A járványterjedés PDE modelljeinek és ezek numerikus megoldásainak kvalitatív tulajdonságai*

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Outline

Motivation

Some historical details

- In the ancient time: Plague of Athens (430-428 BC) (described by Thucydides, no mention of person-to-person contagion)
- The Black Death in the 14th century (the most famous pandemic)
- Yellow Fever epidemic in Philadelphia in 1793 (the first major epidemic in the USA, about 5000 people died out of a population of around 50000)
- Spanish flu pandemic during the World War I (1918-19). More than 30 million people died.
- We have had public health strategy (elimination and control of organisms which cause disease, role of antibiotics) only since the end of World War II.
- There is no end of it (swine flu (2009-10, more than 200000 people died), AIDS, Ebola, etc.)

Black Death (in Europe, 1347-51)

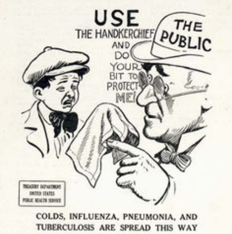
- The plague come from Asia with rat fleas and reached Europe in Sicily in October 1347.
- The disease waved through Europe in four years and reached north-western Russia killing about the 50% of Europe's total population.
- Countries with lower level trade relations with their neighbours were less involved in the disease.

Black Death (in Europe, 1347-51)

Fig. 20.2. Appriximate chronological spread of the Black Death in Europe from 1347–50. (Redrawn from Langer 1964)

Spanish flu, 1918-19

- The most devastating pandemic in the history of the human kind.
- In two years, between 1918 and 1919, more than 30 million people died worldwide, more than those died in the war.
- One-quarter of the USA and one-fifth of the world were infected with the influenza.



Epidemic models

Epidemic models

The goals of the models:

- They are useful to describe and understand disease dynamics.
- They are helpful for prevention of epidemics (e.g. hygiene, calculation of the necessary level of vaccination).
- They help to control the emerging infectious diseases.
- Real life testing is impossible.

$$\Downarrow$$

Mathematical models

Compartmental models

The population is divided into subpopulations. We consider three of them.

1. $I(t)$: infected individuals who can pass on the disease to others;
2. $S(t)$: susceptibles who have yet to contract the disease and become infectious,
3. $R(t)$: members who have been infected but cannot transmit the disease for some reason, e.g., they have been isolated from the rest of the population.

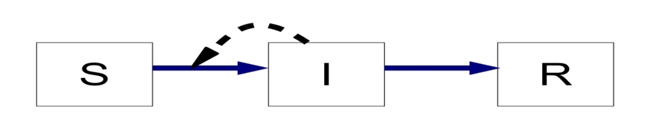
Other classes could be: different states of the disease, latent periods, incubation.

Compartmental models

Assumptions:

- The transmission is horizontal, through direct contact between hosts.
- The mixing of individual hosts is homogeneous.
- Rates of transfer from a compartment are proportional to the population size of the compartment.
- Individuals become infectious upon infection.
- There is no loss of immunity and no possibility of reinfection.
- No input of new susceptibles and no removal from any compartments.
- The total host population remains a constant.

SIR model flow diagram



Blue/solid arrows: movement between classes.
Black/dotted arrow: level of infectious disease influences the rate at which a susceptible individual moves into the infected class.
Assumption: disease confers lifelong immunity. e.g. measles.

SIR model - system of ODEs

Kermack and McKendrick, 1927

$$S' = -aSI,$$
$$I' = aSI - bI,$$
$$R' = bI,$$

$I = I(t)$: number of infective,
$S = S(t)$: number of susceptible and
$R = R(t)$: number of recovered (removed) members.

$a > 0$: contact rate; $b > 0$: recovery coefficient

SIR model - the threshold phenomenon

What happens when I(0) infectives introduced into a population of S(0) susceptibles?

SIR model - the threshold phenomenon

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Two possibilities:

- an epidemic occurs;
- the invasion fades.

SIR model - the threshold phenomenon

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Two possibilities:

- an epidemic occurs;
- the invasion fades.

Second equation (for $I(t)$):

$$I'(t) = I(t)(aS(t) - b).$$

If $S(0) < b/a$ then $I'(0) < 0$ and the infection dies out.

Known as "threshold phenomenon" : susceptibles must exceed a critical threshold for an infection to invade.

(Vaccination policy: if the number of susceptibles is reduced to below the threshold then the disease can be eradicated.)

