Russian Science Foundation

Numerical solution of the optimal control epidemic problem, taking into account age characteristics

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Motivation

$$\begin{cases} \dfrac{dS}{dt} = -\dfrac{\beta I S}{N}, & S(0) = N - I_0, \\ \dfrac{dI}{dt} = \dfrac{\beta I S}{N} - \gamma I, & I(0) = I_0 < N, \\ \dfrac{dR}{dt} = \gamma I, & R(0) = 0. \end{cases}$$

SIS | SIRS | SIRC | SEIR | SEIRD | SEIR-HCD | ...

- Complete immunity is conferred by a single attack, and that an individual is not infective at the moment at which he receives infection.
- No epidemic can occur if the population density is below some threshold value.
- Small increases of the infectivity rate may lead to large epidemics.
- An epidemic, in general, comes to an end, before the susceptible population has been exhausted.

<u>The advantage of SIR models</u>

- Ease of implementation.
- Basis: law of conservation of masses with established relationships to different states of the system.
- Describes large populations (regions, countries).
- Fundamental (to model the spread of another infection in another region, it is sufficient to specify the parameters).

<u>Disadvantages of SIR models</u>

- Describes only 1 peak.
- Changing parameters (virus mutations, restrictive measures, vaccination) leads to the need to re-solve the inverse problem and calculate scenarios with new parameters.

Kermack W.O., McKendrick A.G., A contribution to the mathematical theory of epidemics, 1927

Motivation

$$\frac{\partial u}{\partial t} = d\frac{\partial^2 u}{\partial x^2} + G(u)$$

$$u(x,0) = u_0(x)$$

$u(x,t)$ is the concentration of individuals with a certain gene in the population,
d is the diffusion coefficient,
$G(u)$ is the function of concentration increase per one generation.

Proposed and theoretically investigated a mathematical model based on a parabolic partial derivative equation and applied it to the study of biological problems.

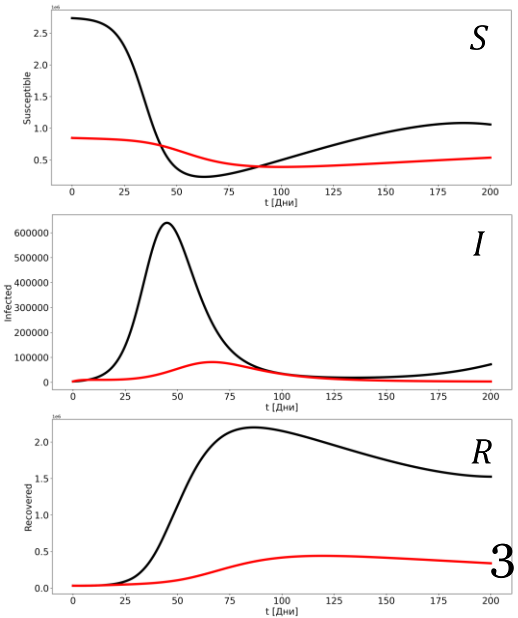
Kolmogorov A.N., Petrovskii I.G., Piskunov N.S., A study of the diffusion equation with increase in the amount of substance, and its application to a biological problem, 1937

Spatial functions can be introduced into the SIR model as follows

$$S(t) = \int_\Omega s(t,x)dx\,, I(t) = \int_\Omega i(t,x)dx\,, R(t) = \int_\Omega r(t,x)dx\,, \ldots$$

$$\frac{dU}{dt} = \Phi(t,U,q), \quad U(t_0) = U_0, \quad U = (S,I,R). \quad \longrightarrow \quad \frac{\partial u}{\partial t} = \Phi(t,u,q) + \nabla(n v \nabla u), \quad u(x,t_0) = u_0(x), \quad u_x(0,t) = u(1,t) = 0, \quad v = (v_s, v_i, v_r).$$

Black line is the ODE
Red line is the PDE



Taking spatial heterogeneity into account allows a more accurate modelling of an epidemic from a spreading center (a large city in the country, a capital city in the region, etc.) with known initial conditions.
However, using the model to describe the second and subsequent waves of the epidemic requires the addition of equations, the introduction of multiple known sources of disease spread $u(x,t_0)$ (the inverse problem of source identification) and computational resources.

Viguerie A., Veneziani A., Lorenzo G. et al. Diffusion-reaction compartmental models formulated in a continuum mechanics framework: application to COVID-19, mathematical analysis, and numerical study, 2020
Aristov V.V., Stroganov A.V., Yastrebov A.D. Simulation of spatial spread of the COVID-19 pandemic on the basis of the kinetic-advection model, 2021

Motivation

$$\partial_t \vec{u} = \nabla(\vec{v}\nabla\vec{u}) + G(\vec{u},\vec{q})$$
$$\vec{u}(x,0) = \vec{u}_0(x)$$
$$\partial_x \vec{u}(0,t) = 0, \vec{u}(1,t) = 0$$

$$+ \quad \int_\Omega u_i(x,t_k)dx = I_k, \quad k = 1,\dots,K$$

Solution of inverse problem:

- does not exist for noisy data I_k^δ
- is not unique for lack of data ($\vec{v} \in \mathbb{R}^d,\ d \gg K$)
- is unstable for $u \in C^2$

Inverse problem: to clarify the velocities $\vec{v}$ rom the additional information I_k

Epidemiology

Li X.-Z., Yang J. and Martcheva M., 2020
Viguerie A., Veneziani A., Lorenzo G. et al., 2020
Krivorotko O.I., Kabanikhin S.I., 2024

