# Lecture 7b:

# **Stochastic Processes**



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Bayesian Data Analysis and Machine Learning for Physical Sciences



# Berkeley Bayesian Data Analysis and Machine Learning for Physical Sciences

Course Map	Module 1	Maximum Entropy and Information, Bayes Theorem
	Module 2	Naive Bayes, Bayesian Parameter Estimation, MAP
	Module 3	MLE, Lin Regression
	Module 4	Model selection I: Comparing Distributions
	Module 5	Model Selection II: Bayesian Signal Detection
	Module 6	Variational Bayes, Expectation Maximization
	Module 7	Hidden Markov Models, Stochastic Processes
	Module 8	Monte Carlo Methods
	Module 9	Machine Learning Overview, Supervised Methods
	Module 10	Unsupervised Methods
	Module 11	ANN: Perceptron, Backpropagation
	Module 12	ANN: Basic Architecture, Regression vs Classification, Backpropagation again
	Module 13	Convolution and Image Classification and Segmentation
	Module 14	Graphs and GNNs
	Module 15	RNNs and LSTMs
	Module 16	Transformer and LLMs

#### <u>Outline</u>

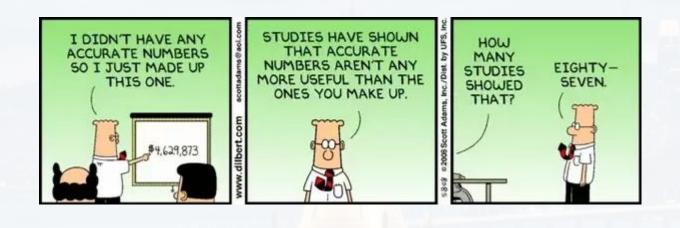
#### The Poissonian Stepper

### **Examples of Stochastic Processes**

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

**Diffusion Processes** 

**Fokker-Planck Equation** 



#### **Outline**

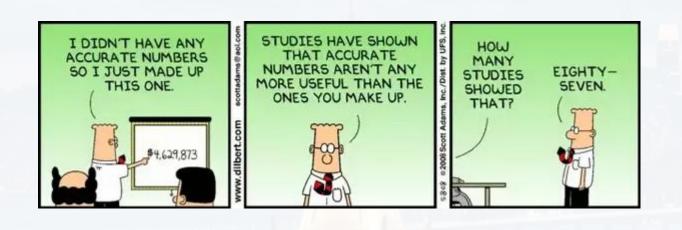
#### The Poissonian Stepper



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

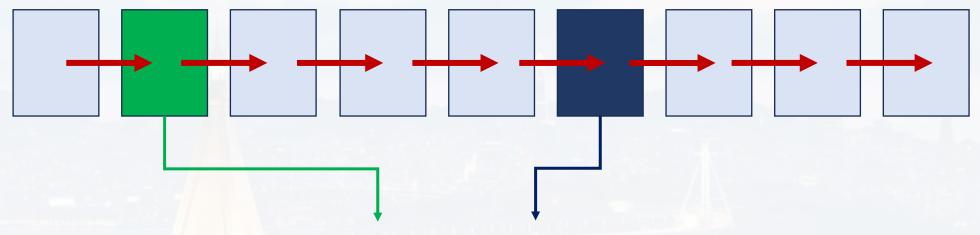
**Diffusion Processes** 

**Fokker-Planck Equation** 



HMM: sequence of states

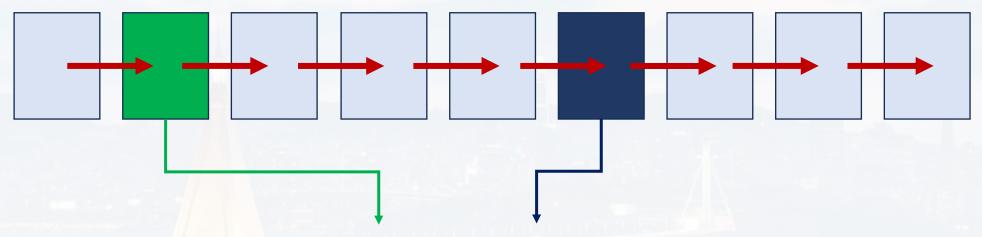
#### set of different states/classes



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

HMM: sequence of states

#### set of different states/classes

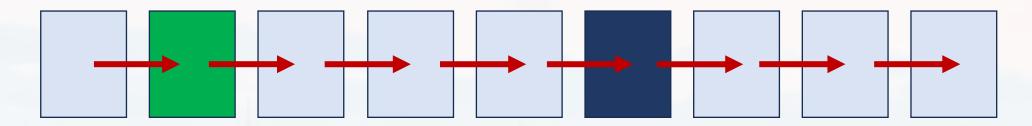


a set of T observations  $O = (O_1, O_2, O_3, \dots O_t, \dots O_T)$  drawing randomly from the states

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!

