“Pattern dynamics” - Spatial population dynamics in terms of individuals

How can “equation-based” models be translated to “individual-based” models?

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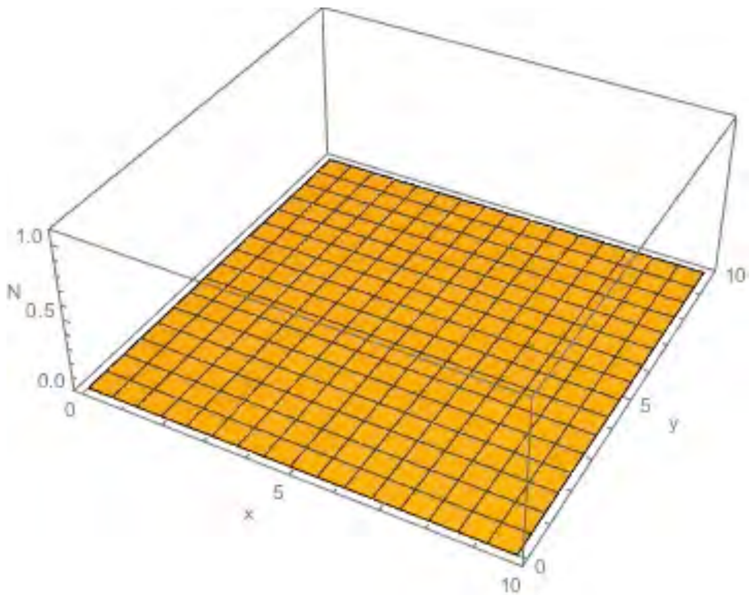
How to model spatial population dynamics?

- Reaction-diffusion model as Partial Differential Equation PDE
- Dynamics of the population density at time *t* and location **x**

$\text{Pop. size: } n(t, \mathbf{x})$

$$\frac{\partial n}{\partial t} = D\left(\frac{\partial^2 n}{\partial x^2} + \frac{\partial^2 n}{\partial y^2}\right) + f(n)$$



$$f(n) = \epsilon(1-n)n$$

Traveling wave

Velocity $2\sqrt{\epsilon D}$

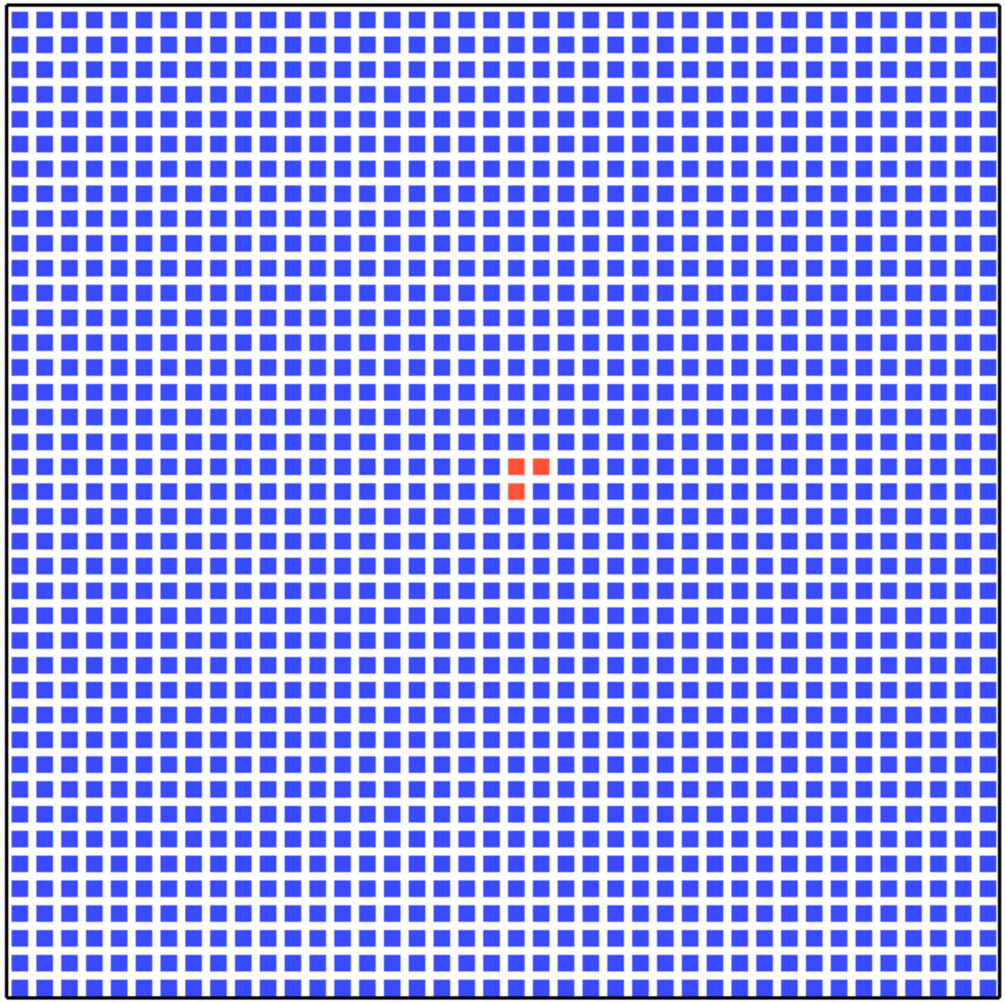
How to model spatial population dynamics?

- Lattice model
- Stochastic transition of a cell between “vacant” and “occupied”
- A vacant site 0 is colonized from adjacent occupied + sites
- An occupied site + goes locally extinct to 0
- How occupied/vacant sites are distributed over space?

0	0	0	0	0
0	+	+	0	0
0	+	0	0	0
0	0	+	0	0
0	0	0	0	0

0 : Vacant
+ : Occupied

Lattice model



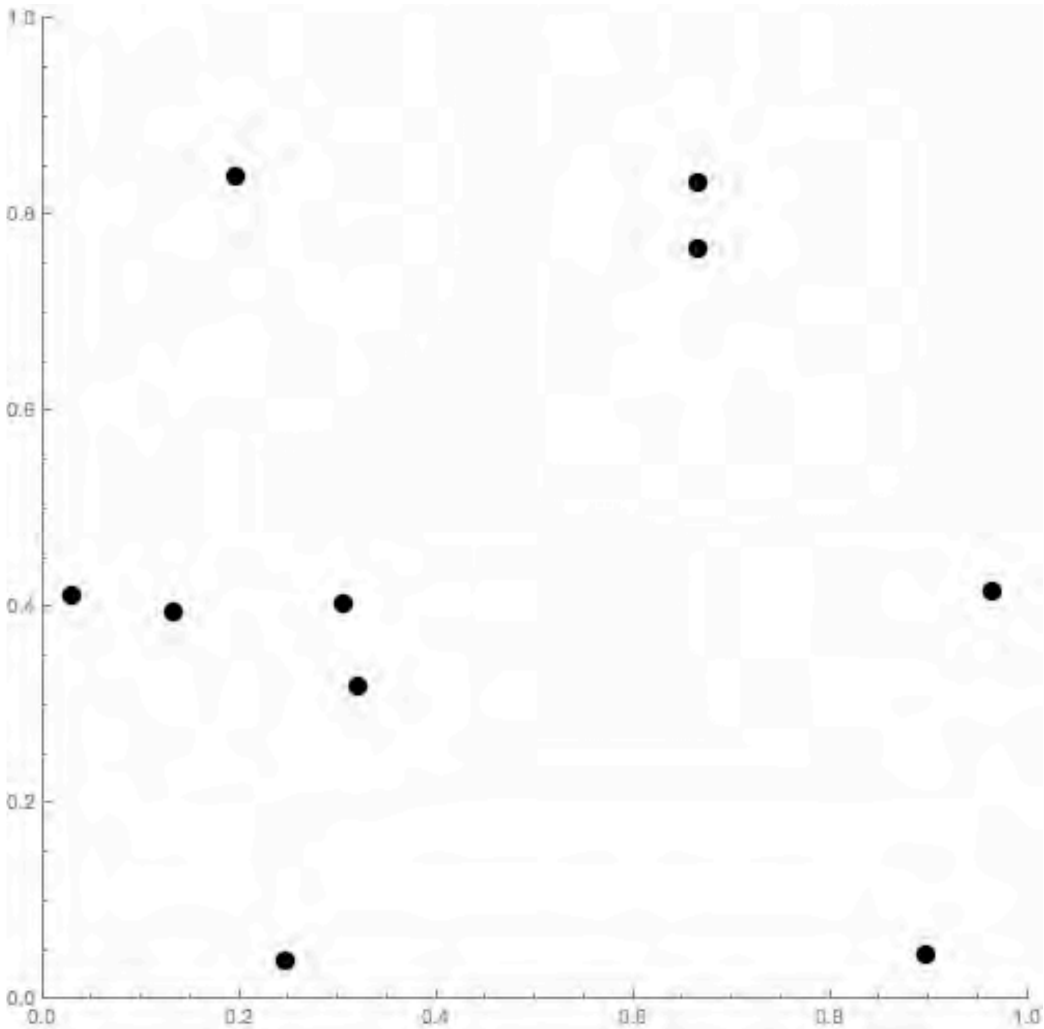
Space size L = 40, Rate colonization = 1.2, Rate extinction = 1
t = 0.0534873, Occupied = 3, Vacant = 1597

0 : Vacant in blue
+ : Occupied in red

Spatial population dynamics as point pattern dynamics

- A mapped point pattern, or point pattern, is a collection of points as individuals located on space
- Each point gives birth, dies, and moves, with a certain rules
- Point pattern dynamics is an individual-based spatial dynamics; each individual has a set of properties that affect birth, death, etc. (age, location, etc.)
- How to analyze point pattern dynamics?
    - Stochastic simulations
    - Analytical approaches to understand simulations

Spatial logistic growth model as a point pattern dynamics



Competition range $\sigma_c = 1.0$, Dispersal range $\sigma_m = 0.03$

Law and Dieckmann 2000
Law et al. 2003

Logistic growth model has been extended as PPD as IBM

An individual-based spatial logistic model

Law and Dieckmann 2000
Law et al. 2003

- An individual is a point on two dimensional space
- Each individual feels "local density"
- Each individual gives birth or dies logistically with rates that depend on its local density
- Newly born individual disperses from its parent

This study revisits the classical logistic growth model in terms of individuals' view point

A point pattern

- A point pattern with *n* individuals

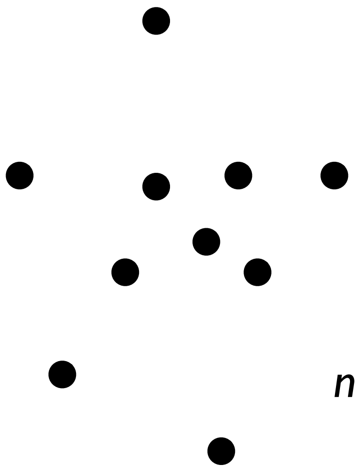
$$p(x) = \sum_{i=1}^{n} \delta_{x_i}(x)$$

$\delta_{x_i}(x) = \delta(x - x_i)$ Dirac delta with peak at the *i*-th individual x_i

$$\delta(x) = \begin{cases} \infty & x = 0 \\ 0 & x \neq 0 \end{cases}$$

$$\int \delta(x)dx = 1$$

$$\int f(x)\delta(x-a)dx = f(a)$$



n = 10

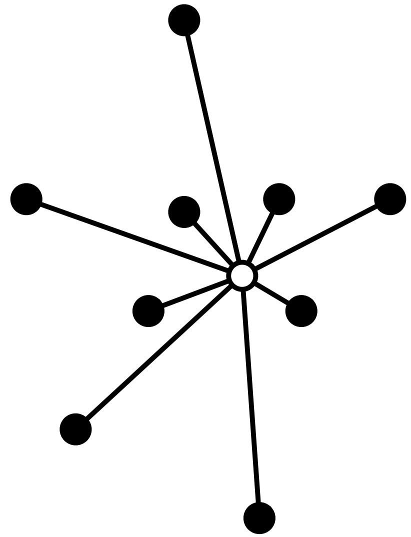
$$\int_\Omega p(x)dx = n$$

Local density

- Define local density of individual *i* as follows

$$N_{local,i} = \int_{\Omega} w_c(|x_i - x|)[p(x) - \delta_{x_i}(x)]dx$$

$$= \sum_{j \neq i} w_c(|x_i - x_j|)$$



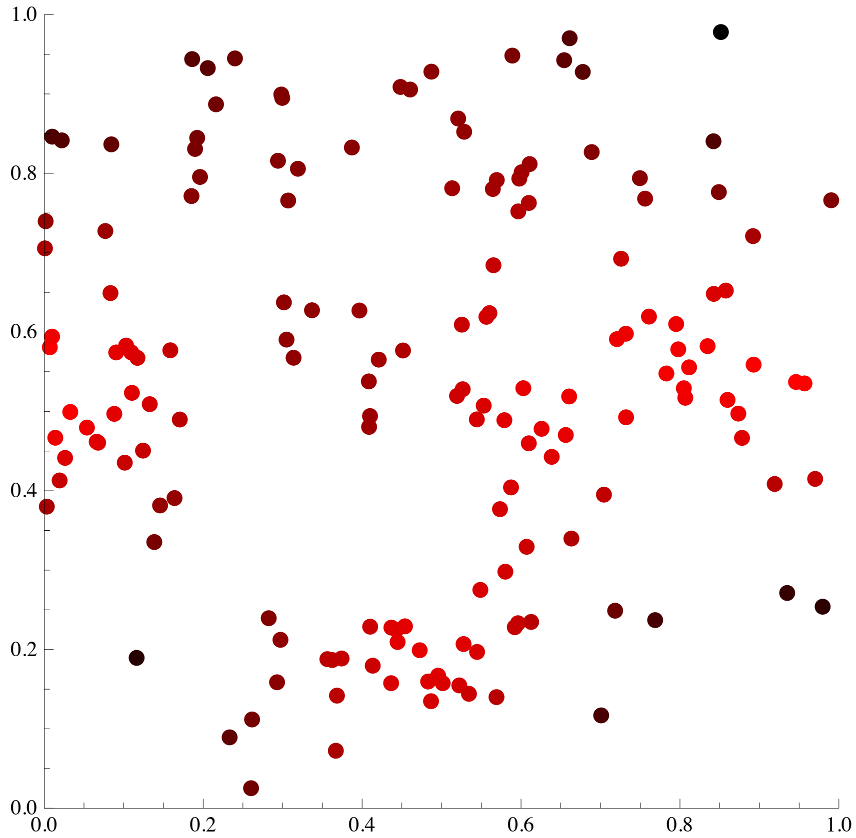
$w_c(d)$ Competition kernel as a function of distance *d*

$$w_c(d) = \frac{1}{2\pi\sigma_c^2} \exp\left[-\frac{d^2}{2\sigma_c^2}\right]$$

σ_c Competition range

Visualized example of local densities

- If surrounded by more neighbors, the local density an individual feels becomes higher



Stochastic process of birth and death of individuals on two dimensional space

- Each individual gives birth or dies with rules
  - Birth rate: $b - b_1 N_{local}$
  - A new born individual disperses from its parent with dispersal kernel $m(d)$
  - Death rate: $d + d_1 N_{local}$

$$m(d) = \frac{1}{2\pi\sigma_m^2} e^{-\frac{d^2}{2\sigma_m^2}}$$

σ_m Dispersal range

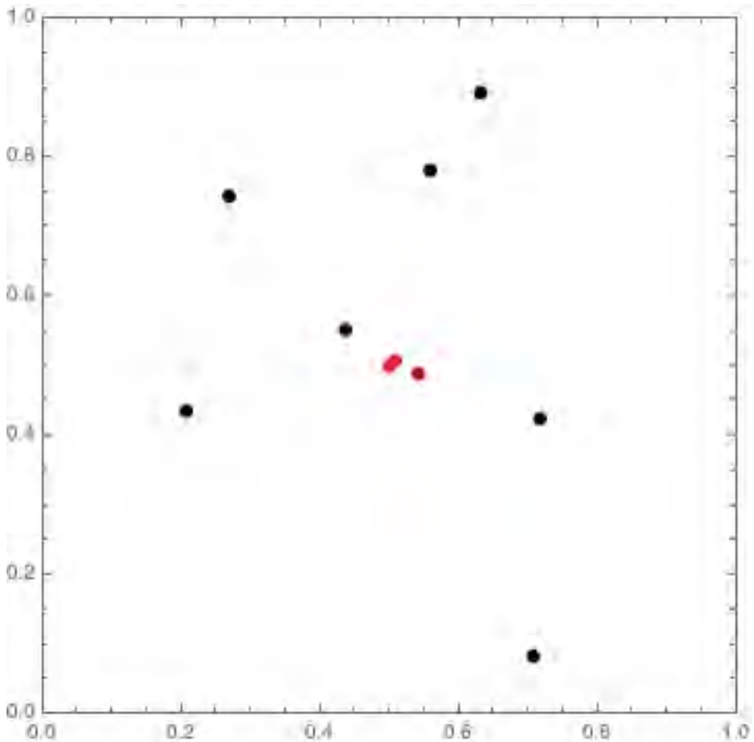
Gillespie algorithm for the stochastic IB spatial logistic model

- 1. Initialization: Set up parameters and initial pp
- 2. Total rate *r*:
  - ΔT = Exp[*r*]

$$r = \sum_{i=1}^{n} (b_1 - b_2 N_{local,i} + d_1 + d_2 N_{local,i})$$

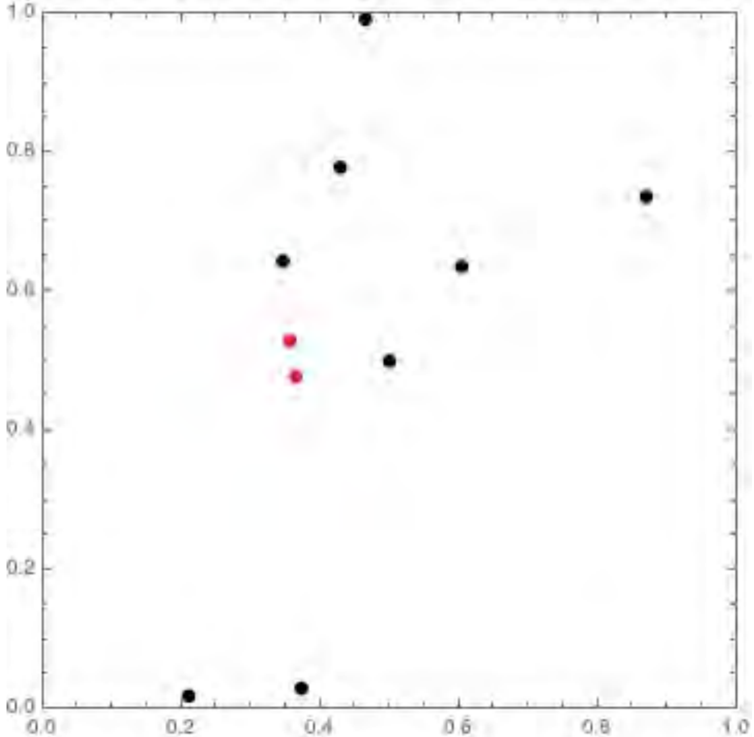
- 3. Advance the time by ΔT and update pp
  - Choose an event (birth or death of a point)
  - If birth, generate a new point from the point with the dispersal kernel
  - if death, delete the point
- Repeat 2 and 3 until a certain time is reached

