Theory and Simulation of individual based models

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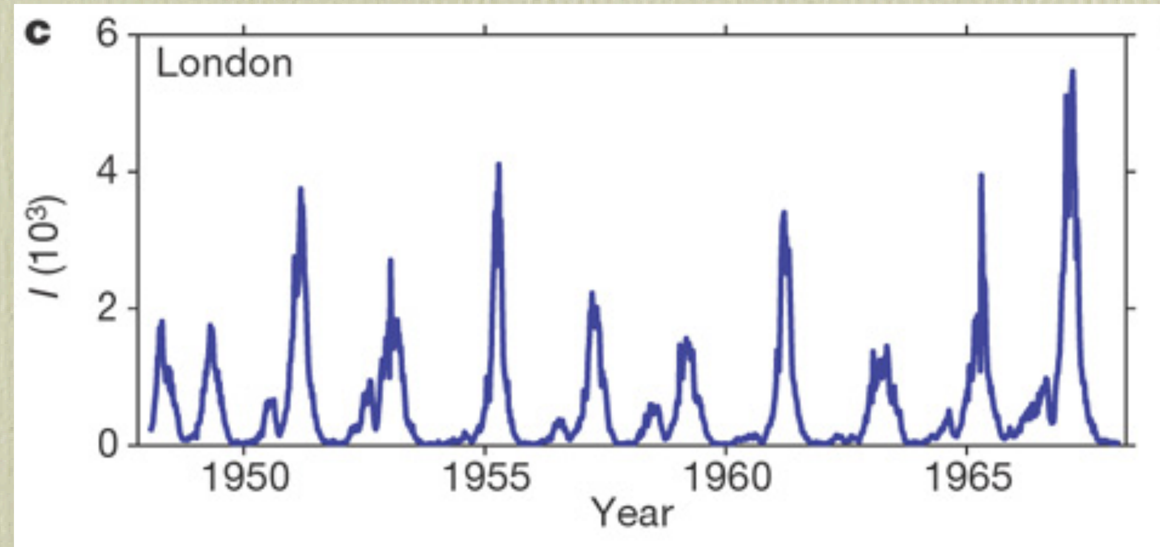
Motivation: what is noise?

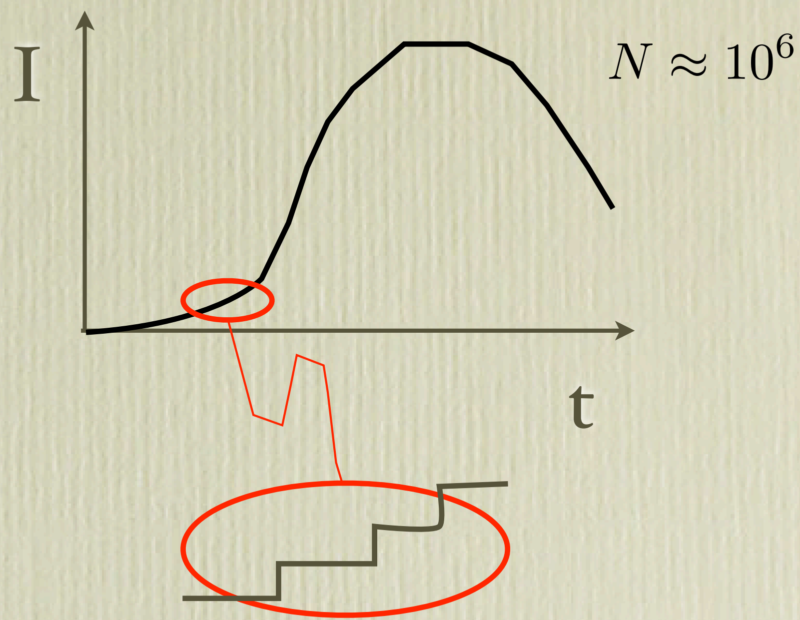
Data:



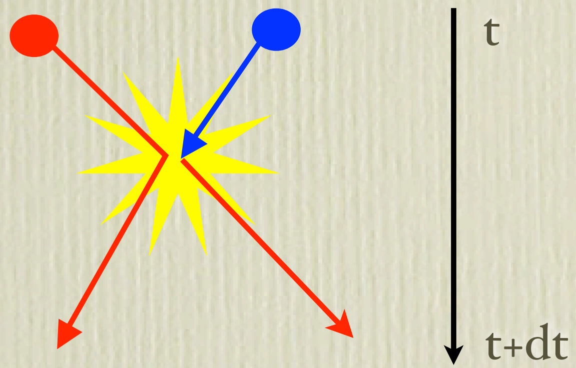
= SI model: $\frac{dI}{dt} = \beta S \frac{I}{N} - \gamma I$ + f(t) + “noise”

Demographic noise

- SI model
$$\frac{dI}{dt} = \beta S \frac{I}{N} - \gamma I$$
means
$$dI = \beta S \frac{I}{N} dt - \gamma I dt$$
but dI = 0,1,2, ...

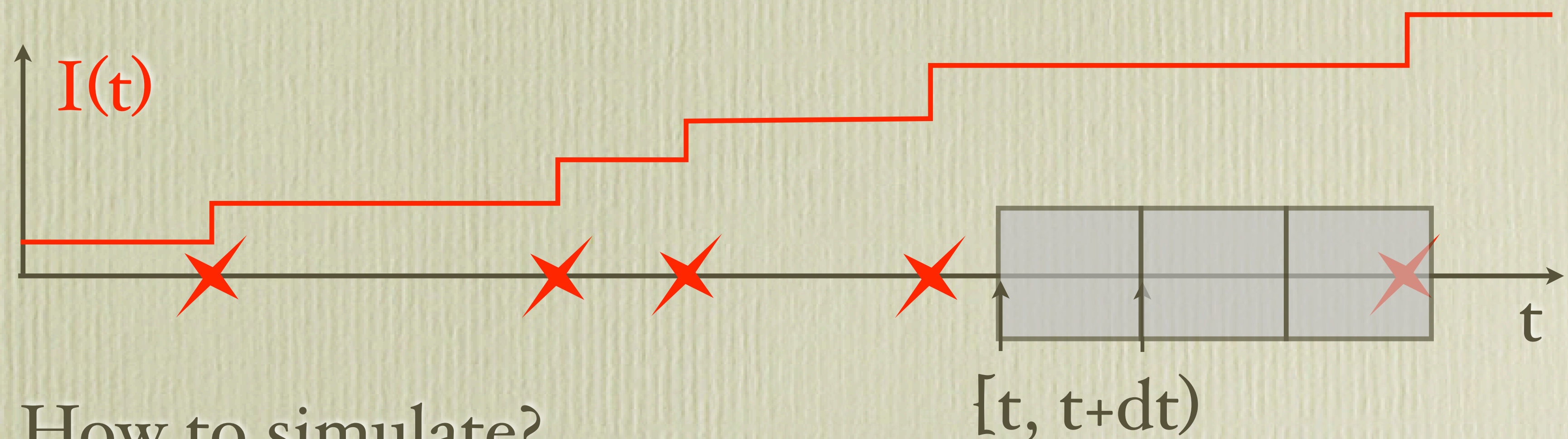


- What is going on at microscopic scale?
Gas of individuals randomly bumping into each other and transmitting the disease



