Optimization of Stochastic Epidemiological Models for Disease Control and Prediction

Dr. Khalil Al Handawi

Joint work with: Prof. Michael Kokkolaras

Journées de l'optimisation 2022

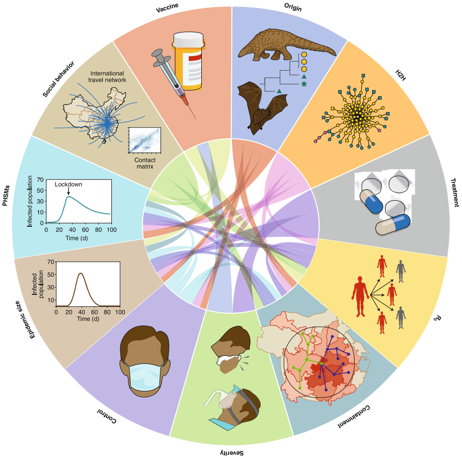
July 24, 2023

Research displinces in epidemiology

Forecasting novel epidemics is a multidisciplinary field involving multiple *targets*

In the early stages of epidemics, we have access to:

Simulation models can be developed based on this information and used in public health and social measures (PHSMs) policy-making.



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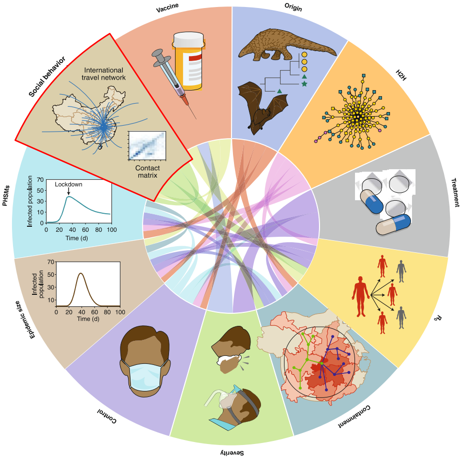

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- **Incidence rate data**

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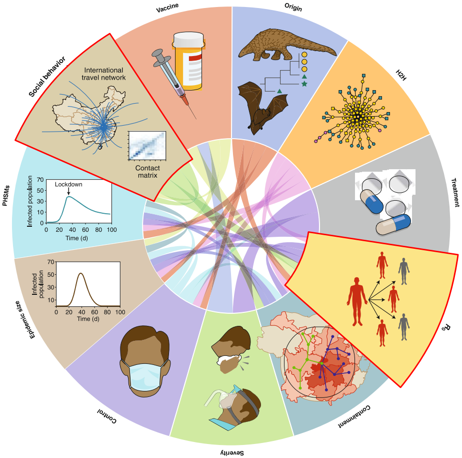

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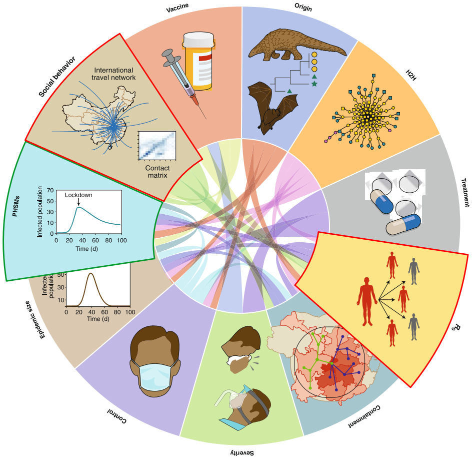
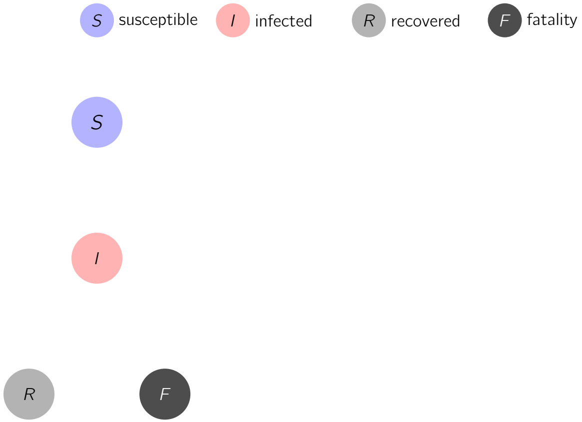