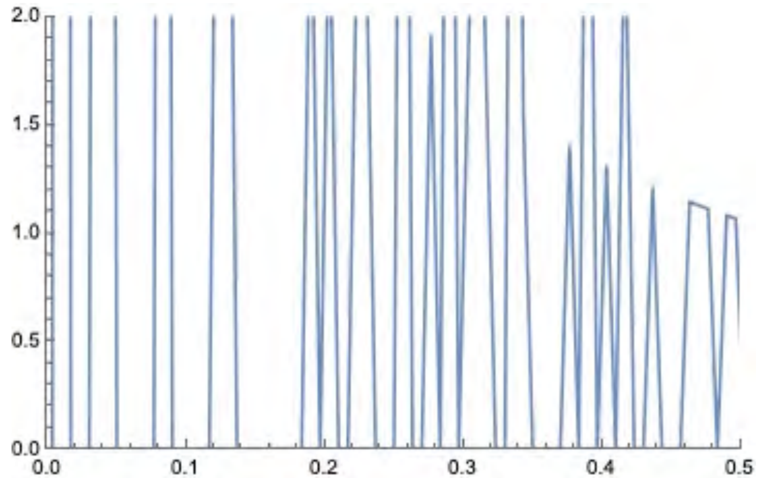
Simulation 1



Competition range $\sigma_c \sim$ dispersal range σ_m

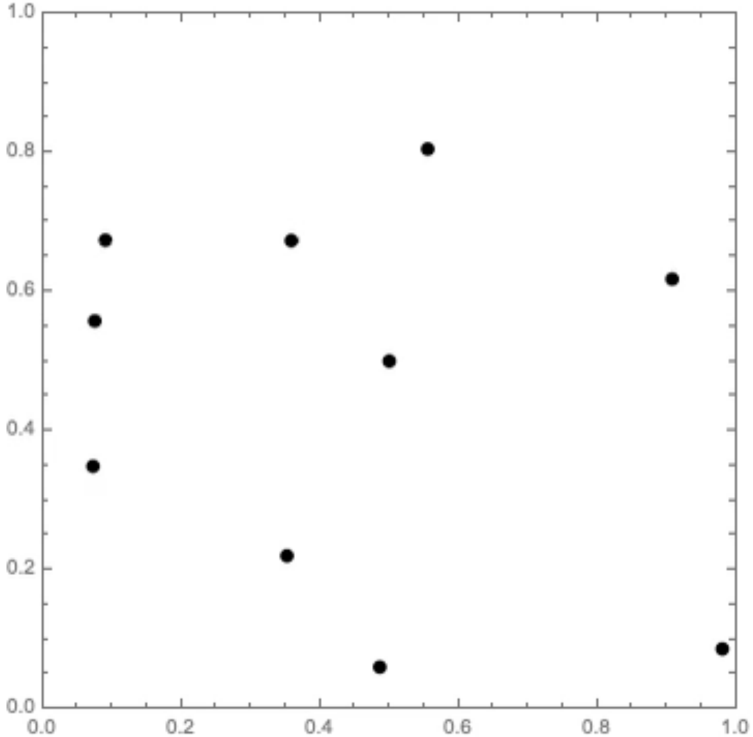
Dynamics of pair correlation function





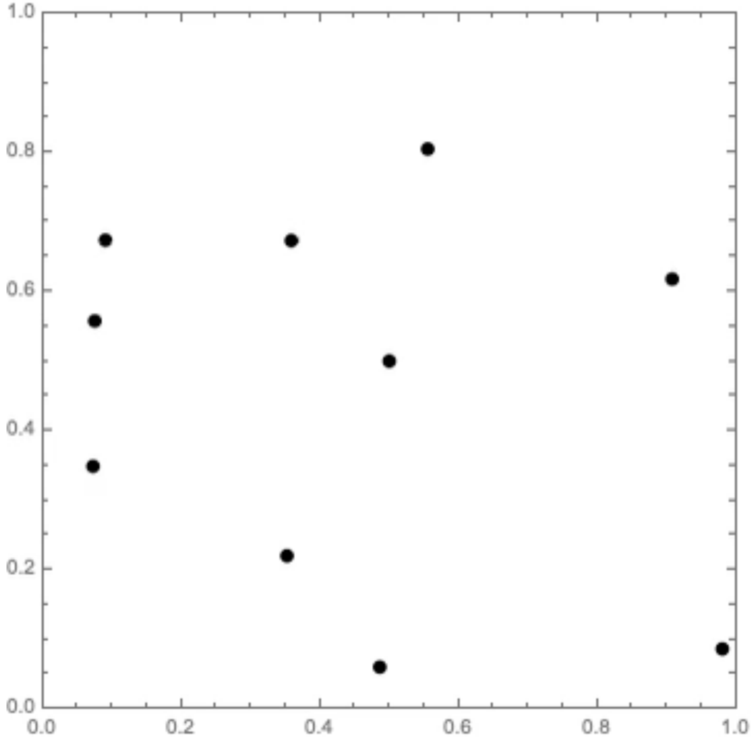
Competition range σ_c ~ dispersal range σ_m

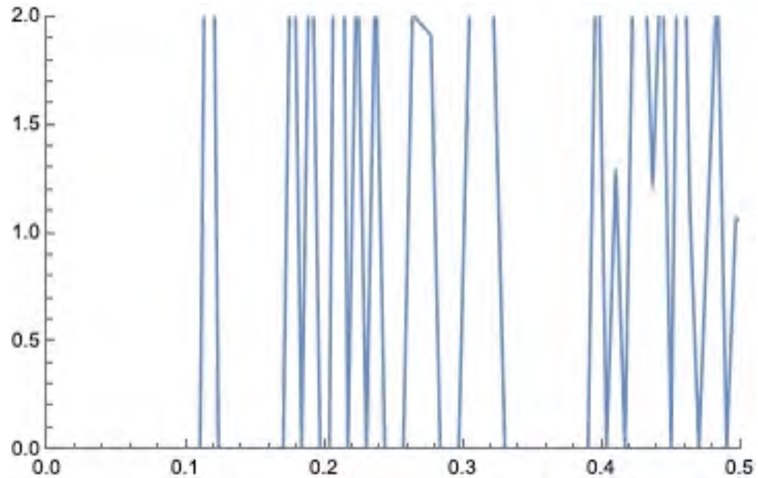
Simulation 2



Competition range σ_c < dispersal range σ_m

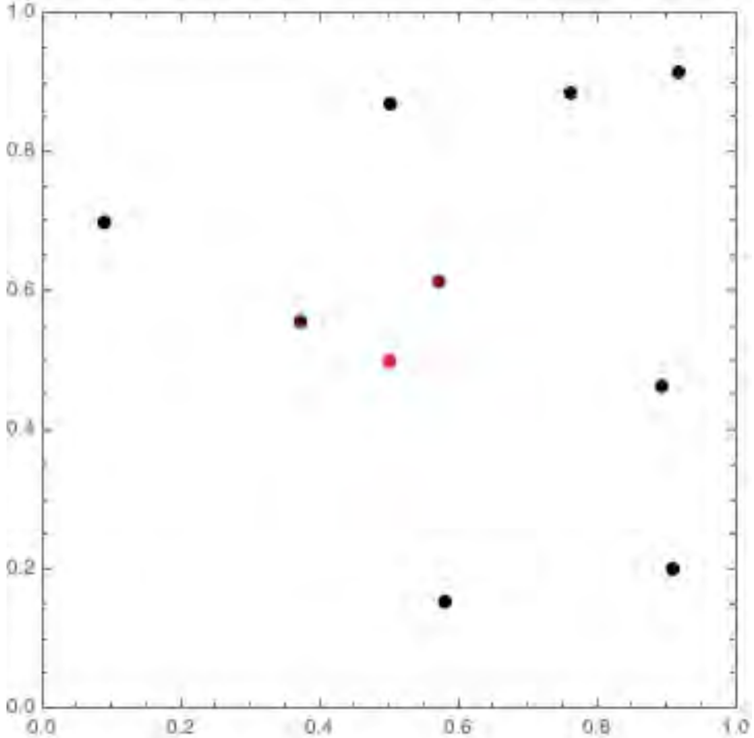
Dynamics of pair correlation function

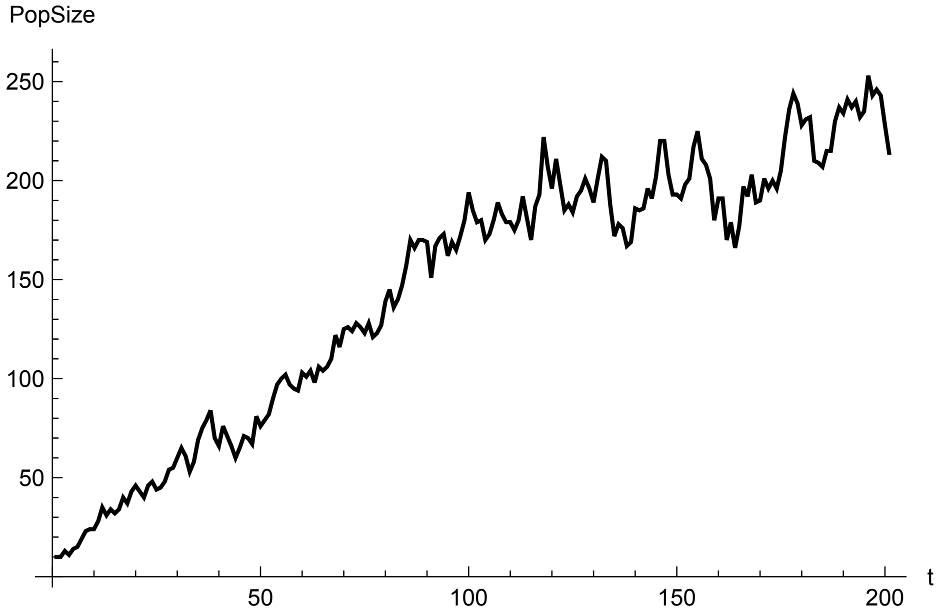




Competition range σ_c < dispersal range σ_m

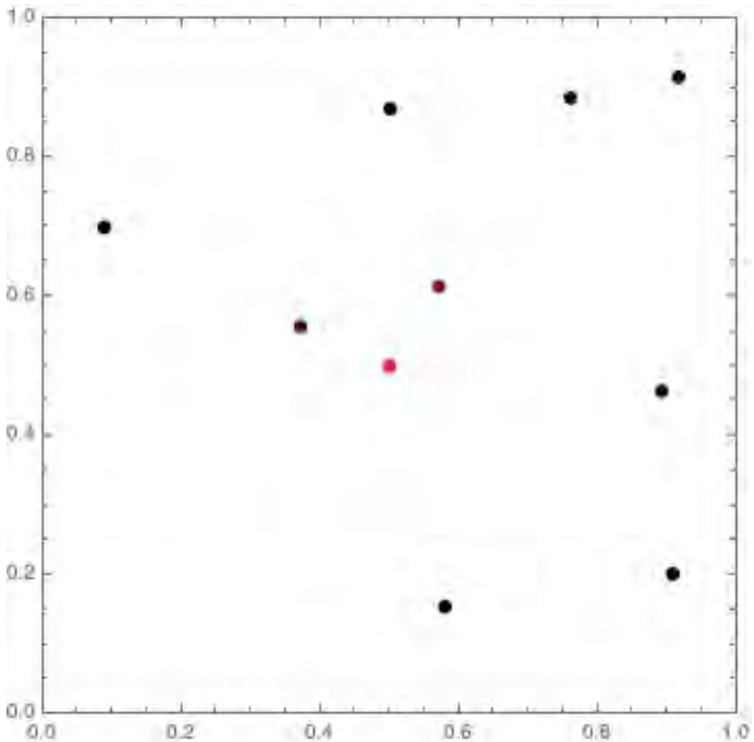
Simulation 3

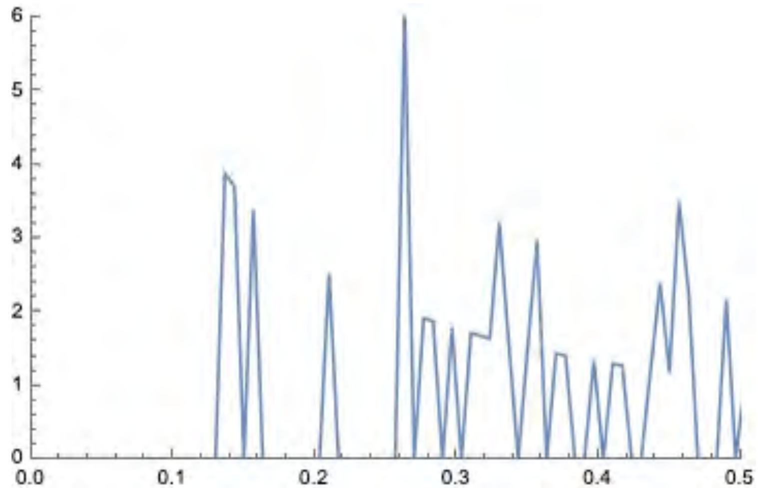




Competition range σ_c > dispersal range σ_m

Dynamics of pair correlation function





Competition range σ_c > dispersal range σ_m

An individual-based spatial logistic model

Law and Dieckmann 2000
Law et al. 2003

- IB spatial logistic model behaves like the classic logistic growth model in terms of the population size
- Competition range σ_c and dispersal range σ_m critically affect population dynamics and pattern dynamics
- $\sigma_c \sim \sigma_m$: Pattern is nearly random, CSR
- $\sigma_c << \sigma_m$: Pattern is regular (over-dispersed)
- $\sigma_c >> \sigma_m$: Pattern is clustered

How can we interpret simulations?

- Simulation is computationally expensive and one realization may not tell full picture of the rules assumed (birth, death, etc., at individual level)
- We need to extract "essence" of the rules from which stochastic simulations are realized
- We want to translate "rules (algorithm)" of birth, death, etc. at individual level into mathematical equations

Moment dynamics of the IB spatial logistic growth model

Law and Dieckmann 2000
Law et al. 2003

N Density of singlets (individuals)

$$\frac{dN}{dt} = (b - d)N - (b_1 + d_1) \int w_c(\xi)C(\xi)d\xi$$

$C(\xi)$ Density of pairs displaced by ξ

When point pattern is CSR, $C(\xi) = N^2$

$$\frac{dN}{dt} = (b - d)N - (b_1 + d_1)N^2$$

Dynamics of the pair density

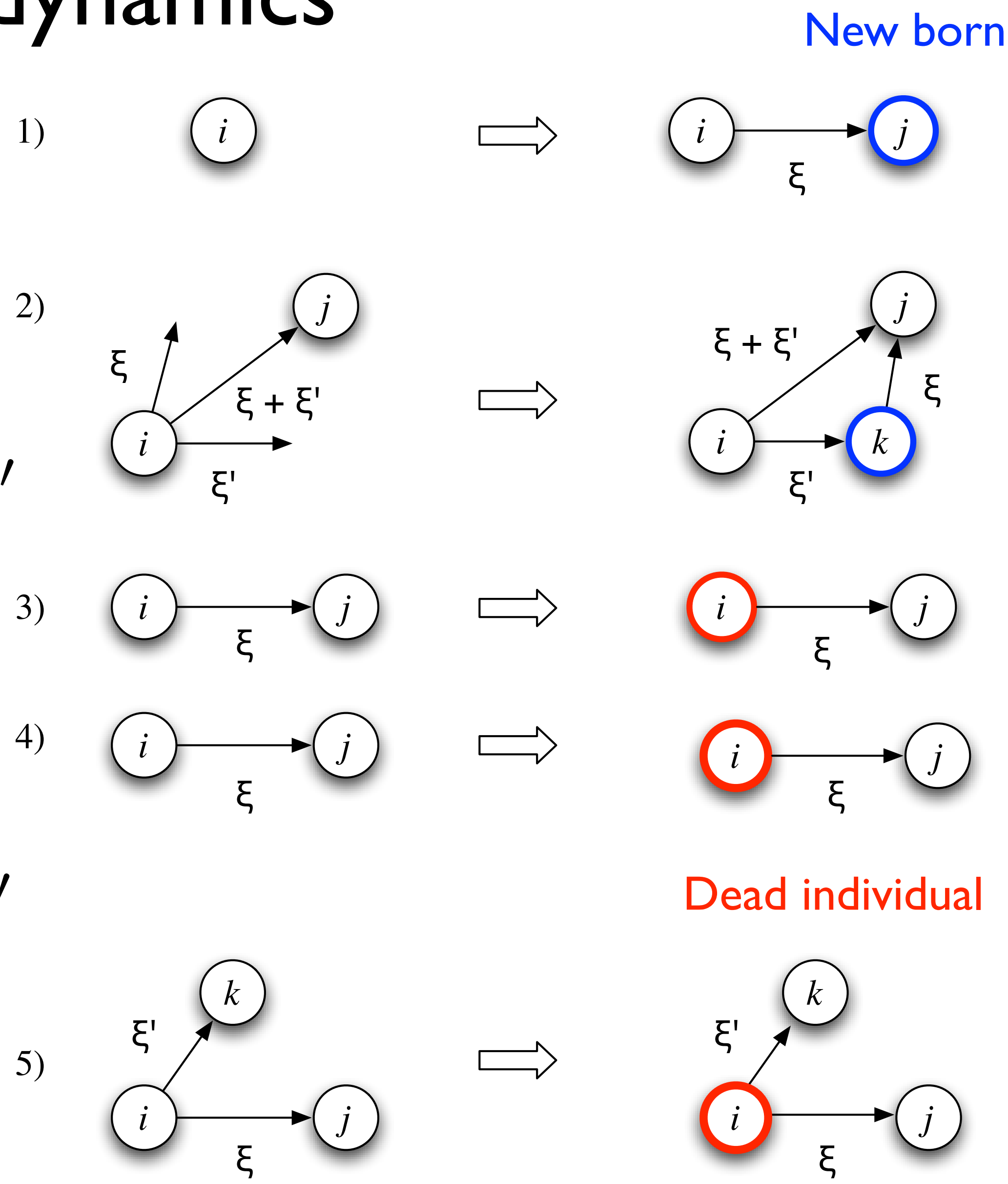
Birth rate is constant *b* (b_1 = 0)