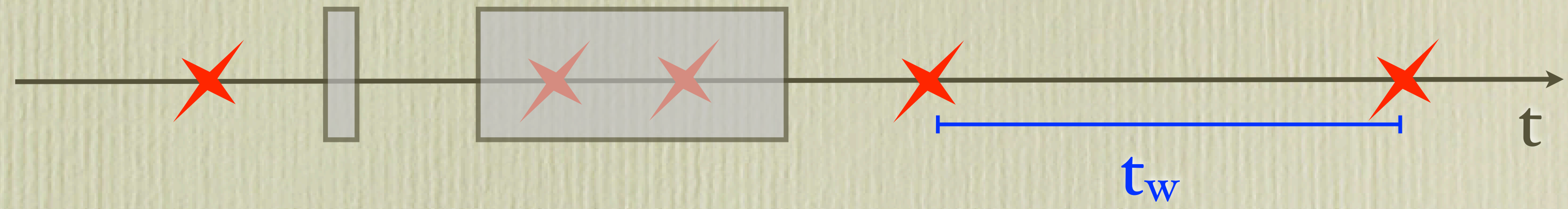
Simplest case: Poisson process

- Infection ($I \to I+1$) event occurs in any interval $[t, t+dt)$ independently with probability $r dt$ ($r>0$)



- How to simulate?
  1 fix dt small
  2 draw a uniform random variable X=`rand()`
  3 event occurs in $[t, t+dt)$ if $X<rdt$
  4 advance time $t \to t+dt$, go back to 2

This is ok in theory but in practice...



- If dt is too large more than one event can occur in [t, t+dt) → dt has to be small
- If dt is very small, most of the time there is no event in [t, t+dt). Simulation is very slow!
- Can we find a more clever way to simulate?
- How much should I wait for the next event?

Waiting time distribution

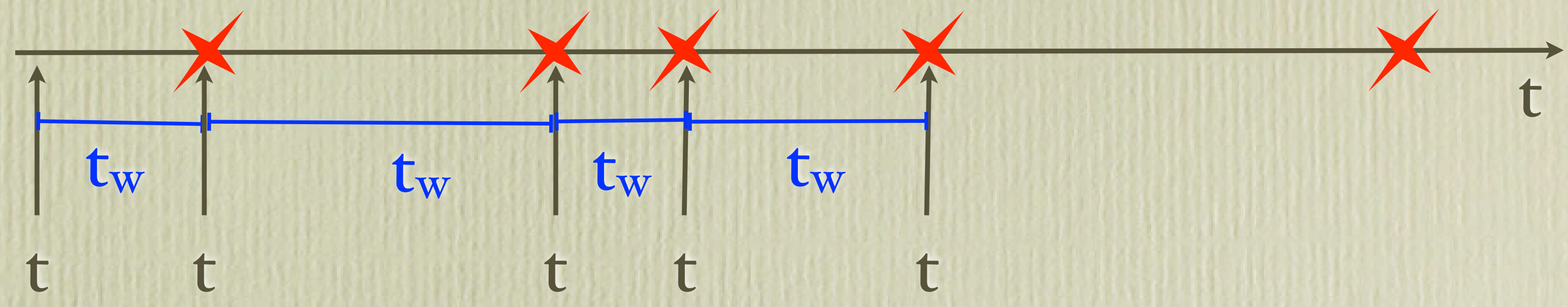
- $P_0(t,t+s)$=probability that no event occur in [t,t+s)
- $P_0(t,t+s)=F(s)$ does not depend on t
- Waiting time: t_w $\quad F(s) = P\{t_w > s\} = \int_s^\infty f(s)ds$
- $F(s_1+s_2)=F(s_1)F(s_2)$ for all $s_1, s_2 > 0$ $\rightarrow F(s) = e^{-rs}$
- pdf of t_w:

$$f(s) = -\frac{dF(s)}{ds} = re^{-rs}$$

- A random variable with this pdf is obtained as

$$t_w = -\log(\texttt{rand}())/r$$

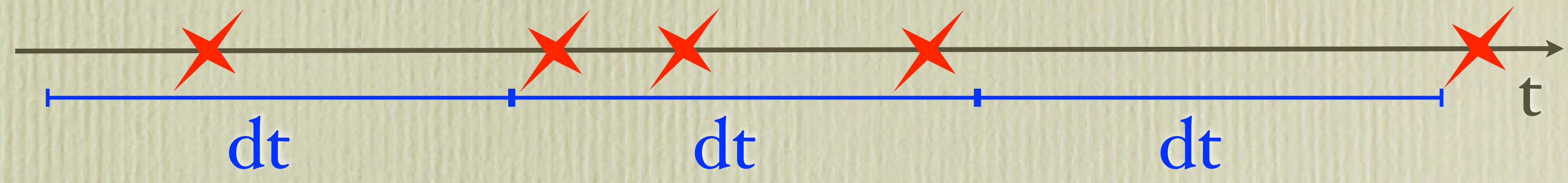
Draw directly the times when events will occur!



- At time t
- draw a waiting time t_w
- advance time to $t+t_w$
- repeat

This is exact!

Fixed dt simulations



- $P_k(u)$=probability of k events in [t,t+u)

$$P_1(\tau) = \int_0^\tau P_0(s) r ds P_0(\tau - s - ds) \cong \int_0^\tau P_0(s) r ds P_0(\tau - s)$$

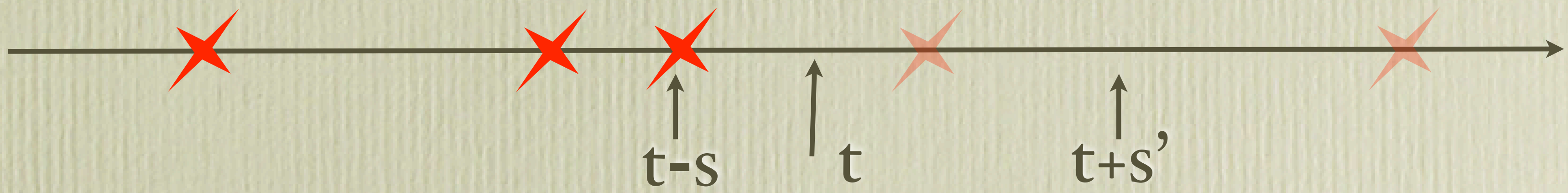
$$\vdots$$

$$P_k(\tau) = \int_0^\tau P_{k-1}(s) r ds P_0(t - s) = \frac{(r\tau)^k}{k!} e^{-r\tau}$$

- Draw k from $P_k(u)$

Note: Poisson process "has no memory"

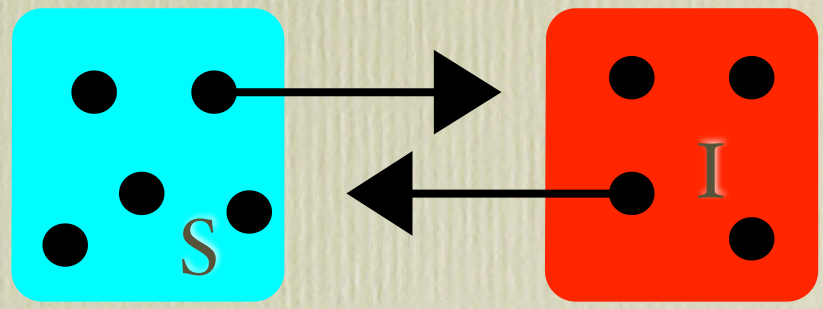
- The average time between events is 1/r
- If I start looking at the process at time t, how much should I wait on average?