Economics

Kabanikhin S., Krivorotko O., Bektemessov Z., Bektemessov M. and Zhang S., 2020

Climate

Pyanova E. A., Penenko V. V. and Faleychik L. M., 2019

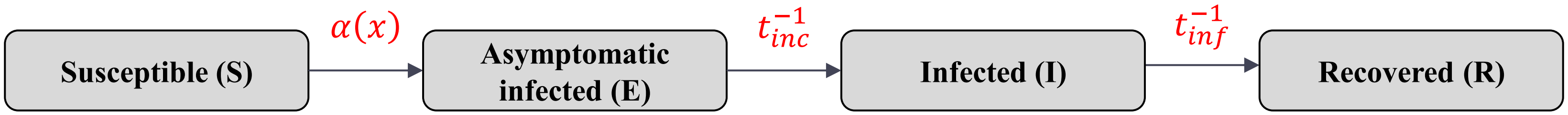
Social networks

Sun W., Qi J. and Zhang J., 2018
Krivorotko O., Zvonareva T., Zyatkov N., 2021

SEIR model

$$
\begin{cases}
\frac{\partial s}{\partial t} = \nabla(n v_s \nabla s) - \alpha(x) s i, \\
\frac{\partial e}{\partial t} = \nabla(n v_e \nabla e) + \alpha(x) s i - t_{inc}^{-1} e, \\
\frac{\partial i}{\partial t} = \nabla(n v_i \nabla i) + t_{inc}^{-1} e - t_{inf}^{-1} i, \\
\frac{\partial r}{\partial t} = \nabla(n v_r \nabla r) + t_{inf}^{-1} i,
\end{cases}
$$

Parameter	Description	Boundaries
v_u	The space velocity of the group u	(0, 1)
$\alpha(x)$	Infection rate between asymptomatic and susceptible populations	(0, 1)
t_{inc}	The duration of incubation period	2-14 days
t_{inf}	The duration of the infection period	2-14 days



Direct problem: find vector $u = (s, e, i, r)$ with known parameters q, v, initial data $s(x,0) = s_0(x), e(x,0) = e_0(x)$, $i(x,0) = i_0, r(x,0) = r_0$ and boundary conditions $\frac{\partial u(0,t)}{\partial x} = 0, u(1,t) = 0.$

Statement of the inverse problem

$$\begin{cases} \frac{\partial s}{\partial t} = \nabla(n v_s \nabla s) - \alpha(x) s i, & s(x,0) = s_0(x), \\ \frac{\partial e}{\partial t} = \nabla(n v_e \nabla e) + \alpha(x) s i - t_{inc}^{-1} e, & e(x,0) = e_0(x), \\ \frac{\partial i}{\partial t} = \nabla(n v_i \nabla i) + t_{inc}^{-1} e - t_{inf}^{-1} i, & i(x,0) = i_0, \\ \frac{\partial r}{\partial t} = \nabla(n v_r \nabla r) + t_{inf}^{-1} i, & r(x,0) = r_0, \\ \frac{\partial u(0,t)}{\partial x} = 0, \quad u(1,t) = 0. \end{cases}$$

+

Additional information:

$$\boldsymbol{I_k} = \int_0^1 i(x, t_k), \qquad k = 1, \dots, K$$

Inverse problem: find $v = (v_s, v_e, v_i)$ using number of symptomatic diagnosed of COVID-19 $\boldsymbol{I_k}$ in K days with known parameters q.

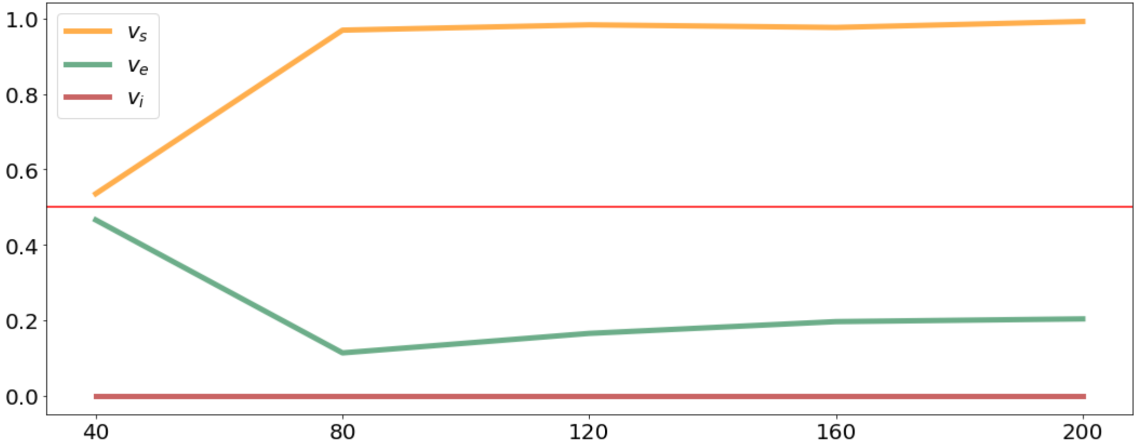
$$J(v) = \sum_{k=1}^{K} \left| \int_0^1 i(x, t_k; v) - \boldsymbol{I_k} \right|^2 \rightarrow \min_{v=(v_s, v_e, v_i)}$$

Sensitivity analysis of the SEIR-HCD model

$$\begin{cases} \dfrac{\partial s}{\partial t} = \nabla(n v_s \nabla s) - \alpha(x) s i, & s(x,0) = s_0(x), \\ \dfrac{\partial e}{\partial t} = \nabla(n v_e \nabla e) + \alpha(x) s i - t_{inc}^{-1} e, & e(x,0) = e_0(x), \\ \dfrac{\partial i}{\partial t} = \nabla(n v_i \nabla i) + t_{inc}^{-1} e - t_{inf}^{-1} i, & i(x,0) = i_0, \\ \dfrac{\partial r}{\partial t} = \nabla(n v_r \nabla r) + t_{inf}^{-1} i, & r(x,0) = r_0, \\ \dfrac{\partial u(0,t)}{\partial x} = 0, \quad u(1,t) = 0. \end{cases}$$

$$S_i = \frac{V_{q_i}\left(E_{Q_i}(f|q_i)\right)}{V(f)}, \qquad f(t) = \int_0^1 i(x,t)\,dx$$

q_i	i-th parameter
Q_i	generated matrix of unknown parameters without q_i
$E_{Q_i}(f\|q_i)$	means that the average value for f is taken over all possible values of Q_i at a fixed q_i
V_{q_i}	variance that is taken over all possible values of q_i
$V(f)$	variance of matrix f



The diffusion coefficients v_e, v_i are not sensitive.