Death rate depends on local density (d_1 > 0)

$$
\begin{aligned}
\frac{d}{dt}C(\xi) = \;& 2bm(\xi)N \\
& + 2b\int m(\xi')C(\xi+\xi')d\xi' \\
& - 2dC(\xi) \\
& - 2d_1 w_c(\xi)C(\xi) \\
& - 2d_1 \int w_c(\xi')T(\xi,\xi')d\xi'
\end{aligned}
$$

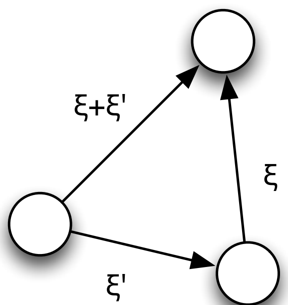
Geometrical interpretation of the pair density dynamics

$$\begin{aligned}\frac{dC(\xi)}{dt} &= 2bm(\xi)N \\ &+ 2b\int m(\xi')C(\xi+\xi')d\xi' \\ &- 2dC(\xi) \\ &- 2d_1 w_c(\xi)C(\xi) \\ &- 2d_1\int w_c(\xi')T(\xi,\xi')d\xi'\end{aligned}$$



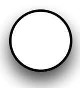
Moment closure

- Density of triplets has to be approximated using the singlet and the pair densities for the moment dynamics to be closed
- How triplet density can be approximated remains an open question
- Several candidates are proposed and evaluated which better explain simulations (Law and Dieckmann 2000, Law et al. 2003)

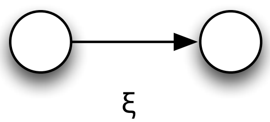


$$T(\xi, \xi') \approx \frac{C(\xi)C(\xi')}{N}$$

N

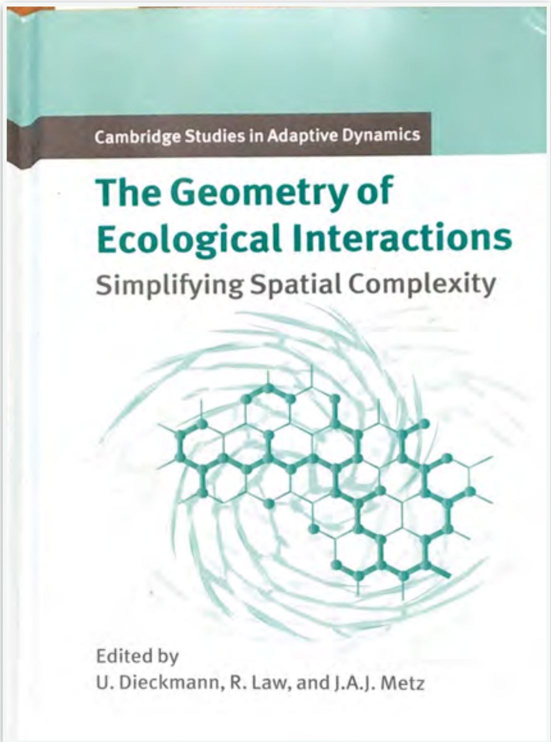


$C(\xi)$



The Method of Moments - How to derive the moment dynamics

- Definition of the moments (1st, 2nd, and 3rd, ...)
- Bookkeeping an individual's fate (birth, death, and movement) naturally leads to the moment dynamics

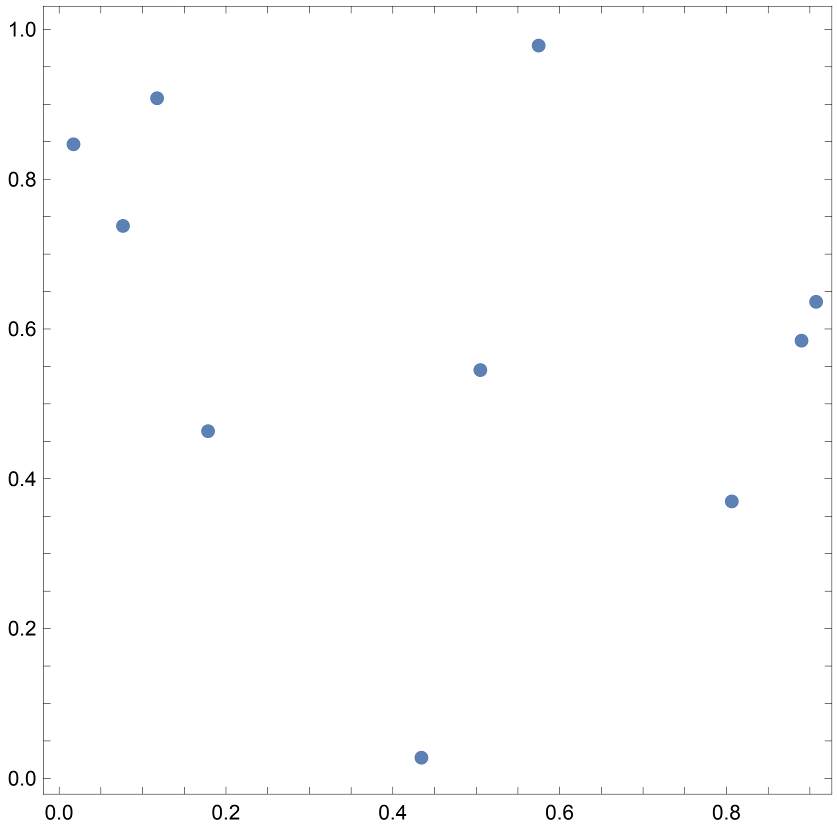


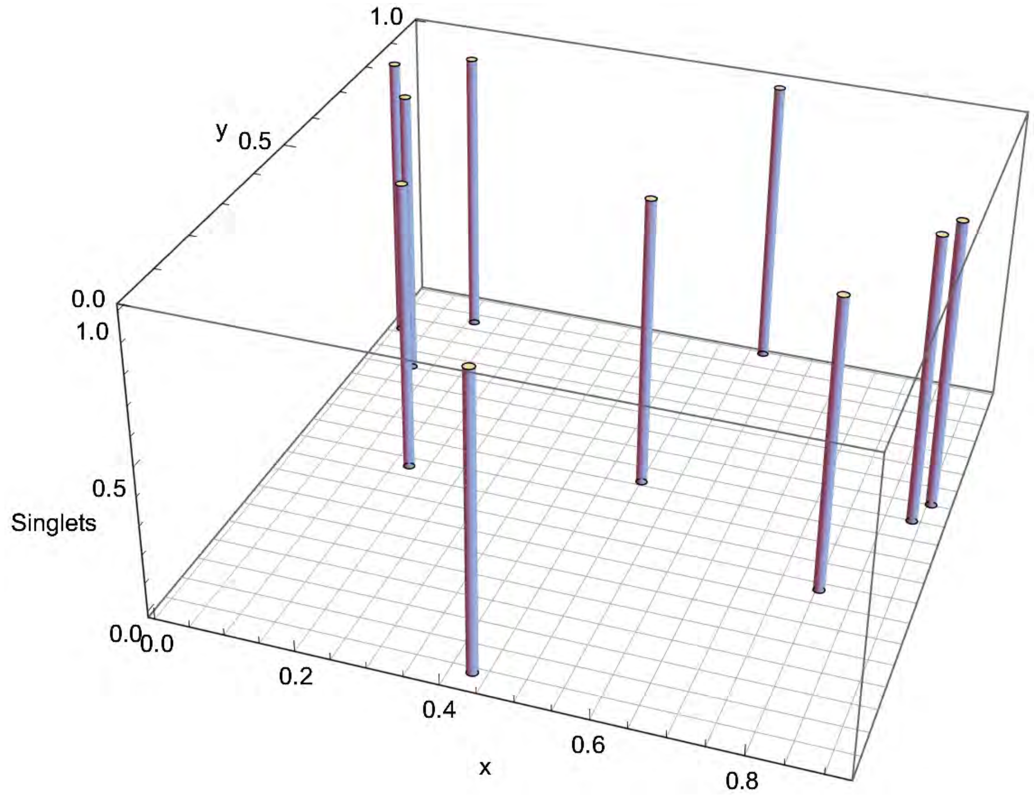
The Geometry of Ecological Interactions
Eds. Dieckmann, Law, Metz
Cambridge University Press 2000
Chapter 14, 21

Definitions of the moments

Assume a point pattern *p*: $$p(x) = \sum_{i=1}^{n} \delta(x - x_i)$$

$$\delta(x - x_i) = \delta_{x_i}(x)$$





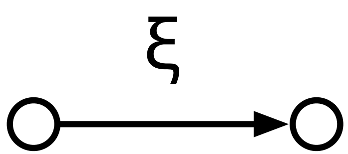
Definitions of the moments

The first moment of the pattern *p* is defined as the singlet density, *N*(*p*)

$$N(p) = \frac{1}{A}\int p(x)dx = \frac{n}{A} \qquad \text{Area } A$$

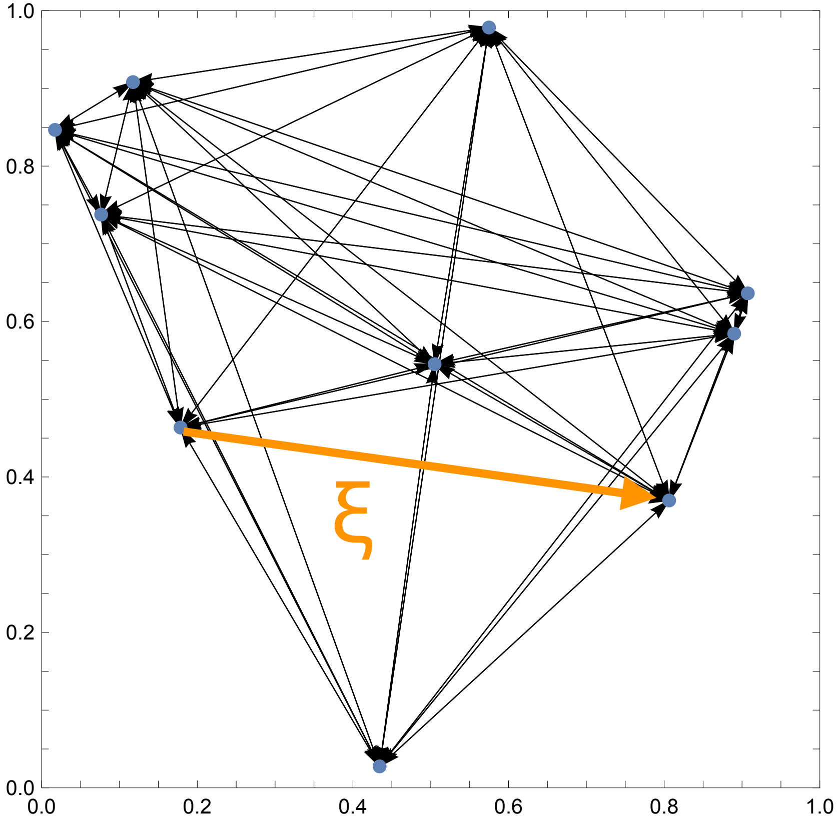
The second moment of the pattern *p* is defined as the density of pairs displaced by ξ, Pair density *C*(ξ, *p*)

$$C(\xi, p) = \frac{1}{A}\int p(x)[p(x+\xi) - \underline{\delta(\xi)}]dx$$



Self-pairs have been removed

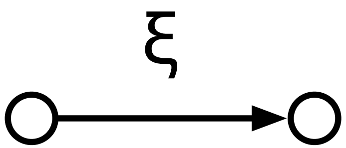
Definitions of the moments



A directed pair displaced by ξ can be picked up by

$$p(x)p(x+\xi)$$

Self-pairs ξ = 0 have to be removed

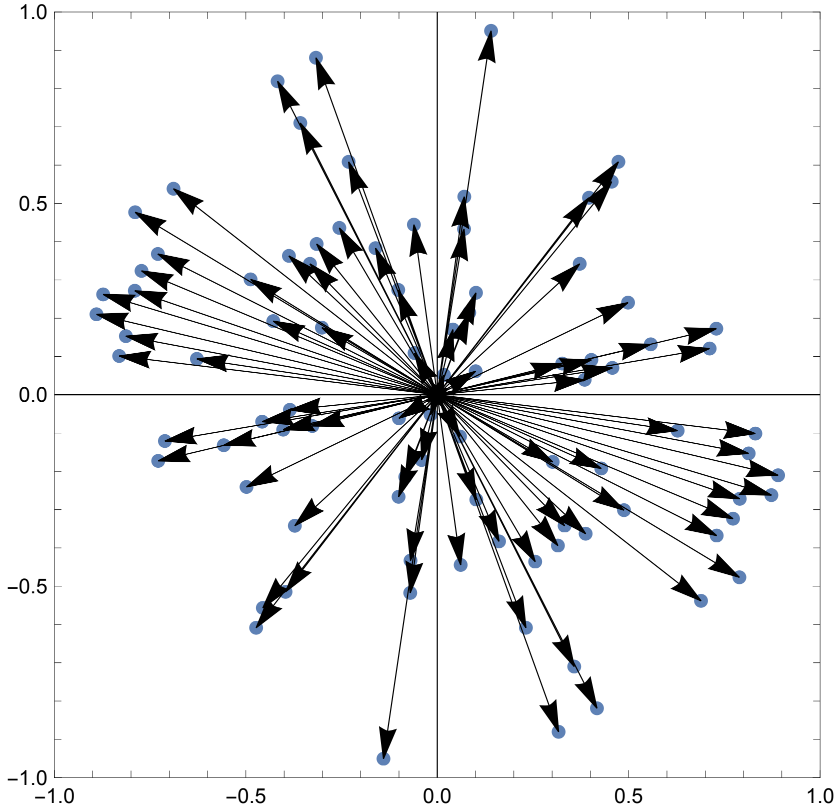


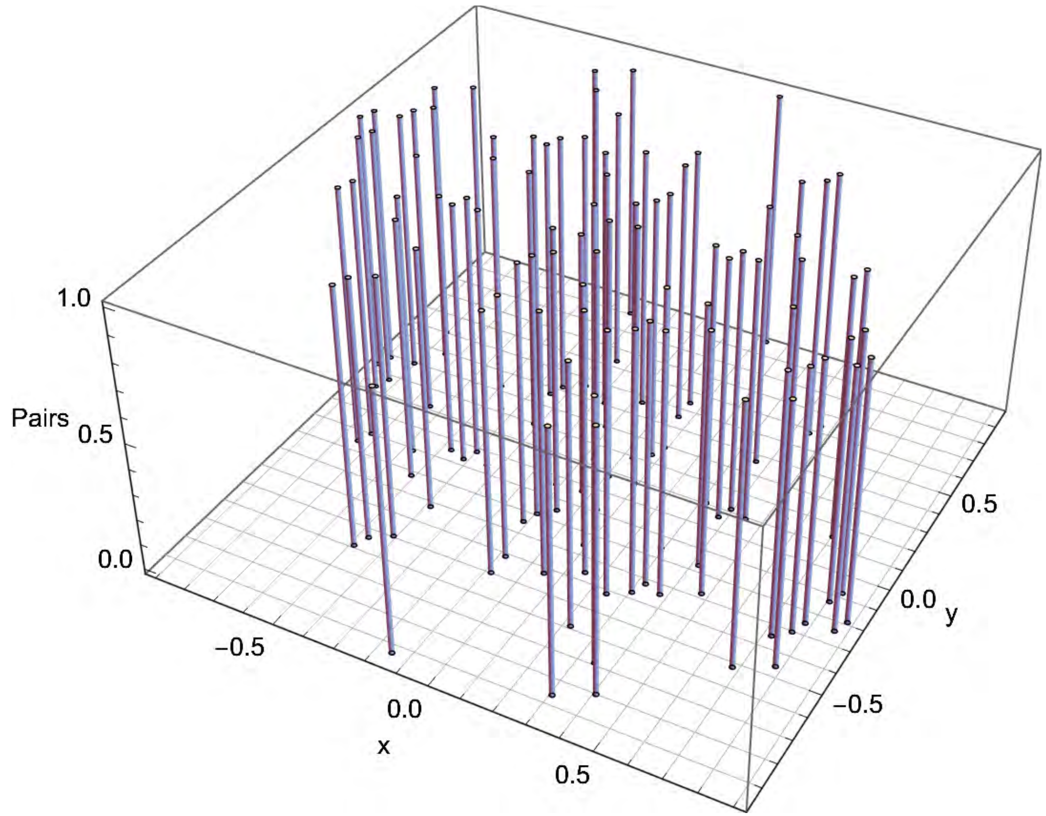
$$C(\xi,p) = \frac{1}{A}\int p(x)[p(x+\xi) - \delta(\xi)]dx$$

Definitions of the moments

The pair density $C(\xi, p)$

$$\int C(\xi,p)d\xi = N(p)(N(p)-1)$$



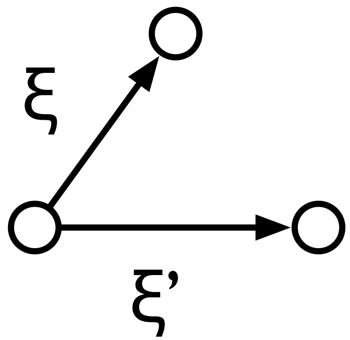


Definitions of the moments

The 3rd moment of the pattern *p* is defined as the density of triplets displaced by ξ and ξ', Triplet density *T*(ξ, ξ', *p*)

$$T(\xi, \xi', p) = \frac{1}{A}\int p(x)[p(x+\xi) - \delta(\xi)][p(x+\xi') - \delta(\xi') - \delta(\xi - \xi')]dx$$

Self-pairs and self-triplet have been removed



Averaged moments

The first moment averaged over realizations

$$N = \int N(p)P(p)dp$$

The second moment averaged over realizations

$$C(\xi) = \int C(\xi, p)P(p)dp$$

where *P*(*p*) is the probability density that a pattern *p* is realized

The pattern dynamics

Point pattern *p* dynamically changes and its probability density *P*(*p*) obeys the pattern dynamics

$$\frac{d}{dt}P(p) = \int \left[w(p|p')P(p') - w(p'|p)P(p)\right] dp'$$

w(*p*' | *p*) is the transition rate that the pattern *p* changes to *p*'

In ecology, the pattern *p* changes to *p*' either by birth, death and movement of an individual

The transition rate

The transition rate *w*(*p*' | *p*) is explicitly given as

$$
\begin{aligned}
w(p'|p) = &\iint \underline{B(x, x', p)} p(x) \Delta(p + \delta_{x'} - p') dx dx' \\
&+ \int \underline{D(x, p)} p(x) \Delta(p - \delta_x - p') dx \\
&+ \iint \underline{M(x, x', p)} p(x) \Delta(p - \delta_x + \delta_{x'} - p') dx dx'
\end{aligned}
$$

where Δ is the generalized delta function (functional)

