Lecture 7b:

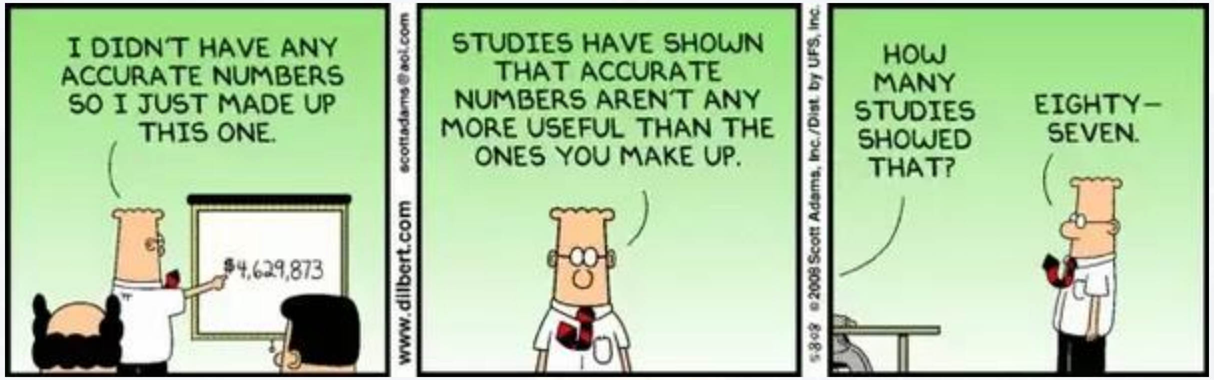
Stochastic Processes

Markus Hohle

University California, Berkeley

Bayesian Data Analysis and Machine Learning for Physical Sciences

Course Map



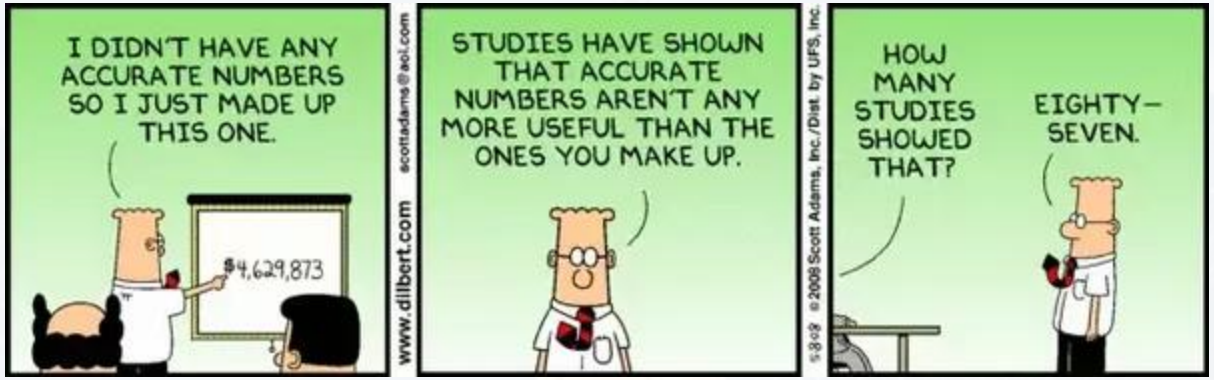
Outline

The Poissonian Stepper

Examples of Stochastic Processes
- Radioactive Decay
- Chem. Reactions
- Predator Prey
- Gene Expression

Diffusion Processes

Fokker-Planck Equation



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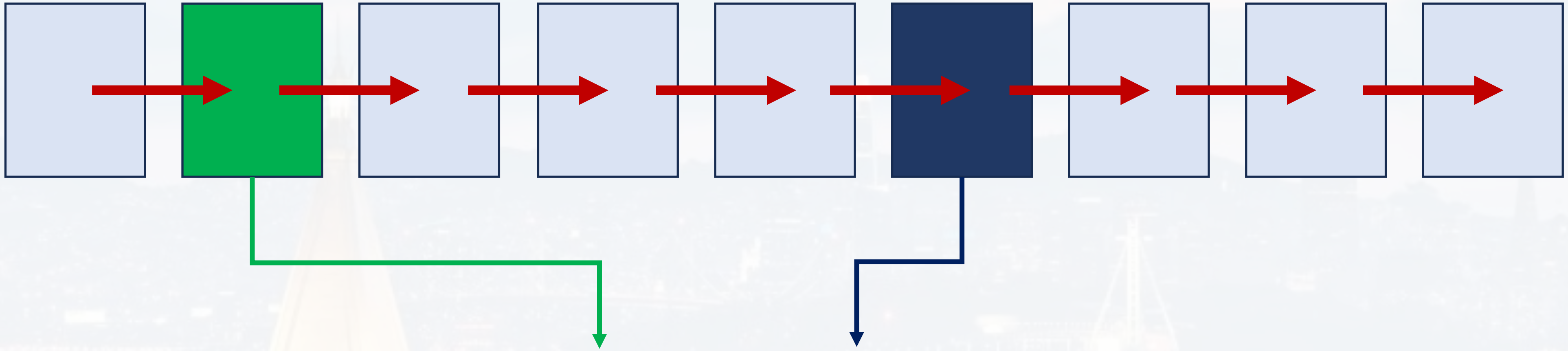
HMM: sequence of states

set of different states/classes

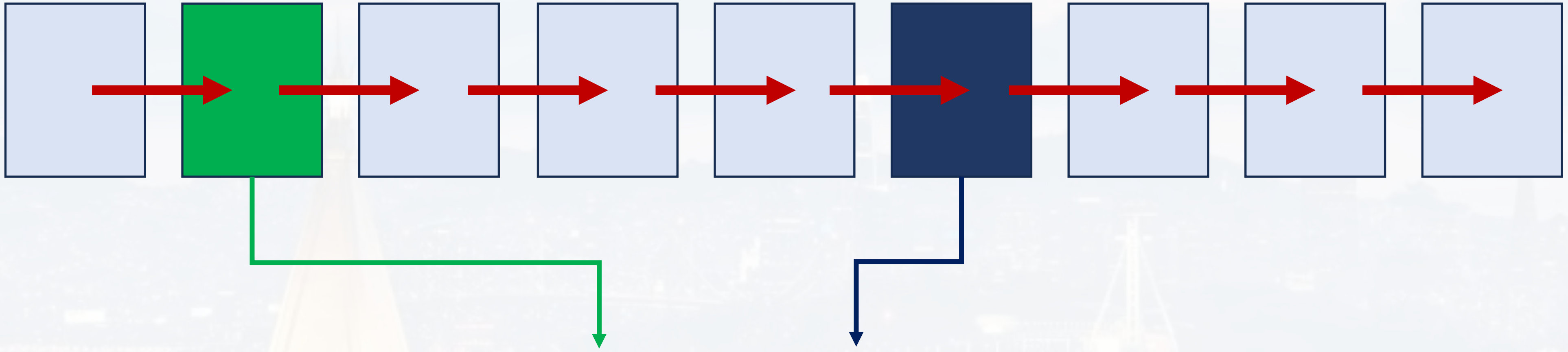


a set of T observations O $\quad O = (O_1, O_2, O_3, \dots O_t, \dots O_T)$ drawing randomly from the states

Stochastic Processes:

HMM: sequence of states

set of different states/classes

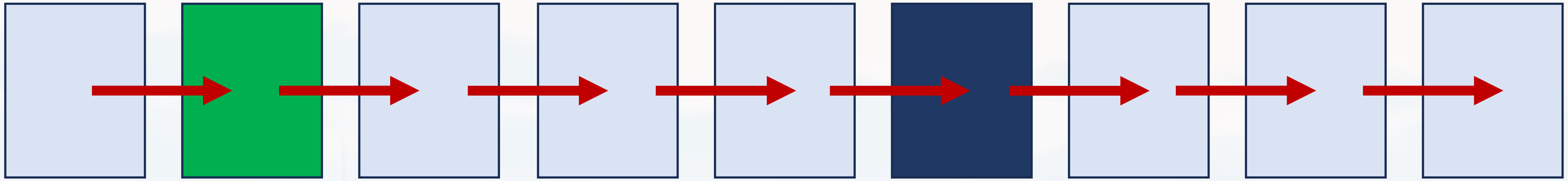


a set of T observations O $\quad O = (O_1, O_2, O_3, \dots O_t, \dots O_T)$ drawing randomly from the states

goal:
- focus on the states
- better understand the processes wrt time t
- model the processes as a function of time t
- later: **Monte Carlo** sampling, but we need to understand the processes first!

Stochastic Processes: The Poissonian Stepper

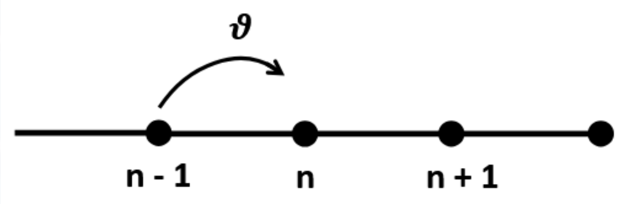
sequence of states, but now: state graph **is not ergodic at all!**

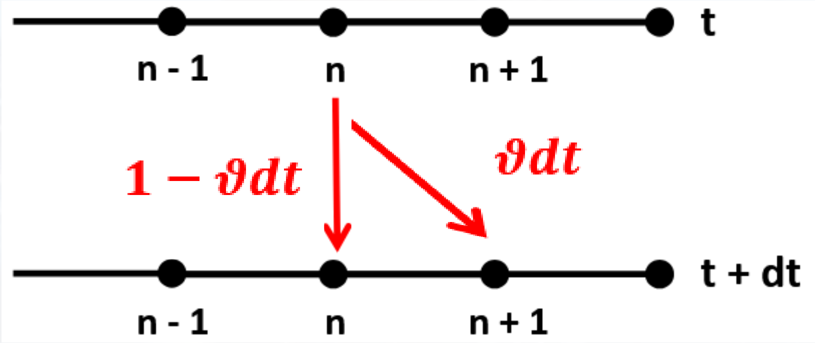


n: different states

ϑ: hopping rate

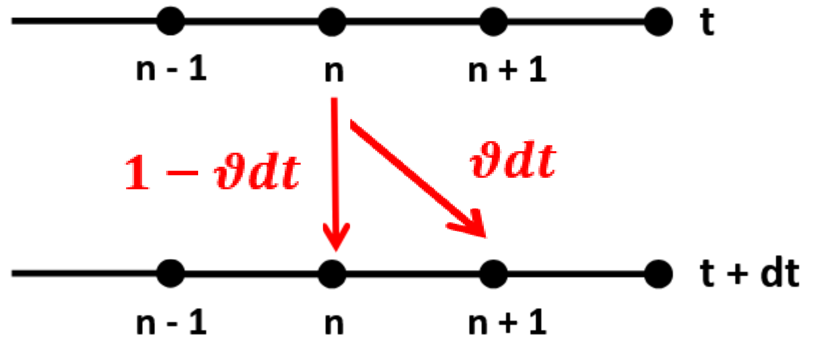
- for now: $\vartheta = const$
- $[\vartheta] = probability/time$





assumption: - we can resolve the process such, that the system performs either **one step** or **no step** within a **timestep** dt