Inclusion of spatial dependence

- Meta-population models. The population is divided into sub-populations according to some geopolitical considerations. $\rightarrow$ Coupled system of ODEs.
- Local infection models (local spatial SIR model - lsSIR) $\rightarrow$ Coupled system of PDEs
  - A member of the population can infect only members in its well defined spatial neighbourhood
  - The speed of the motion of the individuals can be neglected (compared to the speed of the disease)
- Models with diffusion (diffusive spatial SIR model - dsSIR) $\rightarrow$ System of reaction diffusion equations
  - The members propagate according to some diffusion rules.

Local spatial SIR models and their qualitative properties

Inclusion of spatial dependence - IsSIR model

Mathematical model with local infection (Kendall, 1965)

$$S'_t(x,t) = -\left(\int_{K(x)} W(|x'-x|)I(x',t)\,\mathrm{d}x'\right)S(x,t),$$

$$I'_t(x,t) = \left(\int_{K(x)} W(|x'-x|)I(x',t)\,\mathrm{d}x'\right)S(x,t) - bI(x,t),$$

$$R'_t(x,t) = bI(x,t),$$

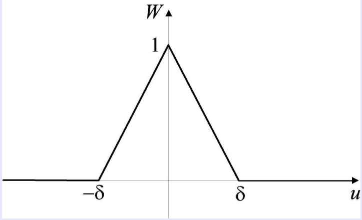
$S = S(x,t)$, $I = I(x,t)$ and $R = R(x,t)$ are now spatial dependent densities.

The nonnegative weighting function W depends only on the distance of the points x' and x, and $K(x)$ is a prescribed neighbourhood of the point x.

Inclusion of spatial dependence - IsSIR model

Simplifications:

- We consider 1D or 2D problems.
- $K(x)$ is a ball around x with radius δ.
- The weighting function is as shown (or its positive multiple)



- I is approximated with its second order spatial Taylor series.

This is an extension of what was proposed in [Jones, Sleeman, 2011] for the one-dimensional case.

Inclusion of spatial dependence - IsSIR model

IsSIR model

$$\begin{aligned} S_t' &= -S\left(\vartheta I + \varphi \Delta_D I\right), \\ I_t' &= S\left(\vartheta I + \varphi \Delta_D I\right) - bI, \\ R_t' &= bI, \end{aligned} \tag{1}$$

where Δ_D is the $D = 1, 2$ dimensional spatial Laplace operator. The homogeneous Dirichlet boundary condition is applied.

$$\vartheta = \int_{K(0)} W(|u|)\,\mathrm{d}u, \quad \varphi = \frac{1}{2}\int_{K(0)} u^2 W(|u|)\,\mathrm{d}u$$

are positive constants that can be computed from the model.

Travelling wave solutions

In order to model epidemic waves we are looking for travelling wave solutions. Let us set

$$S(x,t) = \tilde{S}(x-ct), \quad I(x,t) = \tilde{I}(x-ct), \quad R(x,t) = \tilde{R}(x-ct),$$

where c is the constant wave speed, $\tilde{I}$ and $\tilde{S}$ have the properties

$$\lim_{\xi\to\pm\infty} \tilde{I}(\xi) = 0, \quad \lim_{\xi\to\pm\infty} \tilde{I}'(\xi) = 0, \quad \lim_{\xi\to\infty} \tilde{S}(\xi) = \tilde{S}^{\infty} > 0.$$

Travelling wave solutions

After some manipulations we get:

Form of the system after inserting the wave form solutions

$$\tilde{S}' = \frac{b}{c}\tilde{I} - \frac{c}{\phi}\log(\tilde{S}/\tilde{S}^\infty) + \frac{\theta c}{b\phi}(\tilde{I} + \tilde{S} - \tilde{S}^\infty),$$

$$\tilde{I}' = \frac{c}{\phi}\log(\tilde{S}/\tilde{S}^\infty) - \frac{\theta c}{b\phi}(\tilde{I} + \tilde{S} - \tilde{S}^\infty),$$

$$\tilde{R}' = -\frac{b}{c}\tilde{I}.$$

Travelling wave solutions

Let us introduce the notations

$$\tilde{S}^{-\infty} = \lim_{\xi \to -\infty} \tilde{S}(\xi), \; \tilde{S}^{\infty} = \lim_{\xi \to \infty} \tilde{S}(\xi).$$

Lemma. The necessary condition of the travelling wave solution is

$$\tilde{S}^{\infty} > b/\theta.$$

Moreover

$$\tilde{S}^{-\infty} < b/\theta,$$

that is the epidemic wave does not leave enough susceptible members back to be able to sustain a new wave. If the necessary condition is satisfied then

$$c \geq 2\sqrt{\tilde{S}^{\infty}\phi(\tilde{S}^{\infty}\theta - b)}$$

is a lower bound for the wave speed.