Simulation and modeling of pandemics in early stages

Joint work with: Prof. Michael Kokkolaras

Background: epidemiological models

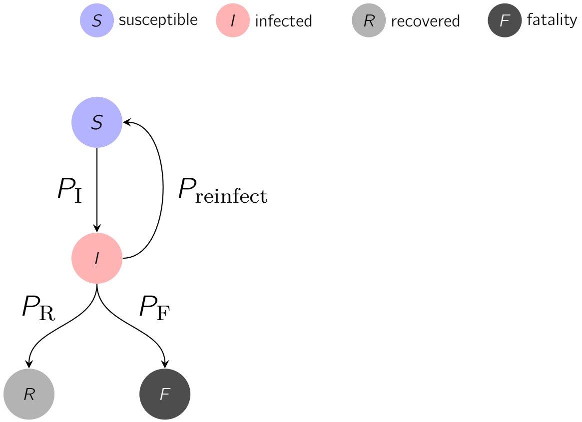
What are compartmental epidemiological models?



Background: epidemiological models

What are compartmental epidemiological models?

- Described by a *stochastic* process



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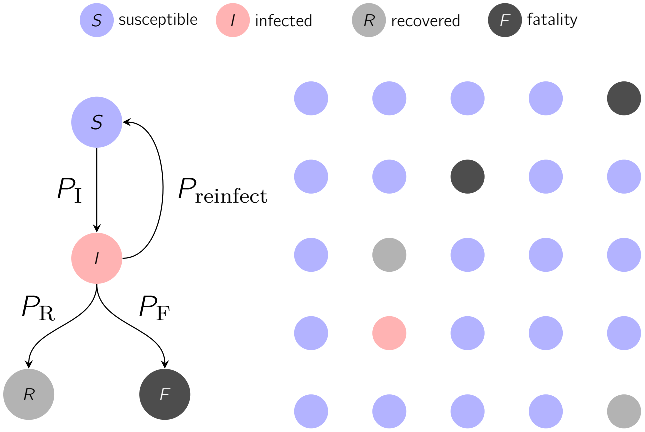
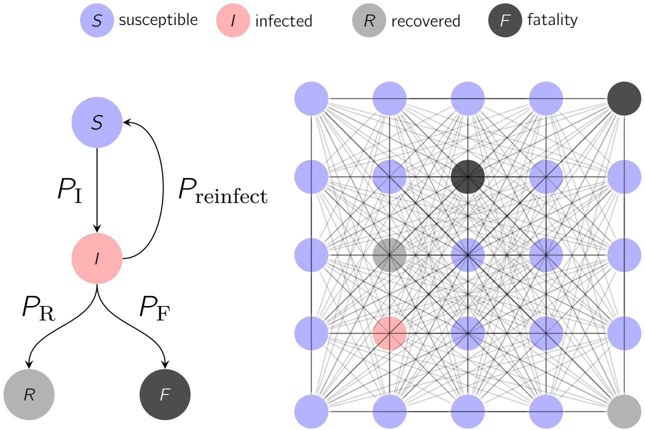


Background: epidemiological models

What are compartmental epidemiological models?

- Described by a *stochastic* process
- Assumes *homogenous* interaction



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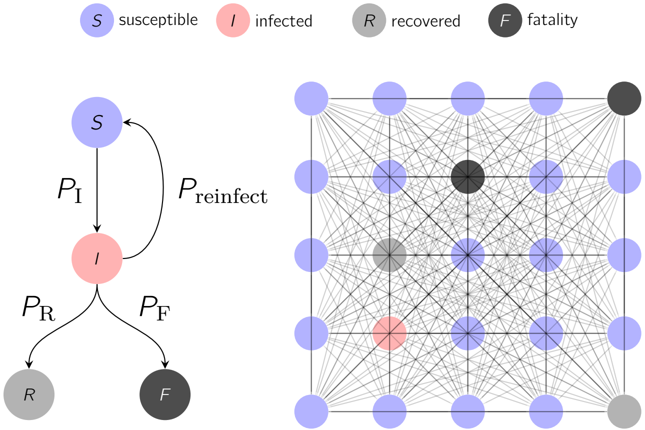
What are compartmental epidemiological models?