Sobol I.M., Sensitivity analysis for non-linear mathematical models, 1993

Results for logistic model

$$\begin{cases} \frac{\partial I}{\partial t} = D\frac{\partial^2 I}{\partial x^2} + \left(1 - \frac{I}{N}\right)\alpha(t)I \\ I(x,1) = \varphi(x), \quad l_1 \le x \le l_2 \\ \frac{\partial I}{\partial x}(l_1,t) = \frac{\partial I}{\partial x}(l_2,t) = 0, \quad t \ge 1 \end{cases}$$

+

Additional information:

$$\sum_{i=1}^{N_1} I(x_i,t_k) = f_k, \qquad k = 1,\dots,N_2$$

$$\min_{q=(\varphi(x_1),\dots,\varphi(x_d))} J(q) = \min_q \left(\sum_{k=1}^{N_2} \left| \sum_{i=1}^{N_1} I(x_i,t_k;q) - f_k \right|^2 \right)$$

Method	$error(q)$	Run time, h
FGM	4.91	0.003
PSO	3.16	0.19
PSO+FGM	8.09	0.64
TT	**0.75**	1.09
TT+FGM	0.93	1.1

$$error(q) = \sum_{i=1}^{6} \frac{|q_i - q_i^{ex}|}{q_i^{ex}}$$

The smallest error value $error_{min}$ is achieved using the TT method.

Tensor Train global optimization (TT)

$$J(q) \to g_a(q)$$

$$g_a(q) = h(J(q) - a)$$

$h(b) = \frac{\pi}{2} - \arctan(b)$, a is some initial approximation to the global minimum of function $J(q)$.

Introduce a grid with n nodes in each of the d directions and tensor $A \in \mathbb{R}^{n^d}$

$$A(i_1, \dots, i_d) = g_a\left(\frac{i_1 - 1}{n - 1}, \dots, \frac{i_d - 1}{n - 1}\right)$$

⇩

The algorithm of the method is based on the sequential approximation of the submatrices of these sweep matrices

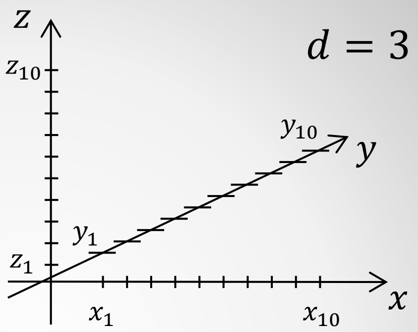
$$A_k(i_1 \dots i_k, i_{k+1} \dots i_d) = A(i_1, \dots, i_d)$$

by the cross method and local optimization of the interpolation nodes obtained by this method.