Birth, death, and movement events

Birth rate (an individual at *x* gives birth to an individual at *x*'):

$$B(x, x', p) =$$
$$\left[b - b_1 \int w_c(x'' - x)[p(x) - \delta_x(x'')]dx'' \right] m^b(x' - x)$$

Death rate (an individual at *x* dies):

$$D(x, p) = d + d_1 \int w_c(x' - x)[p(x) - \delta_x(x')]dx'$$

Movement rate (an individual at *x* moves to *x*')

$$M(x, x', p) = m(x' - x)$$

Derivation of the 1st moment dynamics

$$N = \int N(p)P(p)dp$$

$$\frac{d}{dt}N = \int N(p)\frac{d}{dt}P(p)dp$$

$$\frac{d}{dt}N = \int N(p)\int \left[w(p|p')P(p') - w(p'|p)P(p)\right] dp' dp$$

$$\frac{d}{dt}N = \int \underbrace{\left\{\int \left[N(p') - N(p)\right] w(p'|p)dp'\right\}}_{a_b(p) + a_d(p) + a_m(p)} P(p)dp$$

Derivation of the 1st moment dynamics: contribution of birth

A = 1

$$a_b(p) = \int [N(p') - N(p)]$$

$$\times \iint B(x, x', p)p(x)\Delta(p + \delta_{x'} - p')dxdx'dp'$$

$$= \iint \underline{[N(p + \delta_{x'}) - N(p)]}B(x, x', p)p(x)dxdx'$$

$$= \iint B(x, x', p)p(x)dxdx' \qquad N(p + \delta_{x'}) - N(p) = 1$$

$$= \int \left[b - b_1 \int w_c(x'' - x)\left\{p(x'') - \delta_x(x'')\right\}dx''\right]p(x)dx$$

Derivation of the 1st moment dynamics: contribution of birth

$$a_b(p) = \int \left[b - b_1 \int w_c(x'' - x) \left\{ p(x'') - \delta_x(x'') \right\} dx'' \right] p(x) dx$$

$$= bN(p) - b_1 \iint w_c(x'' - x) p(x) \left\{ p(x'') - \delta_x(x'') \right\} dx dx''$$

$$= bN(p) - b_1 \int w_c(\xi) C(\xi, p) d\xi \qquad\qquad \xi = x'' - x$$

Derivation of the 1st moment dynamics: contributions of death

A = 1

$$
\begin{aligned}
a_d(p) &= \iint [N(p') - N(p)] \\
&\times D(x,p)p(x)\Delta(p - \delta_x - p')dxdp' \\
&= \int \underline{[N(p - \delta_x) - N(p)]} D(x,p)p(x)dx \\
&= -\int D(x,p)p(x)dx \qquad N(p-\delta_x) - N(p) = -1 \\
&= -\int \left[d + d_1 \int w_c(x'-x)[p(x') - \delta_x(x')]dx' \right] p(x)dx \\
&= -dN(p) - d_1 \int w_c(\xi)C(\xi,p)d\xi \qquad \xi = x' - x
\end{aligned}
$$

Derivation of the 1st moment dynamics: contributions of movement

$$
\begin{aligned}
a_m(p) &= \iint [N(p') - N(p)] \\
&\times M(x, x', p) p(x) \Delta(p - \delta_x + \delta_{x'} - p') dx dx' dp' \\
&= \int \underline{[N(p - \delta_x + \delta_{x'}) - N(p)]} M(x, x', p) p(x) dx dx' \\
&= 0 \qquad N(p - \delta_x + \delta_{x'}) - N(p) = 0
\end{aligned}
$$

The 1st moment dynamics

$$\frac{d}{dt}N = \int \{a_b(p) + a_d(p) + a_m(p)\} P(p) dp$$

$$\begin{aligned}\frac{d}{dt}N &= bN - b_1 \int w_c(\xi) C(\xi) d\xi - dN - d_1 \int w_c(\xi) C(\xi) d\xi \\ &= (b-d)N - (b_1 + d_1) \int w_c(\xi) C(\xi) d\xi\end{aligned}$$

Logistic model when $C(\xi) = N^2$

Derivation of the 2nd moment dynamics

$$C(\xi) = \int C(\xi, p) P(p) dp$$

$$\begin{aligned}
\frac{d}{dt} C(\xi) &= \int C(\xi, p) \frac{d}{dt} P(p) dp \\
&= \int C(\xi, p) \int [w(p|p') P(p') - w(p'|p) P(p)] dp' dp \\
&= \iint \{C(\xi, p') - C(\xi, p)\} w(p'|p) dp' P(p) dp \\
&= \int \left\{ a^{(b)}(\xi, p) + a^{(d)}(\xi, p) + a^{(m)}(\xi, p) \right\} P(p) dp
\end{aligned}$$

Term birth	Term death	Term movement

Derivation of the 2nd moment dynamics

Term birth

$$a^{(b)}(\xi,p) = \int \{C(\xi,p') - C(\xi,p)\} \iint B(x,x',p)p(x)\Delta(p+\delta_{x'}-p')dxdx'dp'$$

$$= \iint \underline{\{C(\xi,p+\delta_{x'}) - C(\xi,p)\}} B(x,x',p)p(x)dxdx'$$

$$C(\xi,p+\delta_{x'}) = \int (p(x)+\delta_{x'}(x))[p(x+\xi)+\delta_{x'}(x+\xi)-\delta(\xi)]dx$$

$$= \int p(x)[p(x+\xi)-\delta(\xi)]dx + \int p(x)\delta_{x'}(x+\xi)dx$$

$$+ \int \delta_{x'}(x)p(x+\xi)dx + \int \delta_{x'}(x)\delta_{x'}(x+\xi)dx - \int \delta_{x'}(x)\delta(\xi)dx$$

$$= C(\xi,p) + p(x'-\xi) + p(x'+\xi) + \delta(\xi) - \delta(\xi)$$

$$= C(\xi,p) + p(x'-\xi) + p(x'+\xi)$$

Derivation of the 2nd moment dynamics

Term birth

$$
\begin{aligned}
a^{(b)}(\xi, p) = &+ b \int C(\xi' + \xi, p) m^{(b)}(\xi') d\xi' \\
&+ b \times m^{(b)}(-\xi) N(p) \\
&- b' \iint w(\xi'') m^{(b)}(\xi') T(\xi'', \xi' - \xi, p) d\xi'' d\xi' \\
&- b' \times m^{(b)}(\xi) \int w(\xi'') C(\xi'', p) d\xi'' \\
&- b' \int w(\xi'') m^{(b)}(\xi + \xi'') C(\xi'', p) d\xi'' \\
&+ \langle \xi \to -\xi \rangle
\end{aligned}
$$

Derivation of the 2nd moment dynamics

"Term death" and "Term movement" can be also derived after careful bookkeeping an individual's death and movement

Dynamics of the pair density C(ξ)

How is C(ξ) generated and lost?

$$
\begin{aligned}
\frac{d}{dt}C(\xi) = & + b \times m^{(b)}(-\xi)N \\
& + b \int m^{(b)}(\xi')C(\xi'+\xi)d\xi' \\
& - b' \times m^{(b)}(\xi) \int w(\xi'')C(\xi'')d\xi'' \\
& - b' \int m^{(b)}(\xi+\xi'')w(\xi'')C(\xi'')d\xi'' \\
& - b' \iint m^{(b)}(\xi')w(\xi'')T(\xi'',\xi'-\xi)d\xi''d\xi' \\
& - d \times C(\xi) \\
& - d' \times w(\xi)C(\xi) \\
& - d' \int w(\xi')T(\xi,\xi')d\xi' \\
& - \int m(x')dx'C(\xi) \\
& + \int m(-\xi')C(\xi+\xi')d\xi' \\
& + \langle \xi \to -\xi \rangle
\end{aligned}
$$

birth

death

movement

Dynamics of the pair density $C(\xi)$

Each term of the pair dynamics can be interpreted geometrically

- Terms birth (the pair ξ is generated or generation is inhibited)
  - The singlet *i* gives birth to an individual relative at $-\xi$ with b
  - The point *i* in the pair $\xi + \xi'$ gives birth to an individual relative at ξ' with b
  - Competition within the pair ξ'' inhibits a birth from the point *i* relatively at ξ
  - Competition within the pair ξ'' inhibits a birth from the point *i* relatively at $\xi + \xi''$
  - Competition within the pair ξ'' inhibits a birth from the point *i* relative at ξ' in the triplet $(\xi'', \xi' - \xi)$

Dynamics of the pair density $C(\xi)$

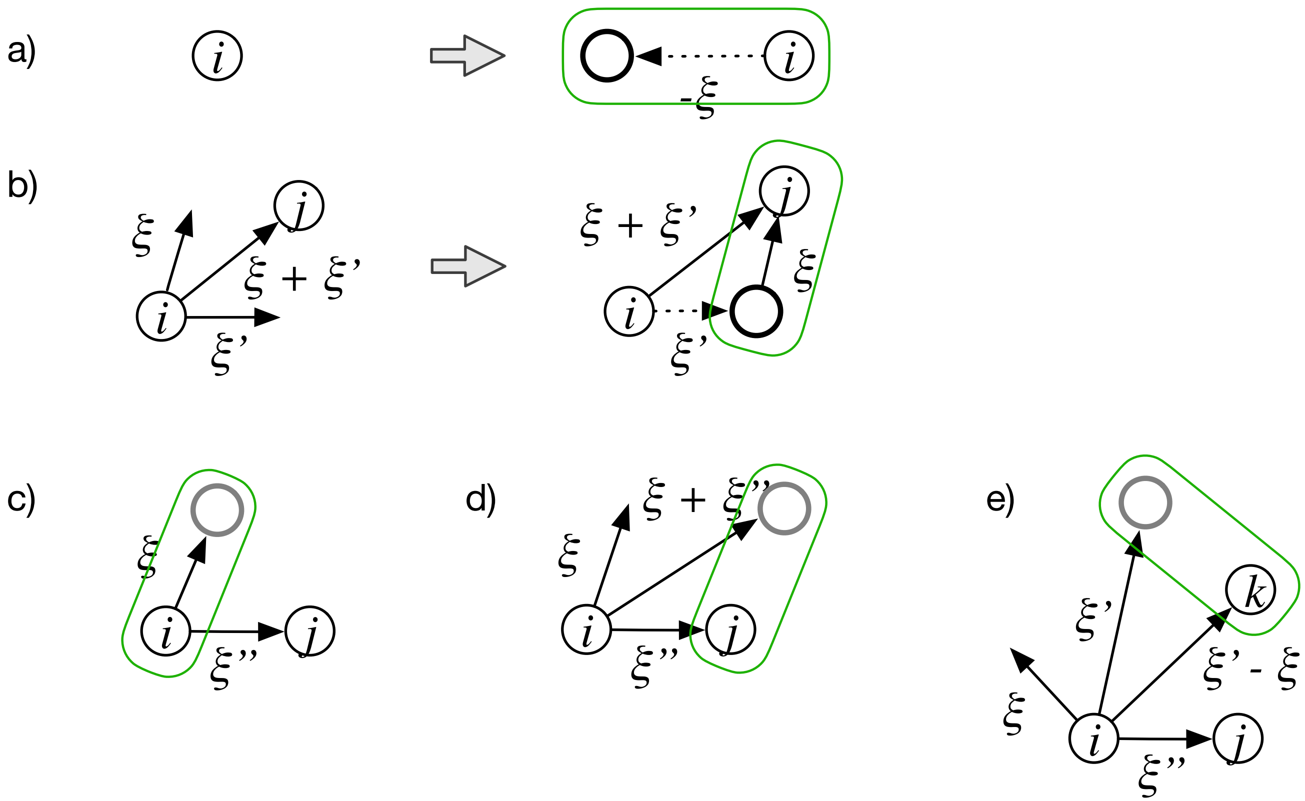
Each term of the pair dynamics can be interpreted geometrically

- Terms death (the pair ξ is lost)
  - The point i in the pair ξ dies with d
  - The point i in the pair ξ dies by competition within the pair
  - The point i in the triplet (ξ, ξ') dies by competition with the point k in the triplet
- Terms movement
  - The point i or j moves and the pair ξ is lost
  - The point j in the pair $\xi + \xi'$ moves by $-\xi'$ and the pair ξ is generated

Dynamics of the pair density C(ξ)

Each term of the pair dynamics can be geometrically interpreted

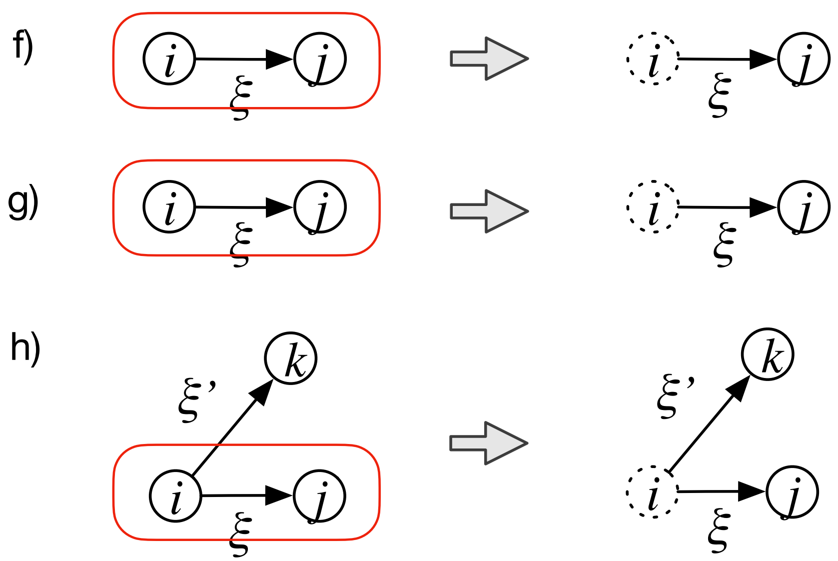
Terms birth



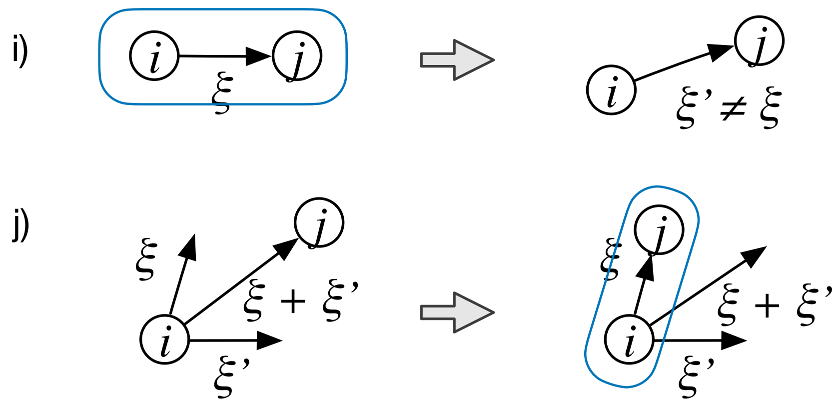
Dynamics of the pair density C(ξ)

Each term of the pair dynamics can be geometrically interpreted

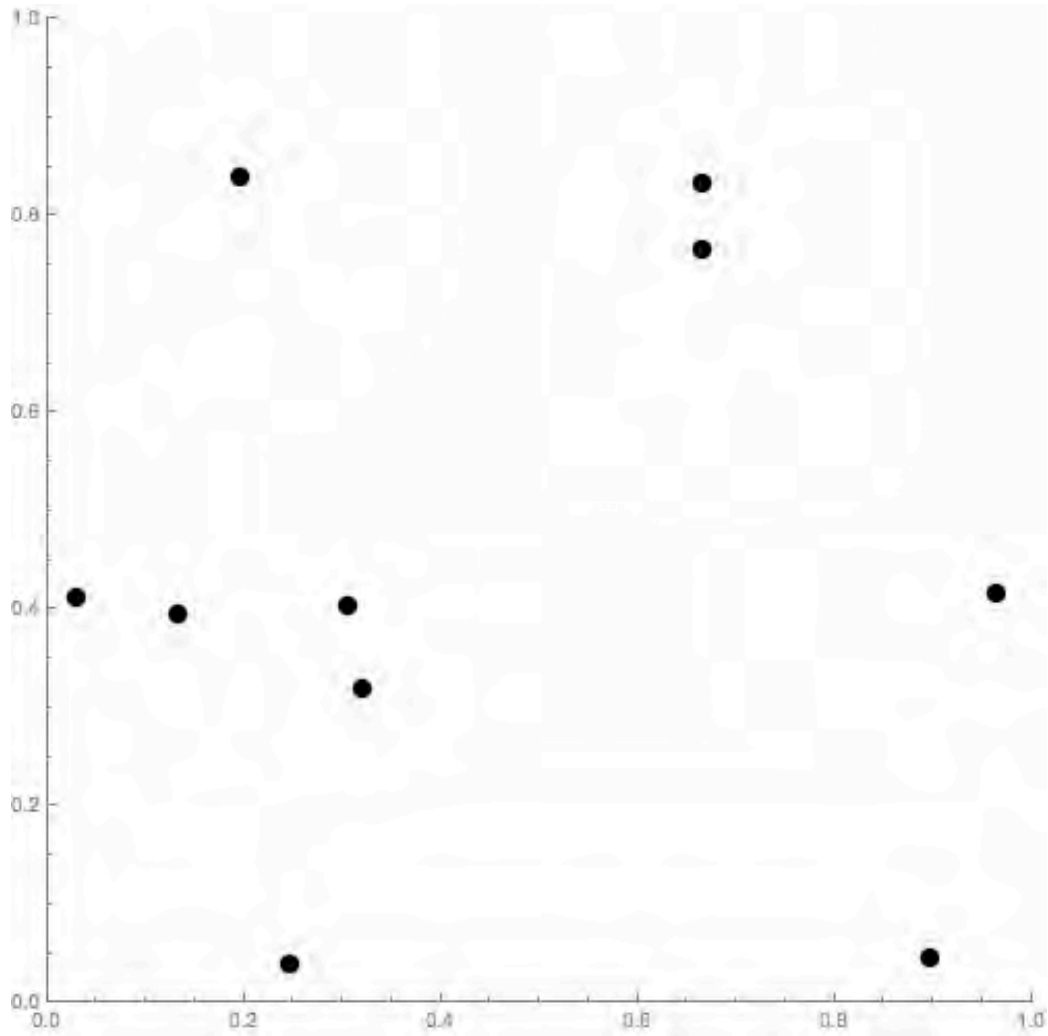
Terms death



Terms movement



Spatial logistic growth model as a point pattern dynamics



Competition range σ_c = 1.0, Dispersal range σ_m = 0.03

Dynamics of the moments

Simple birth and death, no density dependency (b_1 = d_1 = 0)

$$\frac{d}{dt}N = (b-d)N$$

$$\begin{aligned}\frac{d}{dt}C(\xi) = &+ b \times m^{(b)}(-\xi)N \\ &+ b\int m^{(b)}(\xi')C(\xi'+\xi)d\xi' \\ &- d \times C(\xi) \\ &- \int m(x')dx' C(\xi) \\ &+ \int m(-\xi')C(\xi+\xi')d\xi' \\ &+ \langle \xi \to -\xi \rangle\end{aligned}$$