Some qualitative properties of the lsSIR model

lsSIR model

$$
\begin{aligned}
S_t' &= -S\left(\vartheta I + \varphi \Delta_D I\right), \\
I_t' &= S\left(\vartheta I + \varphi \Delta_D I\right) - bI, \\
R_t' &= bI,
\end{aligned}
$$

Our requirements are (investigated in [FH2014] for 1D):

P1 Additivity property
$S + I + R$ is constant at a fixed spatial position.

P2 Monotonicity property
– S monotone decreases in time
– R monotone increases in time

P3 Nonnegativity property
$S > 0$, $I \geq 0$, $R \geq 0$ at $t = 0$
$\Downarrow$
$S, I, R \geq 0$.

Some qualitative properties of the lsSIR model

Theorem. If the condition

$$\vartheta I + \varphi \Delta_D I \geq 0$$

is satisfied for all x and t then properties P2 and P3 are true for the solution of problem (1). Property P1 is true without any restrictions.

Notice that the condition is not an a priori one.

Finite difference schemes for the lsSIR model

In [FH2016, to appear] we gave the conditions of the qualitative properties of the finite difference numerical solutions of the lsSIR model for different boundary conditions.

We generalize the previous results. We give conditions in dimensions $D = 1, 2$.

We solve the problem on $[0, L]$ or on $[0, L] \times [0, L]$. We use the homogeneous Dirichlet boundary condition (outside the considered domain conditions are incompatible with life).

We define a uniform spatial grid
$\omega_h = \{x_k \in [0, L] \,|\, x_k = kh,\ k = 0, \dots, N+1,\ h = L/(N+1)\}$
and a positive time step $\tau > 0$. In 2D, a similar grid is defined.

Explicit Euler method (EEM)

The vector s^n contains the approximations of the S-values at the inner grid points ordered in row-continuous way. The other vectors are defined similarly.
We define the EE difference scheme as follows.

$$\frac{s^{n+1}-s^n}{\tau} = -s^n p^n$$
$$\frac{i^{n+1}-i^n}{\tau} = s^n p^n - bi^n,$$
$$\frac{r^{n+1}-r^n}{\tau} = bi^n,$$

where $p^n = \vartheta i^n + \varphi Q_D i^n$ and Q_D is the discretization matrix of the D dimensional Laplace operator.

How to satisfy the discrete versions of the qualitative properties?

Properties of the EE numerical solution

Theorem. Let us suppose that at the initial state $s^0 \geq 0$, $i^0 \geq 0$, $r^0 \geq 0$, and $p^0 \geq 0$ (a priori condition), moreover assume that

$$\tau \leq \min\left\{\frac{1}{b + 2D\varphi M/h^2}, \frac{1}{M(\vartheta + 2D\varphi/h^2)}\right\},$$

where $M = \max(s^0 + i^0 + r^0)$. Then the EE finite difference scheme satisfies the qualitative properties [P1]-[P3].

Properties of the EE numerical solution

Theorem. Let us suppose that the qualitatively adequate finite difference solution of the sSIR model

- describes a numerical wave of speed c for the infectious individuals,
- this wave has a strictly concave, monotonically decreasing part in the direction of the moving and
- $\tau < h/c$

then the density of the susceptibles must be greater than b/ϑ on that part of the wave profile (compare with the continuous case).

Implicit Euler method (IEM)

We define the IE difference scheme as follows.

$$
\begin{aligned}
\frac{s^{n+1}-s^n}{\tau} &= -s^{n+1}p^n \\
\frac{i^{n+1}-i^n}{\tau} &= s^{n+1}p^n - bi^{n+1}, \\
\frac{r^{n+1}-r^n}{\tau} &= bi^{n+1}.
\end{aligned}
$$

How to satisfy the discrete versions of the qualitative properties?