$d = 3$

$$f(x, y, z) = 2x + yz$$

$$n = 10,$$
$$x, y, z \in [1,10]$$

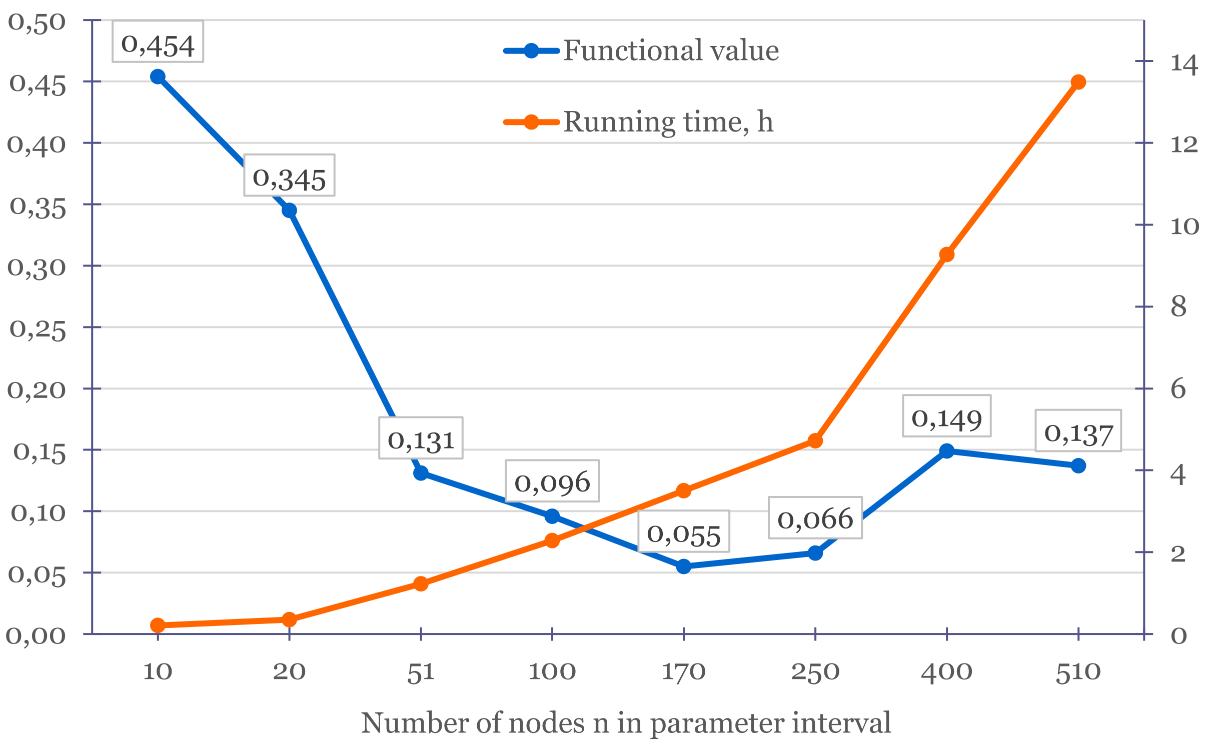


$$A(i, j, k) = f\left(x_i, y_j, z_k\right)$$

$$\begin{pmatrix} A(1,1,1) & \cdots & A(1,10,1) & & A(1,1,10) & \cdots & A(1,10,10) \\ \vdots & \ddots & \vdots & \cdots & \vdots & \ddots & \vdots \\ A(10,1,1) & \cdots & A(10,10,1) & & A(10,1,10) & \cdots & A(10,10,10) \end{pmatrix}$$
$$=$$
$$\begin{pmatrix} 1 & \cdots & 12 & & 12 & \cdots & 102 \\ \vdots & \ddots & \vdots & \cdots & \vdots & \ddots & \vdots \\ 21 & \cdots & 30 & & 30 & \cdots & 120 \end{pmatrix}$$

Oseledets I. V., Tyrtyshnikov E. E., Breaking the curse of dimensionality, or how to use SVD in many dimensions, 2009
Zheltkov D. A., Oferkin I. V. et al., TTDock: a docking method based on tensor train decompositions, 2013

Efficiency of the TT method

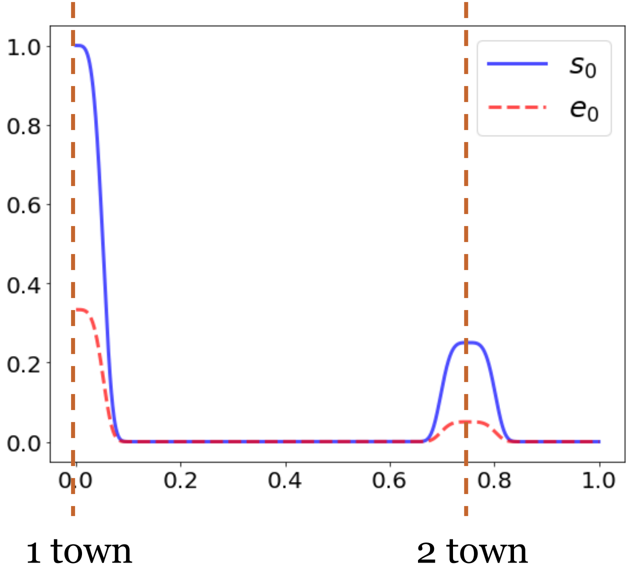


SSCC computing node:
2 Intel Xeon Gold 6248R
processors (3 GHz, 24 cores)
384 GB of main memory

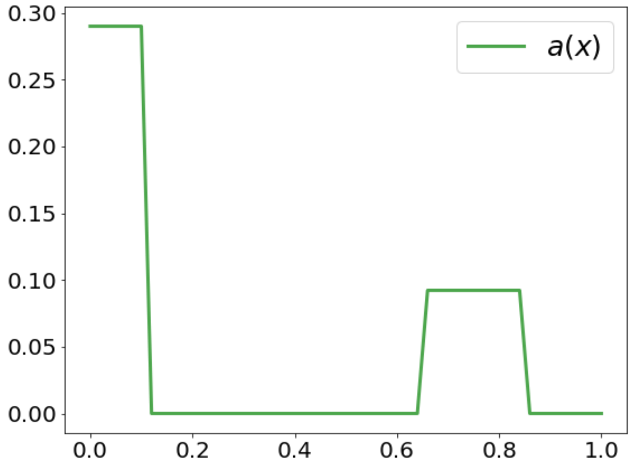
The function value (blue line) decreases as the number of nodes increases. However, as the number of nodes increases, the running time of the program (orange line) critically increases.

Input data

Initial density of susceptible and asymptomatic infected



Infection rate

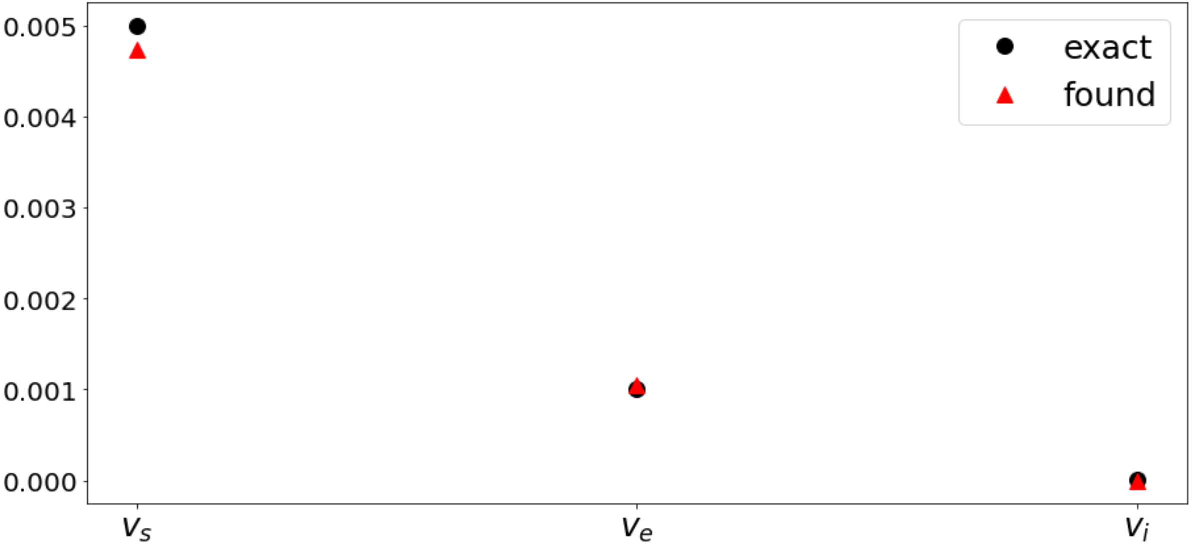


Parameter	Value
t_{inc}	5
t_{inf}	8
N	8380336
I_0	65392
R_0	1002965
v_r	$5 \cdot 10^{-3}$