$P(n, t + dt)$: probability that we observe the system in state n at time $t + dt$



n:	different states
ϑ:	hopping rate $(probability/time)$
dt:	time increment

$P(n, t + dt)$: probability that we observe the system in state n at time $t + dt$

for now, states only change from $n \to n + 1$

$$P(n, t + dt) = P(n - 1, t)\, vdt + P(n, t)\,(1 - vdt)$$

system was in state $n - 1$, but jumped to state n within dt

system was in state n and did not jump within dt

$$= P(n - 1, t)\, vdt + P(n, t) - P(n, t)\, vdt$$

$$P(n, t + dt) \approx P(n, t) + \frac{dP(n, t)}{dt} dt$$

dt is small

$$\boxed{\frac{dP(n, t)}{dt} = \nu\, P(n - 1, t) - \nu\, P(n, t)}$$

Master Equation

Stochastic Processes:

n:	different states
ϑ:	hopping rate ($probability/time$)
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$$\boxed{\frac{dP(n,t)}{dt} = \nu\, P(n-1,t) - \nu\, P(n,t)}$$

Master Equation

$$\frac{d}{dt}P(n,t) = P(jump\ up|\ at\ n-1)\ P(at\ n-1)$$

$$- P(jump\ down|\ at\ n)\ P(at\ n)$$

$$\boxed{\frac{dP(n,t)}{dt} = \nu\, P(n-1,t) - \nu\, P(n,t)}$$

Master Equation

$\boldsymbol{n}$:	different states
$\boldsymbol{\vartheta}$:	hopping rate $(probability/time)$
$\boldsymbol{dt}$:	time increment

goal: find $\mathrm{P}(n,t)$

$\boldsymbol{P(n,t+dt)}$: **probability that we observe the system in state $\boldsymbol{n}$ at time $\boldsymbol{t+dt}$**

real-valued **moment-generating function**

for now, states only change from $\boldsymbol{n \to n+1}$

$$G(z,t) = \sum_{n=0}^{\infty} P(n,t)\, z^n$$

k^{th} moment: $\left.\dfrac{\partial^k G(z,t)}{\partial z^k}\right|_{z=1}$

$$\frac{d}{dt}G(z,t) = \sum_{n=0}^{\infty} \frac{dP(n,t)}{dt}\, z^n = \sum_{n=0}^{\infty} [\nu\, P(n-1,t) - \nu\, P(n,t)] z^n$$

$$= \sum_{n=0}^{\infty} \nu\, P(n-1,t)\, z^n - \sum_{n=0}^{\infty} \nu\, P(n,t)\, z^n$$

both sums have independent indices

$$= \sum_{m=0}^{\infty} \nu\, P(m,t)\, z^{m+1} - \sum_{n=0}^{\infty} \nu\, P(n,t)\, z^n$$

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both sums have independent indices

$$= \sum_{n=0}^{\infty} \nu\, P(n,t)\, z^{n+1} - \sum_{n=0}^{\infty} \nu\, P(n,t)\, z^n$$

$$= \sum_{n=0}^{\infty} \nu\, P(n,t)\,[z^{n+1} - z^n] = \sum_{n=0}^{\infty} \nu\, P(n,t) z^n [z-1] = \nu[z-1]G(z,t)$$

$$\boxed{\frac{dP(n,t)}{dt} = \nu\, P(n-1,t) - \nu\, P(n,t)}$$

Master Equation

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$$\frac{d}{dt}G(z,t) = \nu[z-1]G(z,t)$$

the system always starts at $n = 1$ at $t = 0$

$$P(n \neq 0, t=0) = 0$$

$$P(n = 0, t=0) = 1 \quad \rightarrow \; G(z, t=0) = 1$$

$$G(z,t) = e^{\nu(z-1)t}$$

$$e^{-\nu t}e^{\nu z t} = \sum_{n=0}^{\infty} P(n,t)\, z^n$$

Taylor Series of $e^{\nu z t}$ wrt to z

$$\boxed{\frac{dP(n,t)}{dt} = \nu\, P(n-1,t) - \nu\, P(n,t)}$$

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Taylor Series of $e^{\nu z t}$ wrt to z

$$\boldsymbol{e^{-\nu t}} \sum_{n=0}^{\infty} \frac{\boldsymbol{(\nu t)^n}}{\boldsymbol{n!}} z^n = \sum_{n=0}^{\infty} \boldsymbol{P(n,t)}\, z^n$$

$$\boldsymbol{P(n,t) = \frac{(\nu t)^n}{n!} e^{-\nu t}}$$

Poissonian distribution

Stochastic Processes:

$$\boxed{\frac{dP(n,t)}{dt} = \nu\, P(n-1,t) - \nu\, P(n,t)}$$

Master Equation

$\boldsymbol{n}$:	**different states**
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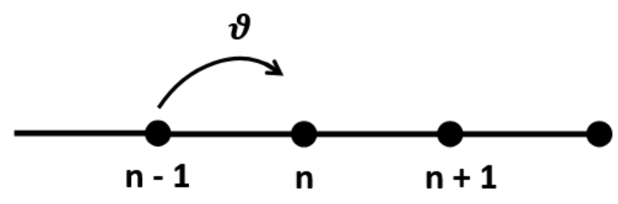
for now, states only change from $\boldsymbol{n \rightarrow n+1}$



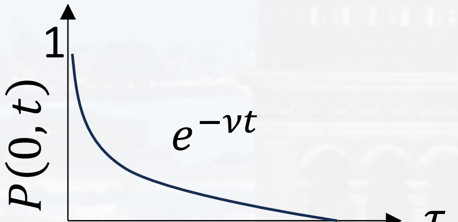
calculating the **waiting time** (time τ *between* two events)

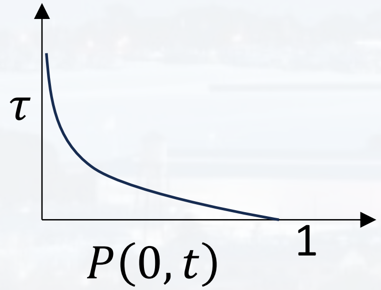
$$P(0,t) = \frac{(\nu t)^0}{0!} e^{-\nu t}$$

$$\tau = -\frac{1}{\nu} ln[P(0,t)]$$

$P(0,t) = e^{-\nu t}$ is the probability that the stepper **has not** moved → cdf

$\bar{P} = 1 - e^{-\nu t}$ is the probability that the stepper **has moved**





see later, Gillespie algorithm

Stochastic Processes:

$$\boxed{\frac{dP(n,t)}{dt} = \nu\, P(n-1,t) - \nu\, P(n,t)}$$

Master Equation

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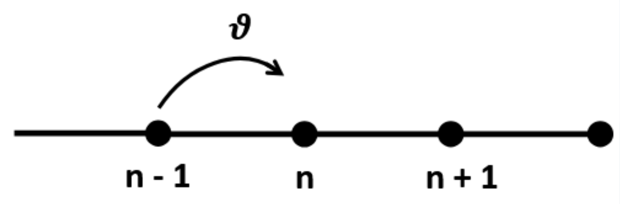
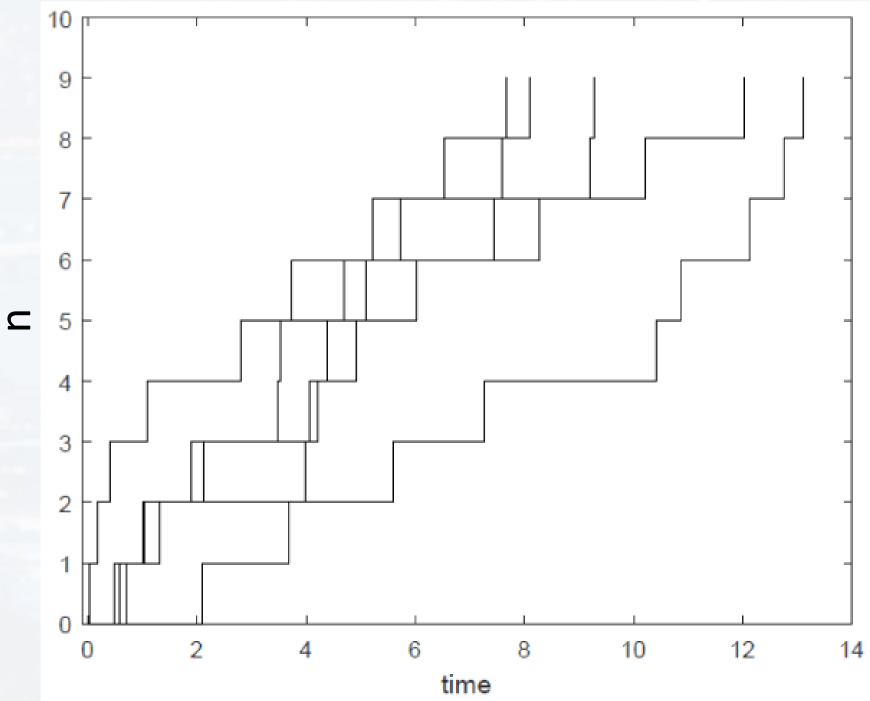
$$P(n,t) = \frac{(\upsilon t)^n}{n!} e^{-\nu t}$$

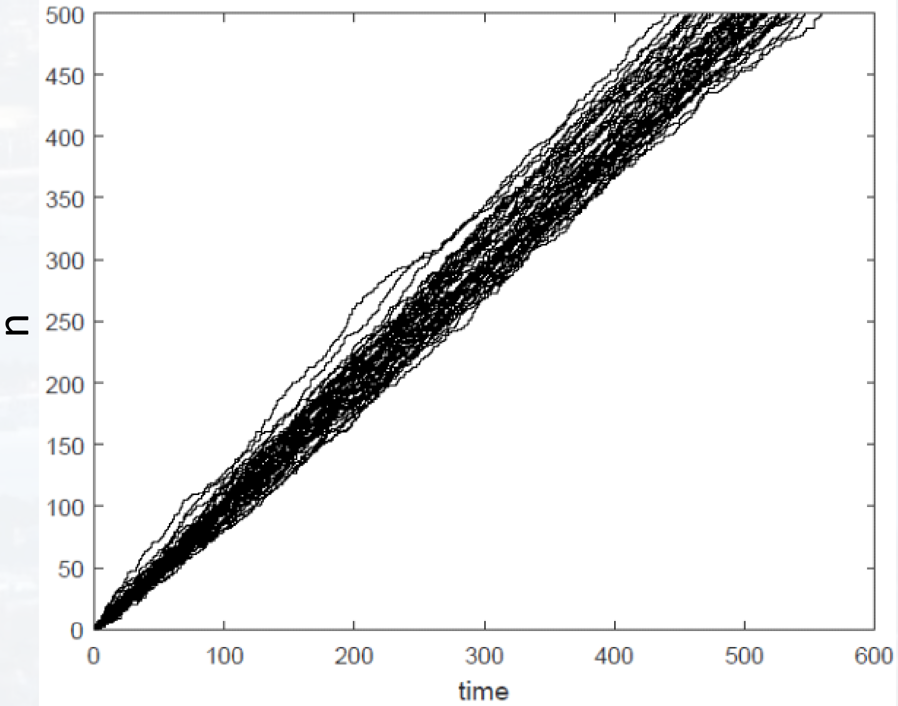
$\boldsymbol{P(n,t+dt)}$: probability that we observe the system in state $\boldsymbol{n}$ at time $\boldsymbol{t+dt}$

