Spreading dynamics in graphs

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February, 9 2016, Rome
Overview

- Reaction Diffusion problem
- Graph theory
- Reaction Diffusion dynamics on graphs
- Relation between topological structure of graphs and reaction dynamics
- Perspectives
Reaction Diffusion problem

Ubiquitous processes including reaction and diffusion that show up as soon as diffusing elements when propagating, get close and react, modifying their state

Two basic approaches:

- Single individuals moving and interacting (agent based description)

- Continuous fields diffusing and interacting in a media represented by mesoscopic and coarse-grained equation (pde description)
Reaction Diffusion problem

\[
\partial_t \theta_{\beta}(\vec{x},t) = \sum_{i,j} \sum_{\gamma} D_{ij}^{\gamma} \partial^2_{ij} \theta_{\gamma}(\vec{x},t) + \alpha_{\beta} F_{\beta}[\theta(\vec{x},t)]
\]

FKPP model
(1937)

\[
\frac{\partial}{\partial t} \theta(x,t) = D \frac{\partial^2}{\partial x^2} \theta(x,t) + \alpha F[\theta(x,t)]
\]

\[\theta(x,t) \in [0,1] \quad F(0) = F(1) = 0 \quad F(\theta) > 0 \text{ if } 0 < \theta < 1\]

\[
\begin{align*}
\frac{d \theta_a}{dt} &= \alpha \theta_a \theta_b \\
\frac{d \theta_b}{dt} &= -\alpha \theta_a \theta_b
\end{align*}
\]

FKPP reaction term

Autocatalytic reaction

\[A + B \rightarrow 2A\]

with probability \(\alpha\)
Reaction Diffusion problem

\[
\frac{\partial}{\partial t} \theta(x,t) = D \frac{\partial^2}{\partial x^2} \theta(x,t) + \alpha \theta(x,t)(1 - \theta(x,t))
\]

\[
\begin{align*}
\theta(x,t) &\to 1 \quad \forall \, x \\
\lim_{t \to \infty} M(t) &= 1 \\
M(t) &\sim 2v_0 t
\end{align*}
\]

\[v_0 = 2 \sqrt{D \alpha F'(0)}\] (localized initial condition)
Topological properties studied with statistical methods for large size networks

Dynamical processes on graphs

Which is the relation?
Graphs

- $N$ sites $i \in V$
- $A_{ij}$ adjacency matrix
- $M$ links $(i, j) \in E$
- $k_i$ degree of connectivity
- $l_{ij}$ Shortest path from $i$ to $j$

$P(k)$ connectivity degree distribution

Average clustering coefficient $\langle C \rangle$

Average minimum distance $\langle L \rangle$
Graphs

\[ k_{nn,i} = \frac{1}{k_i} \sum_{j \in E(i)} k_j \]

\[ k_{nn}(k) = \frac{1}{N} \sum_{i \mid k_i = k} k_{nn,i} \]

\[ r = \frac{\sum_k (k - \langle k \rangle) (k_{nn}(k) - \langle k \rangle) P_l(k)}{\sum_j (j - \langle j \rangle)^2 P_l(j)} \]

Pearson assortativity coefficient

Random graphs

Connections between sites with probability \( p \)

Erdős Renyi graph (1960)

\[ p_c = \ln \frac{N}{N} \]

\( p \sim p_c \rightarrow \) connected graph

\[ P(k) = e^{\langle k \rangle} \frac{\langle k \rangle}{k!} \]

Poisson distribution

\[ \langle C \rangle = p = \frac{\langle k \rangle}{N} \]

\[ \langle I \rangle \approx \frac{\ln(N)}{\ln\langle k \rangle} \]
Toward real networks

Small-World property

Random graphs model

Homogenous

Scale-Free network

\[ \langle k^2 \rangle \gg 1 \]

\[ P(k) = e^{-\langle k \rangle} \frac{\langle k \rangle^k}{k!} \]

Heterogeneous networks

\[ P(k) = k^{-\gamma} \]
Reaction diffusion on graphs

\[ \frac{\partial}{\partial t} \theta_i(t) = w \sum_j L_{ij} \theta_j(t) + \theta_i(t) \left( 1 - \theta_i(t) \right) \]

\[ w = \frac{D}{\alpha} \]

\[ L_{ij} = k_i \delta_{ij} - A_{ij} \]

Many researchers have focused on the dynamics of processes taking place in networks, in some cases trying to understand the relation between dynamics and topological properties.