Properties of the IE numerical solution

Theorem. Let us suppose that at the initial state $s^0 \geq 0$, $i^0 \geq 0$, $r^0 \geq 0$, and $p^0 \geq 0$ (a priori condition), moreover assume that

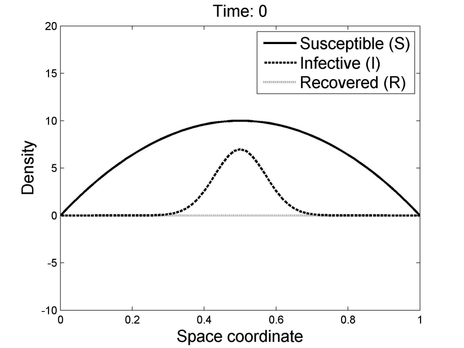
$$\tau \leq \begin{cases} ((2D\varphi/h^2 - \vartheta)M)^{-1}, & \text{if } h < h^\star, \\ \text{arbitrary}, & \text{if } h \geq h^\star, \end{cases}$$

where $h^\star = (2D\varphi/\vartheta)^{1/2}$. Then the IE finite difference scheme satisfies the qualitative properties [P1]-[P3].

Numerical tests

1D example: Parameter setting and initial conditions

We set $L = 1$, $\delta = 0.01$, $b = 0.03$ and the spatial step size is set to $h = 1/60$ ($N = 59$). With this choices we have $\vartheta = \delta$ and $\varphi = \delta^3/12$.



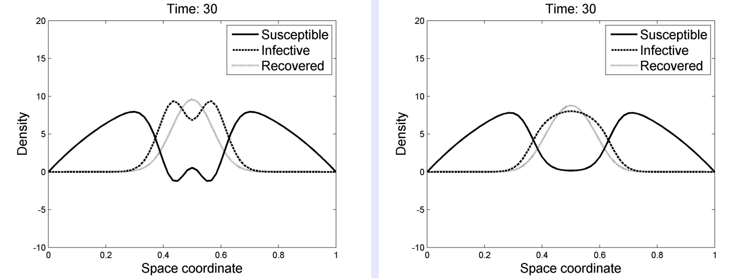
$(M = 17)$

Sufficient conditions (EEM)

The upper bound for the time step is

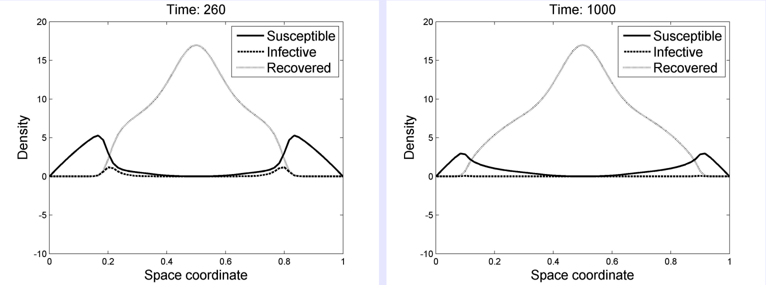
$$\tau \leq 5.5494.$$

$\tau = 15$ (thus above the obtained bound) and $\tau = 5$ cases at $t = 30$.



Numerical wave

Regions where the density of the susceptibles is not greater than $b/\vartheta = 3$ are not able to conduct epidemic waves.



2D example: Parameter setting

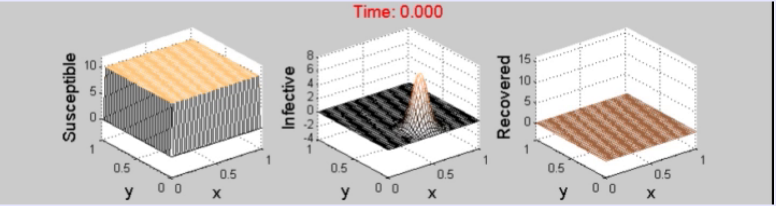
We set $L = 1$, $N = 40$, $b = 0.05$, $\delta = 0.07$, $\varphi = 10\delta^4\pi/40$, $\vartheta = 10\delta^2 * \pi/3$ (W is multiplied by 10). With the initial functions we have $M = 18$.

Using the IE method the sufficient condition for the time step is $\tau \leq 0.7359$.

We will use the time steps $\tau = 0.7$ and $\tau = 10$.