$$i_0 = \frac{I_0}{N}, \qquad r_0 = \frac{R_0}{N}$$

Viguerie A., Veneziani A., Lorenzo G. et al. Diffusion-reaction compartmental models formulated in a continuum mechanics framework: application to COVID-19, mathematical analysis, and numerical study, 2020

Results



Additional information:

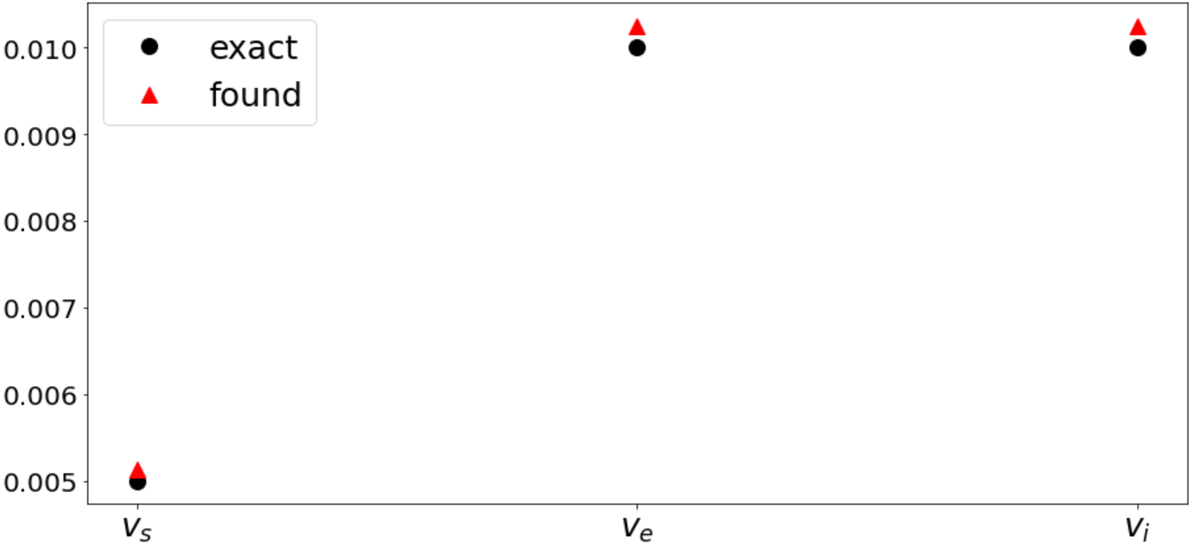
$$I_k = \int_0^1 i(x, t_k)\,, \qquad k = 1, \dots, 200$$

Parameter	Exact value	Found value
v_s	$5 \cdot 10^{-3}$	$4.73 \cdot 10^{-3}$
v_e	$1 \cdot 10^{-3}$	$1.05 \cdot 10^{-3}$
v_i	$1 \cdot 10^{-5}$	0

$$error(q) = \sum_{i=1}^{6} \frac{|q_i - q_i^{ex}|}{q_i^{ex}} = 1.1$$

Parameter v_i is poorly recovered because the value is too small.

Results



Additional information:

$$\boldsymbol{I_k} = \int_0^1 i(x, t_k)\,, \qquad k = 1, \ldots, 200$$

Parameter	Exact value	Found value
v_s	$5 \cdot 10^{-3}$	$5.13 \cdot 10^{-3}$
v_e	$1 \cdot 10^{-2}$	$1.03 \cdot 10^{-2}$
v_i	$1 \cdot 10^{-2}$	$1.03 \cdot 10^{-2}$

$$error(q) = \sum_{i=1}^{6} \frac{|q_i - q_i^{ex}|}{q_i^{ex}} = 0.076$$

The method recovers considered parameters well if their values are not too close to zero.

Conclusion of the section

Taking spatial heterogeneity into account allows a more accurate modelling of an epidemic from a spreading center (a large city in the country, a capital city in the region, etc.) with known initial conditions.

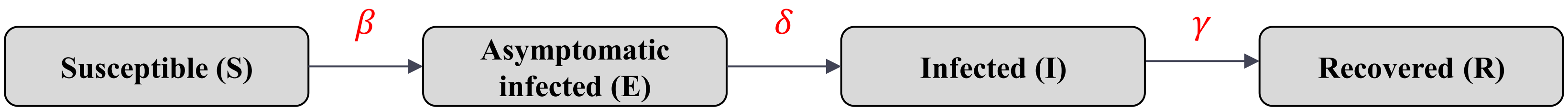
The SEIR model is sensitive to the diffusion coefficients of susceptible group.

The TT method is able to recover the considered parameters well if they are not close to zero.

SEIR model, taking into account age characteristics

$$
\begin{cases}
\frac{\partial S}{\partial t} + v\frac{\partial S}{\partial a} = -\beta\frac{S(a,t)I(a,t)}{N}, \\
\frac{\partial E}{\partial t} + v\frac{\partial E}{\partial a} = \beta\frac{S(a,t)I(a,t)}{N} - \delta E(a,t), \\
\frac{\partial I}{\partial t} + v\frac{\partial I}{\partial a} = \delta E(a,t) - \gamma I(a,t), \\
\frac{\partial R}{\partial t} + v\frac{\partial R}{\partial a} = \gamma I(a,t),
\end{cases}
$$

Parameter	Description
a	Age
β	Infection rate between asymptomatic and susceptible populations
δ^{-1}	The duration of incubation period
γ^{-1}	The duration of the infection period



Direct problem: find vector $X = (S, E, I, R)$ with known parameters q, initial data $X(a, 0) = X_0(a)$ and boundary conditions $\frac{\partial X(a_0,t)}{\partial a} = \frac{\partial X(a_1,t)}{\partial a} = 0$.