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

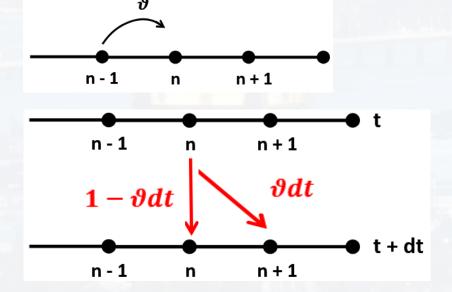


*n*: different states

 $\vartheta$ : hopping rate

- for now:  $\theta = const$ 

 $-[\vartheta] = probability/time$ 



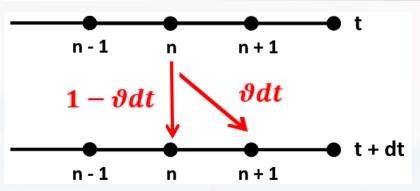
assumption:

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





 $\vartheta$ : hopping rate (probability/time)

dt: time increment

$$P(n, t + dt)$$
:

probability that we observe the system in state n at time t+dt

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

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

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

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

**Master Equation** 



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

**Master Equation** 

different states n:

θ: hopping rate (*probability/time*)

dt: time increment

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



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

#### **Master Equation**

n: ϑ:

different states hopping rate (probability/time)

**dt**: time increment

**goal:** find P(n, t)

P(n, t + dt):

probability that we observe the system in state n at time t+dt

real-valued moment-generating function

$$G(z,t) = \sum_{n=0}^{\infty} P(n,t) z^n$$
  $k^{th}$  moment:  $\frac{\partial^k G(z,t)}{\partial z^k} \bigg|_{z=1}$ 

for now, states only change from 
$$n o n + 1$$

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

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

both sums have independent indices

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



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

**Master Equation** 

different states n: θ:

hopping rate (probability/time) dt: time increment

**goal:** find P(n, t)

P(n, t + dt):

probability that we observe the system in state n at time t + dt

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

$$\frac{d}{dt}G(z,t) = \sum_{n=0}^{\infty} \frac{dP(n,t)}{dt} z^n = \sum_{m=0}^{\infty} v P(m,t) z^{m+1} - \sum_{n=0}^{\infty} v P(n,t) z^n$$

both sums have independent indices

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

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

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

#### **Master Equation**

different states n: θ: hopping rate (*probability/time*)

dt: time increment

**goal:** find P(n, t)

P(n,t+dt):

probability that we observe the system in state n at time t + dt

real-valued moment-generating function

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  $k^{th}$  moment:  $\frac{\partial^k G(z,t)}{\partial z^k} \bigg|_{z=1}$ 

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

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

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

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

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

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

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

Taylor Series of  $e^{vzt}$  wrt to z

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

**Master Equation** 

different states n:

θ: hopping rate (*probability/time*)

dt: time increment

**goal:** find P(n, t)

P(n, t + dt):

probability that we observe the system in state n at time t + dt

real-valued moment-generating function

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

$$G(z,t) = \sum_{n=0}^{\infty} P(n,t) z^n$$
  $k^{th}$  moment:  $\frac{\partial^k G(z,t)}{\partial z^k} \bigg|_{z=1}$ 

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

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

$$G(z,t) = e^{\nu(z-1)t}$$
  $e^{-\nu t}e^{\nu zt} = \sum_{n=0}^{\infty} P(n,t) z^n$  Taylor Series of  $e^{\nu zt}$  wrt to  $z$ 

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

$$P(n,t) = \frac{(vt)^n}{n!}e^{-vt}$$
 Poissonian distribution

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

**Master Equation** 

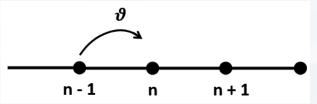
different states n: **ϑ**: hopping rate (*probability/time*) dt: time increment

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

P(n, t + dt):

probability that we observe the system in state n at time t + dt

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



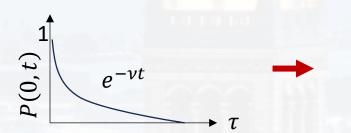
calculating the **waiting time** (time  $\tau$  between two events)

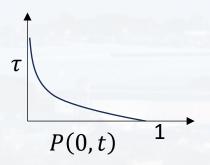
$$P(0,t) = \frac{(vt)^0}{0!} e^{-vt} \qquad \tau = -\frac{1}{v} ln[P(0,t)]$$

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

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

is the probability that the stepper has not moved  $\rightarrow$  cdf





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

see later, Gillespie algorithm



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

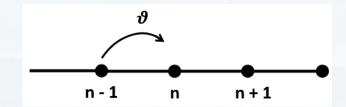
#### **Master Equation**

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

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

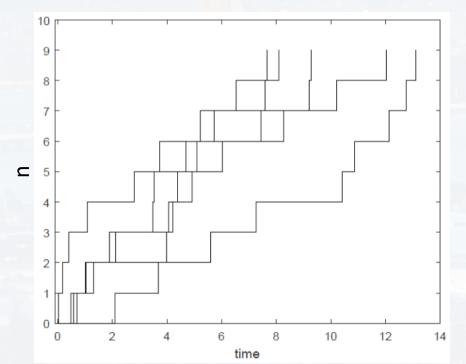
$$P(n, t + dt)$$
:

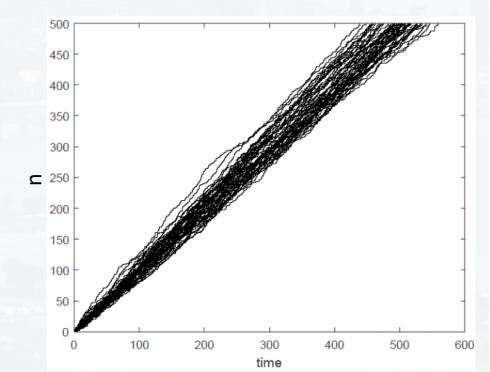
probability that we observe the system in state n at time t+dt