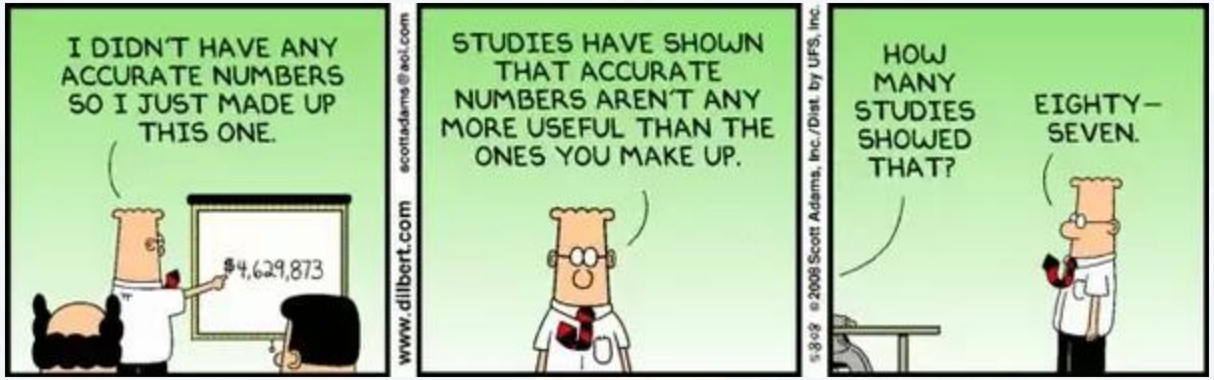


$$\tau = -\frac{1}{\nu} ln[P(0,t)]$$

for now, states only change from $\boldsymbol{n \rightarrow n+1}$







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$A \xrightarrow{k} \emptyset$

n:	different states
ϑ:	hopping rate ($probability/time$)
dt:	time increment

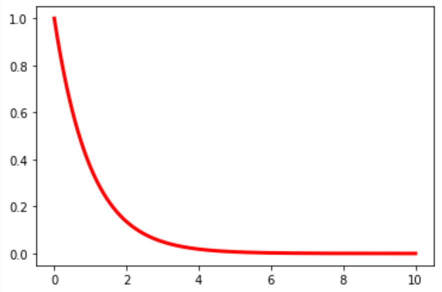
deterministic scenario:

A(t) can be a concentration or a number!

$$\frac{\Delta A(t)}{A(t)} \frac{1}{\Delta t} = -k$$

constant relative change per time step

$$\frac{dA(t)}{A(t)} = -k\, dt$$



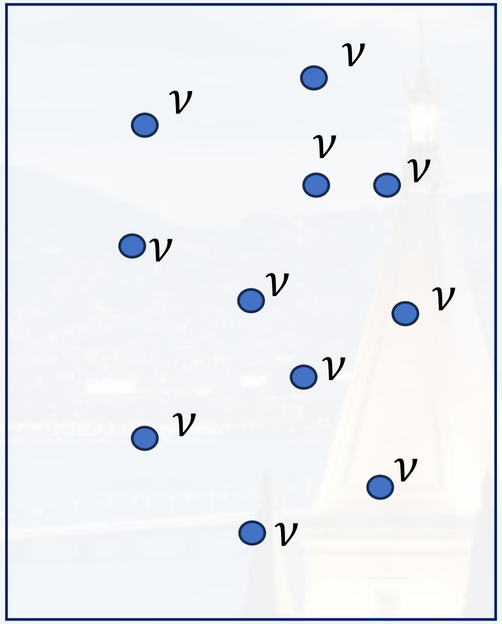
$$A(t) = A(t=0)\, e^{-kt}$$

Stochastic Processes:

$A \xrightarrow{k} \emptyset$ stochastic scenario: number n of particles A

$\boldsymbol{n}$:	**different states**
$\boldsymbol{\vartheta}$:	**hopping rate**
$\boldsymbol{dt}$:	**time increment**
$\tau = -ln[P(0,t)]\,/\nu$:	**waiting time**

t



for $t = 0$ **many** atoms
→ **τ is small**

Δt

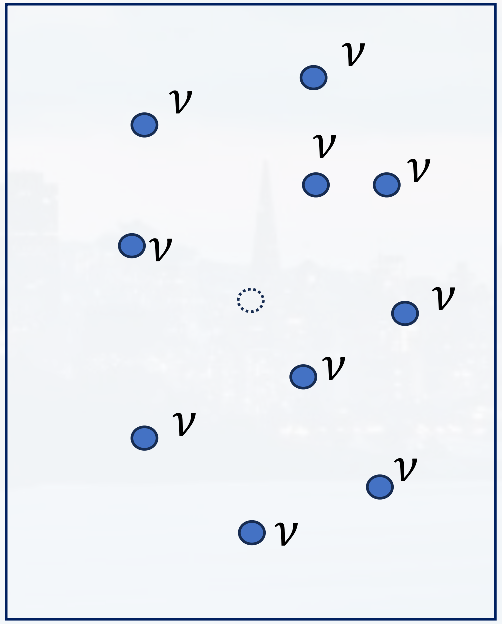
each atom has the probability ν to decay per time

logical ***or*** → **adding** the probabilities

$\nu \rightarrow \nu\, n(t)$

$$\Delta\mathrm{t} = -\frac{1}{\nu\, n(t)} ln[P(0|t)]$$

t + Δt



$$\boxed{\frac{dP(n,t)}{dt} = \nu\,[n+1]P(n+1,t) - \nu\, n\, P(n,t)}$$

Master Equation

path leading from $n+1$, to state n within dt

path leading away from state n

Stochastic Processes:

- Radioactive Decay
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$A \xrightarrow{k} \emptyset$ stochastic scenario:

n:	different states
ϑ:	hopping rate
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$\tau = -ln[P(0,t)]/\nu$:	waiting time

$$\boxed{\frac{dP(n,t)}{dt} = \nu\,[n+1]P(n+1,t) - \nu\, n\, P(n,t)}$$

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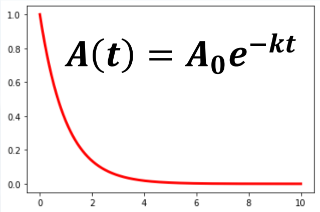
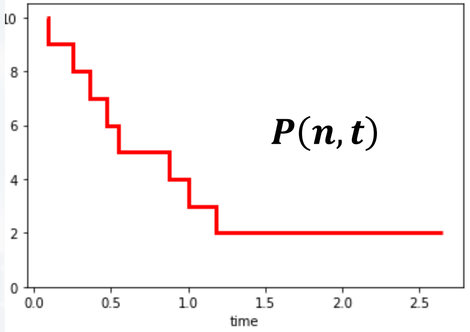
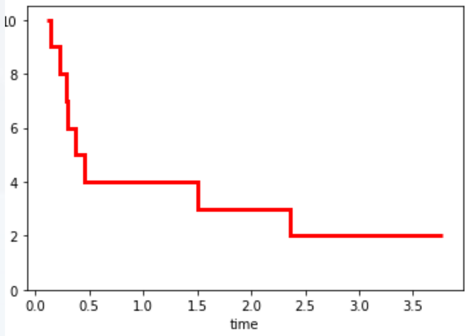
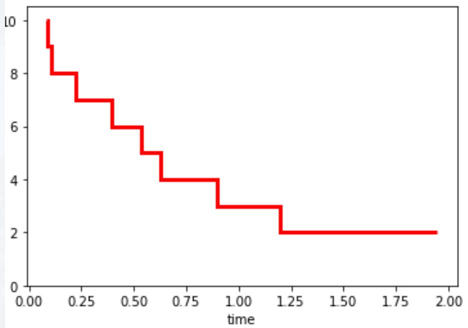








initial conditions:

$$\frac{dP(n,t)}{dt} = -\,\nu n_o P(n,t)$$

$$P(n_o,t) = e^{-\nu n_o t} \qquad P(n_o,t) = 1$$

solving for $P(n,t)$ using the initial conditions,
the master equation and $G(z,t) = \sum_{n=0}^{\infty} P(n,t)\, z^n$ leads to:

$$P(n,t) = e^{-\nu n_o t} \binom{n_o}{n} [1 - e^{-\nu t}]^{n_o - n}$$

mean of n(t) over *n*: $A(t) = \sum_{n=0}^{n_o} n\, P(n,t) \;\; = \sum_{n=0}^{n_o} n\, e^{-\nu n_o t} \binom{n_o}{n} [1 - e^{-\nu t}]^{n_o - n} = n_o e^{-\nu t}$

Stochastic Processes:

Examples

- Radioactive Decay
- Chem. Reactions
- Predator Prey
- Gene Expression

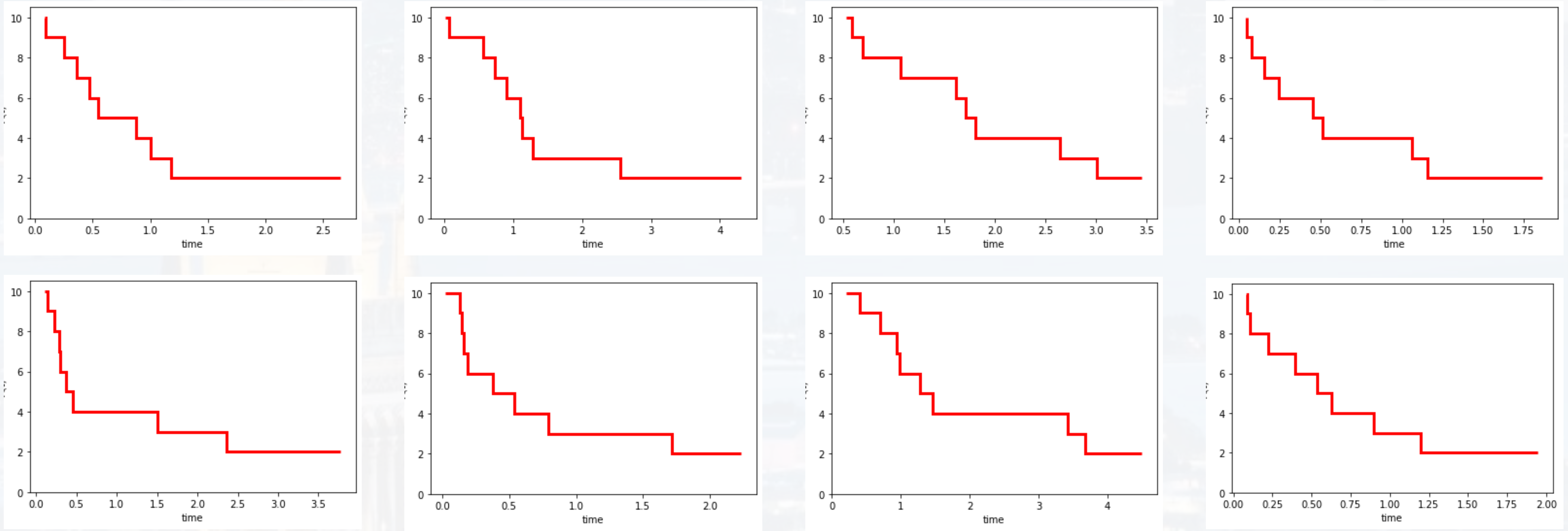
$A \xrightarrow{k} \emptyset$ stochastic scenario:

n:	different states
ϑ:	hopping rate
dt:	time increment
$\tau = -ln[P(0,t)]\,/\nu$:	waiting time

$$\boxed{\frac{dP(n,t)}{dt} = \nu\,[n+1]P(n+1,t) - \nu\, n\, P(n,t)}$$

Master Equation

$$P(n,t) = e^{-\nu n_o t}\binom{n_o}{n}\left[1 - e^{-\nu t}\right]^{n_o - n} \qquad \Delta t = -\frac{1}{\nu\, n(t)}\, ln[P(0|t)]$$



Stochastic Processes:

- **Radioactive Decay**
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$\boldsymbol{n}$:	**different states**
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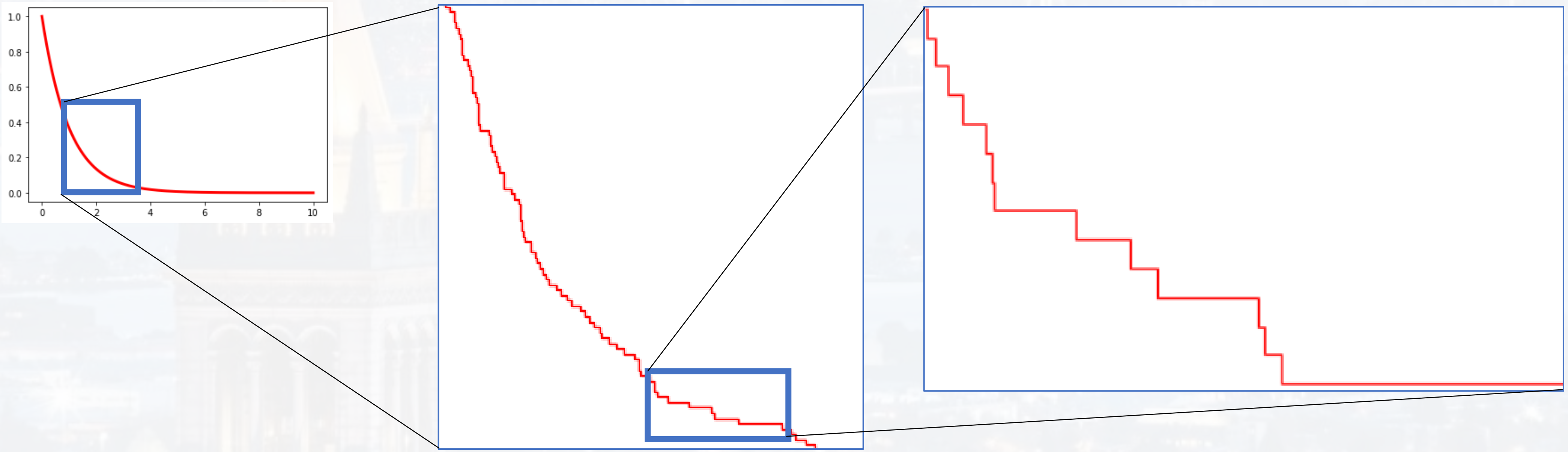
$A \xrightarrow{k} \emptyset$ stochastic scenario:

$$\boxed{\frac{dP(n,t)}{dt} = \nu\,[n+1]P(n+1,t) - \nu\, n\, P(n,t)}$$

Master Equation

$$P(n,t) = e^{-\nu n_o t}\binom{n_o}{n}[1 - e^{-\nu t}]^{n_o - n} \qquad \Delta t = -\frac{1}{\nu\, n(t)} ln[P(0|t)]$$

one run, but large *n*



Stochastic Processes:

- Radioactive Decay
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$$A \underset{k_-}{\overset{k_+}{\rightleftarrows}} B$$

n: number of particles of A

m: number of particles of B

$\boldsymbol{n}$:	**different states**
$\boldsymbol{\vartheta}$:	**hopping rate**
$\boldsymbol{dt}$:	**time increment**
$\boldsymbol{\tau = -ln[P(0,t)]\,/\nu}$:	**waiting time**

$$\nu(A) \rightarrow \nu_+\, n(t) \qquad \nu(B) \rightarrow \nu_-\, m(t) \qquad \nu_{tot} = \nu(A) + \nu(B) = \nu_+\, n(t) + \nu_-\, m(t)$$

$$\boxed{\Delta t = -\frac{1}{\nu_+\, n(t) + \nu_-\, m(t)}\, ln[P(0|t)]}$$

time that elapses until **a** reaction to occur

next: deciding ***which*** reaction should occur (next lecture)

$$\begin{tikzcd} \boxed{n-1, m+1} \arrow[r, shift right, "\nu_-"'] & \boxed{n,m} \arrow[l, shift right, "\nu_+"'] \arrow[r, shift right, "\nu_-"'] & \boxed{n+1, m-1} \arrow[l, shift right, "\nu_+"'] \end{tikzcd}$$

$$\frac{dP(n,m,t)}{dt} = \nu_+\, \boldsymbol{(n+1)P(n+1, m-1, t)} + \nu_-\, \boldsymbol{(m+1)P(n-1, m+1, t)}$$

$$-\nu_+\, \boldsymbol{n\, P(n,m,t)} - \nu_-\, \boldsymbol{m\, P(n,m,t)}$$

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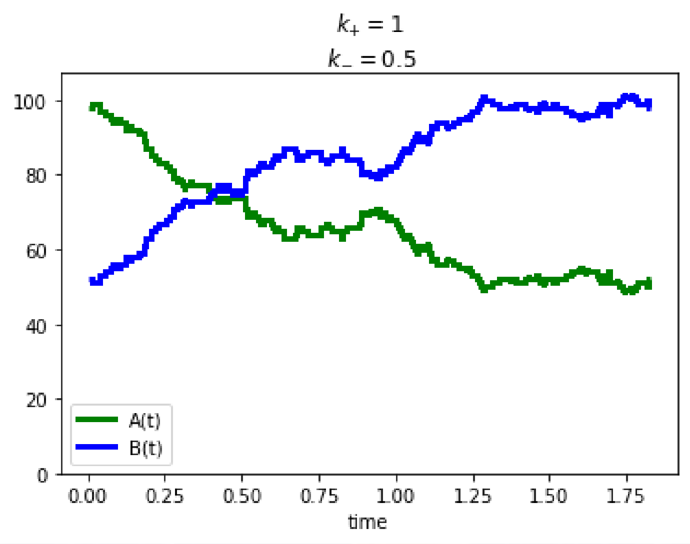
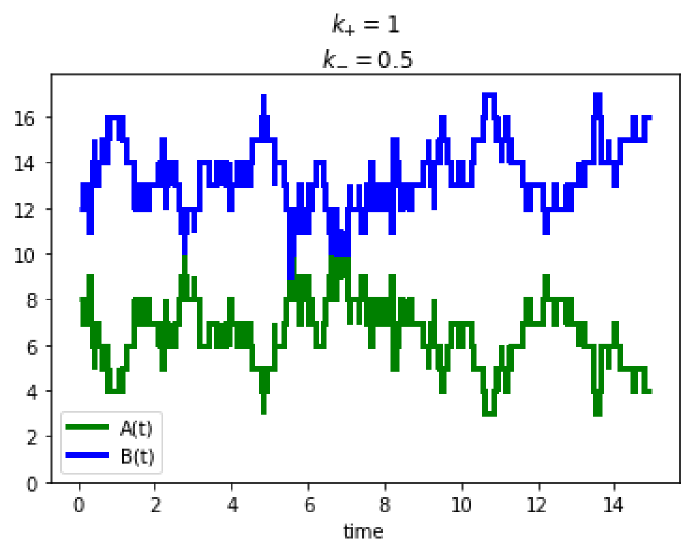
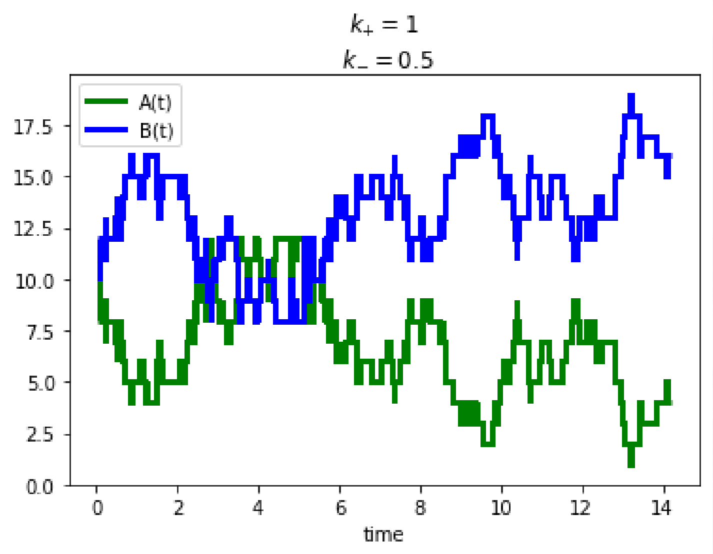
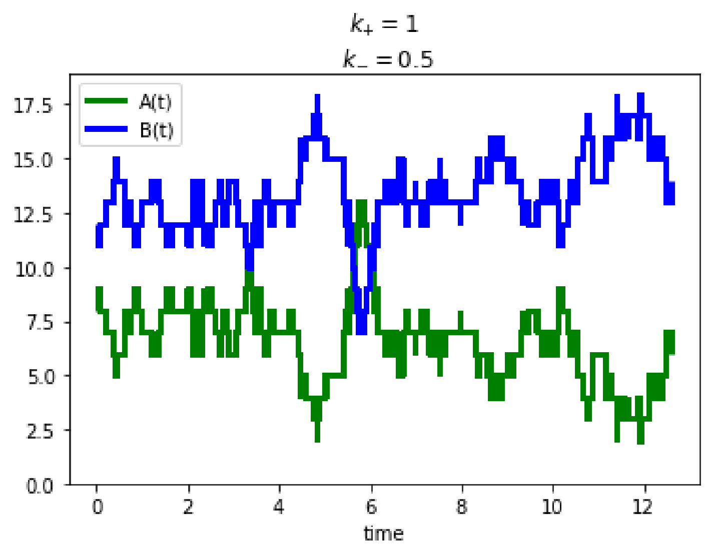


equilibrium at $\frac{A}{B} = \frac{k\_}{k+}$

N = 10







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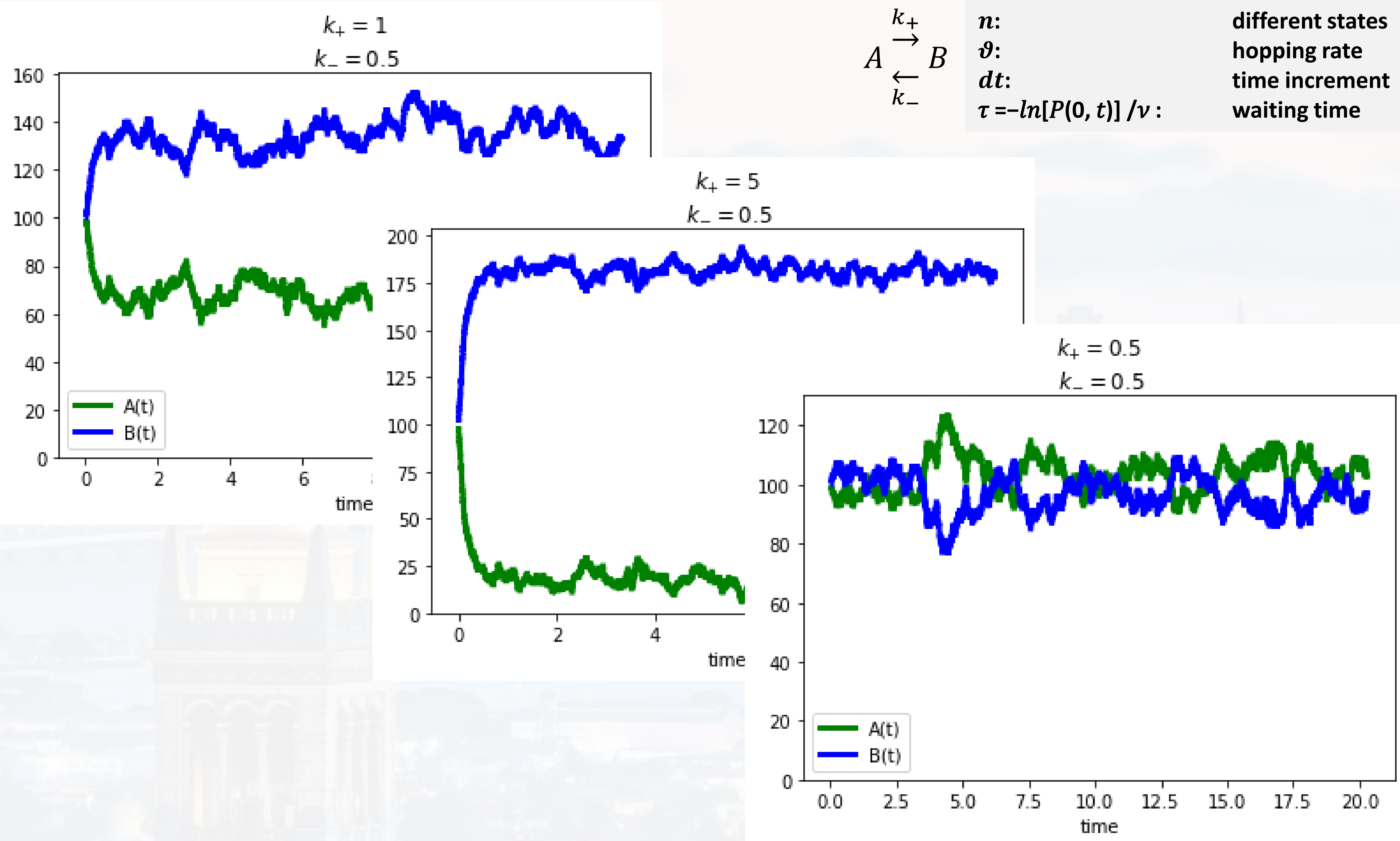

$$A \underset{k_-}{\overset{k_+}{\rightleftarrows}} B$$

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$\tau = -ln[P(0,t)]\,/\nu$:	**waiting time**