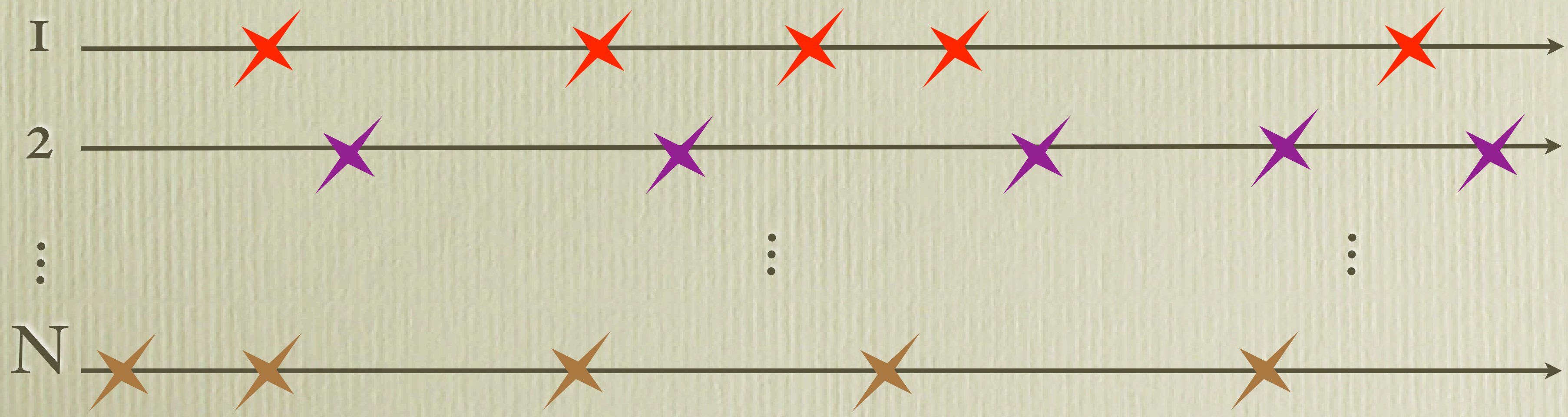
- If I know that the last event occurred at time t-s, what is the probability that the next event will occur after time t+s'?

From one to N processes: e.g. individual based SI model

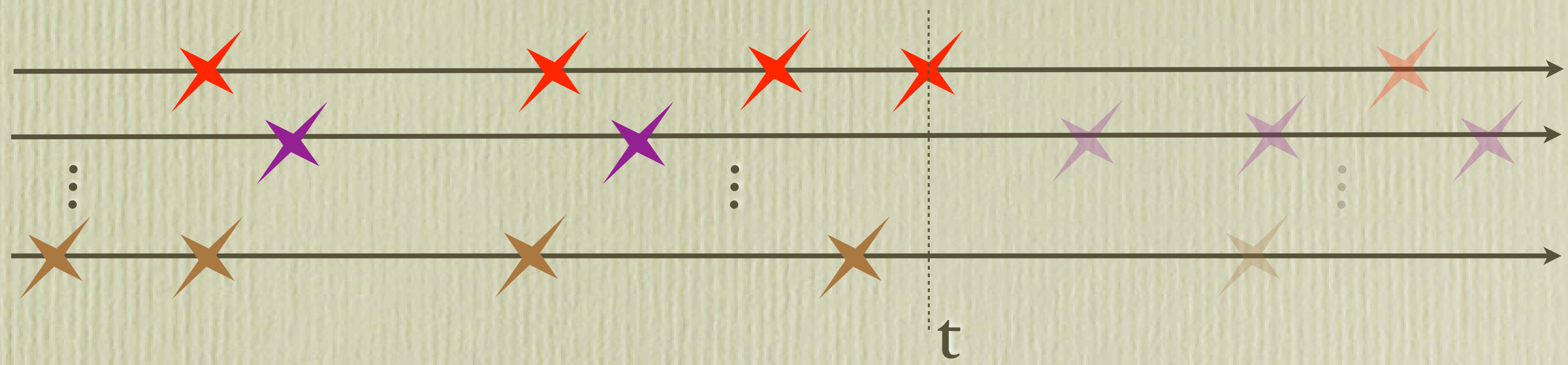
- N individuals, $i=1,2,\ldots,N$
- Each can be either S ($x_i=0$) or I ($x_i=1$)
- In $[t,t+dt)$:
  each $x_i=0$ can become $x_i=1$ with $P(S\rightarrow I)=r_i dt$
  each $x_i=1$ can become $x_i=0$ with $P(I\rightarrow S)=r_i dt$



$r_i=(1-x_i)\beta S/N+\gamma x_i$

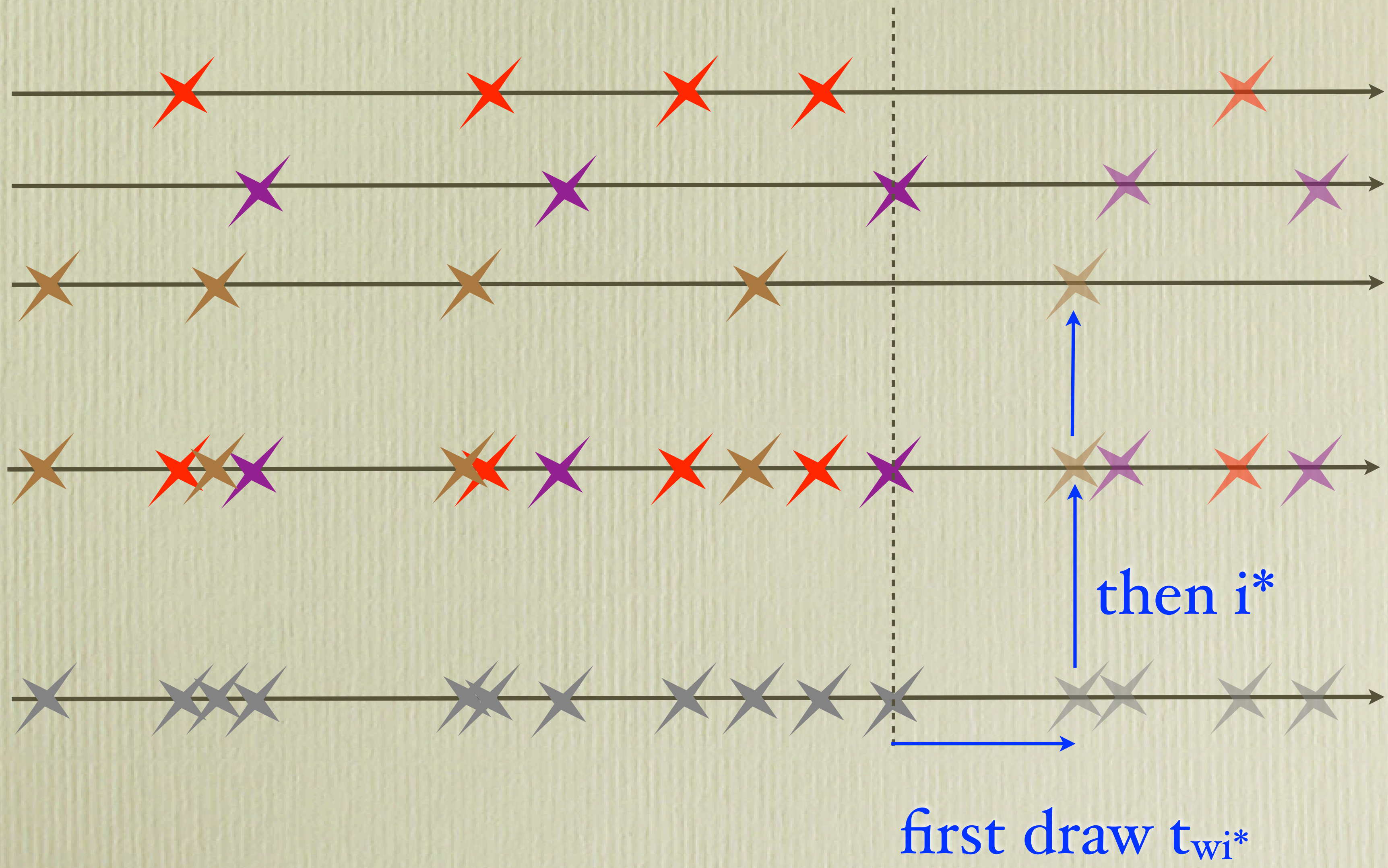


How to make a simulation?