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

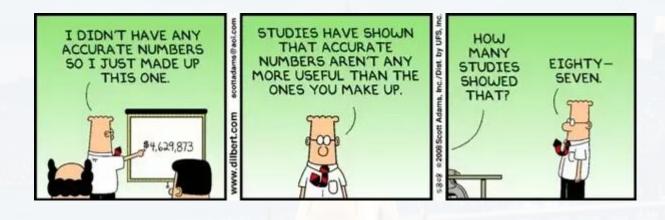
for now, states only change from n o n+1





#### <u>Outline</u>

**The Poissonian Stepper** 



#### **Examples of Stochastic Processes**

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

**Diffusion Processes** 

**Fokker-Planck Equation** 



#### - Radioactive Decay

Chem. Reactions
Predator Prey
Gene Expression

$$A \overset{k}{\to} \emptyset$$

*n*: different states

 $\vartheta$ : hopping rate (probability/time)

dt: time increment

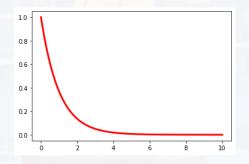
deterministic scenario:

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

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



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



#### - Radioactive Decay

Chem. Reactions
Predator Prey
Gene Expression

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

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

t

\_\_\_\_

 for t = 0 many atoms  $\rightarrow \tau$  is small

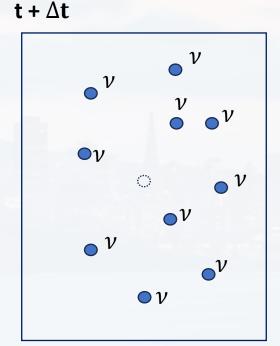
 $\Delta \mathbf{t}$ 

**each** atom has the probability  $\nu$  to decay per time

logical  $or \rightarrow adding$  the probabilities

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

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



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

**Master Equation** 

path leading from n+1, part to state n within dt fr

path leading away from state n



initial conditions:

### Berkeley Stochastic Processes:

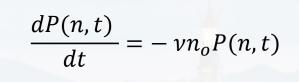
#### - Radioactive Decay

stochastic scenario:

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

#### **Master Equation**

 $A(t) = A_0 e^{-kt}$ 

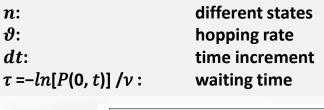


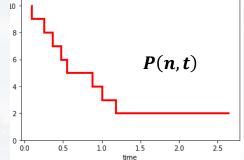
$$P(n_o, t) = e^{-\nu n_o t} \qquad P(n_o, t) = 1$$

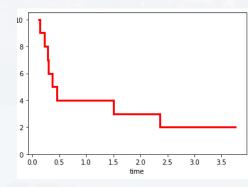
solving for P(n, t) using the initial conditions, the master equation and  $G(z,t) = \sum_{n=0}^{\infty} P(n,t) z^n$  leads to:

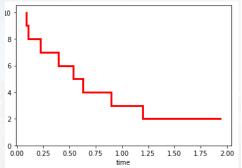
$$P(n,t) = e^{-\nu n_o t} \binom{n_o}{n} [1 - e^{-\nu t}]^{n_o - n}$$

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











#### - Radioactive Decay

stochastic scenario:

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

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

**Master Equation** 

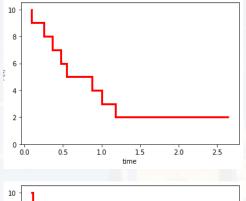
dt:

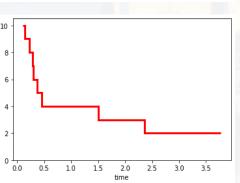
n:

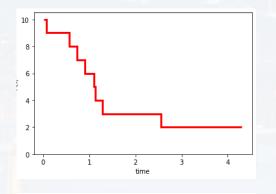
θ:

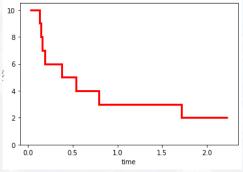
different states hopping rate time increment

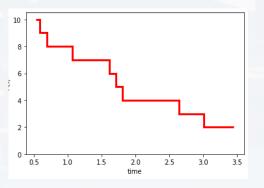
 $\tau = -ln[P(\mathbf{0}, t)] / \nu$ : waiting time