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L: sheep (lambs)
W: wolfs
E: "empty"

$$A \underset{k_-}{\overset{k_+}{\rightleftarrows}} B$$

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ϑ:	hopping rate
dt:	time increment
$\tau = -ln[P(0,t)]\,/\nu$:	waiting time

original model:

$$L + E \xrightarrow{k_1} L + L$$ lambs reproduce

$$W \xrightarrow{k_2} E$$ wolfs starve

$$W + L \xrightarrow{k_3} W + W$$ sometimes a wolf kills a lamb and then reproduces

$$W + L \xrightarrow{k_4} W + E$$ sometimes a wolf just kills a lamb

same:

$$L \xrightarrow{k_1} 2\,L$$

$$L + W \xrightarrow{k_2} 2\,W$$

$$W \xrightarrow{k_3} \Phi$$

Stochastic Processes:

- Radioactive Decay
- Chem. Reactions
- **Predator Prey**
- Gene Expression

L:	sheep (lambs)
W:	wolfs
E:	"empty"

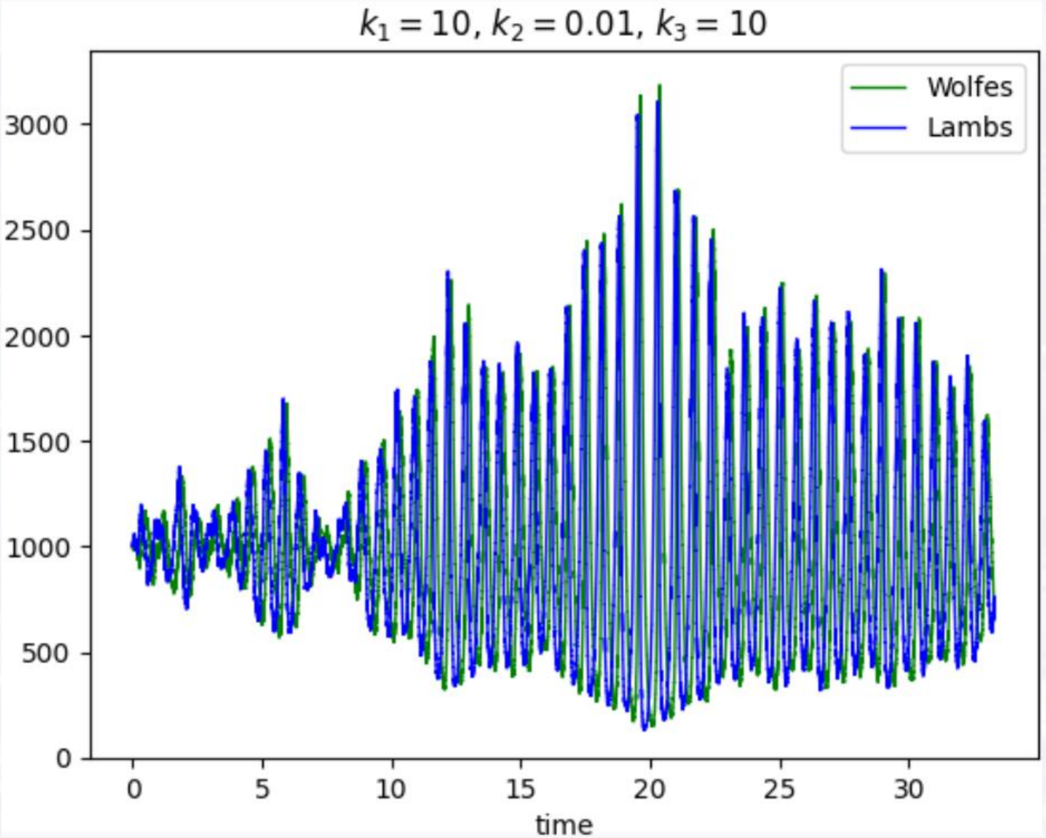
$$L \xrightarrow{k_1} 2\,L$$

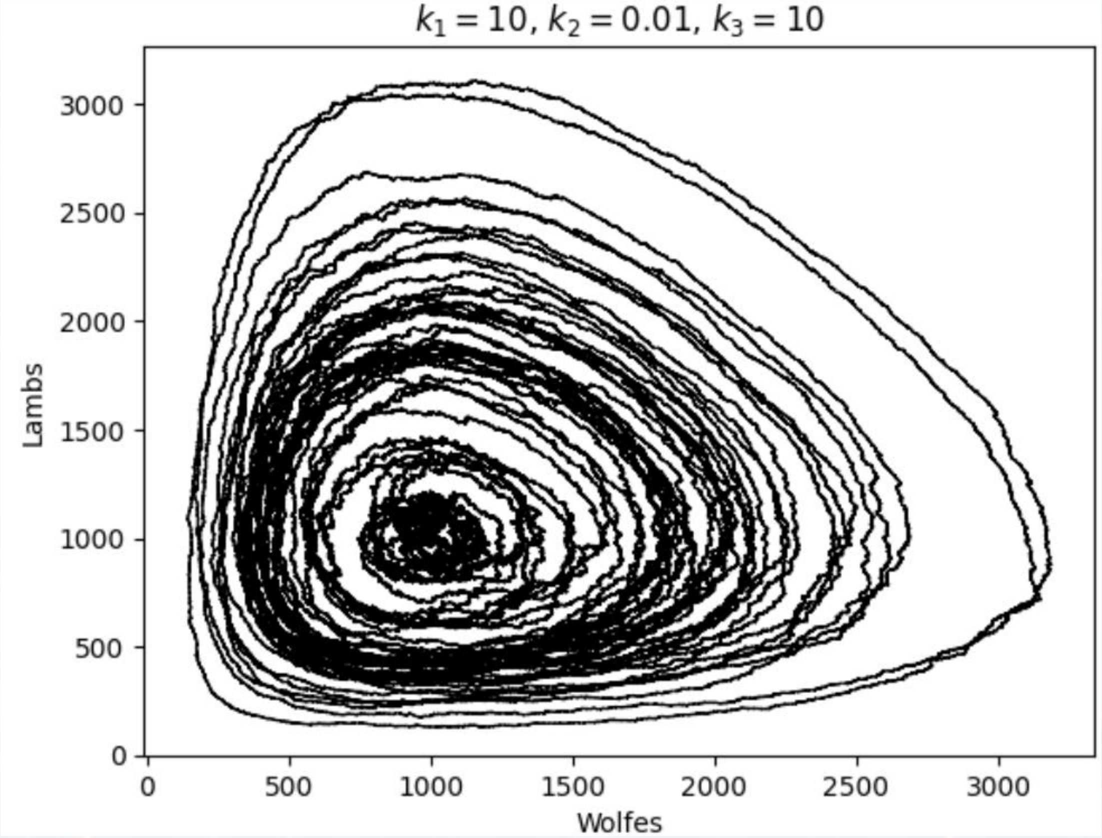
$$L + W \xrightarrow{k_2} 2\,W$$

$$W \xrightarrow{k_3} \Phi$$

$$A \underset{k_-}{\overset{k_+}{\rightleftarrows}} B$$

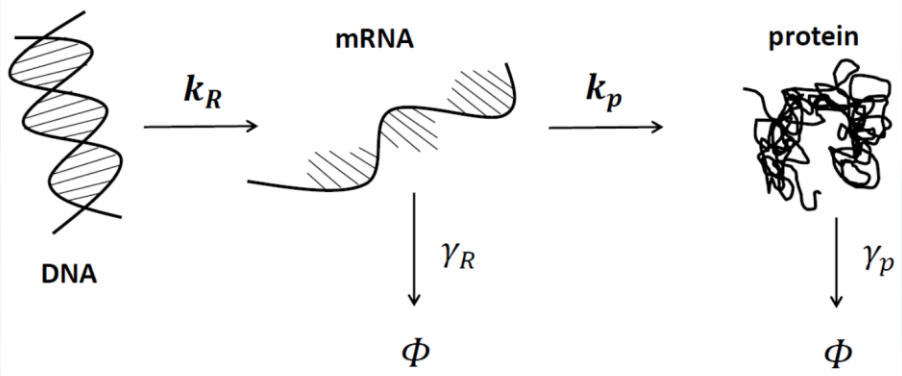
n:	**different states**
ϑ:	**hopping rate**
dt:	**time increment**
$\tau = -ln[P(0,t)]\,/\nu$:	**waiting time**

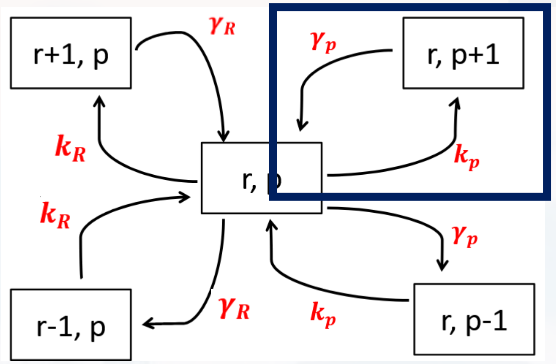




simplest model aka "central dogma"

r: **number of mRNA molecules**
p: **number of protein molecules**



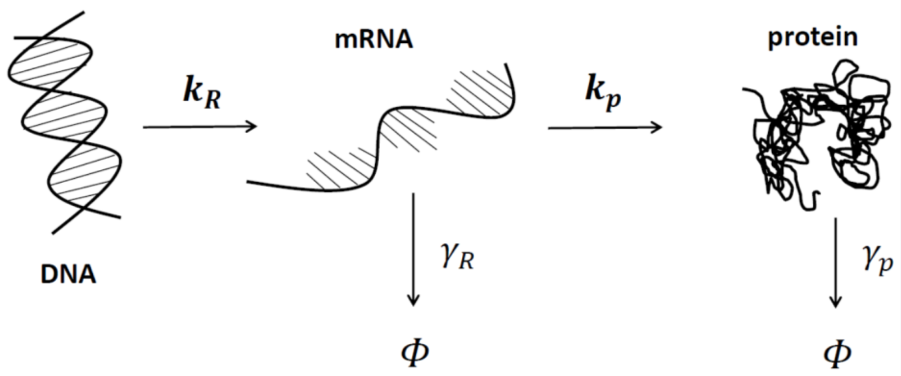


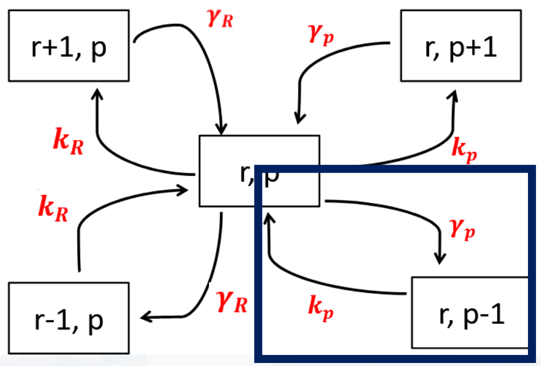
$w(r,p,t)$: probability to observe the system with r mRNA molecules and p protein molecules