- At time time t, for each process i=1,...,N draw a waiting time $t_{w,i}$ from the exponential pdf with rate r_i
- Find the process which occurs next, $i^*=\mathrm{argmin}\{t_{w,i}\}$
- Do process i^* and advance time to $t+ t_{w,i^*}$
- Note:
  - exact
  - need to find the minimum of N variables, O(log N)
  - no need to re-draw waiting times for $i \neq i^*$!

We can do better if we first draw the time to the next event and then find which event is it



In practice:

(this is also called the Gillespie algorithm)

1. Find the probability of the combined process

$$\begin{aligned} P\{t_{w,i^*} > t\} &= P\{t_{w,1} > t, t_{w,1} > t, \ldots, t_{w,N} > t\} \\ &= P\{t_{w,1} > t\} P\{t_{w,1} > t\} \cdots P\{t_{w,N} > t\} \\ &= e^{-r_1 t} e^{-r_1 t} \cdot e^{r_N t} = e^{-\sum_i r_i t} \\ &= e^{-Rt} \end{aligned}$$

$$R = \sum_{i=1}^{N} r_i$$

i.e. draw $t_{wi^*} = -\log(\texttt{rand}())/R$

2. Compute the probability that i*=i

$$P\{i^* = i\} = P\{t_{w,i} < t_{w,j}\ \forall j \neq i\} = \int_0^\infty dt_i r_i e^{-r_i t} \prod_{j \neq i} e^{-r_j t}$$

$$= \frac{r_i}{R}$$

Back to the SI model

- At time t

$$I(t) = \sum_{i=1}^{N} x_i(t), \qquad S(t) = N - I(t) \qquad r_i = \begin{cases} \beta \frac{I}{N} & \text{if } x_i = 0 \\ \mu & \text{if } x_i = 1 \end{cases}$$

- Draw waiting time for next event:

$$t_w = -\frac{1}{R}\log(\texttt{rand}()), \qquad R = \left[\mu + \beta\left(1 - \frac{I}{N}\right)\right] I$$

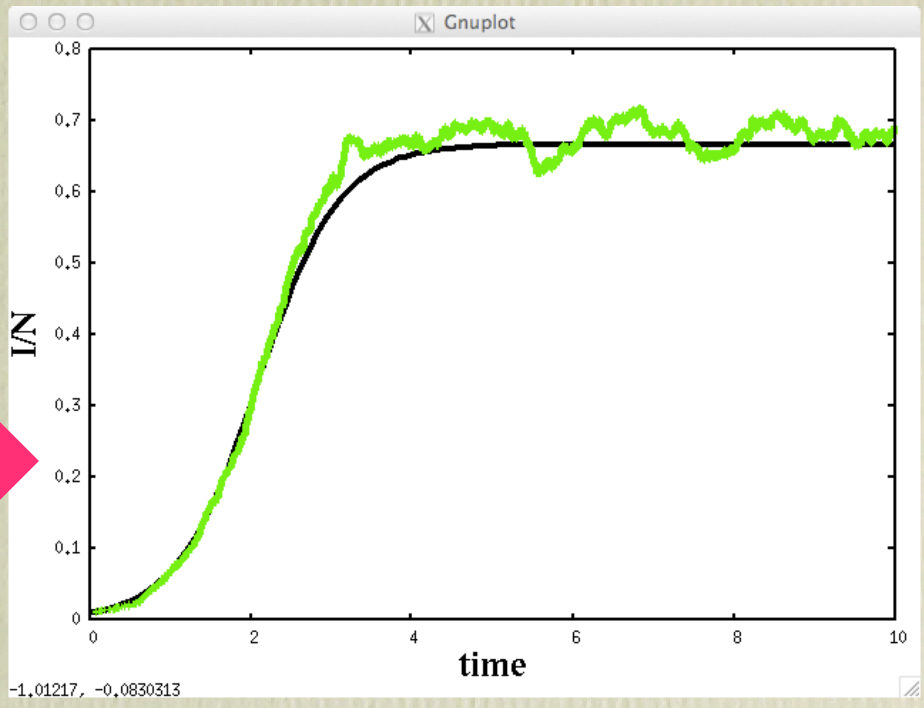
- Draw i* ...

- ... or

$$I(t + t_w) = \begin{cases} I(t) - 1 & \text{with probability } \mu I/R \\ I(t) + 1 & \text{else} \end{cases}$$

Let's write a program:

```
      N=1000
      I=10
      beta=3.0
      mu=1.0
      t=0.0
10    R=(mu+beta*(1-float(I)/N))*I
      dt=-log(ran2(idum))/R
      t=t+dt
      print *,t,I
      if (ran2(idum).lt.mu*I/R) then
         I=I-1
      else
         I=I+1
      end if
      print *,t,I
      if (I.gt.0.and.t.lt.100) go to 10
      end
```