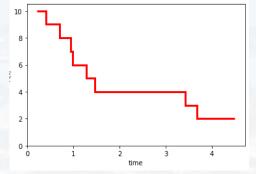


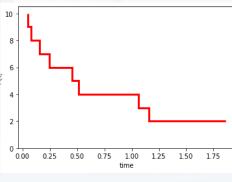


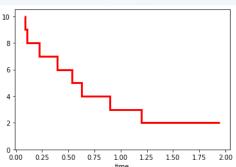














#### - Radioactive Decay

Chem. Reactions
Predator Prey
Gene Expression

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

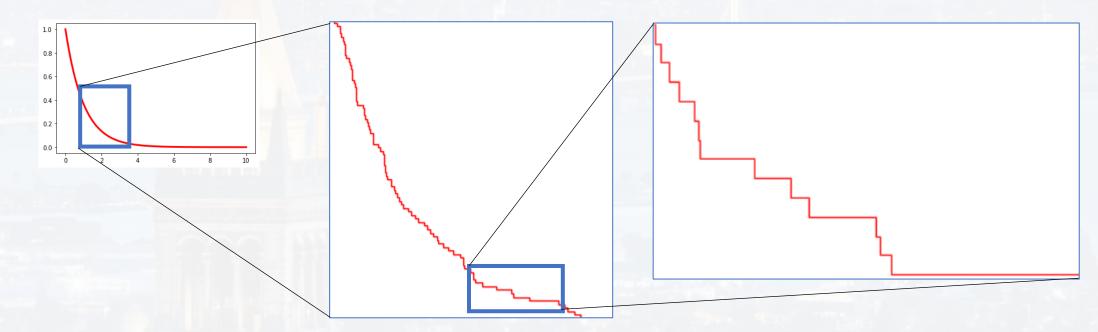
$$\frac{dP(n,t)}{dt} = \nu [n+1]P(n+1,t) - \nu n P(n,t)$$

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

n:different states $\vartheta$ :hopping ratedt:time increment $\tau = -ln[P(0, t)] / v$ :waiting time

Master Equation

one run, but large n



- Chem. Reactions

number of particles of A n: number of particles of B m:

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

$$\nu(A) \rightarrow \nu_+ n(t)$$

$$\nu(A) \rightarrow \nu_+ n(t) \qquad \nu(B) \rightarrow \nu_- m(t)$$

$$v_{tot} = v(A) + v(B) = v_{+} n(t) + v_{-} m(t)$$

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

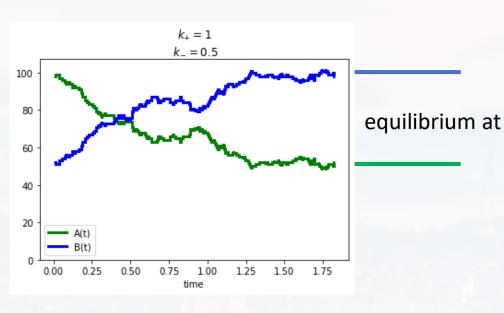
time that elapses until a reaction to occurs

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

$$\nu_{+}$$
  $\nu_{-}$   $n,m$   $\nu_{-}$   $n+1, m-1$ 

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

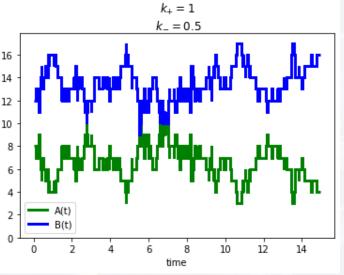
- Chem. Reactions

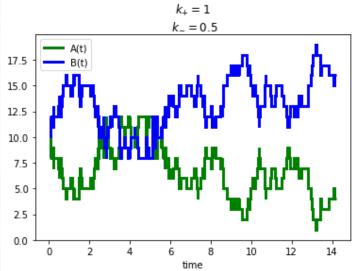


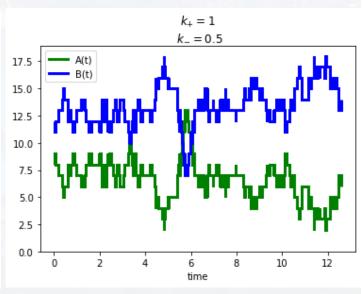
n: dt:  $\tau = -ln[P(\mathbf{0}, t)] / \nu$ :

different states hopping rate time increment waiting time

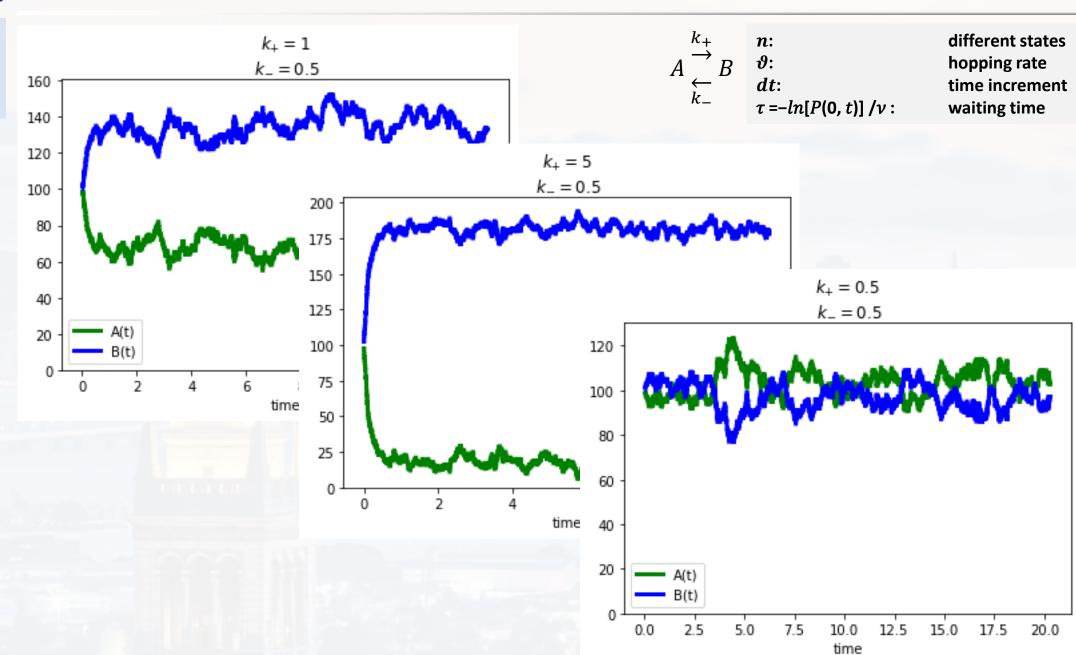
N = 10







- Chem. Reactions





- Predator Prey

L: sheep (lambs)

