# Density dependent Markov chains and their approximations 

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## Outline

1. Markov chains
2. Density dependent Markov chains (DDMC)
3. Approximations of DDMCs
3.1 Deterministic approximation with ODEs
3.2 Stochastic approximation with SDEs
4. Conclusions

## 1. Continuous time Markov chains

- discrete state space
- continuous time process, $Z(t)$
- enjoys the Markov property

$$
\begin{aligned}
& \operatorname{Pr}(Z(s+t)=j \mid Z(s)=i,\{Z(u): 0 \leq u<s\})= \\
& \operatorname{Pr}(Z(s+t)=j \mid Z(s)=i)
\end{aligned}
$$

- this memoryless property implies that holding times are exponential


## 1. Continuous time Markov chains

- a CTMC is usually specified through its infinitesimal generator

$$
Q=\left(\begin{array}{cccccc}
-q_{1} & q_{1,2} & q_{1,3} & & q_{1, n-1} & q_{1, n} \\
q_{2,1} & -q_{2} & q_{2,3} & \ldots & q_{2, n-1} & q_{2, n} \\
q_{3,1} & q_{3,2} & -q_{3} & & q_{3, n-1} & q_{3, n} \\
& & & \ddots & & \\
q_{n-1,1} & q_{n-1,2} & q_{n-1,3} & \ldots & -q_{n-1} & q_{n-1, n} \\
q_{n, 1} & q_{n, 2} & q_{n, 3} & \ldots & q_{n-1, n} & -q_{n}
\end{array}\right)
$$

with

$$
q_{i}=\sum_{j} q_{i, j}
$$

## 1. $M / M / 1$ queue

- queue fed by Poisson process with exponential server

$$
Q=\left(\begin{array}{cccccc}
-\lambda & \lambda & 0 & \cdots & & \\
\mu & -\lambda-\mu & \lambda & 0 & \ldots & \\
0 & \mu & -\lambda-\mu & \lambda & 0 & \cdots \\
& & & \ddots & & \\
& & & 0 & \mu & -\lambda-\mu \\
& \cdots & \cdots & 0 & \mu & -\mu
\end{array}\right)
$$

## 1. Analysis of CTMCs

- two ways of thinking what happens in a CTMC:
- first choose sojourn time according to $q_{i}$ and then the next state according to $q_{i, j} / q_{i}$
- generate exponential random variables according to $q_{i, j}$ and then select the smallest of them to specify the next state
- transient probabilities calculated through matrix exponential

$$
P(t)=[\operatorname{Pr}(X(t)=j \mid X(0)=i)]=e^{t Q}=\sum_{n=0}^{\infty} \frac{Q^{n} t^{n}}{n!}
$$

- steady state by linear system

$$
\pi Q=0, \quad \sum_{i} \pi_{i}=1
$$

## 1. Randomization

- several ways of calculating matrix exponential: Moler, C. and C. Van Loan. 2003. Nineteen dubious ways to compute the exponential of a matrix, twenty-five years later. SIAM Review 45, 3V49.
- randomization is best suited to CTMCs

$$
P(t)=\sum_{n=0}^{\infty}(I+Q / q)^{n} \frac{e^{-q t}(q t)^{n}}{n!}
$$

with $q>\max _{i} q_{i}$

## 2. Density dependent Markov chains

- we consider the class of density dependent Markov chains
- describe the interaction of groups of identical objects
- informally: the intensities of the interactions can be expressed as a function of the density of the objects present in the considered area or volume
- (instead of expressed as a function of the number of objects itself)


## 2. Density dependent Markov chains

- formally a sequence of density dependent Markov chains is:
- indexed by a parameter, denoted by $N$ (area or volume or total number of objects)
- has state space $\mathcal{S}^{[N]} \subseteq \mathbb{Z}^{k}$ ( $k$ groups of identical objects)
- the transition intensities are in the form:

$$
q_{r, r+m}^{[N]}=N f\left(\frac{r}{N}, m\right)
$$

- by relaxing the above form we obtain the class of nearly density dependent Markov chains with transition intensities in the form

$$
q_{r, r+m}^{[N]}=N f\left(\frac{r}{N}, m\right)+N g(r / N, m, N)
$$

with $g(r / N, m, N) \in O(1 / N)$

## 2. Example

- epidemic model with susceptible (S) and infected (I) individuals distributed over an area split into $N$ equally sized cells
- a state is a pair $(i, j)$
- three kinds of transitions:
- 1. susceptible individuals grows:

$$
\emptyset \rightarrow S
$$

with intensity

$$
q_{(i, j),(i+1, j)}^{[N]}=N \lambda_{1}
$$

because the larger the area the higher the intensity

## 2. Example

- three kinds of transitions:
- 2. one susceptible individual becomes infected:

$$
S+2 I \rightarrow 3 I
$$

with intensity

$$
\begin{aligned}
q_{(i, j),(i-1, j+1)}^{[N]}= & \frac{i j(j-1)}{2} \frac{1}{N^{3}} N \lambda_{2}= \\
& N\left(\frac{\lambda_{2}}{2} \frac{i}{N}\left(\frac{j}{N}\right)^{2}\right)-N\left(\frac{1}{N} \frac{\lambda_{2}}{2} \frac{i}{N} \frac{j}{N}\right)
\end{aligned}
$$