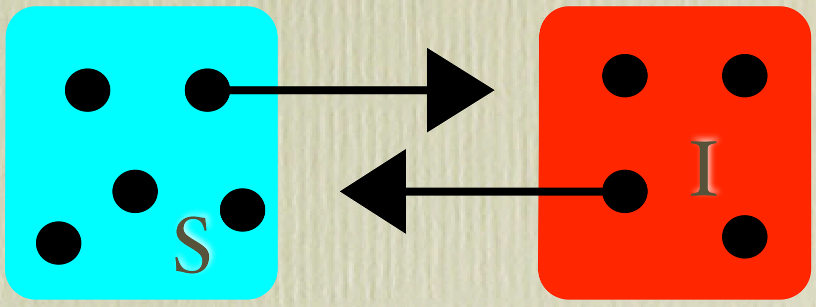


Note: seasonality

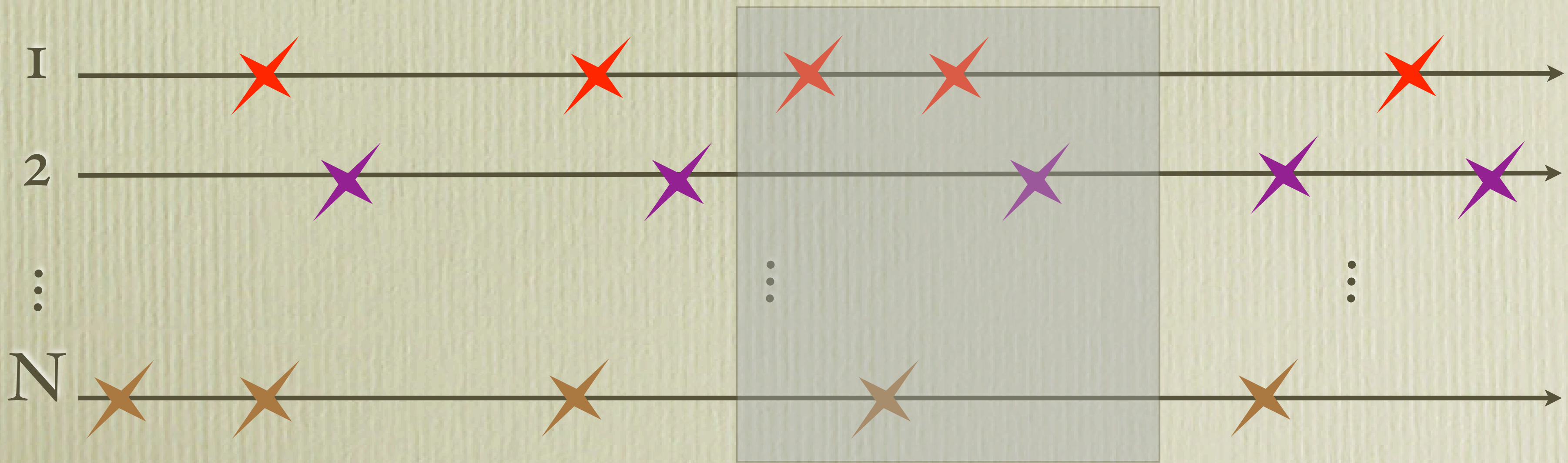
- Seasonality: if rates $r_i(t)$ depend on t things get more complex ...
- Yet as long as $r_i(t)$ does not change significantly over times of order t_{wi^*} one can consider r_i as constant
- $t_{wi^*} \sim 1/N$ so if $dr_i/dt << N$ all is fine

Question: Why can't I take a fixed dt?

$$I(t) = \sum_{i=1}^{N} x_i(t), \qquad S(t) = N - I(t)$$



$$r_i = \begin{cases} \beta \frac{I}{N} & \text{if } x_i = 0 \\ \mu & \text{if } x_i = 1 \end{cases}$$

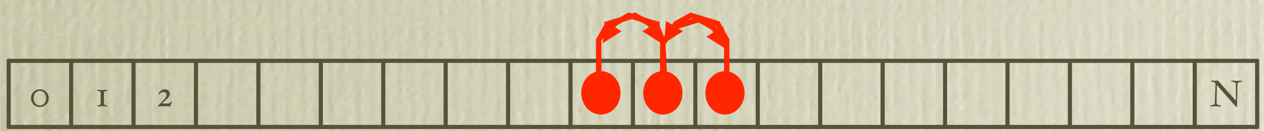


The Master equation

- P(I,t) = probability of I infected individuals
- Two processes: I⇒I+1 or I⇒I-1

$$w(I \to I+1) = \beta I \left(1 - \frac{I}{N}\right), \qquad w(I \to I-1) = \mu I$$

$$\frac{\partial P(I,t)}{\partial t} = P(I-1,t)w(I-1 \to I) + P(I+1,t)w(I+1 \to I)$$
$$-P(I,t)w(I \to I+1) - P(I,t)w(I \to I-1)$$



I-1, I, I+1

Seasonality without seasons

n predators, m preys

transition rates:

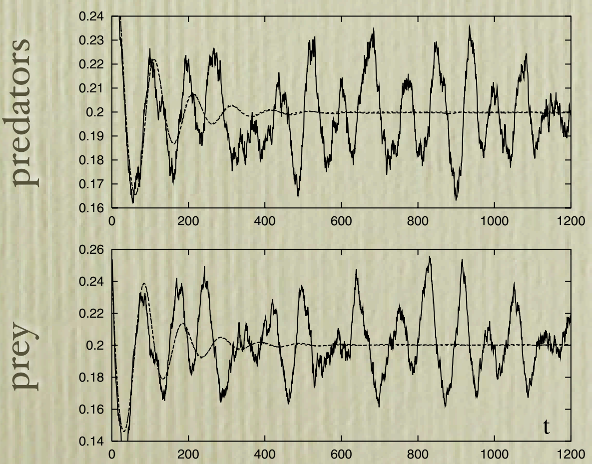
$$w[(n,m) \to (n'm')] = T(n'm'|n,m)$$

$$T(n-1,m|n,m) = d_1 n,$$

$$T(n,m+1|n,m) = 2b\frac{m}{N}(N-n-m),$$

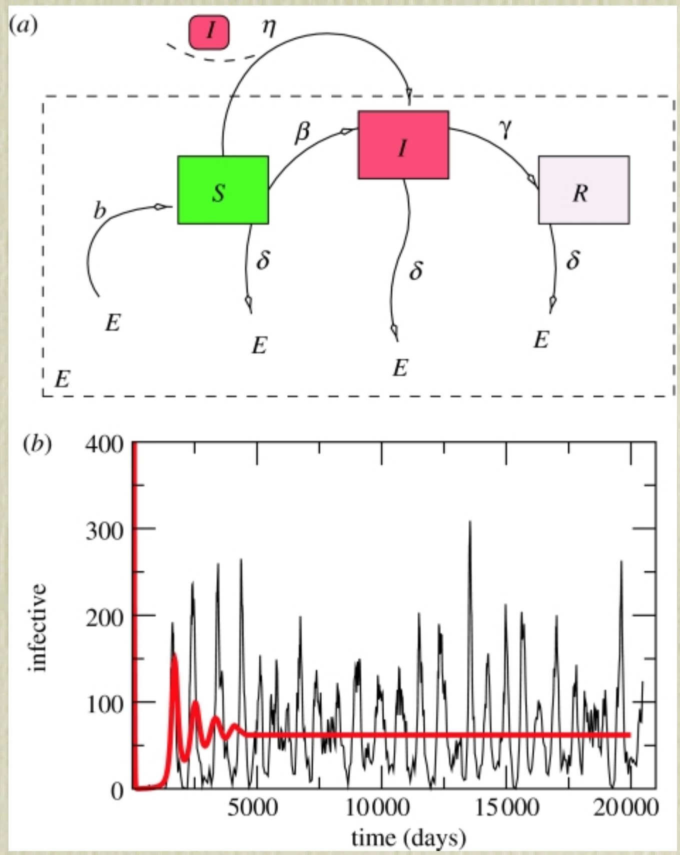
$$T(n,m-1|n,m) = 2p_2\frac{nm}{N} + d_2 m,$$