Dynamics of the moments

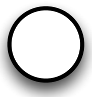
No birth and no death (*b* = *d* = 0)

$$N = \text{const.}$$

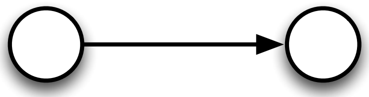
$$\begin{aligned}\frac{d}{dt}C(\xi) = &- \int m(x')dx'C(\xi) \\ &+ \int m(-\xi')C(\xi+\xi')d\xi' \\ &+ \langle \xi \to -\xi \rangle\end{aligned}$$

Quantification of point pattern

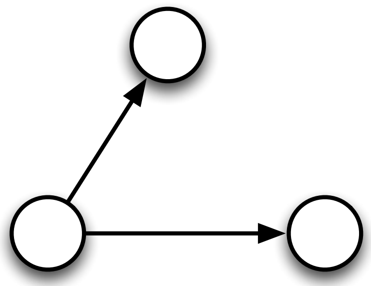
- 1st order (Number of points)
- 2nd order (Number of pairs displaced with a certain distance)
- 3rd order (Number of triplets with a certain configuration)



Number of points
as a scalar



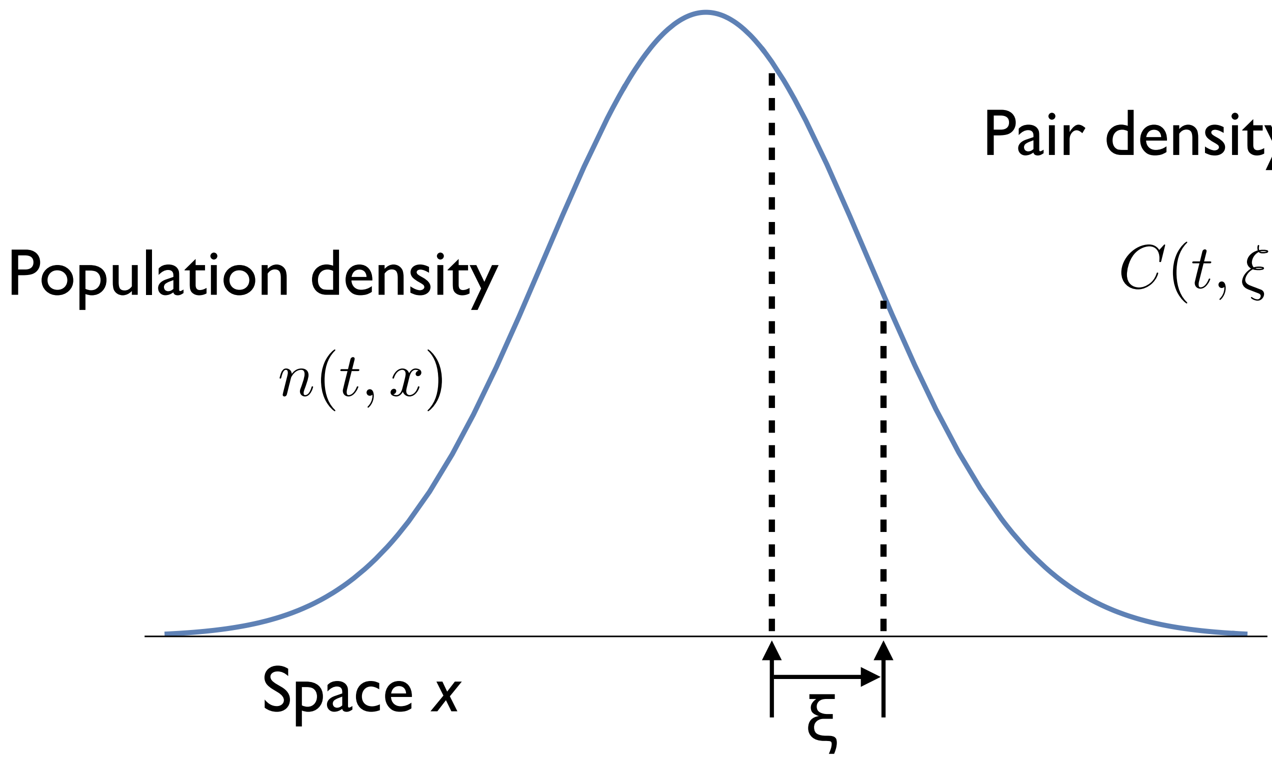
Number of pairs as a
function of a vector



Number of triplets as a
function of two vectors

How is the Method of Moments related to other models (e.g., RD)

- 1st order (Number of points) as the total density
- 2nd order (Number of pairs displaced with a certain distance) lacks information of points' location



Pair density ξ

$$C(t,\xi) = \int n(t,x)n(t,x+\xi)dx$$

$$n(t,x) \Leftrightarrow C(t,\xi)$$

?

Application to competition, predator-prey models, epidemic models, etc.

- ANY non-spatial population models as ODE can be readily extended to point pattern dynamics
  - Lotka-Volterra competition/predator-prey model
  - Expressions have been derived (Dieckmann and Law 2000)
- Epidemic dynamics SIS, SIR, SEIR, etc., where individuals' "status" changes + birth, death, and movement
- With individuality explicitly considered, can we obtain novel insights that models without individuality fail to capture?

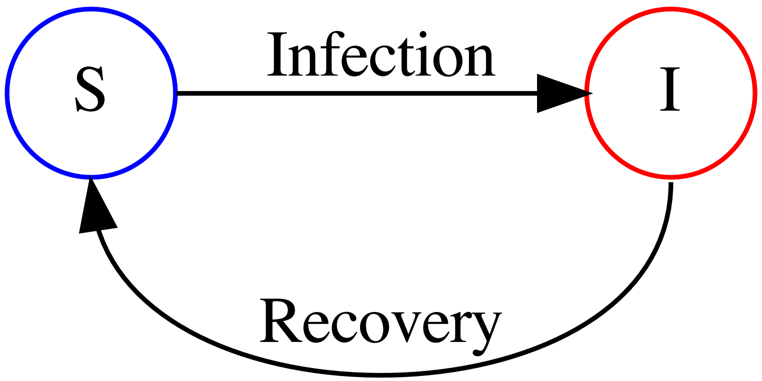
Spatial SIS model as point pattern dynamics

Hamada and Takasu J theor biol 2019
doi.org/10.1016/j.jtbi.2019.02.005

- SIS model: Susceptible becomes Infectious becomes Susceptible
- An individual is a point; points do not move and no birth and no death occur
- Status of a point is *S* or *I*
- An infectious *I* infects nearby *S* with the infection rate β(*d*) that depends on the distance *d* to *S*
- An infectious *I* recovers to *S* with the recovery rate γ

Classical SIS model as ODE (non spatial)

- Essentially the same as the classical logistic growth model



$$\frac{dS}{dt} = -\beta SI + \gamma I$$

$$\frac{dI}{dt} = \beta SI - \gamma I$$

$$\frac{dI}{dt} = (\beta N - \gamma)\left(1 - \frac{I}{N - \gamma/\beta}\right) I \qquad N = S + I \text{ const.}$$

The disease is endemic when $\beta N/\gamma > 1$

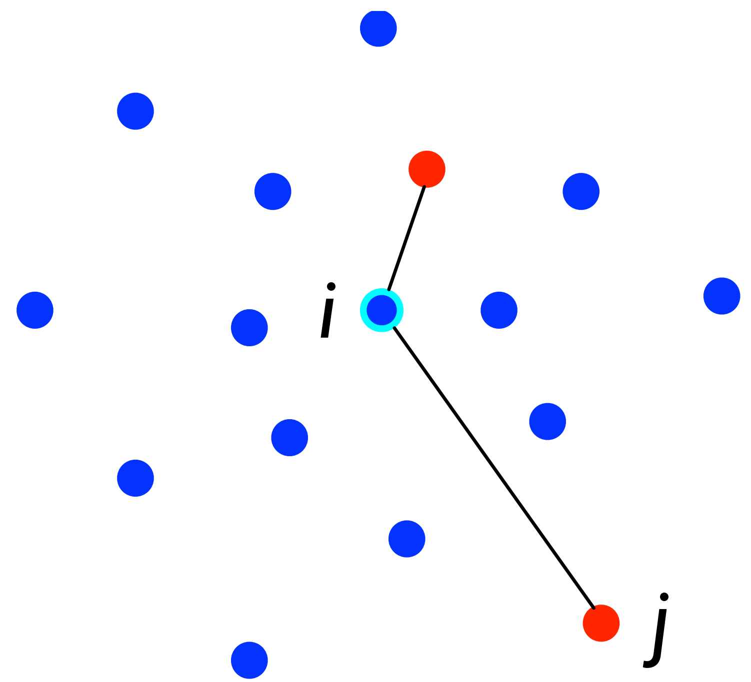
Infection rate depends on the distance to *I*

- The rate of a focal *S* to be infected is given as the sum of infection rates to *I* in neighbor
- Each *S* has its own rate to become *I*

The rate of a focal individual *i* in *S* to be *I*

$$B_i(S \to I) = \sum_{j \in I} \beta(d_{ij})$$

$$\text{E.g. } \beta(d) = \frac{\beta_0}{2\pi\sigma_I^2} \exp\left[-\frac{d^2}{2\sigma_I^2}\right]$$

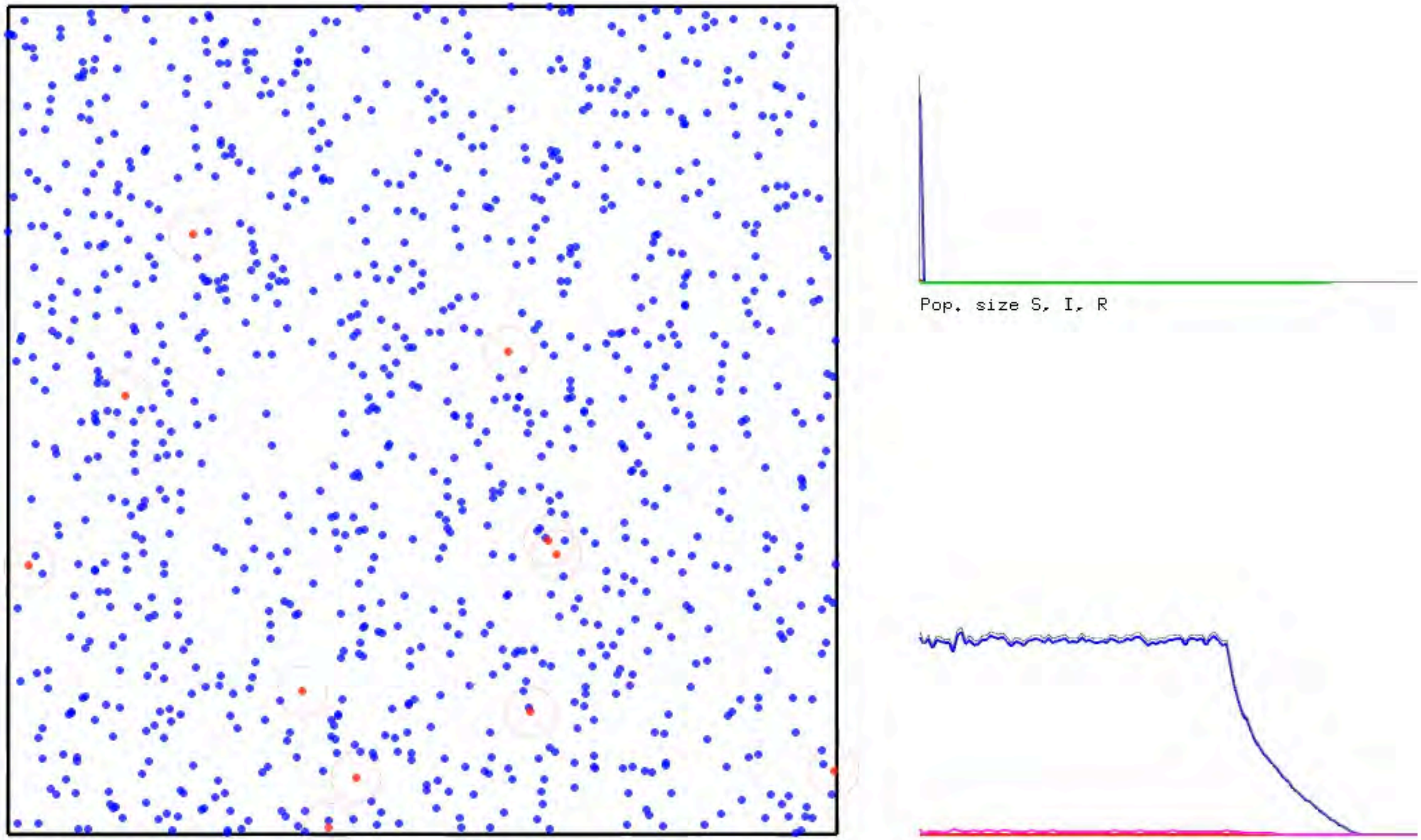


S in blue, *I* in red

Gillespie algorithm for the SIS p.p. dynamics

- Calculate rates of change (infection and recovery) for each individual
  - Possible status changes: *S* to *I* and *I* to *S*
- Determine the inter-event time Δt ~ Exponentially distributed with the total rate
- Advance the time by Δt
- Choose an event among possible events (a point *S* becomes *I*, or a point *I* becomes *S*)
- Repeat the above steps

SIS model simulation 1



Direct algorithm

PCF S-S, I-I, S-I (I-S), and all pairs

Space size L = 1, Range competition = 0.02, Range dispersal = 0.02, Range infection = 0.01, Beta = 1.2, Gamma = 5.1, CELLS = 12

t = 2.29109e-05, pop size total = 1010, S = 999, I = 11, R = 0

Analytical model of the stochastic SIS point pattern dynamics

- The point pattern is static (no birth, death, and movement) but "mark" of a point stochastically changes between *S* and *I*
- Size of the state space Ω is 2^n (*n*: Number of points)
- Status of the marked point pattern stochastically changes in the state space Ω (too large!)
- We focus on singlets and pairs

Analytical model of the stochastic SIS point pattern dynamics

- Each point is indexed by *i* (*i* = 1, 2, 3, ..., *n*)
- There are *n*(*n*–1) directed pairs. Each directed pair is indexed by *i* and *j* (*i* ≠ *j*) or *l* (*l* = 1, 2, 3, ..., *n*(*n*–1))

$P_{iS},\ P_{iI}$: Probability that point *i* is in *S* and *I*, respectively

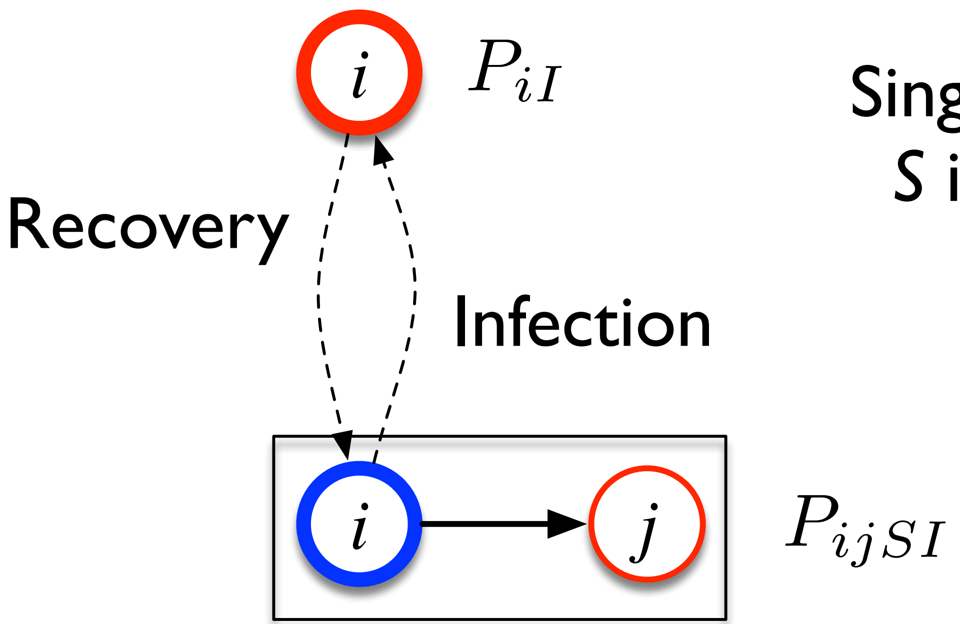
$P_{ijSS},\ P_{ijSI},\ P_{ijIS},\ P_{ijII}$: Probability that directed pair *i*-*j* is in *S*-*S*, *S*-*I*, *I*-*S*, and *I*-*I*, respectively

$P_{\xi_{ij},SS} \quad \xi_{ij} = x_j - x_i$

$P_{\xi_l,SS}$

Transitions of singlet status

Status of a focal singlet *i* changes either by infection or recovery



Singlets in circle:
S in blue and *I* in red

$j \neq i$

Pairs in rectangle

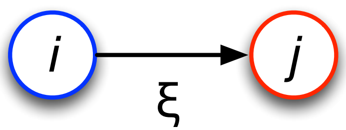
Singlet dynamics

- A point *i* in *S* becomes *I* with the rate $B_i(S \to I)$ (infection from points $j \neq i$ in *I*)
- A point *i* in *I* becomes *S* with the recovery rate $B_i(I \to S) = \gamma$

$$B_i(S \to I) = \sum_{j \neq i} \beta(|-\xi_{ij}|) P_{ijSI} \qquad \xi_{ij} = x_j - x_i$$

$$\frac{d}{dt} P_{iS} = -\sum_{j \neq i} \beta(|-\xi_{ij}|) \underline{P_{ijSI}} + \gamma P_{iI}$$

Pair probability is involved



Singlet dynamics

- Averaged singlet probabilities as mean-field dynamics

$$\langle P_S \rangle = \frac{1}{n} \sum_{i=1}^{n} P_{iS} \qquad \langle P_I \rangle = \frac{1}{n} \sum_{i=1}^{n} P_{iI}$$

$$\frac{d}{dt} \langle P_S \rangle = -\frac{1}{n} \sum_{i=1}^{n} \sum_{j \neq i} \beta(| - \xi_{ij}|) P_{ijSI} + \gamma \langle P_I \rangle$$

If we assume $P_{ijSI} = P_{iS} \times P_{jI} = \langle P_S \rangle \langle P_I \rangle$

$$\frac{d}{dt} \langle P_S \rangle = -\beta \langle P_S \rangle \langle P_I \rangle + \gamma \langle P_I \rangle$$