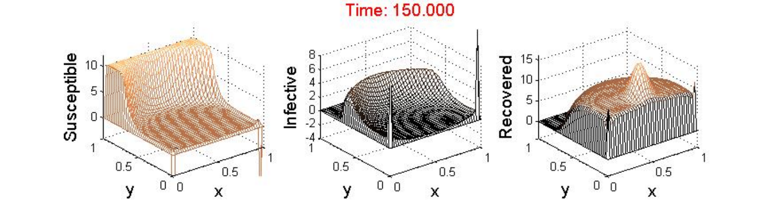
Correct numerical solution (IEM)

$\tau = 0.7$



Incorrect numerical solution (IEM)

$\tau = 10$



Diffusive spatial SIR model and its qualitative properties

Continuous model with diffusion

Problem in the previous model: to preserve the qualitative properties additional condition:

$$\vartheta I + \varphi \Delta_D I \geq 0$$

for all (x, t) on the solution domain.

Continuous model with diffusion

Problem in the previous model: to preserve the qualitative properties additional condition:

$$\vartheta I + \varphi \Delta_D I \geq 0$$

for all (x, t) on the solution domain.

We extend the SIR model in two directions:

- S, I and R depend on both space and time variables;
- there is spatial motion (due to the diffusion).

Mathematical model: system of nonlinear PDEs.

Continuous model with diffusion

Mathematical model with spatial dependence and with diffusion

$$
\begin{aligned}
S_t'(x,t) &= d_1 S_{xx}''(x,t) - kI(x,t)S(x,t),\\
I_t'(x,t) &= d_2 I_{xx}''(x,t) + kI(x,t)S(x,t) - \gamma I(x,t),\\
R_t'(x,t) &= d_3 R_{xx}''(x,t) + \gamma I(x,t).
\end{aligned}
$$

$S = S(x,t)$, $I = I(x,t)$ and $R = R(x,t)$ are the space dependent densities.

Here $x \in [0, L]$ + initial conditions + Neumann boundary condition

Notation: dsSIR

Some qualitative properties of the dsSIR model

dsSIR model

$$S'_t = d_1 S''_{xx} - kIS,$$
$$I'_t = d_2 I''_{xx} + kIS - \gamma I,$$
$$R'_t = d_3 R''_{xx} + \gamma I.$$

There is spatial motion $\Rightarrow$ new functions:

$\tilde{S}(t) = \int_0^L S(x,t)dx$, $\tilde{I}(t) = \int_0^L I(x,t)dx$
$\tilde{R}(t) = \int_0^L R(x,t)dx$.

- [P1] Additivity property:
  $N(t) = \tilde{S}(t) + \tilde{I}(t) + \tilde{R}(t) = constant$.
- [P2] Monotonicity property: $\tilde{S}(t)$ monotone decreases and $\tilde{R}(t)$ monotone increases in time.
- [P3] Nonnegativity property
  $S(x,0) > 0$, $I(x,0) \geq 0$, $R(x,0) \geq 0 \Rightarrow S(x,t)$, $I(x,t)$, $R(x,t) \geq 0$ for all (x,t).

Some qualitative properties of the dsSIR model

Theorem. The dsSIR model has unique (local) solution, and it possesses the required qualitative properties [P1]-[P3].

The statement is true in any space dimension, i.e., we may assume that $x \in \Omega$, where $\Omega \subset \mathbb{R}^D$ with $D \geq 1$.

Discrete dsSIR model with diffusion

We define a shifted uniform spatial grid

$$\omega_h = \{x_j = h/2 + jh,\ j = -1, 0, \dots, N,\ h = L/N\}$$

and a positive time step $\tau > 0$. (Higher dimensions similar meshes are used.)

We apply the notations $s_j^n \approx S(x_j, n\tau)$, etc.

Finite difference scheme with explicit Euler method

We define the difference scheme by using the EEM:

$$\frac{s_j^{n+1}-s_j^n}{\tau}=d_1\frac{s_{j+1}^n-2s_j^n+s_{j-1}^n}{h^2}-ks_j^n i_j^n,$$

$$\frac{i_j^{n+1}-i_j^n}{\tau}=d_2\frac{i_{j+1}^n-2i_j^n+i_{j-1}^n}{h^2}+ks_j^n i_j^n-\gamma i_j^n,$$

$$\frac{r_j^{n+1}-r_j^n}{\tau}=d_3\frac{r_{j+1}^n-2r_j^n+r_{j-1}^n}{h^2}+\gamma i_j^n,$$

$j=0,\ldots,N-1$, $n=0,1,\ldots$.