$$T(n+1,m-1|n,m) = 2p_1\frac{nm}{N},$$



A.J. McKane, T.J. Newman Phys. Rev. Lett. 2005

Epidemics: (open) SIR model

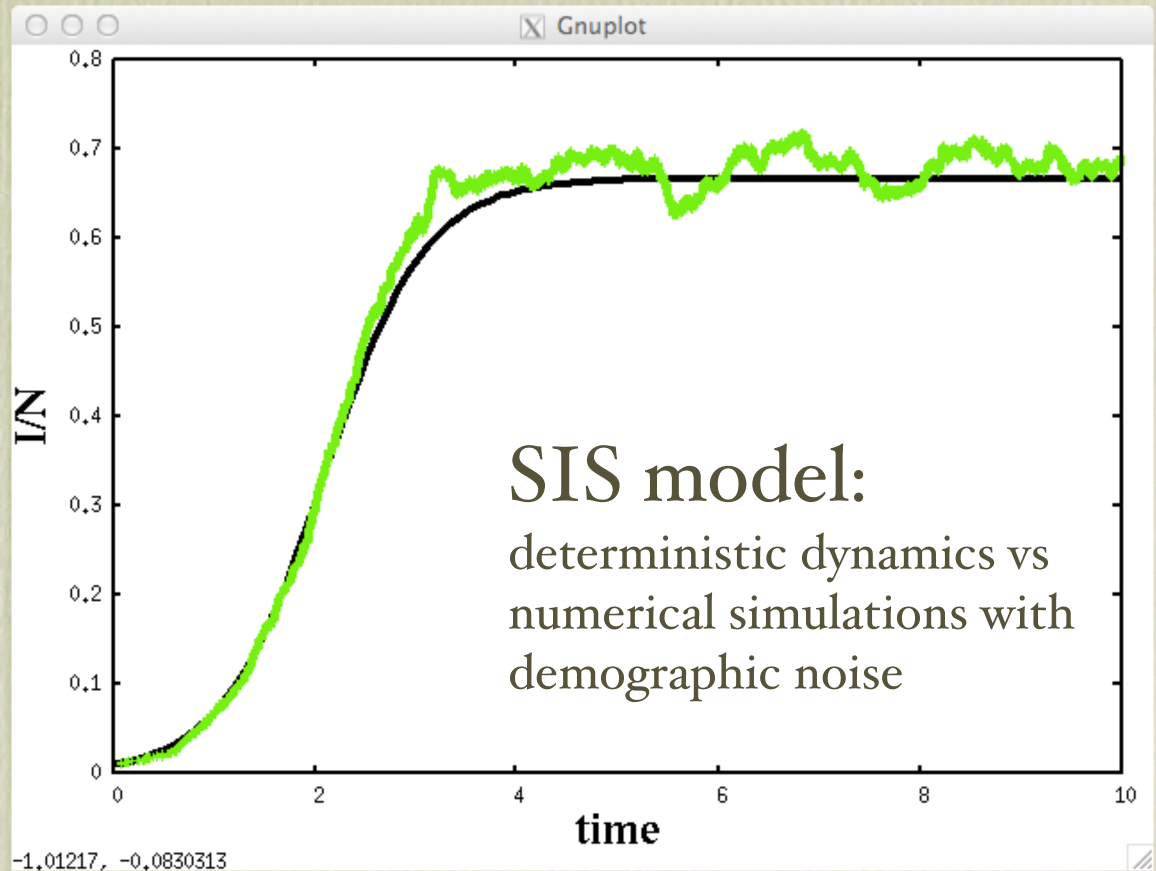


D. Alonso, A.J. McKane, M. Pascual Interface 2007

Lecture II Stochastic differential equations

Can we describe stochastic fluctuations with differential equations?

$$\frac{dI}{dt} = \beta I \left(1 - \frac{I}{N}\right) - \mu I + \dots$$



Summary

- Effect of noise = the accumulation of random shocks
  $\Rightarrow$ sums of random variables

  $\Rightarrow$ Central Limit Theorem

- As a consequence, the "noise" that can be added to the differential equation has specific math properties (Wiener process), mainly:

$$dW^2 = dt$$

- This has consequences in how you deal with (stochastic) differential equations (e.g. demographic noise, random shocks, etc) and how you integrate them

Preliminary:
random integrals and sums

$$dy = \beta y\,(1-y)\,dt - \mu y dt + \text{"noise"}, \qquad y = I/N$$

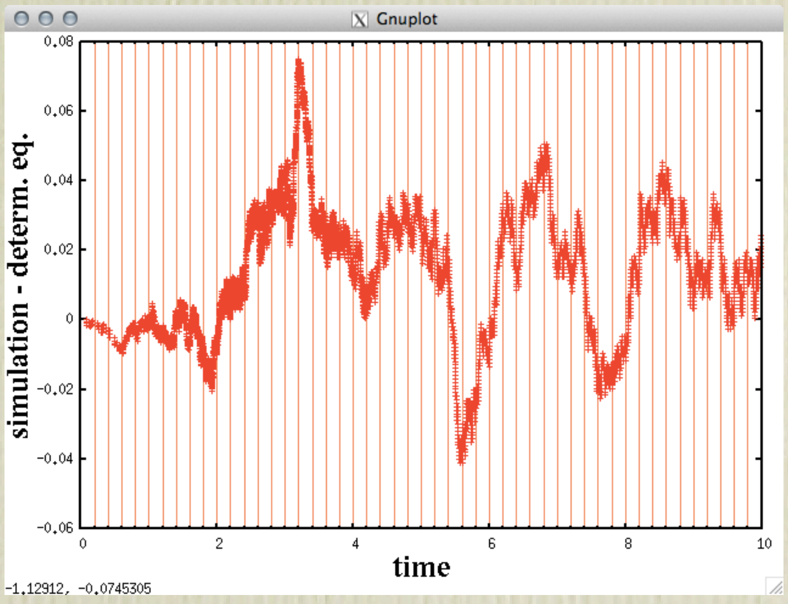
- In order to give a meaning to this, I have to tell you how to compute a solution with $y(t_0)=y_0$

$$y(t) = y_0 + \int_{t_0}^{t} \{\beta y(t')\,[1-y(t')] - \mu y(t')\}\,dt' + \int_{t_0}^{t} \text{"noise"}$$

- From integrals to sums

$$\int_{t_0}^{t} \text{"noise"} = \sum_{i=1}^{N} X_i,$$

$$N = (t-t_0)/dt, \qquad X_i = \int_{t_i}^{t_i+dt} \text{"noise"}$$



The Central Limit Theorem

- If X_i are i.i.d. $E[X_i]$ and the variance $V[X_i]$ is finite, then

$$\sum_{i=1}^{N} X_i = NE[X_i] + \sqrt{NV[X_i]}Z, \quad \text{where} \quad p(z) = \frac{1}{\sqrt{2\pi}} e^{-z^2/2}$$

- In our case, $N=(t-t_0)/dt$ and $E[X_i]=0$, in order to define a continuum time limit $dt \to 0$ we need

$$\lim_{dt\to 0} V[X_i]/dt \quad \text{finite}$$

- Rescaling time: The Wiener process

$$X_i = \int_{t_i}^{t_i+dt} \text{"noise"} = dW(t) = \sqrt{dt}Z, \qquad \int_{t_0}^{t} dW = W(t) - W(t_0) = \sqrt{t-t_0}Z$$

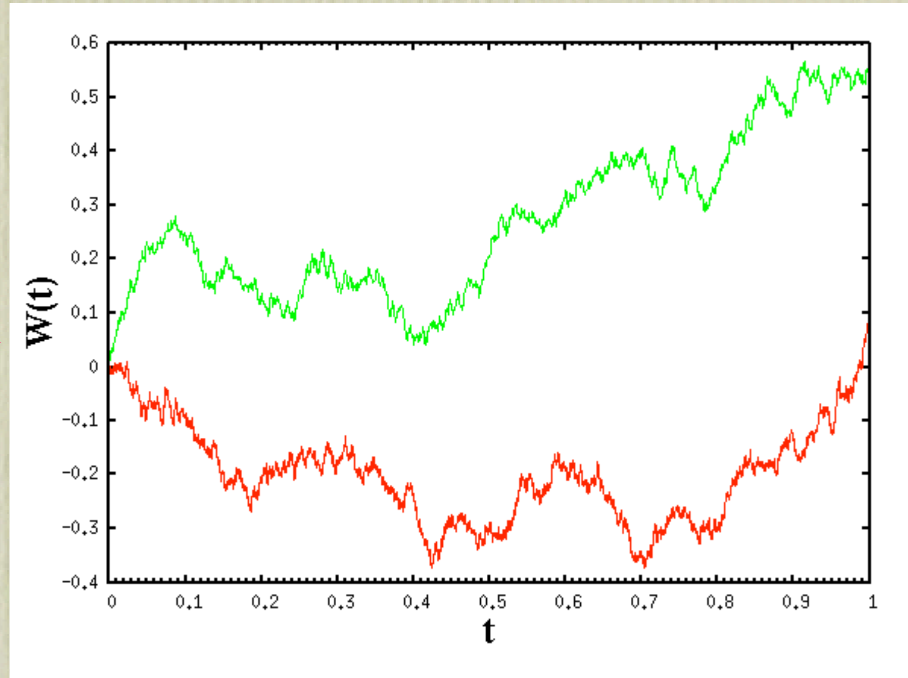
(i.i.d. = independent and identically distributed)