Age-dependent SEIR model with control

$$\begin{cases} \dfrac{\partial S}{\partial t} + v\dfrac{\partial S}{\partial a} = -\beta\big(1 - u_1(a,t)\big)\dfrac{S(a,t)I(a,t)}{N}, \\ \dfrac{\partial E}{\partial t} + v\dfrac{\partial E}{\partial a} = \beta\big(1 - u_1(a,t)\big)\dfrac{S(a,t)I(a,t)}{N} - \delta E(a,t), \\ \dfrac{\partial I}{\partial t} + v\dfrac{\partial I}{\partial a} = \delta E(a,t) - \gamma I(a,t) - u_2(a,t)I(a,t), \\ \dfrac{\partial R}{\partial t} + v\dfrac{\partial R}{\partial a} = \gamma I(a,t) + u_2(a,t)I(a,t), \end{cases}$$

Parameter	**Description**
$u_1(s,t)$	Prevention (medical mask, hand washing, social distancing)
$u_2(s,t)$	Quarantine and medical treatment for infectious populations

Direct problem: $J(u_1,u_2) = \iint\limits_{\Omega} \left(c_1 I(s,t) + \frac{1}{2}\left(c_2 u_1^2(s,t) + c_3 u_2^2(s,t)\right)\right) dtds \to \min$

number of infected people throughout the observation period

cost of financing programs to limit the spread of the epidemic

Age-dependent SEIR model with control

$$\begin{cases} \frac{\partial S}{\partial t} + v\frac{\partial S}{\partial a} = -\beta\big(1 - u_1(a,t)\big)\frac{S(a,t)I(a,t)}{N}, \\ \frac{\partial E}{\partial t} + v\frac{\partial E}{\partial a} = \beta\big(1 - u_1(a,t)\big)\frac{S(a,t)I(a,t)}{N} - \delta E(a,t), \\ \frac{\partial I}{\partial t} + v\frac{\partial I}{\partial a} = \delta E(a,t) - \gamma I(a,t) - u_2(a,t)I(a,t), \\ \frac{\partial R}{\partial t} + v\frac{\partial R}{\partial a} = \gamma I(a,t) + u_2(a,t)I(a,t), \end{cases}$$

$$u_1^*(a,t) = \min\left(1, \max\left(0, \frac{\beta S(a,t)I(a,t)\big(\lambda_1(a,t) - \lambda_2(a,t)\big)}{c_2 N}\right)\right),$$
$$u_2^*(a,t) = \min\left(1, \max\left(0, \frac{I(a,t)\big(\lambda_4(a,t) - \lambda_3(a,t)\big)}{c_3}\right)\right).$$

$$\begin{cases} \frac{\partial \lambda_1}{\partial t} + v\frac{\partial \lambda_1}{\partial a} = \beta\big(1 - u_1(a,t)\big)\frac{I(a,t)}{N}\big(\lambda_1(a,t) - \lambda_2(a,t)\big), \\ \frac{\partial \lambda_2}{\partial t} + v\frac{\partial \lambda_2}{\partial a} = \delta\big(\lambda_2(a,t) - \lambda_3(a,t)\big), \\ \frac{\partial \lambda_3}{\partial t} + \frac{v\partial \lambda_3}{\partial a} = \beta\big(1 - u_1(a,t)\big)\frac{S(a,t)}{N}\big(\lambda_1(a,t) - \lambda_2(a,t)\big) + \big(\gamma + u_2(a,t)\big)\big(\lambda_3(a,t) - \lambda_4(a,t)\big) - c_1, \\ \frac{\partial \lambda_4}{\partial t} + v\frac{\partial \lambda_4}{\partial a} = 0, \end{cases}$$