Neumann b.c.: $s_{-1}^n=s_0^n,\quad s_{N-1}^n=s_N^n$, etc.

How to satisfy the discrete versions of the qualitative properties?

Qualitative properties of finite difference scheme with explicit Euler method

Notation:

$$s(n) = h \sum_{j=0}^{N-1} s_j^n, \quad i(n) = h \sum_{j=0}^{N-1} i_j^n, \quad r(n) = h \sum_{j=0}^{N-1} r_j^n,$$

$$N(n) = s(n) + i(n) + r(n).$$

Discrete qualitative properties:

- [P1] $N(n) = \text{constant}$.
- [P2] $s(n)$ monotone decreases and $r(n)$ monotone increases,
- [P3] $s_j^0 \geq 0; i_j^0 \geq 0; r_j^0 \geq 0 \quad \Rightarrow \quad s_j^n \geq 0; i_j^n \geq 0; r_j^n \geq 0$ for all n.

Qualitative properties of finite difference scheme with explicit Euler method

- [P1] $(N(n) = N^\star = \text{constant})$: without any condition
- [P3] (nonnegativity):

$$\tau < \min\left\{\frac{h^2}{2d_1 + hkN^\star}; \frac{h^2}{2d_2 + h^2\gamma}; \frac{h^2}{2d_3}\right\};$$

- [P2] (monotonicity): without any condition.

Condition for the Courant number $q = \tau/h^2$.

Finite difference scheme with implicit-explicit Euler method (IMEX)

We define the difference scheme by using the IMEX:

$$\frac{s_j^{n+1}-s_j^n}{\tau}=d_1\frac{s_{j+1}^{n+1}-2s_j^{n+1}+s_{j-1}^{n+1}}{h^2}-ks_j^n i_j^n,$$
$$\frac{i_j^{n+1}-i_j^n}{\tau}=d_2\frac{i_{j+1}^{n+1}-2i_j^{n+1}+i_{j-1}^{n+1}}{h^2}+ks_j^n i_j^n-\gamma i_j^n,$$
$$\frac{r_j^{n+1}-r_j^n}{\tau}=d_3\frac{r_{j+1}^{n+1}-2r_j^{n+1}+r_{j-1}^{n+1}}{h^2}+\gamma i_j^n,$$

$j=0,\dots,N-1$, $n=0,1,\dots$.

+Neumann b.c.: $s_{-1}^n=s_0^n,\quad s_{N-1}^n=s_N^n$, etc. +initial condition

How to satisfy the discrete versions of the qualitative properties?

Qualitative properties of finite difference scheme with IMEX method

The above model: SLAE of the form $\mathbf{A}\mathbf{x} = \mathbf{b}$, where $\mathbf{A}$ is an M-matrix.

- [P1] ($N(n) = N^\star = constant$): without any condition
- [P3] (non-negativity): we should guaranty: $\mathbf{b} \geq \mathbf{0}$. The condition:
$$\tau < \min\left\{\frac{h}{kN^\star}; \frac{1}{\gamma}\right\};$$
- [P2] (monotonicity): without any condition.

Condition: $\dfrac{\tau}{h} \sim \dfrac{1}{kN^\star}$

Qualitative properties of finite difference scheme with IMEX method

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- [P2] (monotonicity): without any condition.

Condition: $\dfrac{\tau}{h} \sim \dfrac{1}{kN^\star}$

$\Rightarrow$ there is no condition for the Courant number.

Continuous model with diffusion in higher dimensions

Let $\Omega = [0, L]^2 \subset \mathbb{R}^2$ and Δ_2 the 2-dimensional Laplace operator.

Mathematical model with space dependence and with diffusion in $\mathbb{R}^2$

$$S'_t(x,t) = d_1 \Delta_2 S(x,t) - kI(x,t)S(x,t),$$
$$I'_t(x,t) = d_2 \Delta_2 I(x,t) + kI(x,t)S(x,t) - \gamma I(x,t),$$
$$R'_t(x,t) = d_3 \Delta_2 R(x,t) + \gamma I(x,t).$$

$S = S(x,t)$, $I = I(x,t)$ and $R = R(x,t)$ are the space dependent densities.

Here $x \in \Omega$ + initial conditions + Neumann boundary condition.

The qualitative properties P1-P3 are valid.