If sums of random variables are appropriately rescaled, the result is independent of dt

$$\int_{t_0}^{t} \text{"noise"} = \sum_{i=1}^{N} X_i,$$

$$N = (t - t_0)/dt, \qquad X_i = \int_{t_i}^{t_i+dt} \text{"noise"}$$

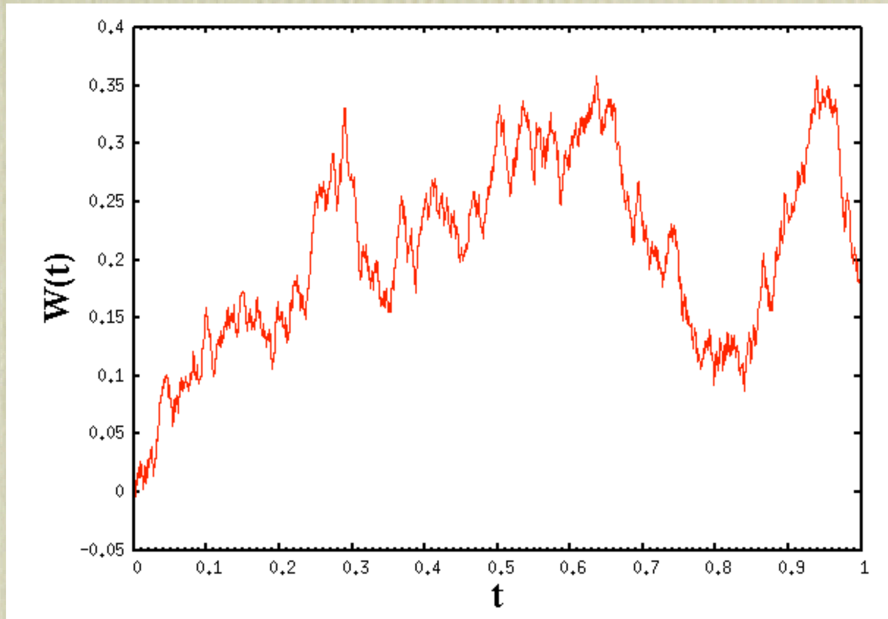
```
read *,dt,idum

N=1.d0/dt
Sum=0
do i=1,N
   X=ran2(idum)-0.5
   Sum=Sum+X
   print *,i*dt,sqrt(dt)*Sum
end do

end
```



Which has been generated with $dt=10^{-3}$ and which with $dt=10^{-4}$?

The Wiener process

$$W(t) = \sum_{i=1}^{t/dt} \sqrt{dt} Z_i, \qquad Z_i \quad \text{i.i.d. Gaussian with} \quad E[Z_i] = 0 \quad V[Z_i] = 1$$



- W(t) is continuous (a.s.)
- W(t) has independent increments

$$\Rightarrow E[W(t_1)W(t_2)] = \min\{t_1, t_2\}$$

- W(t) is nowhere differentiable

$$dW \sim \sqrt{dt} \quad \Rightarrow \quad \frac{dW}{dt} \sim \frac{1}{\sqrt{dt}}$$

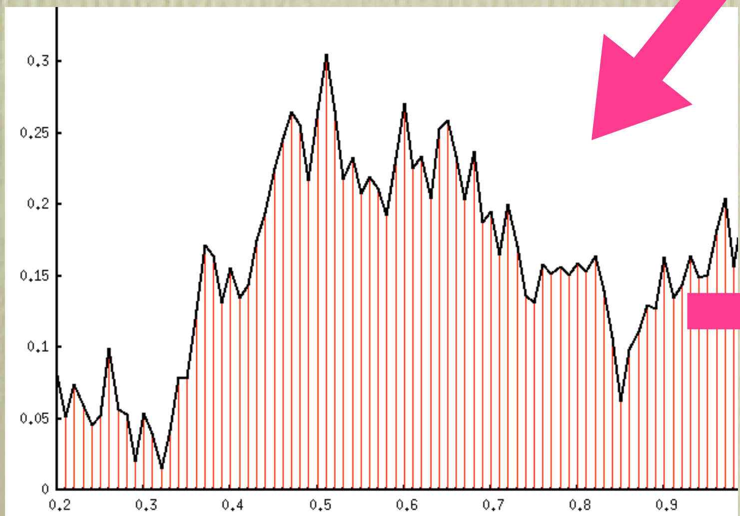
Stochastic differential equations

$$dy = a(y,t)dt + b(y,t)dW$$

- This means

$$y(t) = y(t_0) + \underbrace{\int_{t_0}^{t} a(y(t'),t')dt'}_{\text{Lebesgue integral}} + \underbrace{\int_{t_0}^{t} b(y(t'),t')dW(t')}_{\text{stochastic integral}}$$

?



$$\int_{t_0}^{t} a(y(t'),t')dt' = \lim_{N\to\infty} \sum_{i=1}^{N} a(y(\tau_i),\tau_i)dt_i$$

$$t_0 < t_1 < \dots < t_N = t, \quad dt_i = t_i - t_{i-1}$$

$$t_{i-1} \le \tau_i \le t_i$$

$$\int_{t_0}^{t} b(y(t'),t')dW(t') = \lim_{N\to\infty} \sum_{i=1}^{N} b(y(\tau_i),\tau_i)dW_i$$

$$t_0 < t_1 < \dots < t_N = t, \quad dW_i = W(t_i) - W(t_{i-1})$$

$$t_{i-1} \le \tau_i \le t_i$$

The stochastic integral depends on how the midpoint is chosen

- Stochastic integrals are random variables

$$\int_{t_0}^{t} G(t')dW(t') = Y \quad \Leftrightarrow \quad E\left[\left(\int_{t_0}^{t} G(t')dW(t') - Y\right)^2\right] = 0$$

- Stochastic integral depends on the choice of the midpoint. Example: G(t)=W(t)

$$\int_{t_0}^{t} W(t')dW(t') = \lim_{N\to\infty} \sum_{i=1}^{N} W(\tau_i)dW_i$$

$$t_0 < t_1 < \ldots < t_N = t, \qquad dW_i = W(t_i) - W(t_{i-1})$$

$$\tau_i = \alpha t_i + (1-\alpha)t_{i-1}$$

$$\Rightarrow \quad E\left[\int_{t_0}^{t} W(t')dW(t')\right] = \alpha(t - t_0)$$

Need a prescription

- Ito prescription: $\alpha = 0, \qquad \tau_i = t_{i-1}$

  New term appears in integrals, e.g.

  $$\int_{t_0}^{t} W(t')dW(t') = \frac{W^2(t) - W^2(t_0)}{2} - \frac{t - t_0}{2}$$

  because

  $$df(W) = f'(W)dW + \frac{1}{2}f"(W)dt$$

  Differential equations have to be integrated as in Euler scheme

  $$x(t + dt) = x(t) + a[x(t), t]dt + b[x(t), t]dW(t)$$

  $$dW(t) \;\; \text{independent of} \;\; x(t)$$

- Under other prescriptions (e.g. $\alpha = 1/2$) the rules of integration and differentiation change

Ito formula: dW^2=dt

- Change of variables: y=f(x)

$$dx = a(x,t)dt + b(x,t)dW$$

$$\begin{aligned} dy &= f(x+dx) - f(x) \\ &= \left[[f'(x)a(x,t) + \frac{1}{2} f"(x) b^2(x,t) \right] dt + f'(x)b(x,t)dW \end{aligned}$$

Examples of SDE

- $dx = a(t)dt + b(t)dW$
- $dx = x dW$
- $dx = -kx dt + s\, dW$
- ...