W: wolfs

E: "empty"

 $A \overset{k}{\underset{k}{\leftarrow}}$ 

n 19

dt

 $\tau = -ln[P(\mathbf{0}, t)] / v$ :

different states hopping rate time increment waiting time

original model:

$$L + E \stackrel{k_1}{\rightarrow} L + L$$

 $W \stackrel{k_2}{\to} E$ 

$$W + L \stackrel{k_3}{\to} W + W$$

$$W + L \stackrel{k_4}{\rightarrow} W + E$$

lambs reproduce

wolfs starve

sometimes a wolf kills a lamb and then reproduces

sometimes a wolf just kills a lamb

same:

$$L\stackrel{k_1}{\longrightarrow} 2\,L$$

$$L+W\stackrel{k_2}{\longrightarrow} 2\,W$$

$$W \stackrel{k_3}{\longrightarrow} \Phi$$



- Predator Prey

L: sheep (lambs)

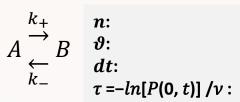
W: wolfs

E: "empty"

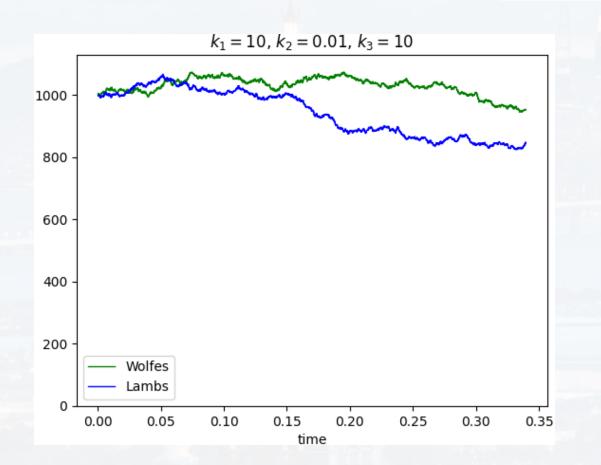
$$L\stackrel{k_1}{\longrightarrow} 2\,L$$

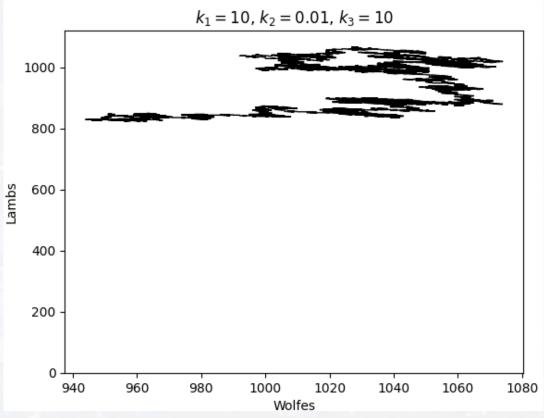
$$L+W\stackrel{k_2}{\longrightarrow} 2\,W$$

$$W\stackrel{k_3}{\longrightarrow} \Phi$$



different states hopping rate time increment waiting time





- Predator Prey

L: sheep (lambs)

W: wolfs

E: "empty"

$$L\stackrel{k_1}{\longrightarrow} 2\,L$$

$$L+W\stackrel{k_2}{\longrightarrow} 2\,W$$

$$W\stackrel{k_3}{\longrightarrow} \Phi$$

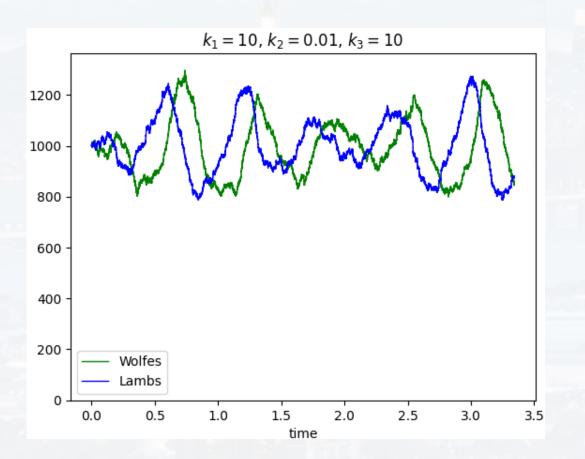
$$A \stackrel{k_+}{\rightarrow} B$$

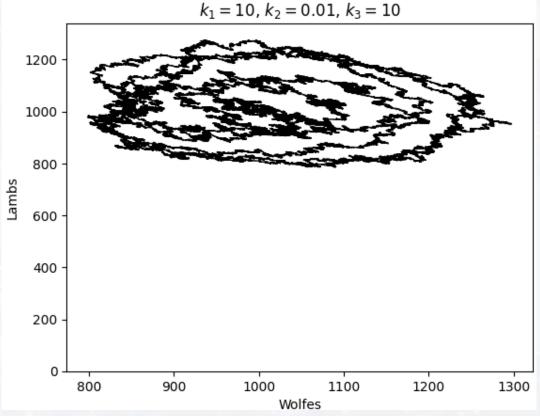
n:

θ:

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

different states hopping rate time increment waiting time







- Predator Prey

L: sheep (lambs)

W: wolfs

E: "empty"

$$L\stackrel{k_1}{\longrightarrow} 2\,L$$

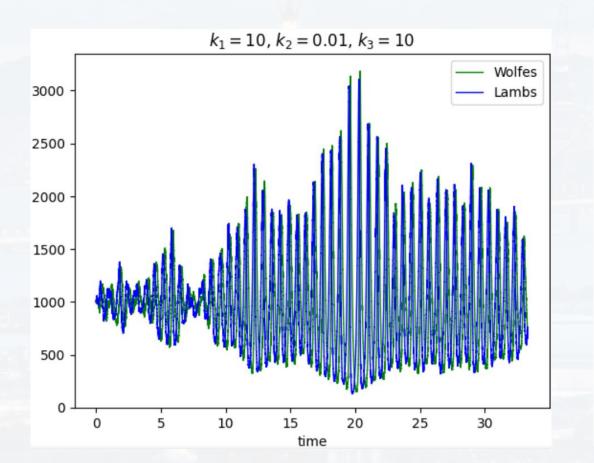
$$L+W\stackrel{k_2}{\longrightarrow} 2\,W$$

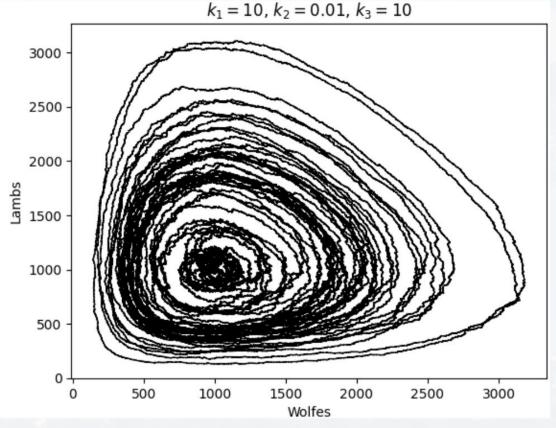
$$W \stackrel{k_3}{\longrightarrow} \Phi$$

$$A \xrightarrow{k_{+}} B \xrightarrow{n:} \theta:$$

$$\leftarrow k_{-} B \xrightarrow{dt:} \tau = -ln[P(0, t)] / v:$$

different states hopping rate time increment waiting time

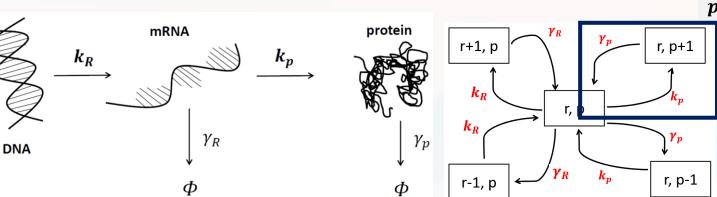




- Radioactive Decay - Chem. Reactions

- Gene Expression

simplest model aka "central dogma"



number of mRNA molecules number of protein molecules

r:

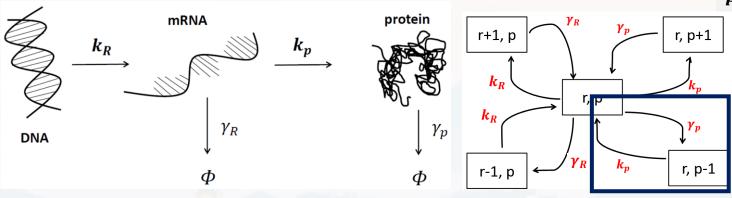
$$\frac{dw(r,p,t)}{dt} = \gamma_P (p+1)w(r,p+1,t) - k_p r w(r,p,t)$$

- Radioactive Decay - Chem. Reactions

- Gene Expression

simplest model aka "central dogma"

r: number of mRNA moleculesp: number of protein molecules



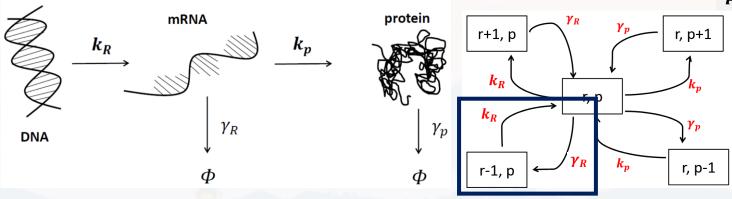
$$\frac{dw(r, p, t)}{dt} = \gamma_P (p+1)w(r, p+1, t) - k_p r w(r, p, t) + k_p r w(r, p-1, t) - \gamma_P p w(r, p, t)$$

- Radioactive Decay - Chem. Reactions

- Gene Expression

simplest model aka "central dogma"

r: number of mRNA moleculesp: number of protein molecules



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

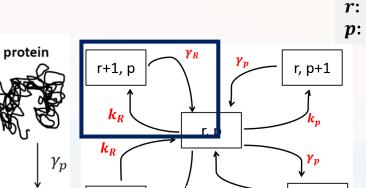
$$+ k_p r w(r, p-1, t) - \gamma_P p w(r, p, t)$$