$$\frac{dw(r,p,t)}{dt} = \gamma_P\,(p+1)w(r,p+1,t) - k_p\, r\, w(r,p,t)$$

simplest model aka "central dogma"

r: number of mRNA molecules
p: number of protein molecules





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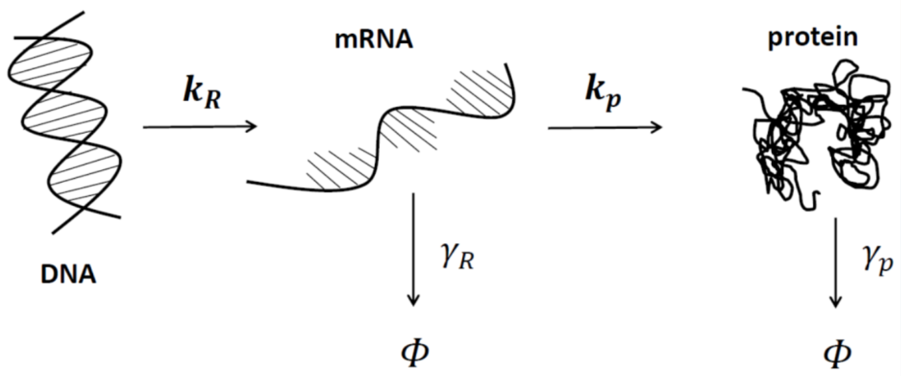
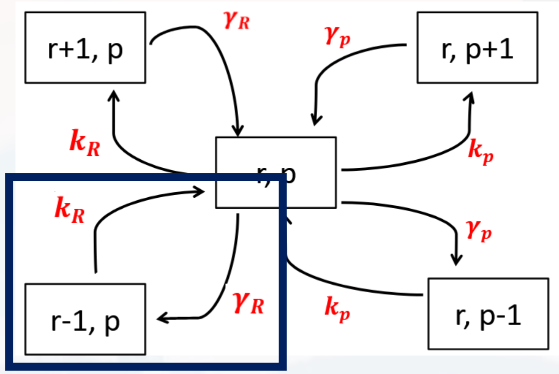
$$\frac{dw(r,p,t)}{dt} = \gamma_P\,(p+1)w(r,p+1,t) - k_p\,r\,w(r,p,t)$$

$$+\,k_p\,r\,w(r,p-1,t) - \gamma_P p\,w(r,p,t)$$

r: number of mRNA molecules
p: number of protein molecules

simplest model aka “central dogma”





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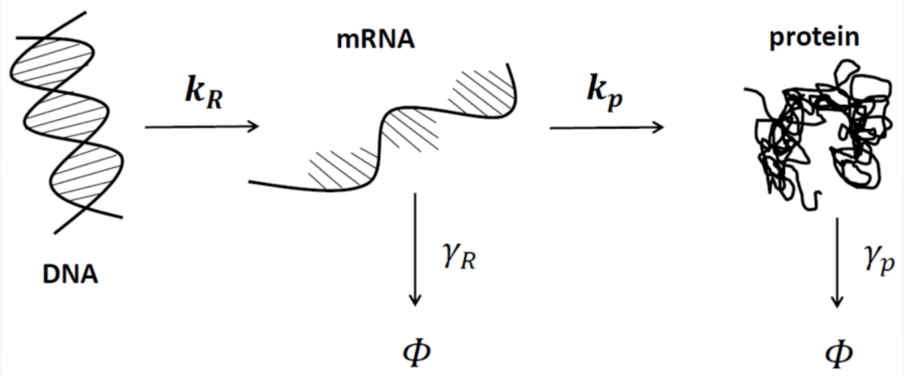
$$\frac{dw(r,p,t)}{dt} = \gamma_P\,(p+1)w(r,p+1,t) - \ k_p\, r\, w(r,p,t)$$

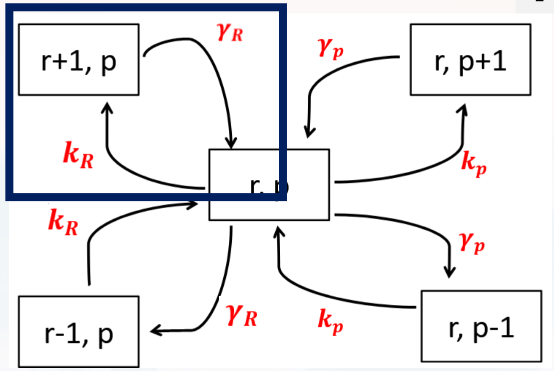
$$+\,k_p\, r\, w(r,p-1,t) - \ \gamma_P p\, w(r,p,t)$$

$$+\,k_R\, w(r-1,p,t)\ - \gamma_R\, r\, w(r,p,t)$$

simplest model aka “central dogma”

r:	**number of mRNA molecules**
p:	**number of protein molecules**





$w(r,p,t)$: probability to observe the system with r mRNA molecules and p protein molecules

$$\frac{dw(r,p,t)}{dt} = \gamma_P\,(p+1)w(r,p+1,t) - k_p\, r\, w(r,p,t)$$

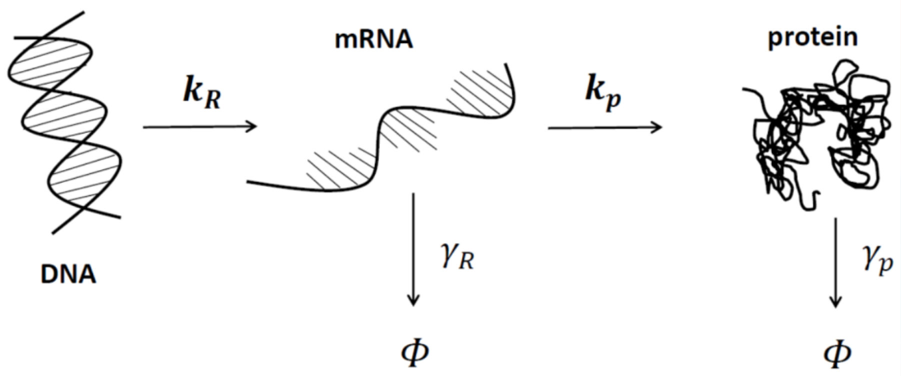
$$+\, k_p\, r\, w(r,p-1,t) - \gamma_P p\, w(r,p,t)$$

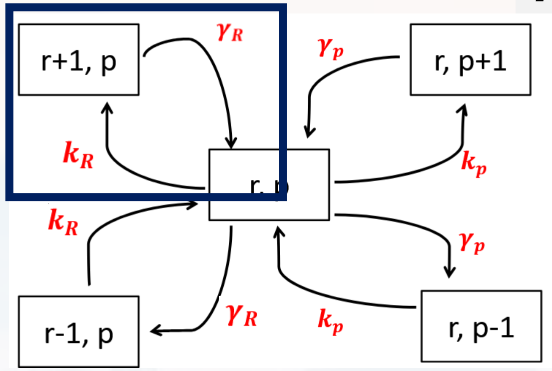
$$+\, k_R\, w(r-1,p,t) - \gamma_R\, r\, w(r,p,t)$$

$$+\, \gamma_R (r+1)\, w(r+1,p,t) - k_R\, w(r,p,t)$$

simplest model aka “central dogma”

$\boldsymbol{r}$:	**number of mRNA molecules**
$\boldsymbol{p}$:	**number of protein molecules**





$w(r,p,t)$: probability to observe the system with *r* mRNA molecules and *p* protein molecules

$$\frac{dw(r,p,t)}{dt} = k_R\, w(r-1,p,t) + \gamma_R(r+1)w(r+1,p,t) + k_P\, r\, w(r,p-1,t)$$

$$+\gamma_P(p+1)\, w(r,p+1,t) - [k_R + \gamma_R\, r + k_P\, r + \gamma_P\, p]\, w(r,p,t)$$

$$G(y,z,t) = \sum_{r,p=0}^{\infty} w(r,p,t)\, y^r z^p \qquad G(y=1,z=1,t) = \sum_{r,p=0}^{\infty} w(r,p,t) = 1$$

simplest model aka "central dogma"

r:	number of mRNA molecules
p:	number of protein molecules

$$\frac{dw(r,p,t)}{dt} = k_R\, w(r-1,p,t) + \gamma_R (r+1) w(r+1,p,t) + k_P\, r\, w(r,p-1,t)$$
$$+ \gamma_P (p+1)\, w(r,p+1,t) - [k_R + \gamma_R\, r + k_P\, r + \gamma_P\, p]\, w(r,p,t)$$

$$G(y,z,t) = \sum_{r,p=0}^{\infty} w(r,p,t)\, y^r z^p \qquad G(y=1,z=1,t) = \sum_{r,p=0}^{\infty} w(r,p,t) = 1$$

expressing the generating function in terms of the master equation

$$\frac{\partial G(y,z,t)}{\partial t} = G(y,z,t)\,[k_R\, y - k_R] + \frac{\partial G(y,z,t)}{\partial y}[\gamma_R + k_P\, yz - \gamma_R y - k_P y] + \frac{\partial G(y,z,t)}{\partial z}[\gamma_P - \gamma_P\, z]$$

Stochastic Processes:

simplest model aka "central dogma"

r: number of mRNA molecules
p: number of protein molecules

expressing the generating function in terms of the master equation

$$\frac{\partial G(y,z,t)}{\partial t} = G(y,z,t)\,[k_R\, y - k_R] + \frac{\partial G(y,z,t)}{\partial y}[\gamma_R + k_P\, yz - \gamma_R y - k_P y] + \frac{\partial G(y,z,t)}{\partial z}[\gamma_P - \gamma_P\, z]$$

in equilibrium $\frac{\partial G(y,z,t)}{\partial t} = 0$ and calculating the moments:

$$\left.\frac{\partial}{\partial y}G(y,z,t)\right|_{y=z=1} = \langle r \rangle$$

$$\left.\frac{\partial}{\partial z}G(y,z,t)\right|_{y=z=1} = \langle p \rangle$$

$$\begin{aligned}\left.\frac{\partial^2}{\partial z^2}G(y,z,t)\right|_{y=z=1} &= \sum_{r,p=0}^{\infty} \frac{\partial}{\partial z}\left.\left[p\, w(r,p,t)\, y^r\, z^{p-1}\right]\right|_{y=z=1} \\ &= \sum_{r,p=0}^{\infty} \left(p^2 - p\right)\, w(r,p,t) \\ &= \langle p^2 \rangle - \langle p \rangle\end{aligned}$$

$$\left.\frac{\partial^2}{\partial y^2}G(y,z,t)\right|_{y=z=1} = \langle r^2 \rangle - \langle r \rangle$$

$$\left.\frac{\partial^2}{\partial y \partial z}G(y,z,t)\right|_{y=z=1} = \langle rp \rangle$$