Back to SIS model: what are a and b?

$$I(t) = Ny(t) = \sum_{i=1}^{N} x_i(t), \qquad \Rightarrow dI = \sum_{i=1}^{N} dx_i \cong NE[dx_i] + \sqrt{NV[dx_i]}Z$$

Central Limit Theorem

$$dx_i = \begin{cases} 1 & \text{with prob.} \quad \beta \frac{I}{N}(1-x_i)dt \\ -1 & \text{with prob.} \quad \mu x_i dt \\ 0 & \text{else} \end{cases}$$

$$E[dx_i] = \beta \frac{I}{N}\left(1 - \frac{I}{N}\right)dt - \mu \frac{I}{N}dt$$

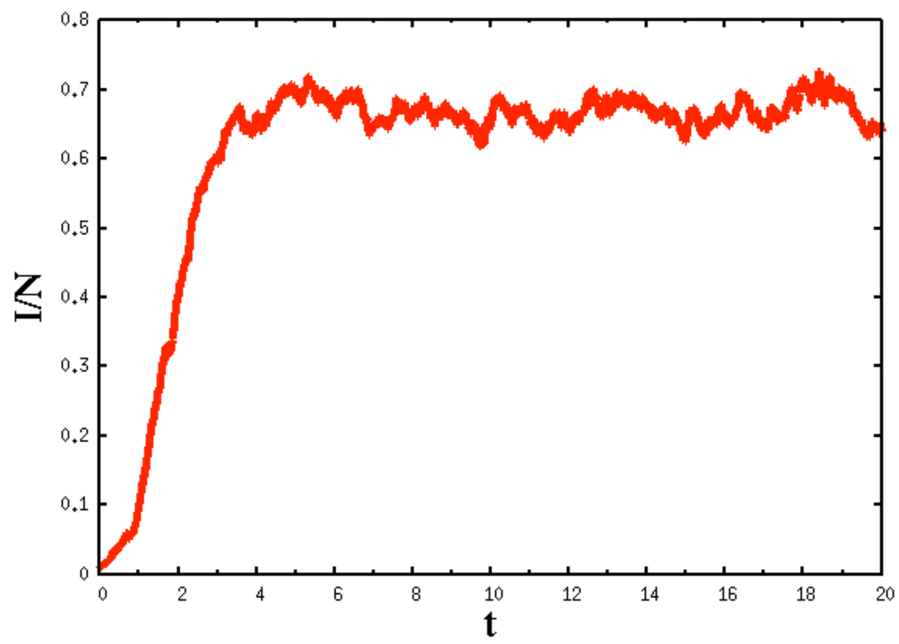
$$\begin{aligned} V[dx_i] &= E[dx^2] - E[dx]^2 \\ &= \beta \frac{I}{N}\left(1 - \frac{I}{N}\right)dt + \mu \frac{I}{N}dt + O(dt^2) \end{aligned}$$

Therefore:

$$dy = [\beta(1-y) - \mu]\, y dt + \frac{1}{\sqrt{N}}\sqrt{[\beta(1-y) + \mu]\, y}dW$$

In FORTRAN this means:

```
      read *,dt,idum

      N=1000

      y=0.01
      beta=3.0
      mu=1.0

      t=0.0
10    dW=sqrt(dt)*gasdev(idum)
      y=y+(beta*(1-y)-mu)*y*dt+sqrt((beta*(1-y)+mu)*y/N)*dW
      t=t+dt
      print *,t,y
      if (y.gt.0.and.t.lt.100) go to 10

      end
```



Van Kampen's system size (or small noise) expansion

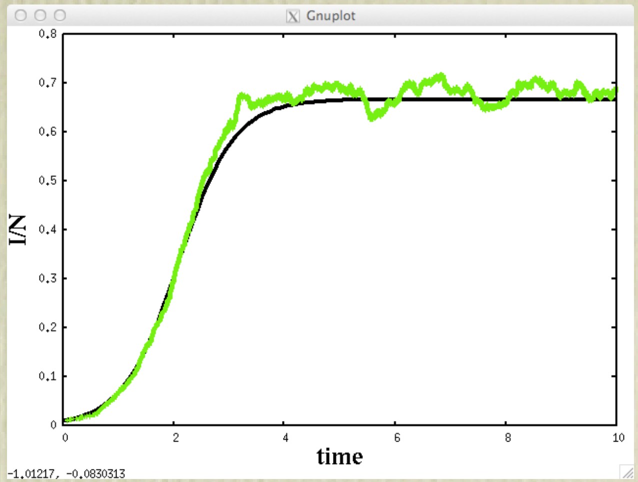
$$dy = \left[\beta\left(1-y\right)-\mu\right]ydt + \frac{1}{\sqrt{N}}\sqrt{\left[\beta\left(1-y\right)+\mu\right]y}dW$$

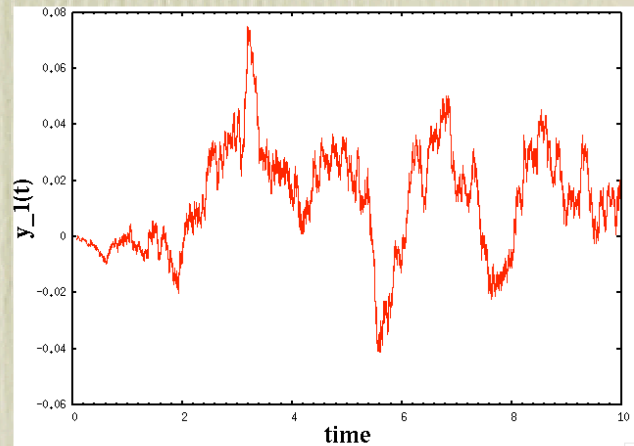
$$\frac{dy_0}{dt} = \left[\beta\left(1-y_0\right)-\mu\right]y_0$$

$$dy = y_0(t)dt + \frac{1}{\sqrt{N}}dy_1(t) + O(1/N)$$

$$dy_1 = \left.\frac{\partial a(y,t)}{\partial y}\right|_{y_0(t)} y_1(t)dt + \frac{b(y_0,t)}{\sqrt{N}}dW$$

$$= -[\mu + \beta(2y_0 - 1)]y_i dt + \frac{\sqrt{[\beta(1-y_0)+\mu]y_0}}{\sqrt{N}}dW$$





References

- C. W. Gardiner C.W. (1985) Handbook of stochastic methods, Springer (chap. 3 & 4)
- van Kampen N.G., (1992). Stochastic processes in physics and chemistry, North Holland, Amsterdam.