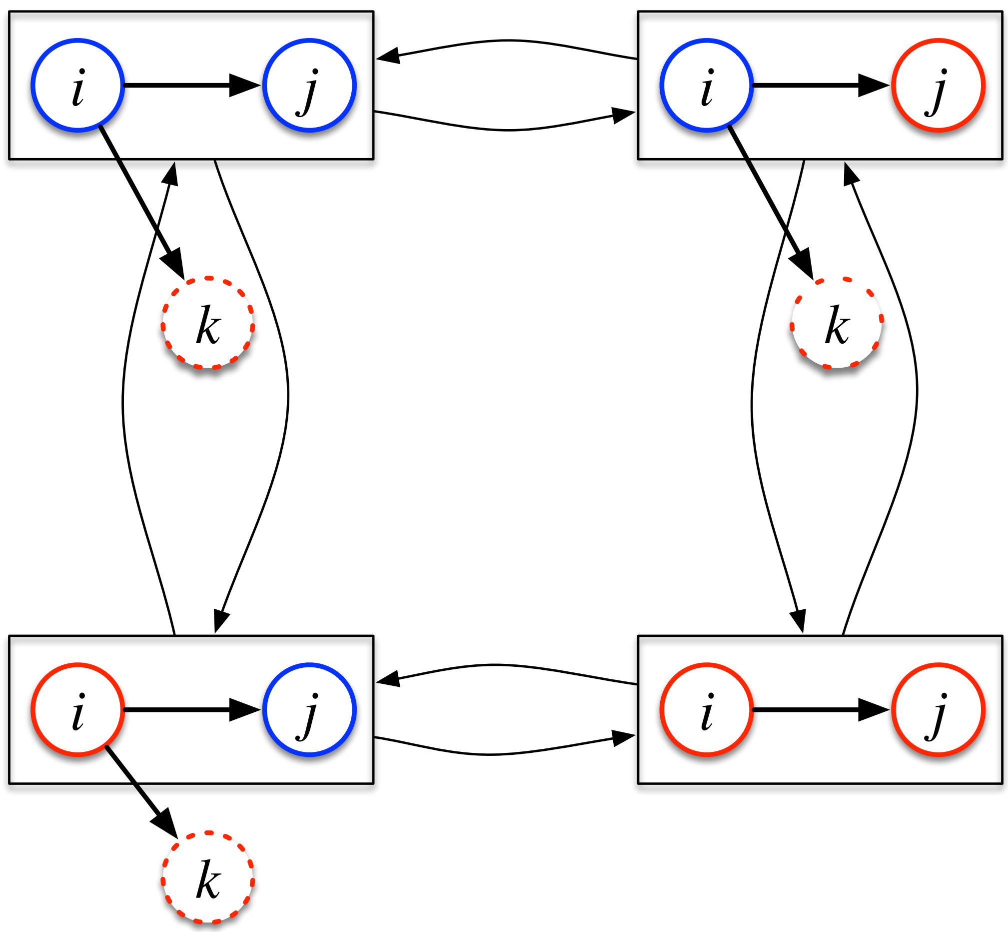
ODE model!

Pair dynamics

Status of a focal pair *i–j* changes either by infection or recovery of a singlet in the pair

Singlets in circle:
S in blue and *I* in red

Pairs in rectangle:
S-S, S-I, I-S, I-I

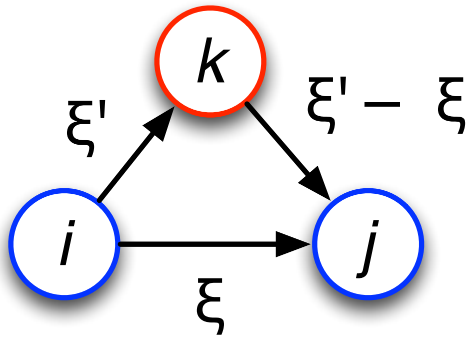


Pair dynamics

- Dynamics of the pair probability *S-S*

$$\frac{d}{dt}P_{ijSS} = \gamma P_{ijSI} + \gamma P_{ijIS} - \sum_{k \neq i,j} \beta(| - \xi_{ik}|)\underline{P_{ijkSSI}} - \sum_{k \neq i,j} \beta(| - \xi_{jk}|)\underline{P_{ijkSSI}}$$

Triplet probability is involved



Pair dynamics

- Dynamics of the pair probability *S-I* and *I-S*

$$\frac{d}{dt}P_{ijSI} = \gamma P_{ijII} - \gamma P_{ijSI} - \beta(|-\xi_{ij}|)P_{ijSI}$$
$$- \sum_{k\neq i,j} \beta(|-\xi_{ik}|)\underline{P_{ijkSII}} + \sum_{k\neq i,j} \beta(|-\xi_{jk}|)\underline{P_{ijkSSI}}$$

$$\frac{d}{dt}P_{ijIS} = \gamma P_{ijII} - \gamma P_{ijIS} - \beta(|\xi_{ij}|)P_{ijIS}$$
$$- \sum_{k\neq i,j} \beta(|-\xi_{jk}|)\underline{P_{ijkISI}} + \sum_{k\neq i,j} \beta(|-\xi_{ik}|)\underline{P_{ijkSSI}}$$

Pair dynamics

- Dynamics of the pair probability *I-I*

$$\frac{d}{dt}P_{ijII} = -2\gamma P_{ijII} + \beta(|-\xi_{ij}|)P_{ijSI} + \beta(|\xi_{ij}|)P_{ijIS}$$
$$+ \sum_{k\neq i,j} \beta(|-\xi_{ik}|)\underline{P_{ijkSSI}} + \sum_{k\neq i,j} \beta(|-\xi_{jk}|)\underline{P_{ijkISI}}$$

Pair dynamics

$$\frac{d}{dt}P_{ijSS} = \gamma P_{ijSI} + \gamma P_{ijIS} - \sum_{k\neq i,j} \beta_{ik}\underline{P_{ijkSSI}} - \sum_{k\neq i,j} \beta_{jk}\underline{P_{ijkSSI}}$$

$$\frac{d}{dt}P_{ijSI} = \gamma P_{ijII} - \gamma P_{ijSI} - \beta_{ij}P_{ijSI} - \sum_{k\neq i,j} \beta_{ik}\underline{P_{ijkSII}} + \sum_{k\neq i,j} \beta_{jk}\underline{P_{ijkSSI}}$$

$$\frac{d}{dt}P_{ijIS} = \gamma P_{ijII} - \gamma P_{ijIS} - \beta_{ij}P_{ijIS} - \sum_{k\neq i,j} \beta_{jk}\underline{P_{ijkISI}} + \sum_{k\neq i,j} \beta_{ik}\underline{P_{ijkSSI}}$$

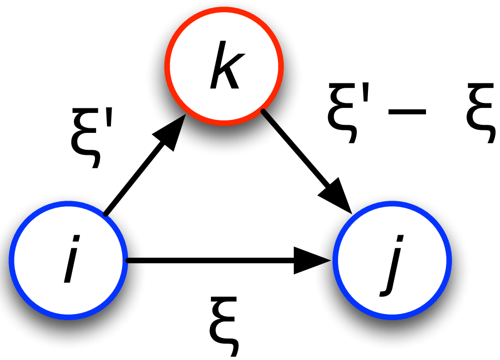
$$\frac{d}{dt}P_{ijII} = -2\gamma P_{ijII} + \beta_{ij}P_{ijSI} + \beta_{ij}P_{ijIS} + \sum_{k\neq i,j} \beta_{ik}\underline{P_{ijkSSI}} + \sum_{k\neq i,j} \beta_{jk}\underline{P_{ijkISI}}$$

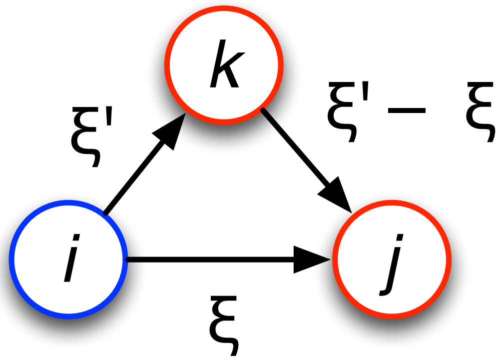
$$\beta_{ij} = \beta(|-\xi_{ij}|) = \beta(|\xi_{ij}|)$$

Moment closure

- The dynamics is not closed; triplet probabilities appear
- Triplet probabilities are approximated as follows

$$P_{ijkSSI} = \frac{P_{\xi,SS}P_{\xi',SI}}{\langle P_S \rangle} \qquad P_{ijkSII} = \frac{P_{\xi,SI}P_{\xi',SI}}{\langle P_S \rangle}$$





Pair dynamics after closure

$$\frac{d}{dt}P_{ijSS} = \gamma P_{ijSI} + \gamma P_{ijIS} - 2\frac{P_{ijSS}}{P_S}\boxed{\sum_{k\neq i,j}\beta_{ik}P_{ikSI}}$$

$$\frac{d}{dt}P_{ijSI} = \gamma P_{ijII} - \gamma P_{ijSI} - \beta_{ij}P_{ijSI} - \frac{P_{ijSI}}{P_S}\boxed{\sum_{k\neq i,j}\beta_{ik}P_{ikSI}} + \frac{P_{ijSS}}{P_S}\boxed{\sum_{k\neq i,j}\beta_{ik}P_{ikSI}}$$

$$\frac{d}{dt}P_{ijIS} = \gamma P_{ijII} - \gamma P_{ijIS} - \beta_{ij}P_{ijIS} - \frac{P_{ijIS}}{P_S}\boxed{\sum_{k\neq i,j}\beta_{ik}P_{ikSI}} + \frac{P_{ijSS}}{P_S}\boxed{\sum_{k\neq i,j}\beta_{ik}P_{ikSI}}$$

$$\frac{d}{dt}P_{ijII} = -2\gamma P_{ijII} + \beta_{ij}P_{ijSI} + \beta_{ij}P_{ijIS} + 2\frac{P_{ijSI}}{P_S}\boxed{\sum_{k\neq i,j}\beta_{ik}P_{ikSI}}$$

$$\beta_{ij} = \beta(|-\xi_{ij}|) = \beta(|\xi_{ij}|)$$

Pair dynamics after closure

$$\boxed{\sum_{k\neq i,j} \beta_{ik} P_{ikSI}} \approx \frac{1}{n}\sum_{i=1}^{n}\sum_{k\neq i,j} \beta_{ik} P_{ikSI} = \gamma \langle P_I \rangle$$

Mean field over *i*

Singlet equilibrium

$$\frac{d}{dt}\langle P_S \rangle = -\frac{1}{n}\sum_{i=1}^{n}\sum_{j\neq i} \beta(|-\xi_{ij}|) P_{ijSI} + \gamma \langle P_I \rangle = 0$$

Pair dynamics after closure

$$\frac{d}{dt}P_{ijSS} = \gamma P_{ijSI} + \gamma P_{ijIS} - 2\frac{P_{ijSS}}{P_S}\boxed{\gamma P_I}$$

$$\frac{d}{dt}P_{ijSI} = \gamma P_{ijII} - \gamma P_{ijSI} - \beta_{ij}P_{ijSI} - \frac{P_{ijSI}}{P_S}\boxed{\gamma P_I} + \frac{P_{ijSS}}{P_S}\boxed{\gamma P_I}$$

$$\frac{d}{dt}P_{ijIS} = \gamma P_{ijII} - \gamma P_{ijIS} - \beta_{ij}P_{ijIS} - \frac{P_{ijIS}}{P_S}\boxed{\gamma P_I} + \frac{P_{ijSS}}{P_S}\boxed{\gamma P_I}$$

$$\frac{d}{dt}P_{ijII} = -2\gamma P_{ijII} + \beta_{ij}P_{ijSI} + \beta_{ij}P_{ijIS} + 2\frac{P_{ijSI}}{P_S}\boxed{\gamma P_I}$$

Pair dynamics is given as a linear combination of pairs

Pair dynamics after closure

$$\begin{pmatrix} -2\frac{\gamma P_I}{P_S} & \gamma & \gamma & 0 \\ \frac{\gamma P_I}{P_S} & -\gamma-\beta_{ij}-\frac{\gamma P_I}{P_S} & 0 & \gamma \\ \frac{\gamma P_I}{P_S} & -\frac{\gamma P_I}{P_S} & -\gamma-\beta_{ij} & \gamma \\ 0 & \beta_{ij}+2\frac{\gamma P_I}{P_S} & \beta_{ij} & -2\gamma \end{pmatrix} \begin{pmatrix} P_{ijSS} \\ P_{ijSI} \\ P_{ijIS} \\ P_{ijII} \end{pmatrix} = \mathbf{0}$$

$$P_{ijSS} + P_{ijSI} + P_{ijIS} + P_{ijII} = 1$$

Equilibrium pair probabilities can be uniquely determined as function of singlets P_S and P_I

Equilibrium of the analytical model

- The dynamics of singlets and pairs looks formidable
- Equilibrium pair probabilities can be explicitly solved

$$
\begin{aligned}
P_{\xi_l,SS} &= \frac{\gamma P_S^2}{\gamma + \beta(|\xi_l|) P_S P_I} \\
P_{\xi_l,SI} &= \frac{\gamma P_S P_I}{\gamma + \beta(|\xi_l|) P_S P_I} \\
P_{\xi_l,IS} &= \frac{\gamma P_S P_I}{\gamma + \beta(|\xi_l|) P_S P_I} \\
P_{\xi_l,II} &= \frac{\gamma P_I^2 + \boxed{\beta(|\xi_l|) P_S P_I}}{\gamma + \beta(|\xi_l|) P_S P_I}
\end{aligned}
$$

Infectious *I*s tend to be clustered by the factor β

Equilibrium of the analytical model

- Averaged singlet probabilities P_S and P_I can be solved from the singlet dynamics

$$0 = \frac{d}{dt}\langle P_S \rangle = -\frac{1}{n}\sum_{i=1}^{n}\sum_{j\neq i}\beta(|-\xi_{ij}|)P_{ijSI} + \gamma\langle P_I \rangle$$

$$\gamma P_I = \frac{1}{n}\sum_{i=1}^{n}\sum_{j\neq i}\beta(|-\xi_{ij}|)\boxed{P_{ijSI}}$$

$$= \frac{1}{n}\sum_{l=1}^{n(n-1)}\beta(r_l)\frac{\gamma P_S P_I}{\gamma + \beta(r_l)P_S P_I}$$

Equilibrium of the analytical model

$$1 = \frac{1}{n}\sum_{l=1}^{n(n-1)} \frac{\beta(r_l)(1-P_I)}{\gamma + \beta(r_l)(1-P_I)P_I}$$

$$\approx (n-1)\int_0^\infty \frac{\beta(r)(1-P_I)}{\gamma + \beta(r)(1-P_I)P_I} 2\pi r dr \quad \text{for CSR}$$

$$\approx (n-1)\int_0^\infty \frac{\beta(r)(1-P_I)}{\gamma + \beta(r)(1-P_I)P_I} 2\pi r \underline{g(r)} dr \quad \text{for general pp}$$

for 2 dimensional pp

$g(r)$: PCF of the point pattern used

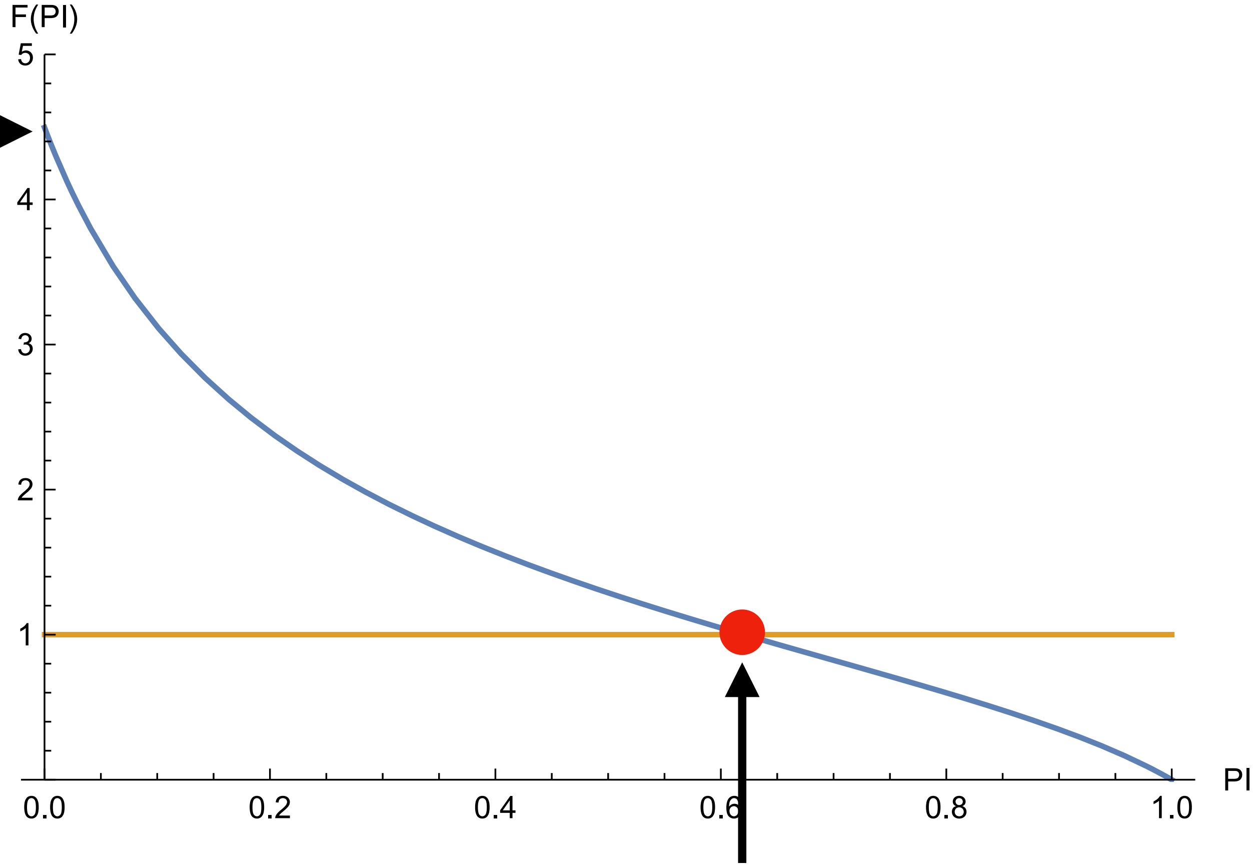
The r.h.s. $F(P_I)$ is monotonically decreasing function of P_I