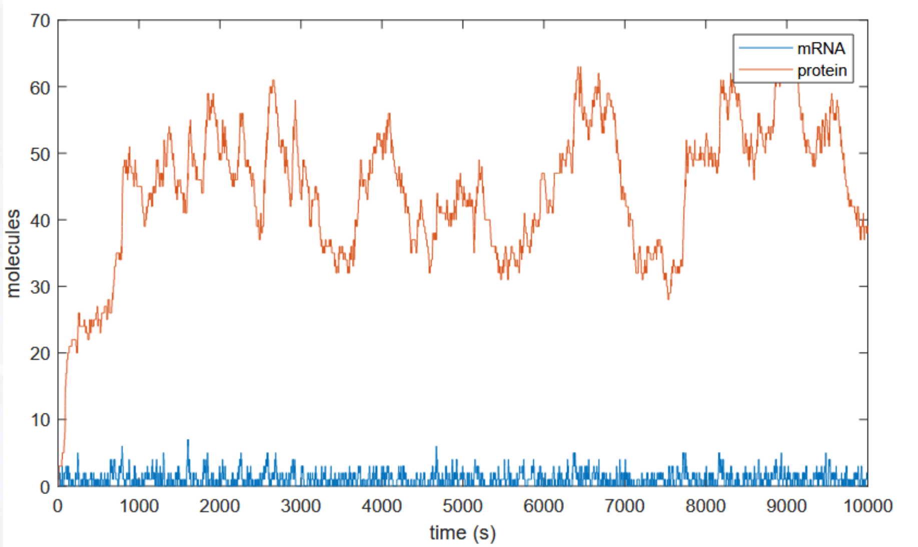
- Radioactive Decay
- Chem. Reactions
- Predator Prey
- **Gene Expression**

simplest model aka “central dogma”

r: **number of mRNA molecules**
p: **number of protein molecules**

in equilibrium $\frac{\partial G(y,z,t)}{\partial t} = 0$ and calculating the moments,
we find

$$\langle r\rangle = \frac{k_R}{\gamma_R} \qquad \langle p\rangle = \frac{k_P\, k_R}{\gamma_P\, \gamma_R} \qquad \sigma_r^2 = \langle r\rangle \qquad \langle pr\rangle = \frac{k_R\langle p\rangle + k_P\langle r\rangle\,(\langle r\rangle + 1)}{\gamma_R + \gamma_P} \qquad \sigma_p^2 = \frac{k_P}{\gamma_P}\langle pr\rangle + \langle p\rangle + \langle p\rangle^2$$



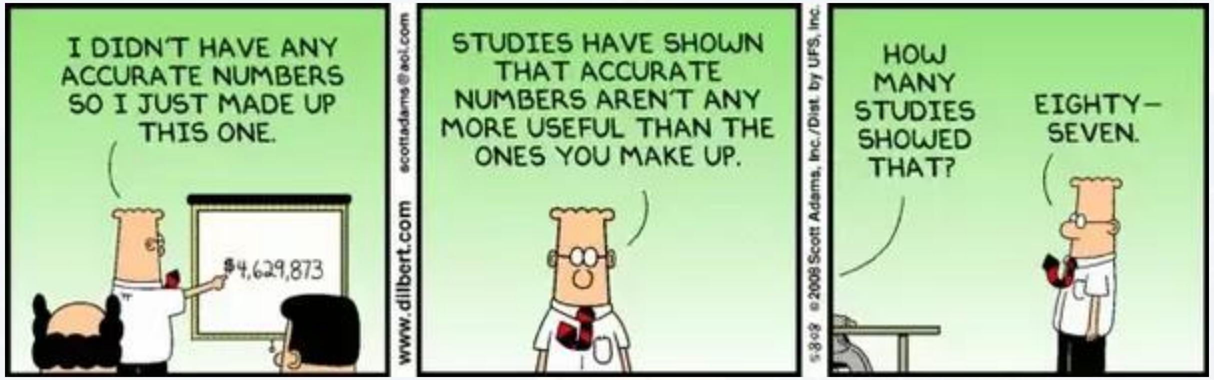
one mRNA molecule produces ≈ 50 protein molecules

We need a model for the expression noise in order to compare differential expression of different samples!

noise for r is poissonian, but not for p

$$\overbrace{\frac{\sigma_3^2}{\langle n_3\rangle^2}}^{\text{Total protein noise}} = \overbrace{\underbrace{\frac{1}{\langle n_3\rangle}}_{\text{Poisson}}}^{\text{From individual births and deaths}} + \overbrace{\underbrace{\frac{1}{\langle n_2\rangle}}_{\text{Poisson}}\underbrace{\frac{\tau_2}{\tau_3+\tau_2}}_{\text{One-step time-averaging}}}^{\text{From spontaneous mRNA noise}} + \overbrace{\underbrace{\frac{1-P_{\mathrm{on}}}{\langle n_1\rangle}}_{\text{Binomial}}\underbrace{\frac{\tau_2}{\tau_2+\tau_3}\,\frac{\tau_1}{\tau_1+\tau_3}\,\frac{\tau_1+\tau_3+\tau_1\tau_3/\tau_2}{\tau_1+\tau_2}}_{\text{Two-step time-averaging}}}^{\text{From forced mRNA noise, originating in gene activation-inactivation}}$$

actual model (Physics of Life Reviews 2 (2005) 157–175)



<u>Outline</u>

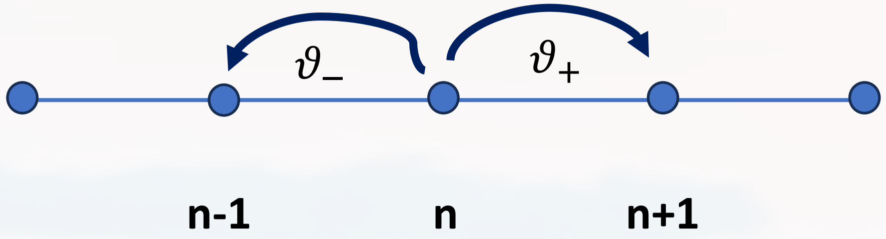
The Poissonian Stepper

Examples of Stochastic Processes
- Radioactive Decay
- Chem. Reactions
- Predator Prey
- Gene Expression

Diffusion Processes

Fokker-Planck Equation

Stochastic Processes:



$\boldsymbol{n}$:	**state**
$\boldsymbol{\vartheta_+}$:	**hopping rate n→ n+1**
$\boldsymbol{\vartheta_-}$:	**hopping rate n→ n-1**
c:	**concentration**
D:	**diffusion constant**

$$\frac{d}{dt}P(n,t) = \vartheta_+ P(n-1,t) + \vartheta_- P(n+1,t) - \vartheta_- P(n,t) - \vartheta_+ P(n,t)$$

in case $\vartheta_- = \vartheta_+ = \vartheta$

$$\frac{d}{dt}P(n,t) = \vartheta\, P(n-1,t) + \vartheta\, P(n+1,t) - 2\vartheta P(n,t)$$

$$= \vartheta[P(n-1,t) + P(n+1,t) - 2P(n,t)]$$

$$\left.\frac{d^2 f}{dx^2}\right|_{x=x_0} = \lim_{\Delta x \to 0} \frac{f(x_0+\Delta x) - 2f(x_0) + f(x_0-\Delta x)}{\Delta x^2}$$

$$\frac{\partial}{\partial t}P(n,t) = \vartheta \frac{\partial^2}{\partial n^2}P(n,t)$$

$$\frac{\partial}{\partial t}P(n,t) = \vartheta\, \Delta P(n,t)$$

$$\frac{\partial c(x,y,z,t)}{\partial t} = D\, \Delta c(x,y,z,t)$$

Fick's 2nd law

$$\frac{\partial c(x,y,z,t)}{\partial t} = D\,\Delta c(x,y,z,t)$$

Fick's 2nd law

$\boldsymbol{n}$:	**state**
$\boldsymbol{\vartheta_{+}}$:	**hopping rate n→ n+1**
$\boldsymbol{\vartheta_{-}}$:	**hopping rate n→ n-1**
c:	**concentration**
D:	**diffusion constant**

The Laplace operator indeed describes diffusion!

numerically:

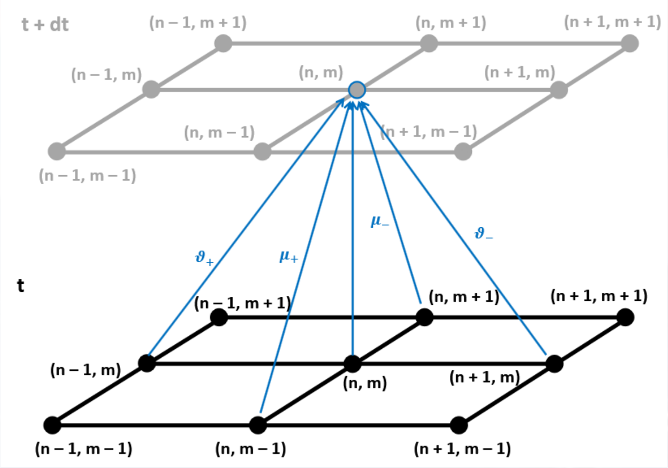
$$c(x_0, y_0, t_0 + \Delta t) =$$

We can calculate c in the ***future***

$$2\Delta t D\left[\frac{c(x_0 + \Delta x,\ y_0, t_0)\ - 2c(x_0,\ y_0, t_0) + c(x_0 -\ \Delta x,\ y_0, t_0)}{\Delta x^2} + \right.$$

$$\left.\frac{c(x_0,\ y_0 +\ \Delta y, t_0)\ - 2c(x_0,\ y_0\ , t_0) + c(x_0,\ y_0 +\ \Delta y, t_0)}{\Delta y^2}\right]$$

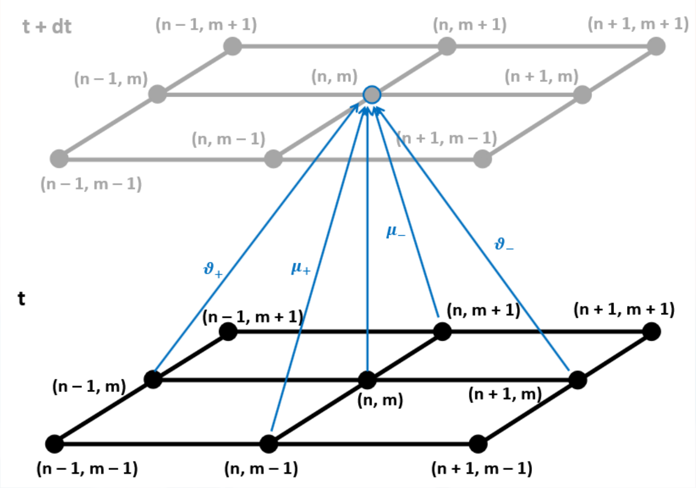
$$+\ c(x_0, y_0, t_0 -\ \Delta t)$$



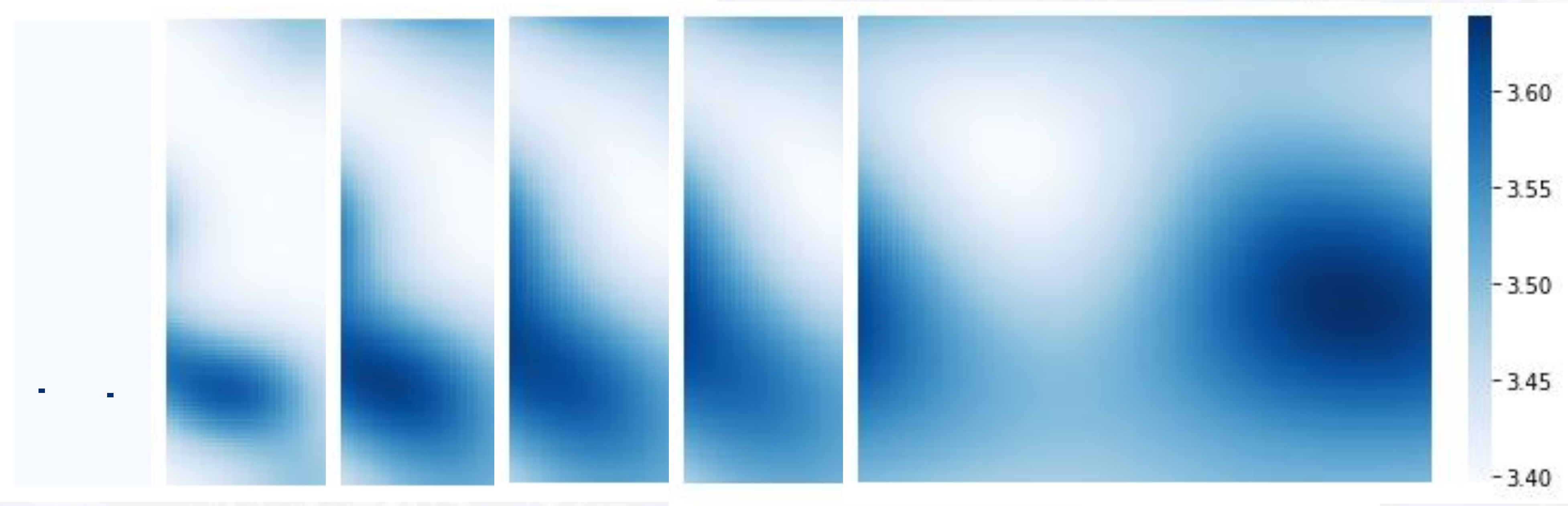
by using all adjacent ***current*** values

