - \lambda_2 \int_0^\infty e^{-(\lambda_1 + \lambda_2) x_2} dx_2 = 1 - \frac{\lambda_2}{\lambda_1 + \lambda_2} \\ &= \frac{\lambda_1}{\lambda_1 + \lambda_2}. \end{split}$$

Assume that X_1, \ldots, X_n are independent and that $X_i \sim exp(\lambda_i)$, i = 1, ..., n.

$$\mathbb{P}(\min_{1 \le i \le n} X_i > x) = \mathbb{P}\left(\bigcap_{i=1}^n \{X_i > x\}\right)$$
$$= \prod_{i=1}^n \mathbb{P}(X_i > x)$$
$$= \prod_{i=1}^n e^{-\lambda_i x}$$
$$= e^{-(\sum_{i=1}^n \lambda_i)x}.$$

Thus, we have shown that $\min_{1 \le i \le n} X_i \sim exp\left(\sum_{i=1}^n \lambda_i\right)$.

The following result combines the two previous results.

Assume that X_1, \ldots, X_n are independent and that $X_i \sim exp(\lambda_i)$, i = 1, ..., n. We want to calculate the probability that X_i is the smallest of all the variables, i.e., that $X_i < X_j$ for all $j \neq i$.

$$\mathbb{P}\left(X_{i} < X_{j} \text{ for all } j \neq i\right) = \mathbb{P}\left(X_{i} < \min_{j \neq i} X_{j}\right)$$

$$= \frac{\lambda_{i}}{\lambda_{i} + \sum_{j \neq i} \lambda_{j}}$$

$$= \frac{\lambda_{i}}{\sum_{j=1}^{n} \lambda_{j}}$$

Proposition 5.2

Assume that X_1, \ldots, X_n are independent and that $X_i \sim exp(\lambda_i)$, i = 1, ..., n. Then mini $X_i \sim exp(\sum_{i=1}^n \lambda_i)$. Moreover, min_i X_i and the rank order of X_1, \ldots, X_n are independent.

PROOF: Since the exponential distribution is memoryless, we get that:

$$\mathbb{P}(X_{i_1} < \dots < X_{i_n} \mid \min_{1 \le i \le n} X_i > t)$$

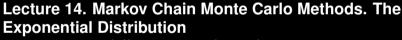
$$= \mathbb{P}\left(X_{i_1} < \dots < X_{i_n} \mid \bigcap_{i=1}^n X_i > t\right)$$

$$= \mathbb{P}\left(X_{i_1} - t < \dots < X_{i_n} - t \mid \bigcap_{i=1}^n X_i > t\right)$$

$$= \mathbb{P}(X_{i_1} < \dots < X_{i_n}).$$

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