Equilibrium of the analytical model

$$F(0) = (n-1)\frac{\beta_0}{\gamma}$$

$$\text{for CSR}$$

$$(n-1)\frac{\beta_0}{\gamma} > 1$$

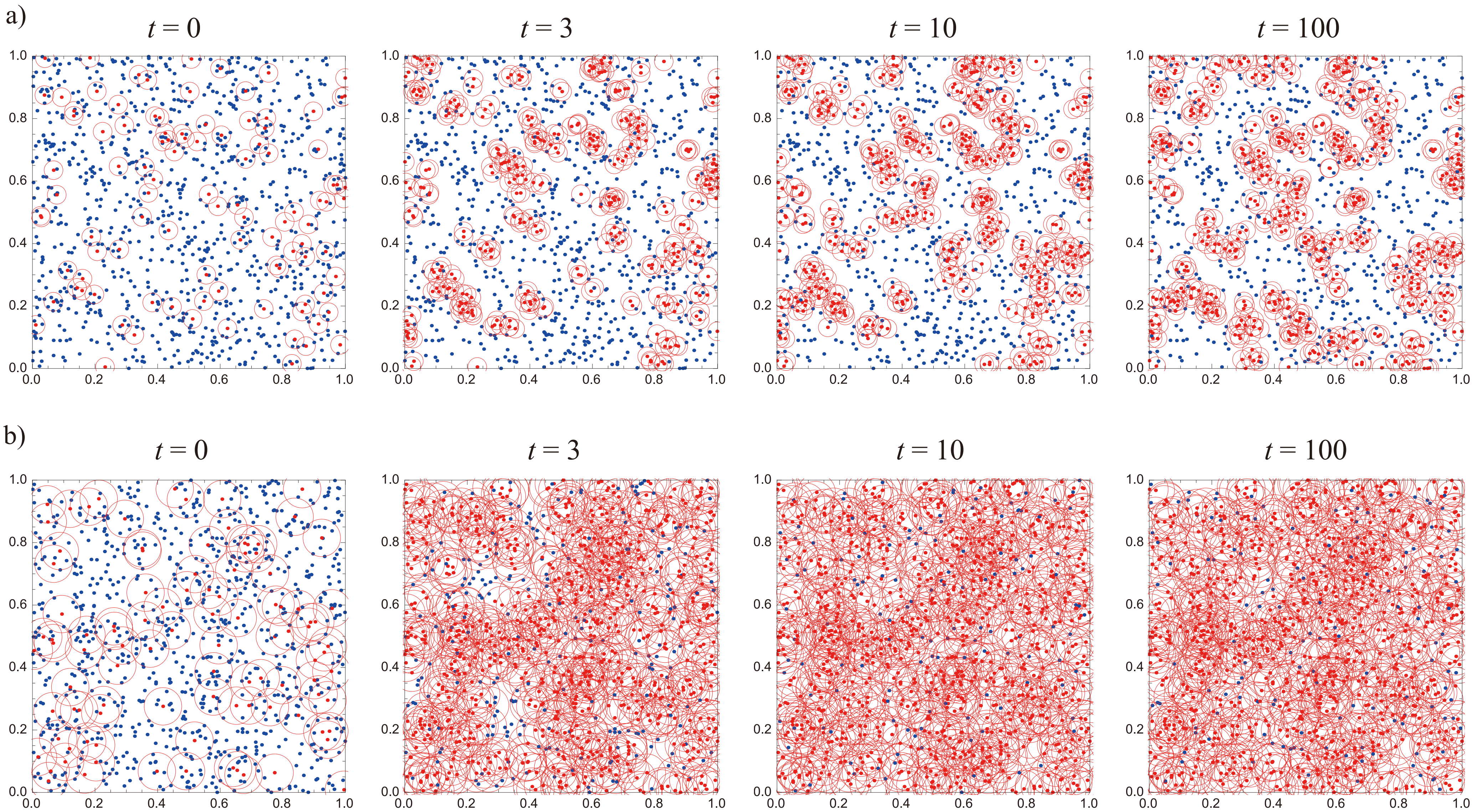


$$P_I^*$$

$$F(1) = 0$$

The r.h.s. $F(P_I)$ is monotonically decreasing function of P_I

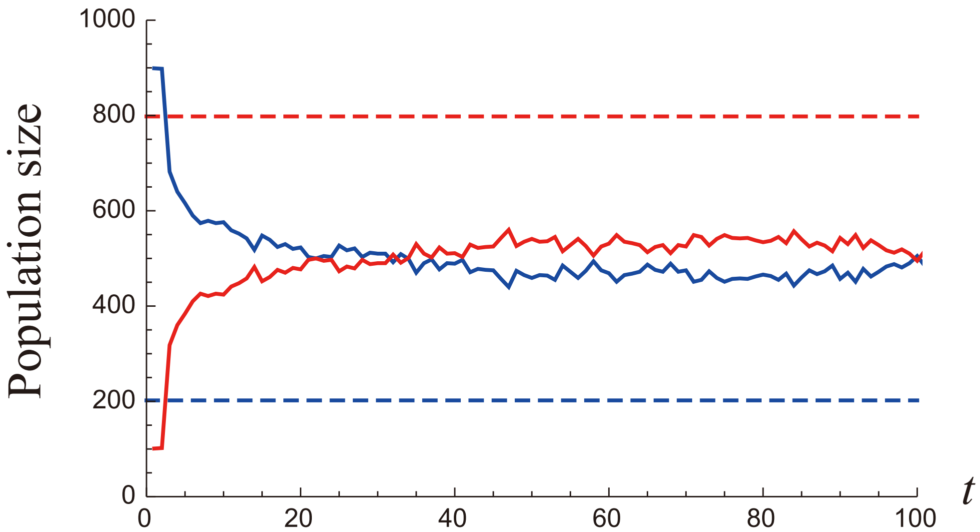
Simulations



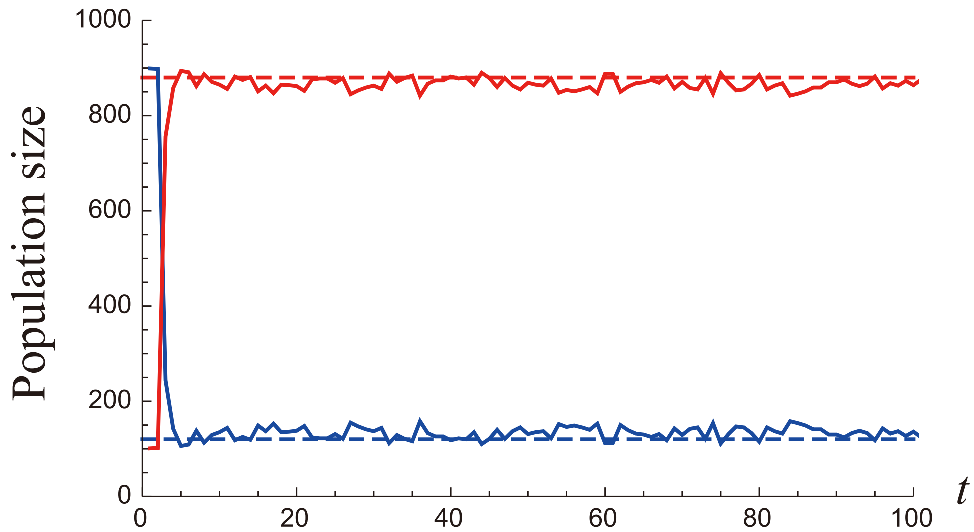
a) Infection range is small σ_I = 0.01, b) large σ_I = 0.02

Simulations and singlet abundance at equilibrium

a)

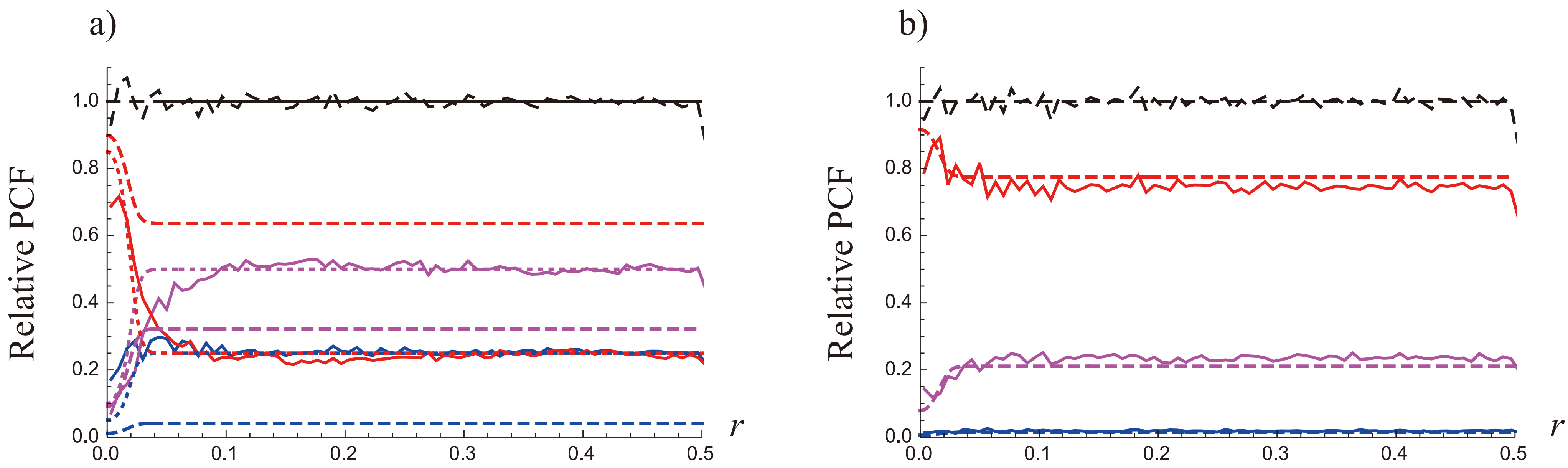


b)



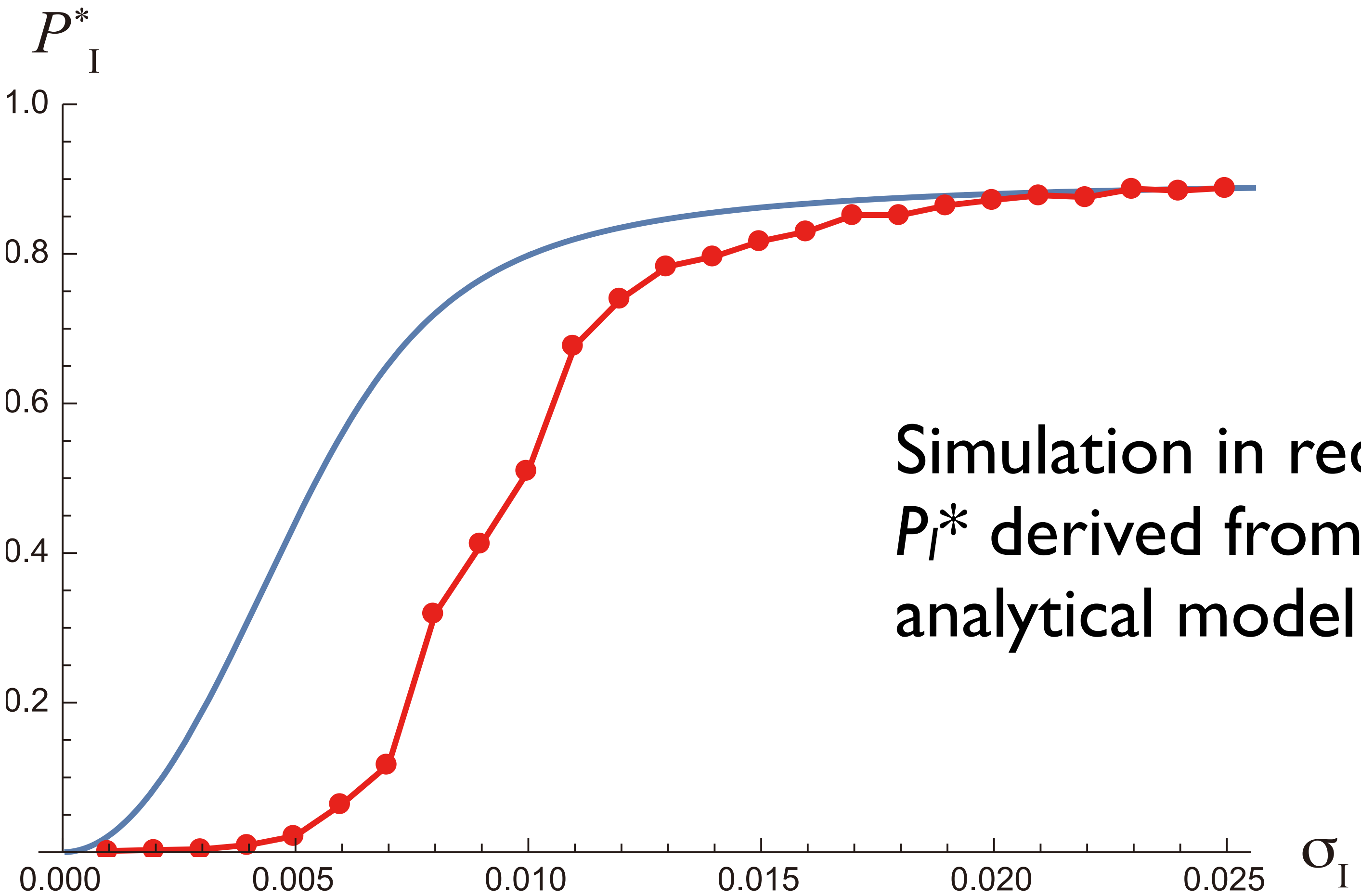
a) Infection range is small $\sigma_I = 0.01$, b) large $\sigma_I = 0.02$

Simulations and pair abundance at equilibrium



a) Infection range is small $\sigma_I = 0.01$, b) large $\sigma_I = 0.02$

Dependency of the equilibrium P_I* on the infection range σ_I



Simulation in red
P_I* derived from the analytical model in blue

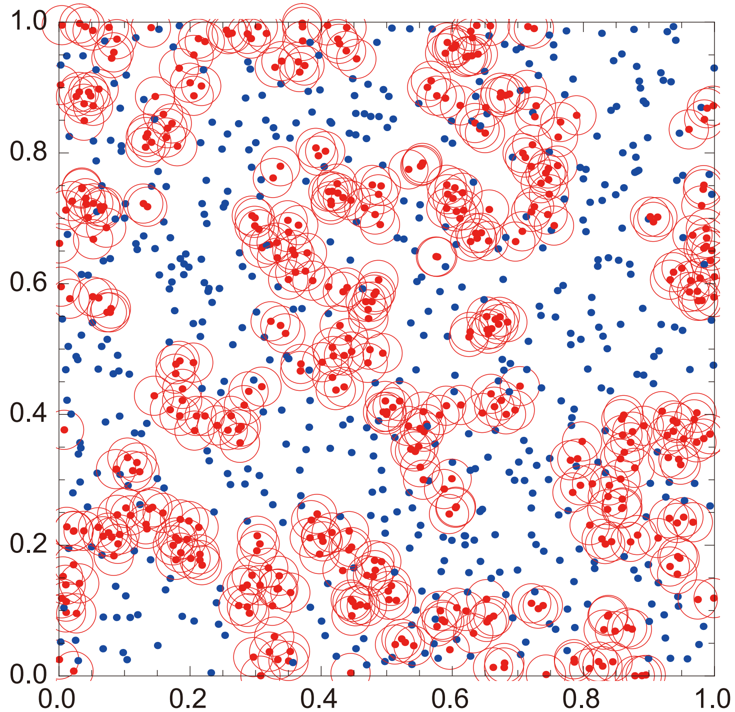
Performance of the analytical model

- Equilibrium can be derived analytically to some extent with the simple closure
- The analytical model describes simulations very well when infection range is large enough, e.g, $\sigma_I = 0.02$
- It fails when infection range becomes smaller $\sigma_I = 0.01$

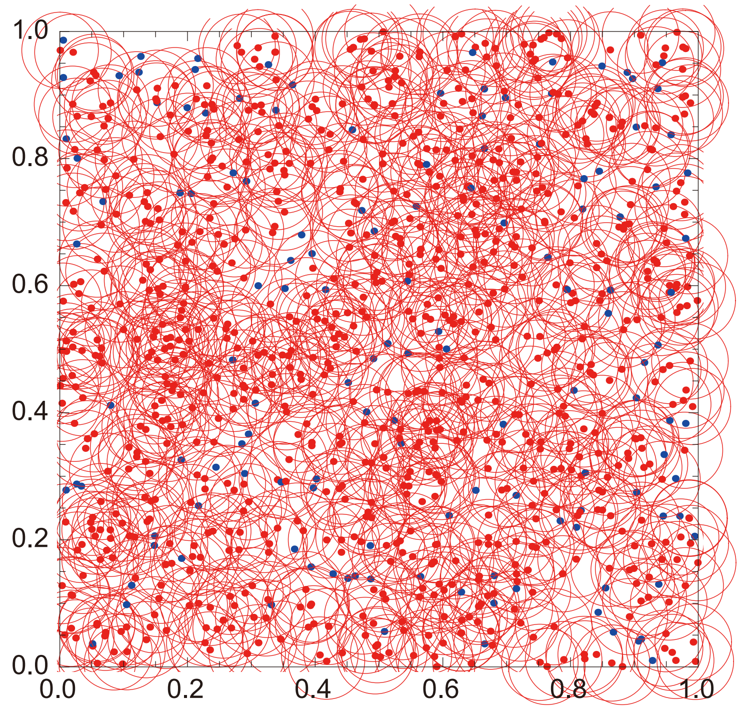
Performance of the analytical model

- The failure can be explained by continuum percolation known as Gillbert disc model; Given a large number of disks, there exists a threshold for the disk radius beyond which all disks are connected or overlapped with each other

$\sigma_I = 0.01$



$\sigma_I = 0.02$



Summary

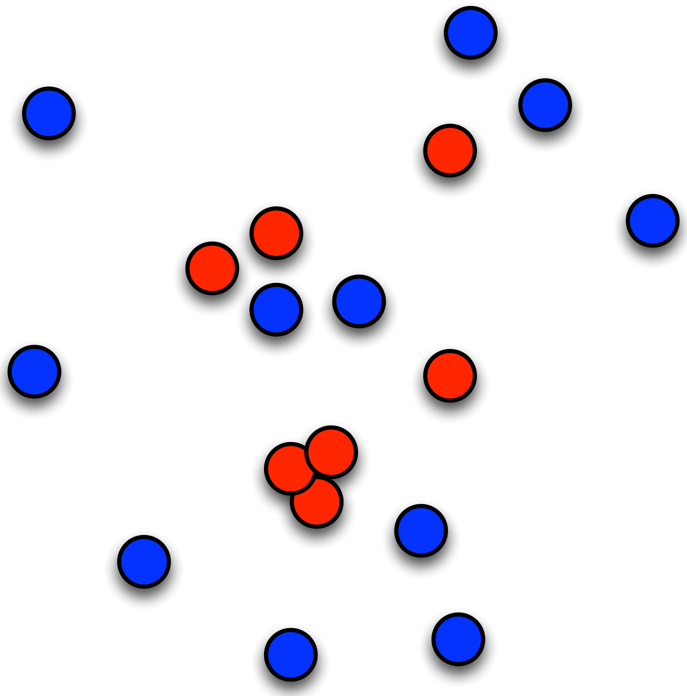
- Spatial SIS model is revisited as a point pattern dynamics
- Equilibrium pair probabilities are analytically tractable
  - Infectious are clustered with the order of the infection kernel $\beta(r)$ that can be arbitrary
  - Base point pattern can be arbitrary (CSR, Clumped, etc.)
  - Assuming equilibrium, $\beta(r)$ could be estimated from an observed point pattern

Discussion

- Epidemic dynamics goes parallel with colonization and local extinction dynamics in meta-population ecology
- An empty site becomes occupied by colonization from other occupied sites by distance-dependent dispersal
- An occupied site becomes empty by local extinction
- Colonization = Infection, Local extinction = Recovery
- Dispersal kernel is often difficult to estimate empirically
- Assuming that the system has reached equilibrium, cross PCFs (presence/absence of a species in sites) can be used to estimate dispersal kernel

Discussion

- Spatial distribution of local sites is easily obtained (GIS, etc.)
- Colonization rate *c*(*r*) or dispersal ability (infection rate in this talk) determines the point pattern at equilibrium
- —> Huong-san presentation!