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

- Radioactive Decay - Chem. Reactions

- Gene Expression

simplest model aka "central dogma"



r, p-1

number of mRNA molecules number of protein molecules

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

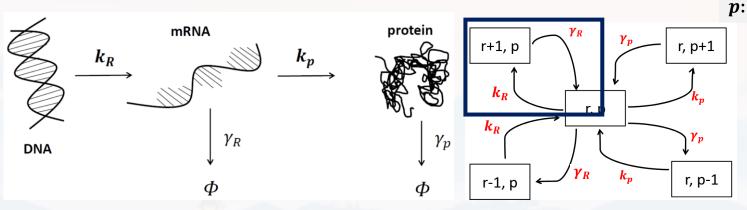
- Radioactive Decay - Chem. Reactions

- Gene Expression

simplest model aka "central dogma"



number of mRNA molecules number of protein molecules



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

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

- Radioactive Decay - Chem. Reactions - Predator Prev

- Gene Expression

simplest model aka "central dogma"

r: number of mRNA moleculesp: 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

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

- Radioactive Decay
- Chem. Reactions
- Predator Prev

- Gene Expression

simplest model aka "central dogma"

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

expressing the generating function in terms of the master equation

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

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

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

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

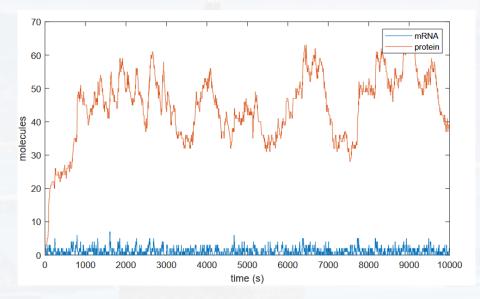
- Gene Expression

simplest model aka "central dogma"

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

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!

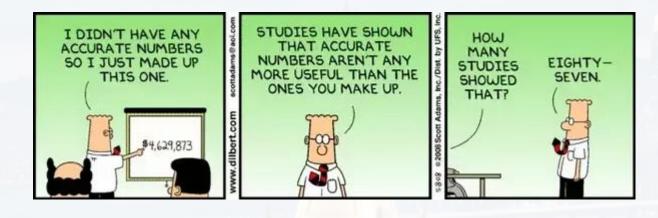
noise for r is poissonian, but not for p

Total protein noise
$$\frac{\sigma_3^2}{\langle n_3 \rangle^2} = \underbrace{\frac{1}{\langle n_3 \rangle}}_{\text{Poisson}} + \underbrace{\frac{1}{\langle n_2 \rangle}}_{\text{Poisson}} \underbrace{\frac{\tau_2}{\tau_3 + \tau_2}}_{\text{Poisson}} + \underbrace{\frac{1}{\langle n_2 \rangle}}_{\text{Poisson}} \underbrace{\frac{\tau_2}{\tau_3 + \tau_2}}_{\text{Poisson}} + \underbrace{\frac{1}{\langle n_2 \rangle}}_{\text{Binomal}} \underbrace{\frac{\tau_2}{\tau_2 + \tau_3}}_{\text{Binomal}} \underbrace{\frac{\tau_1}{\tau_1 + \tau_3}}_{\text{Two-step}} \underbrace{\frac{\tau_1}{\tau_1 + \tau_2}}_{\text{time-averaging}} = \mathbf{a}_{\text{time-averaging}}$$

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

#### <u>Outline</u>

**The Poissonian Stepper** 



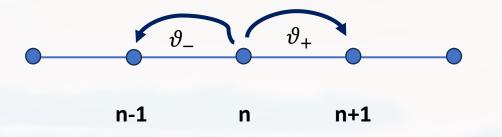
**Examples of Stochastic Processes** 

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

**Diffusion Processes** 

**Fokker-Planck Equation** 





n: state
 ϑ<sub>+</sub>: hopping rate n→ n+1
 ϑ<sub>-</sub>: 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  $\vartheta_{-} = \vartheta_{+} = \vartheta$ 

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

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

$$\frac{d^2 f}{dx^2} \bigg|_{x=x_0} = \lim_{\Delta x \to 0} \frac{f(x_0 + \Delta x) - 2f(x_0) + f(x_0 - \Delta x)}{\Delta x^2} \qquad \frac{\partial}{\partial t} P(n, t) = \vartheta \frac{\partial^2}{\partial n^2} P(n, t)$$

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

$$\frac{\partial c(x, y, z, t)}{\partial t} = D \Delta c(x, y, z, t)$$
 Fick's 2<sup>nd</sup> law

diffusion constant

$$\frac{\partial c(x, y, z, t)}{\partial t} = D \Delta c(x, y, z, t)$$
 Fick's 2<sup>nd</sup> law

The Laplace operator indeed describes diffusion!

numerically:

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

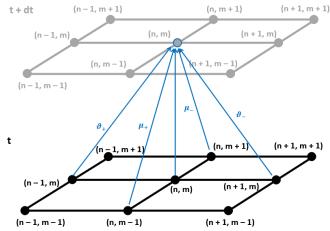
We can calculate *c* in the *future* 

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

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

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

n:state $\vartheta_+$ :hopping rate  $n \rightarrow n+1$  $\vartheta_-$ :hopping rate  $n \rightarrow n-1$ c:concentration