- Described by a *stochastic* process
- Assumes *homogenous* interaction
- Deterministic response for large N



Background: epidemiological models

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- Described by a *stochastic* process
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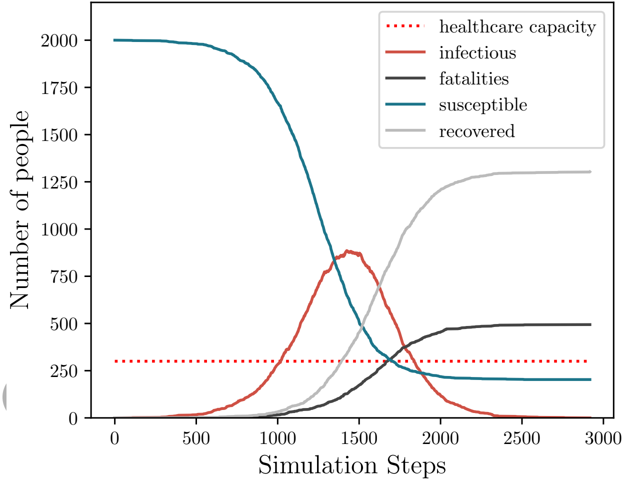
- Deterministic response for large N

$$\frac{dS}{dt} = -\frac{\beta IS}{N},$$

$$\frac{dI}{dt} = \frac{\beta IS}{N} - \gamma I,$$

$$\frac{dR}{dt} = \gamma I,$$

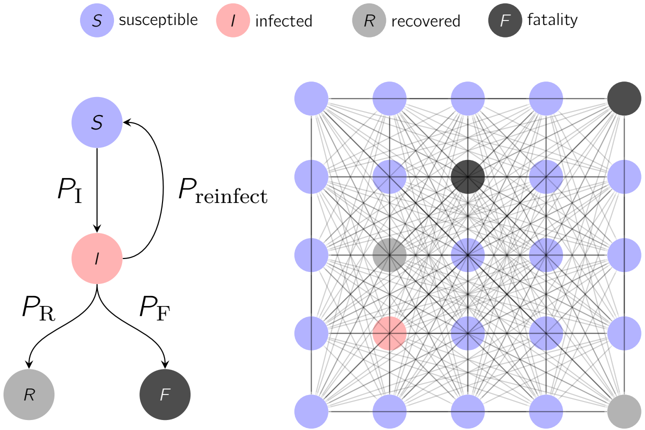
where $N = S + I + R$, β controls infection spread, and γ controls recovery rate



Background: epidemiological models

What are compartmental epidemiological models?

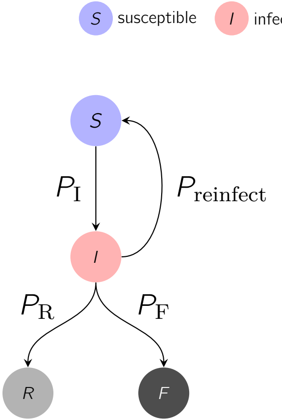
✓ Analytical solutions are available

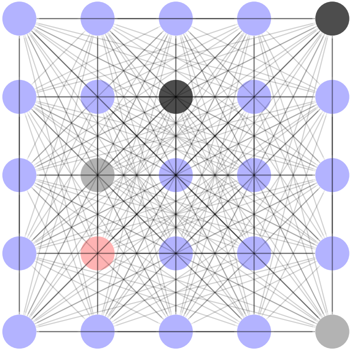


Background: epidemiological models

What are compartmental epidemiological models?