because

$$
\frac{i j(j-1)}{2} \frac{1}{N^{3}}
$$

is the probability that one $S$ and 21 meet in a given cell

## 2. Example

- three kinds of transitions:
- 3. infected individuals can become immune:

$$
I \rightarrow \emptyset
$$

with intensity

$$
q_{(i, j),(i, j-1)}^{[N]}=j \lambda_{3}=q_{(i, j),(i, j-1)}^{[N]}=N \lambda_{3} \frac{j}{N}
$$

because every I individually gets immune with intensity $\lambda_{3}$

## 3. Fluid approximation

- the considered approximations are fluid
- in order to compare models with different values of $N$ we work with the density process:

$$
Z^{[N]}(t)=X^{[N]}(t) / N
$$

### 3.1 Deterministic approximation

- if the initial state that tends to $z_{0}$ as $N$ tends to infinity:

$$
\lim _{N \rightarrow \infty} Z^{[N]}(0)=z_{0}
$$

- then the density process tends to the solution of

$$
d z(t)=\sum_{l \in C} I f(z(t), I) d t, \quad z(0)=z_{0}
$$

### 3.1 Deterministic approximation

- difference between the deterministic approximation and the original stochastic behavior is characterized by

$$
\sup _{t \leq T}\left|Z^{[N]}(t)-z(t)\right|=O(1 / \sqrt{N}) \text { a.s. }
$$

i.e., the error of the deterministic approximation decreases as $1 / \sqrt{N}$

- for any $\epsilon$ there exists $M_{\epsilon}$ such that

$$
P\left(\frac{\sup _{t \leq T}\left|Z^{[N]}(t)-z(t)\right|}{1 / \sqrt{N}}>M_{\epsilon}\right)<\epsilon
$$

### 3.1 Deterministic approximation

- the deterministic approximation provides a single trajectory
- usually considered as the approximate mean
- important characteristics, like significant variance or bimodality or non-deterministic cycle times, can be lost
- these can be present even with very large values of $N$


### 3.1 Lotka-Volterra predator-prey reactions

- models predator pray interactions:

$$
X \rightarrow 2 X, X+Y \rightarrow 2 Y, Y \rightarrow \emptyset
$$

with initial state

$$
(N, N)
$$

and intensities

$$
(10,20 / N, 10)
$$

- accordingly the density process starts from $(1,1)$


### 3.1 Lotka-Volterra predator-prey reactions

With the previous parameters the deterministic approximation oscillates regularly forever:


### 3.1 Lotka-Volterra predator-prey reactions

Compared to $N=50$ :





### 3.1 Lotka-Volterra predator-prey reactions

Compared to $N=100$ :





### 3.1 Lotka-Volterra predator-prey reactions

Compared to $N=500$ :





### 3.1 Lotka-Volterra predator-prey reactions

Compared to $N=2000$ :




### 3.1 Lotka-Volterra predator-prey reactions

Distribution of the largest difference between the ODE and the original behaviour with $N=100,200,1000,2000$ :





### 3.1 Lotka-Volterra predator-prey reactions

Mean error as function of $N$ and its best least square $1 / \sqrt{N}$ fit:


### 3.1 Lotka-Volterra predator-prey reactions

$M_{\epsilon}$ in function of $N$ for which

$$
P\left(\frac{\sup _{t \leq T}\left|Z^{[N]}(t)-z(t)\right|}{1 / \sqrt{N}}>M_{\epsilon}\right)=\epsilon
$$

for $\epsilon=0.05,0.1,0.15,0.2,0.25$ :


### 3.2 Stochastic approximation with SDEs

- approximation with stochastic differential equations:
$d Y^{[N]}(t)=\sum_{l \in C} I f\left(Y^{[N]}(t), l\right) d t+\sum_{l \in C} \frac{l}{\sqrt{N}} \sqrt{f\left(Y^{[N]}(t), l\right)} d W_{l}(t)$
where $W_{l}(t)$ with $I \in C$ are independent standard one-dimensional Brownian motions
- maintains stochasticity: provides distributions
- explicitly uses $N$ (in case of the deterministic approximation $N=\infty$ )
- has better convergence:

$$
\sup _{t \leq T}\left|Z^{[N]}(t)-Y^{[N]}(t)\right|=O(\log N / N) \text { a.s. }
$$

for corresponding pairs of trajectories

### 3.2 Lotka-Volterra predator-prey reactions

Trajectories with $N=50$ :





### 3.2 Lotka-Volterra predator-prey reactions

Trajectories with $N=200$ :





### 3.2 Lotka-Volterra predator-prey reactions

Trajectories with $N=500$ :





### 3.2 Lotka-Volterra predator-prey reactions

Trajectories with $N=2000$ :





### 3.2 Lotka-Volterra predator-prey reactions

Pmf with $N=200,500,1000,2000$ :





### 3.2 Lotka-Volterra predator-prey reactions

Difference in the mean as function of $N$ :


## 4. Conclusions

- exact simulation of CTMC becomes slower with increasing $N$
- for fixed step size, simulation of SDE becomes more accurate as $N$ increases
- ranges of $N$ :
- small $N$ : use an analytical approach (randomization)
- larger $N$ : simulate the Markov chain
- even larger $N$ but still important stochastic behavior: use diffusion approximation
- huge $N$, no stochasticity: use deterministic approximation