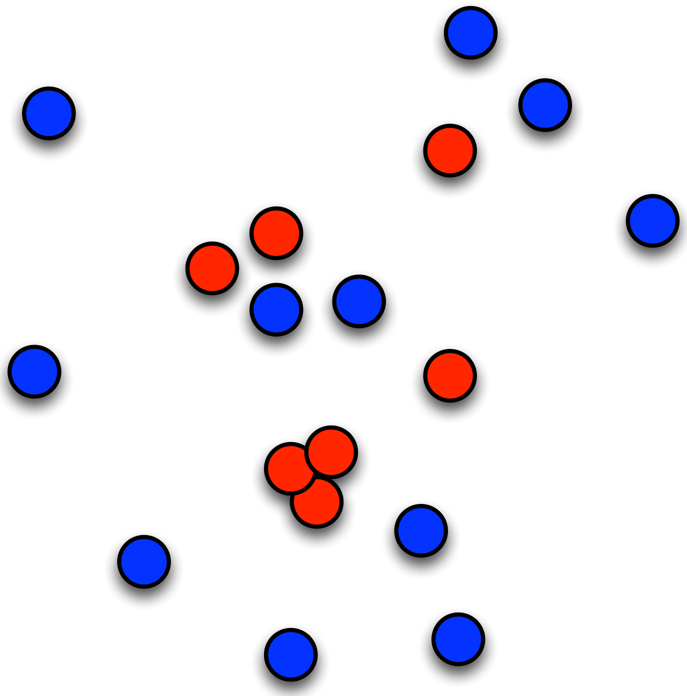


Occupied sites +

Sites potentially occupied but empty now 0

Discussion

- Relative correlation function of thee types of pairs, 0-0, 0-+ (+-0) and +-+ infers the functional form of the infection kernel $k(r)$

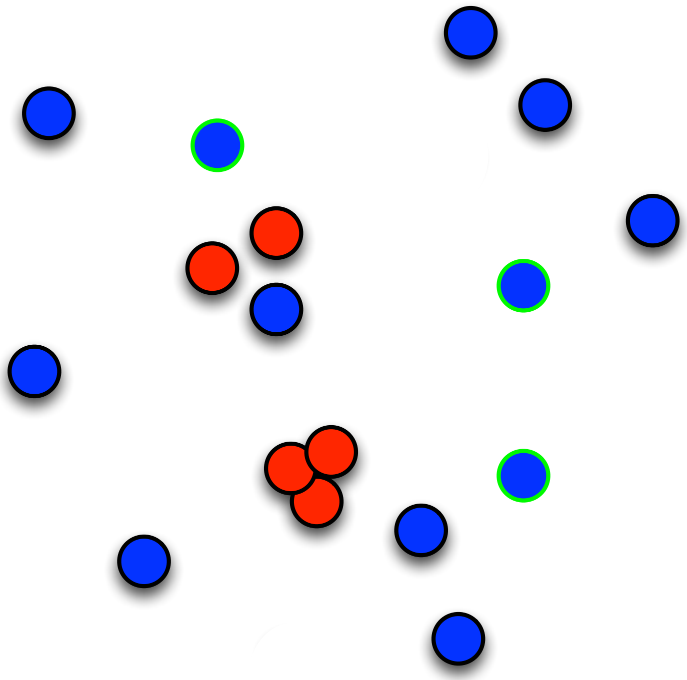


Occupied sites +

Sites potentially occupied but empty now 0

Discussion

- Effect of local site destruction/renewal can be readily handled (death and birth of local sites or patch dynamics)
- Could be useful for designing conservation management



Occupied sites +

Sites potentially occupied but empty now 0

Epidemiological models as point pattern dynamics

- Given an initial spatial pattern with a certain structure,
  - What is the condition for the infection to spread?
  - How are the infectious distributed?
- How do birth and death (ignored so far) affect the disease spread and the infectious distribution at equilibrium?
- Epidemic models as point pattern dynamics ~ Epidemic on metric (dynamic) network

Epidemiological models as point pattern dynamics

- Various ODE models have been analyzed; SIS (this study), SIR, SIRS, SEIR, etc.
- ALL of these can be readily extended to marked point pattern dynamics
- Realistic assumptions can be easily implemented, e.g., time to recovery, etc.

Equation-based and Individual-based models

- In Mathematical biology/Biological mathematics, equation-based models (ODE, PDE, etc.) have been extensively studied
- Many of them, however, are based on very simple (and thus unrealistic) assumptions
- There still remains an open space to explore population dynamics in terms of "individuals"

Moment dynamics

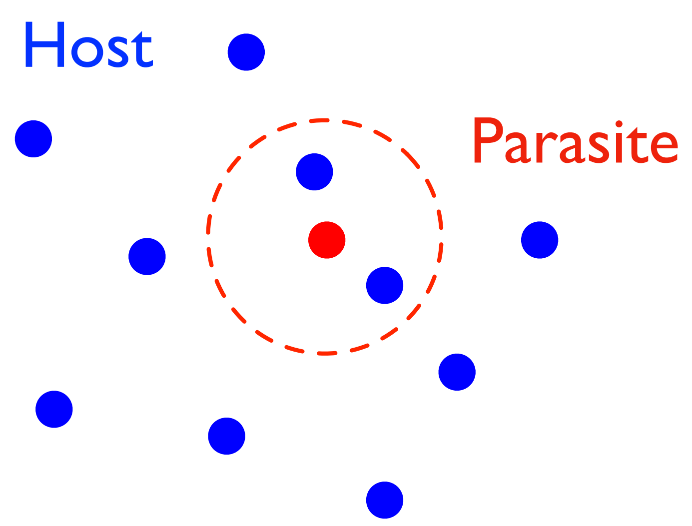
- Stochastic simulation is now easy to carry out
- However, understanding stochastic simulations is difficult because realizations differ from one to one
- We need <u>analytical approach</u> to understand stochastic simulations
- Derivation of the 1st moment (averaged pop size) and 2nd moment (averaged pair density) is a challenge
- Bolker and Pacala (1997), Bolker (1999)
- Law and Dieckmann (2000), Law et al. (2003)

Nicholson-Bailey model as PPD

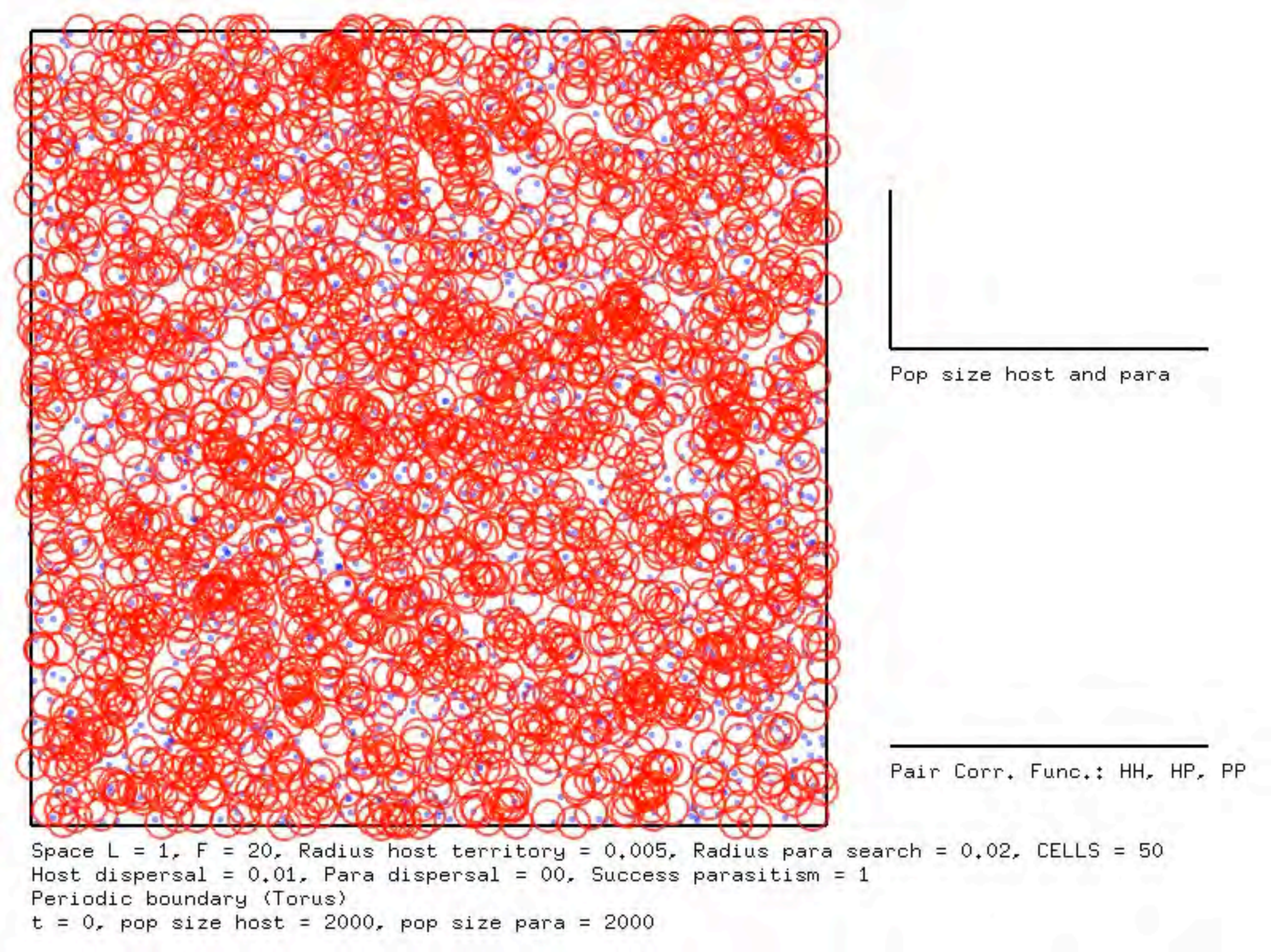
- Nicholson-Bailey model as host-parasite dynamics in discrete time
- NB model as point pattern dynamics can show spatially specific patterns

$$H_{t+1} = R \exp^{-aP_t} H_t$$

$$P_{t+1} = c(1 - \exp^{-aP_t})H_t$$

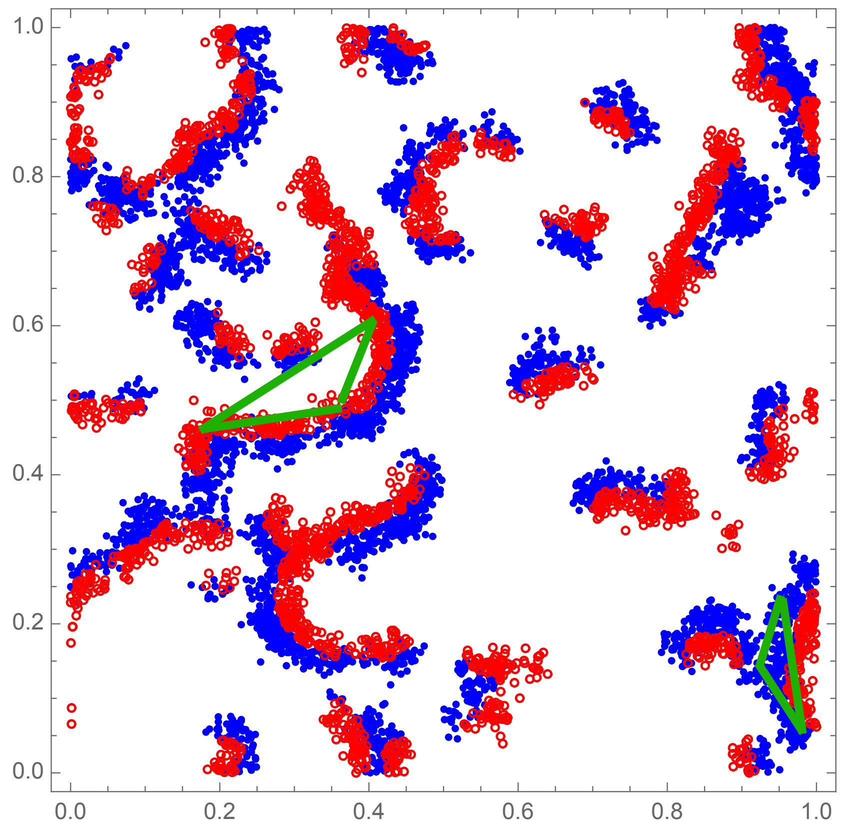


Nicholson-Bailey model as PPD

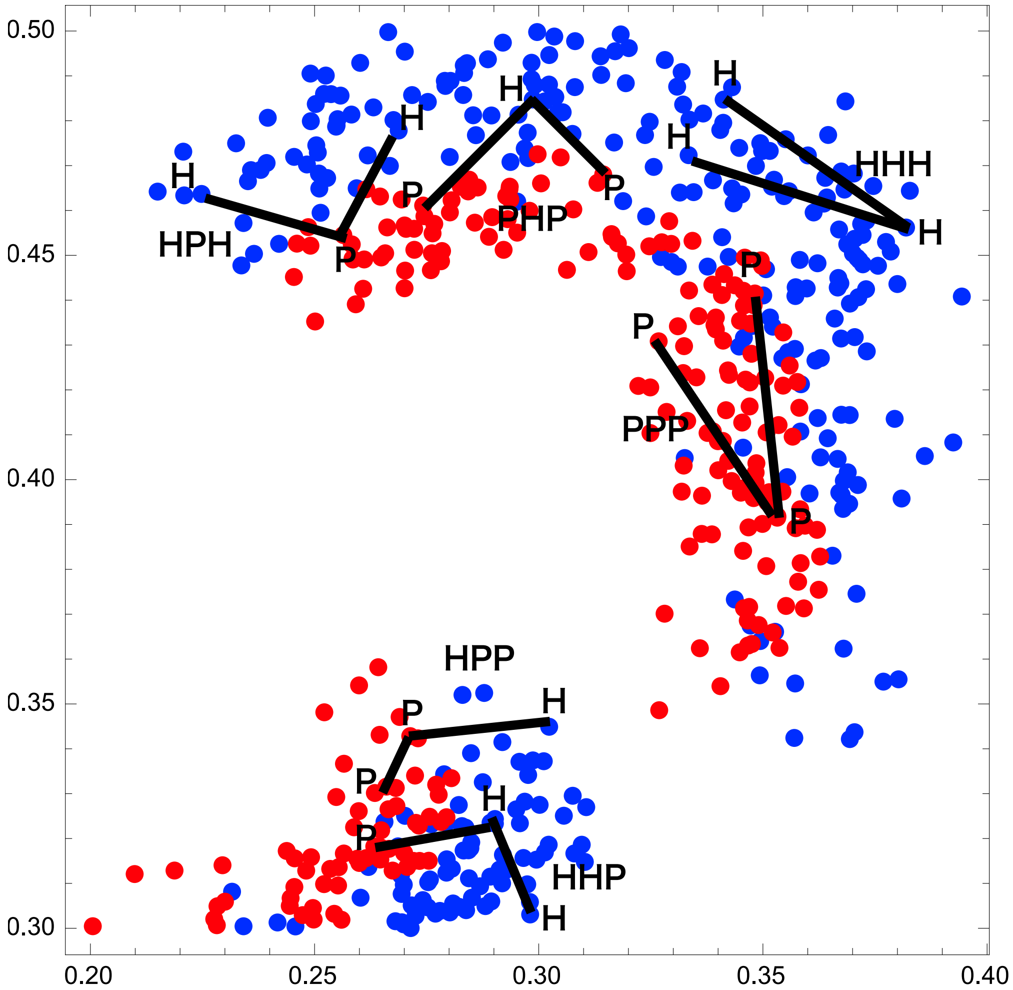


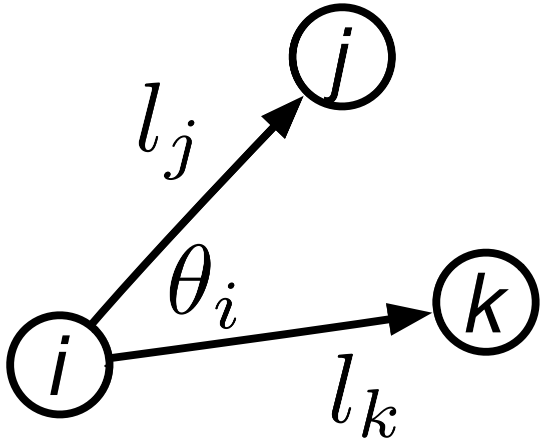
Higher order structure of point pattern

- Focus on triplets made of three points
- Measure a triplet with “shape” and “size”
- Flat triplets will dominate at a certain size



Higher order structure of point pattern





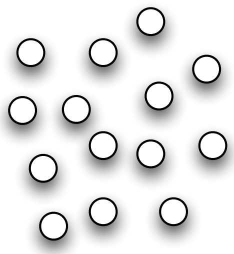
Shape I as the angle
Size S as the average edge

$$\left(\theta_i, \frac{l_j + l_k}{2}\right)$$

How can we understand the world?

- A big challenge to revisit “equation-based” population dynamics models in terms of “individual-based”

Individual-level



What type of individuals?
How many?
Where?
How do they interact?
IBM!

Population-level

Population size

Observed population dynamics

Mathematical models based on simple assumptions for the sake of mathematics (not necessarily for biology)

Derivation of analytical models to fully understand the dynamics

$$\frac{dn}{dt} = f(n)n$$

$$\frac{\partial n}{\partial t} = \Delta n + f(n)$$

$$n_{t+1} = f(n_t)n_t$$

$$?$$