Algorithm

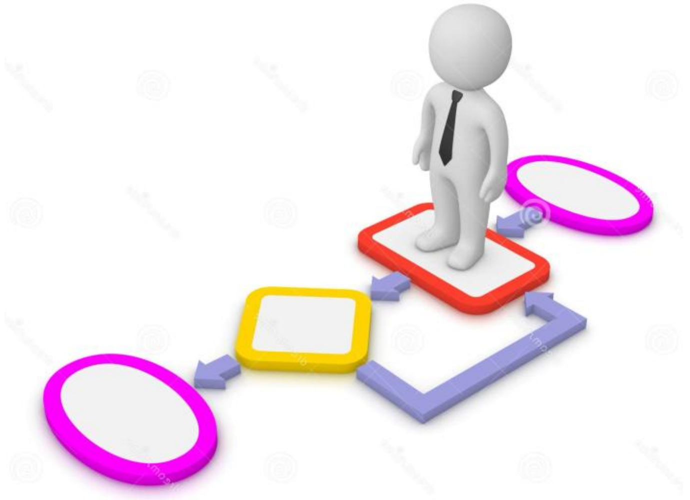
$u_i(a,t)$ is the control functions,

$X = (S, E, I, R)$ is the solution of SEIR,

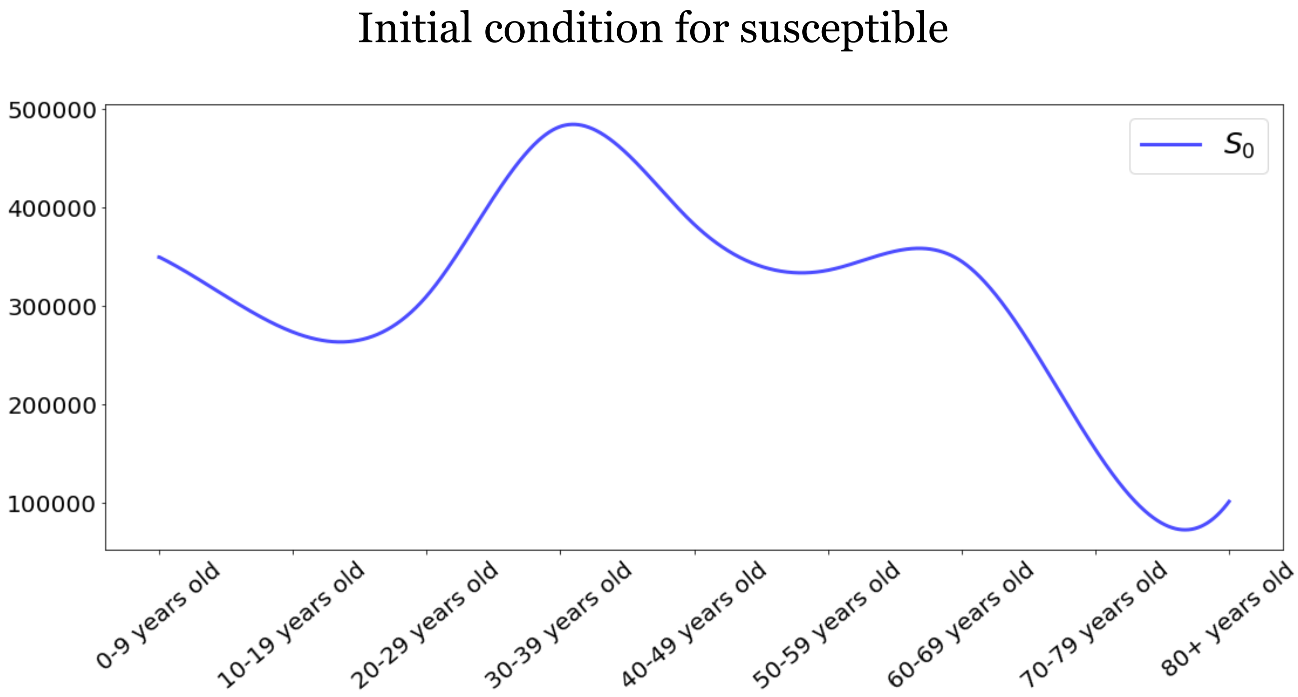
$J(u_1, u_2)$ is the cost function,

$\lambda_k(a,t)$ is the solution of adjoint system.

0) Put $u_i = 0, i = 1,2$.
1) $n = 0$, obtain X and $J_0 = J(u_1, u_2)$.
2) $n = n + 1$, calculate $\lambda_k, k = 1,2,3,4$.
3) Obtain new u_i.
4) Obtain new X.
5) Obtain new $J_n = J(u_1, u_2)$.
6) If $|J_n - J_{n-1}| < \varepsilon$ then X is a solution.
   Otherwise go to 2.



Input data

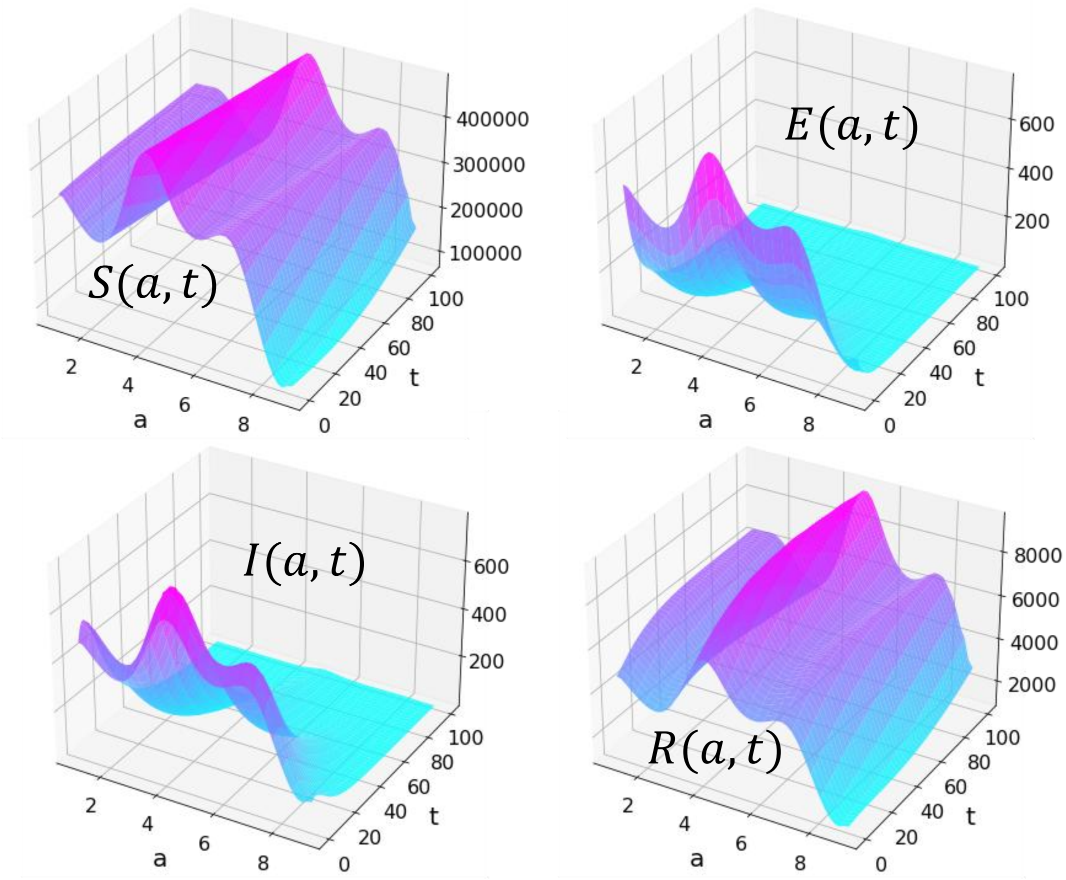


Parameter	Value
β	0.385
δ	1/5
γ	1/8
N	2780292
v	0.01

The functions E_0, I_0, R_0 are proportional to S_0.