Qualitative properties of finite difference scheme in 2D

Mesh with step-size h in both direction.
Notations:

$$s(n) = h^2 \sum_{j=0}^{N-1} \sum_{l=0}^{N-1} s_{j,l}^n, \quad \text{etc.}$$

- Finite difference discretized model with EEM:
  - [P1] ($N(n) = N^\star = \text{constant}$): without any condition
  - [P3] (non-negativity):

$$\tau < \min\left\{ \frac{h^2}{2^2 d_1 + kN^\star}; \frac{h^2}{2^2 d_2 + h^2\gamma}; \frac{h^2}{2^2 d_3} \right\};$$

  - [P2] (monotonicity): without any condition.

Condition for the Courant number $q = \tau/h^2$.

Finite difference discretized model in 2D with implicit-explicit Euler method

- Finite difference discretized model with IMEX:
  - [P1] ($N(n) = \mathrm{constant}$): without any condition
  - [P3] (non-negativity):

$$\tau < \min\left\{\frac{h^2}{kN^\star};\ \frac{1}{\gamma}\right\};$$

  - [P2] (monotonicity): without any condition.

Condition: $\dfrac{\tau}{h^2} \sim \dfrac{1}{kN^\star}$

Finite difference discretized model in 2D with implicit-explicit Euler method

- Finite difference discretized model with IMEX:
  - [P1] ($N(n) = \text{constant}$): without any condition
  - [P3] (non-negativity):

$$\tau < \min\left\{\frac{h^2}{kN^\star}; \frac{1}{\gamma}\right\};$$

  - [P2] (monotonicity): without any condition.

Condition: $\dfrac{\tau}{h^2} \sim \dfrac{1}{kN^\star}$

$\Rightarrow$ There is condition for the Courant number.

Numerical tests

2D example: Parameter setting

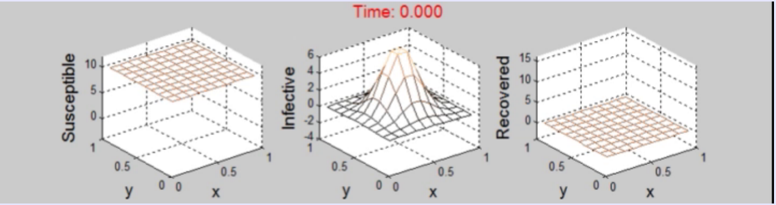
We set $L = 1$, $N = 10$, $k = 0.05$, $d_1 = d_2 = d_3 = 0.01$, $\gamma = 0.07$, and hence $N^\star = 11.2533$.

We apply the IMEX method.

The sufficient condition for $\tau = 0.0177$. We will apply two time steps: $\tau = 0.017$ and $\tau = 2.5$.

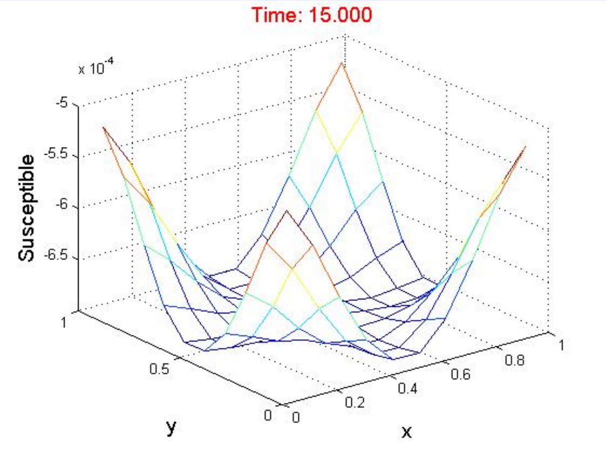
Correct numerical solution (IMEX)

$\tau = 0.017$



Incorrect numerical solution (IMEX)

$\tau = 2.5$



Summary

- We have formulated the basic qualitative properties of the continuous and discrete epidemic models.
- We have constructed different discrete models (lsSIR, dsSIR) in 1D and 2D.
- We gave *a priori* checkable sufficient condition for the discrete model to guarantee the qualitative properties.
- We checked the sharpnes of the sufficient bounds on numerical examples.

Future work

- More complex discrete models (not only diffusion).
- Construction and analysis of new lsSIR models (from the integral equaion).
- Generalization of the dsSIR model for variable diffusion coefficients.
- Consideration of lsSIR and dsSIR models with variable step-size.
- Other qualitative properties?

Thank you for your attention