and the immediate ***past*** value

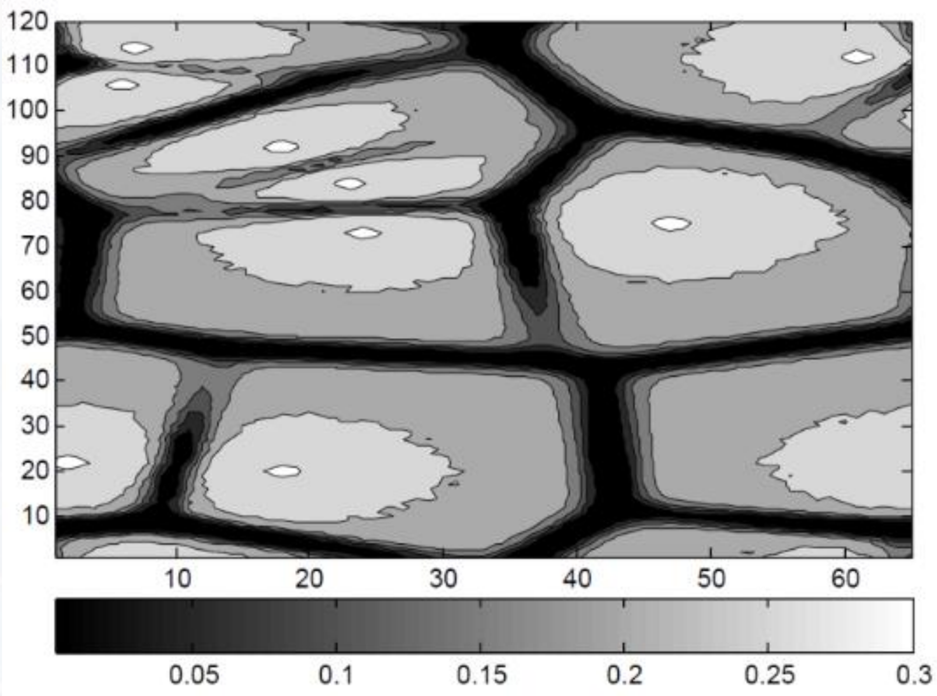
Stochastic Processes:

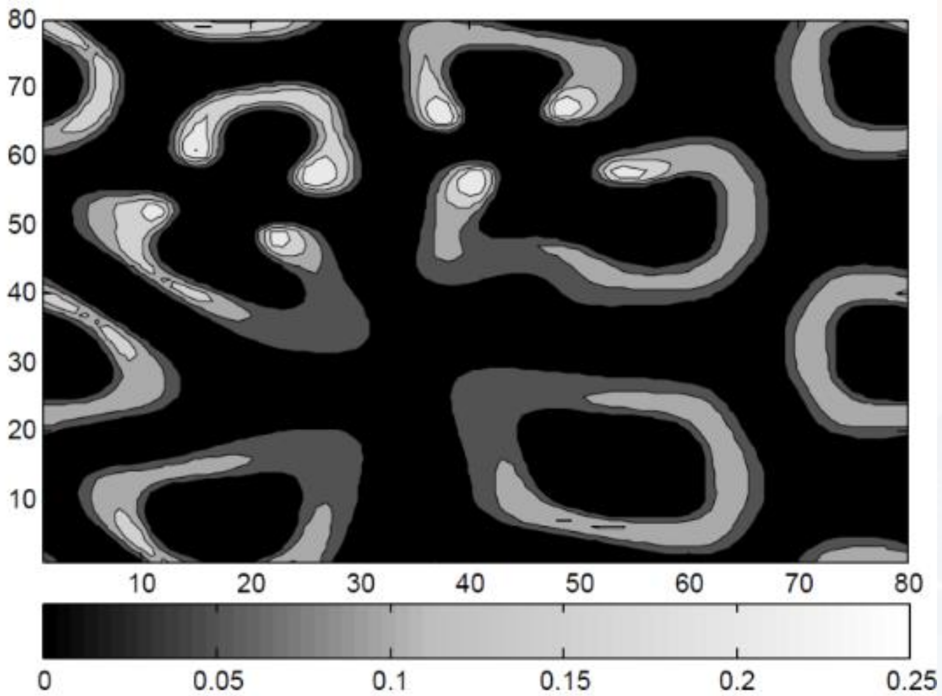


initial condition

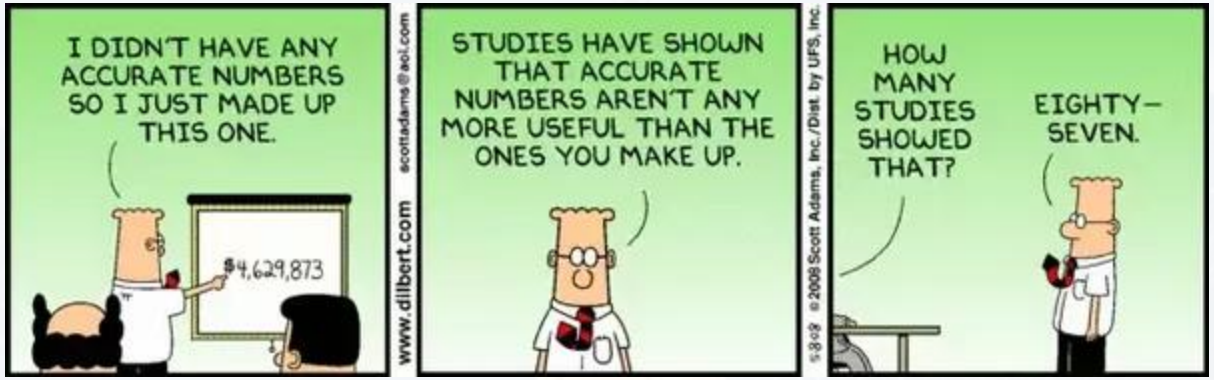


modelling fur and skin pattern:





Outline



The Poissonian Stepper

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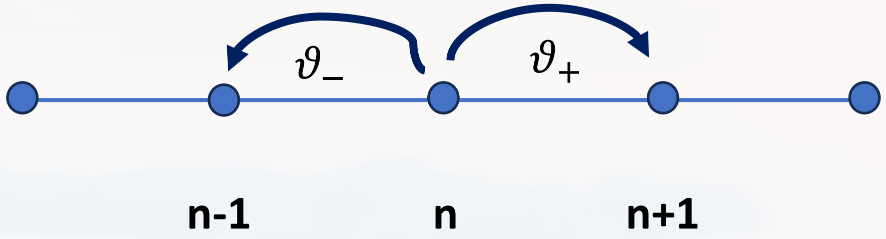
Diffusion Processes

Fokker-Planck Equation



$\boldsymbol{n}$:	state
$\boldsymbol{\vartheta_+}$:	hopping rate n→ n+1
$\boldsymbol{\vartheta_-}$:	hopping rate n→ n-1
c:	concentration
D:	diffusion constant

$$\frac{d}{dt}P(n,t) = \vartheta_+\, P(n-1,t) \; + \vartheta_-\, P(n+1,t) \; - \vartheta_-\, P(n,t) \; - \vartheta_+\, P(n,t)$$

$$\frac{d}{dt}P(n,t) = -\frac{\vartheta_+ - \vartheta_-}{2}[P(n+1,t) - P(n-1,t)] \; + \frac{\vartheta_+ + \vartheta_-}{2}[P(n+1,t) \; + \; P(n-1,t) \; - \; 2P(n,t)]$$

$$\frac{\partial}{\partial t}P(n,t) = -\frac{\vartheta_+ - \vartheta_-}{2}\frac{\partial}{\partial n}P(n,t) + \frac{\vartheta_+ + \vartheta_-}{2}\frac{\partial^2}{\partial n^2}P(n,t)$$

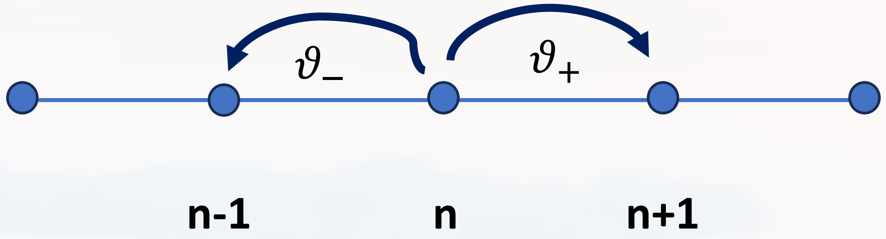
drift term with $v = \frac{\vartheta_+ - \vartheta_-}{2}$

diffusion term as before

$$\frac{\partial c(x,y,z,t)}{\partial t} = -\vec{v}\cdot grad\; c(x,y,z,t) \; + D\, \Delta c(x,y,z,t)$$

Smoluchowski equation

Stochastic Processes:



n:	state
ϑ_+:	hopping rate n→ n+1
ϑ_-:	hopping rate n→ n-1
c:	concentration
D:	diffusion constant

$$\frac{\partial}{\partial t}P(n,t) = -\frac{\vartheta_+ - \vartheta_-}{2}\frac{\partial}{\partial n}P(n,t) + \frac{\vartheta_+ + \vartheta_-}{2}\frac{\partial^2}{\partial n^2}P(n,t)$$

$$\frac{\partial c(x,y,z,t)}{\partial t} = -\vec{v}\cdot grad\ c(x,y,z,t) + D\,\Delta c(x,y,z,t)$$

Smoluchowski equation

both, ϑ_+ and ϑ_- can be functions of *n*, hence of *x*

$$\frac{\partial P(\vec{x},t)}{\partial t} = -\sum_{i=1}^{N}\frac{\partial}{\partial x_i}\left[v_i(\vec{x},t)P(\vec{x},t)\right] + \sum_{i=1}^{N}\sum_{j=1}^{N}\frac{\partial^2}{\partial x_i \partial x_j}\left[D_{ij}(\vec{x},t)P(\vec{x},t)\right]$$

Fokker-Planck equation

$$i\hbar\frac{\partial\Psi(\vec{x},t)}{\partial t} = \left[\frac{-\hbar^2}{2m}\Delta + V(\vec{x},t)\right]\Psi(\vec{x},t)$$

Schrödinger equation

Thank you very much for your attention!