Krivorotko O. , Sosnovskaia M., Kabanikhin S. Agent-based mathematical model of COVID-19 spread in Novosibirsk region: Identifiability, optimization and forecasting, 2023

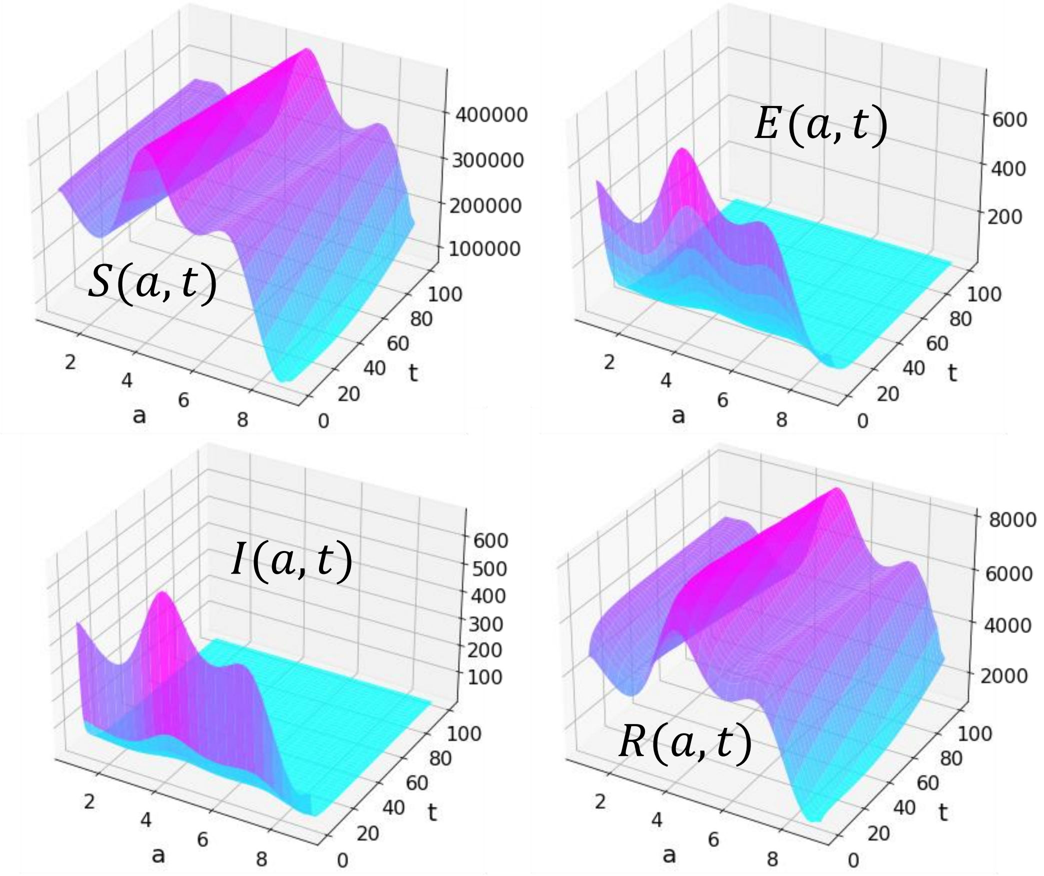
Numerical experiments without control

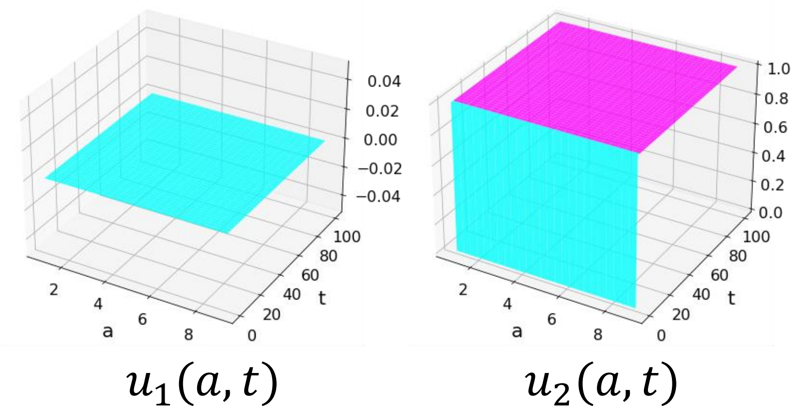


$$u_1(a,t) = u_2(a,t) = 0$$

For the selected parameters of the SEIR model, the number of sensitive patients almost does not change, the asymptomatic ones decrease, the infected ones first increase, then also decrease and move into the group of recovered ones.

Numerical experiments with control





For the selected parameters of the SEIR model with control, the number of asymptomatic and infected decreases faster. This is achieved in the absence of restrictive measures ($u_1(a,t) = 0, \forall a,t$) and maximum quarantine measures and effective treatment of infected people ($u_2(a,t) = 1, t \neq 0$).

Conclusion

Taking age heterogeneity into account allows a more accurate modelling of an epidemic.

For the selected parameters of the SEIR model with control, the number of asymptomatic and infected decreases faster. This is achieved in the absence of restrictive measures and maximum quarantine measures and effective treatment of infected people.

Thank you for your attention!

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