Assortative network \rightarrow Slower spreading \rightarrow Disassortative network \rightarrow Faster spreading

RD in Erdös Renyi graph

\[ N(l) \sim l^{d_i} \quad (\text{in graphs}) \quad \rightarrow \quad N(l) = e^{cl} \quad (d_i = \infty) \quad \rightarrow \quad M(t) \sim e^{\alpha t} \]

\[ \alpha \sim \ln \langle k \rangle \]

Dual structured graphs

Local structure
Graph with M sites with nearest neighbour connections

N sites randomly chosen (N<M)

A type
Randomly chosen connections among the N sites with probability p
Dual structured graphs

Local structure
Graph with M sites with nearest neighbour connections

N sites randomly chosen (N<M)

B type
Randomly chosen connections between the N sites and the remaining M-N sites with probability q
Dual structured graphs

\[
M/N = 10^{-2}
\]

\[
P = 2 \, p_c
\]

Assortativity

\[
r_A \sim 0.83
\]

\[
r_B \sim 0.04
\]

Graphs with two-folded structure of connections

(epidemological diffusion inside infrastructure network, protein folding structure...)

\[
\langle k \rangle_{ran}^a = p(N-1) = q(M-N) = \langle k \rangle_{ran}^b
\]

\[
q = \frac{p(N-1)}{M-N}
\]

\[
P(k)
\]

\[
r \langle k \rangle
\]

\[
\langle l \langle k \rangle \rangle
\]

\[
\frac{10^2}{10^1} \quad 10^0 \quad 10^{-1}
\]

\[
0 \quad 5 \quad 10 \quad 15 \quad 20 \quad 25 \quad 30 \quad 35
\]

\[
0 \quad 10^{-5} \quad 10^{-4} \quad 10^{-3} \quad 10^{-2} \quad 10^{-1} \quad 10^0 \quad 10^1
\]

\[
0 \quad 0.2 \quad 0.4 \quad 0.6 \quad 0.8 \quad 1
\]

\[
0 \quad 10 \quad 20 \quad 30 \quad 40 \quad 50 \quad 60
\]

\[
0 \quad 10 \quad 20 \quad 30 \quad 40 \quad 50 \quad 60
\]
RD in dual structured graphs

\[ M^s(t) = \sum_i \theta_i(t) \quad M(t) = \frac{1}{n_s} \sum M^s(t) \]

\[ T^s(\Theta) = \min \{ t | M^s(t) \geq \Theta \} \quad T(\Theta) = \frac{1}{n_s} \sum T^s(\Theta) \]

From a first insight we have agreement with [1] (more assortative slower spreading)

\[ C(T(\Theta), x) = \frac{1}{n_s} \sum (T^s(\Theta) - T(\Theta))(x^s - x) \]

The average minimum distance have a better correlation with large filling time of the system
RD in dual structured graphs

Ring distance structure
\[ R_i(l) = \{ j \in V | l_{ij} = l \} \]

Cumulative ring distance
\[ G_i(l) = \{ j \in V | l_{ij} \leq l \} \]

Percentage up to \( l \)
\[ S_i(l) = \frac{|G_i(l)|}{M} \]

Filling time up to \( l \)
\[ T_i(l) = \frac{S_i(l)}{v_0} \]

Filling time up to \( l \)
\[ T_{mf}(\Theta) = \frac{1}{\alpha} \log \frac{\Theta(1 - M(0))}{M(0)(1 - \Theta)} \]

\[ T_{lp} \sim \frac{\Theta}{\sqrt{\alpha}} \]

\[ \text{Ring assortativity} \]
\[ r_i(l) = \frac{\sum_{k \in G_i(l)} (k - \langle k \rangle)(k_{nn}(k) - \langle k \rangle)P_i(k)}{\sum_{j \in G_i(l)} (j - \langle j \rangle)^2 P_i(j)} \]
Perspectives

- Understand the relation between topological properties of the graphs and dynamical behaviour.

- Study the problem in more realistic situations, using different reacting terms, and building real network structures. For instance in network as real transport infrastructures connections, or introducing RD epidemiological model, like SIR or SIS [3].

- Study RD problems on graphs with an agent based approach [4], passing from pde equations to stochastic processes, stressing effects of RD on a discrete population, or to analyze populations made of a few number of elements.