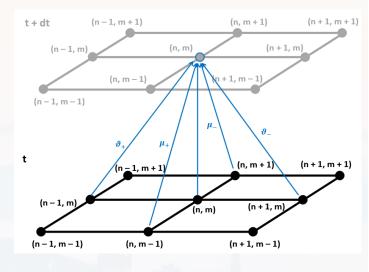


by using all adjacent current values

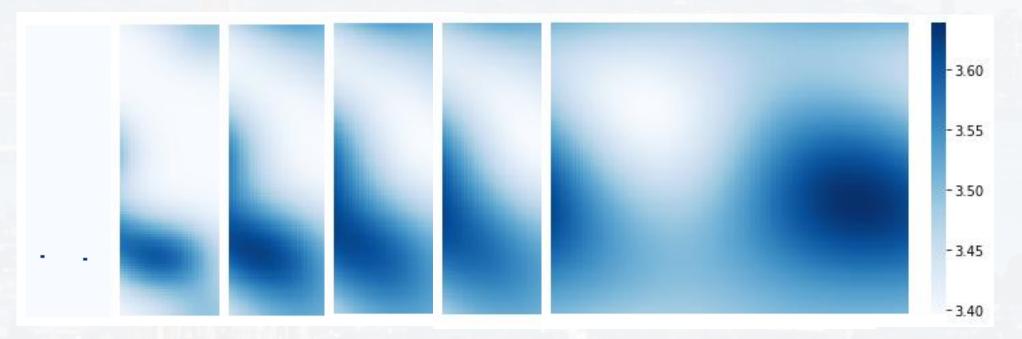
D:

and the immediate *past* value

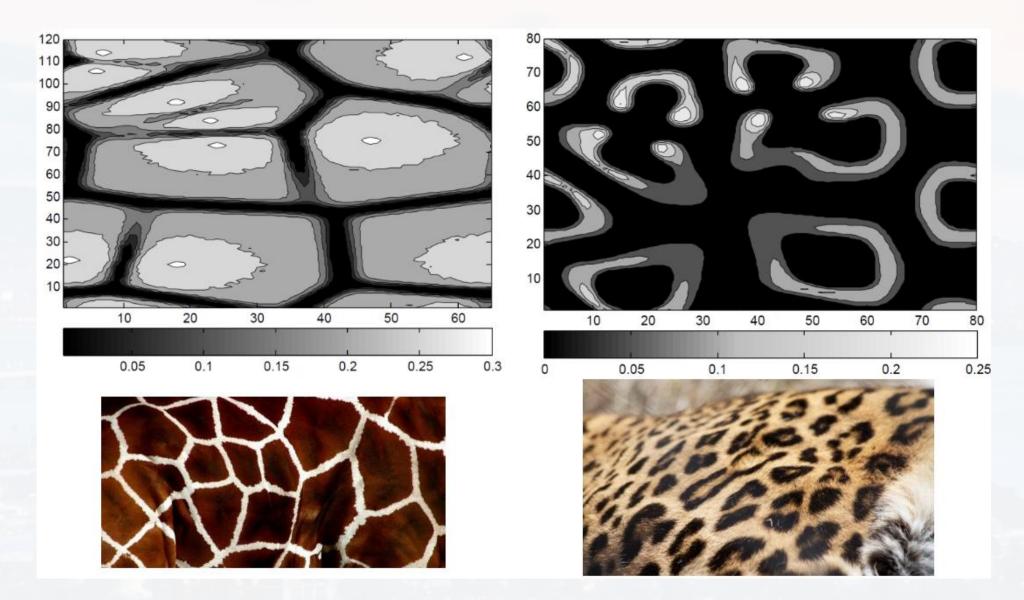




#### initial condition



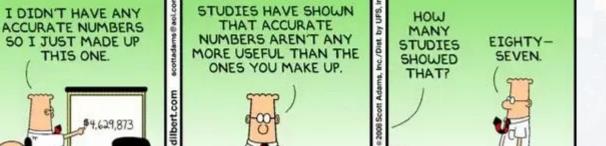
#### modelling fur and skin pattern:



THIS ONE.

#### <u>Outline</u>

**The Poissonian Stepper** 

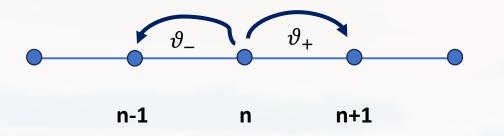


**Examples of Stochastic Processes** 

**Diffusion Processes** 

**Fokker-Planck Equation** 





state n:

 $\vartheta_+$ : hopping rate  $n \rightarrow n+1$ 

hopping rate  $n \rightarrow n-1$ 

c: concentration

D: diffusion constant

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

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

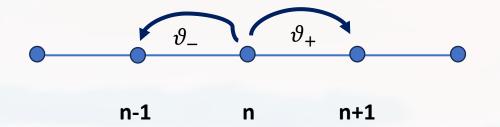
$$\frac{\partial}{\partial t}P(n,t) = -\frac{\vartheta_{+} - \vartheta_{-}}{2}\frac{\partial}{\partial n}P(n,t) + \frac{\vartheta_{+} + \vartheta_{-}}{2}\frac{\partial^{2}}{\partial n^{2}}P(n,t)$$

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** 





$$n$$
:state $\vartheta_+$ :hopping rate  $n \rightarrow n+1$  $\vartheta_-$ :hopping rate  $n \rightarrow n-1$ c:concentration

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

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

Smoluchowski equation

both,  $\vartheta_+$  and  $\vartheta_-$  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!