- ✓ Analytical solutions are available
- ✓ Captures large-scale population dynamics



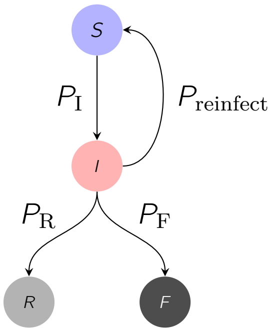


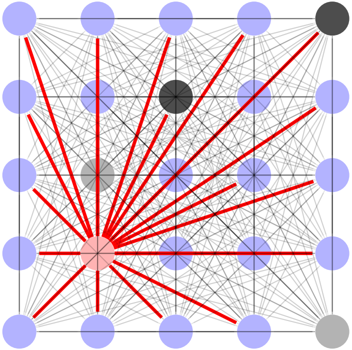
Background: epidemiological models

What are compartmental epidemiological models?

- ✓ Analytical solutions are available
- ✓ Captures large-scale population dynamics
- ✘ Does not account for *geography*

S susceptible I infected R recovered F fatality

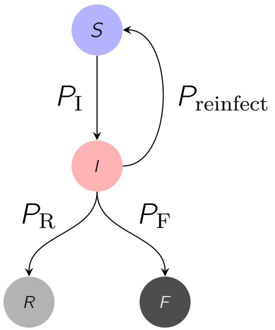


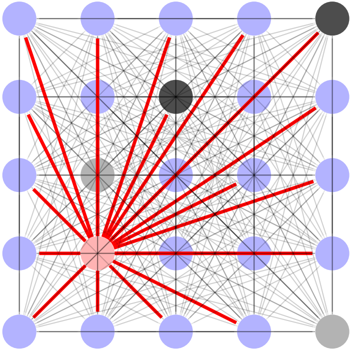


Background: epidemiological models

What are compartmental epidemiological models?

- ✓ Analytical solutions are available
- ✓ Captures large-scale population dynamics
- ✘ Does not account for *geography*
- ✘ Cannot model effect of intervention policies





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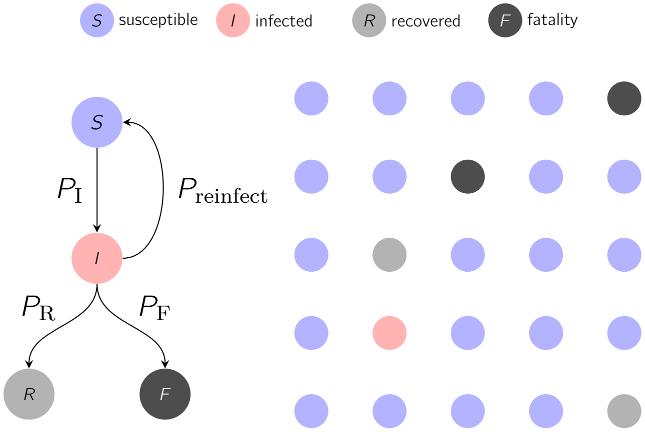

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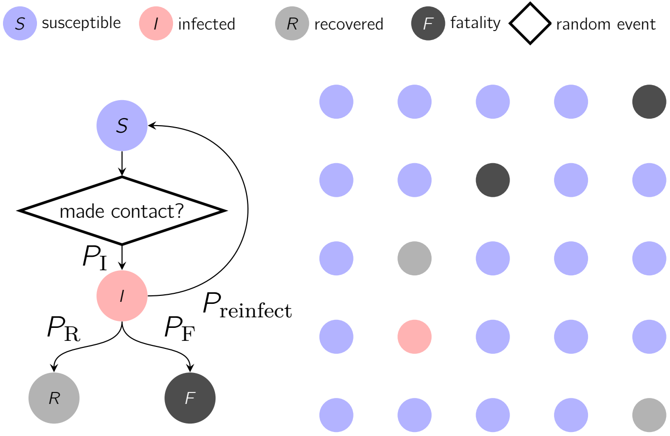
What are agent-based epidemiological models?

- *Stochastic* process



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What are agent-based epidemiological models?

- *Stochastic* process
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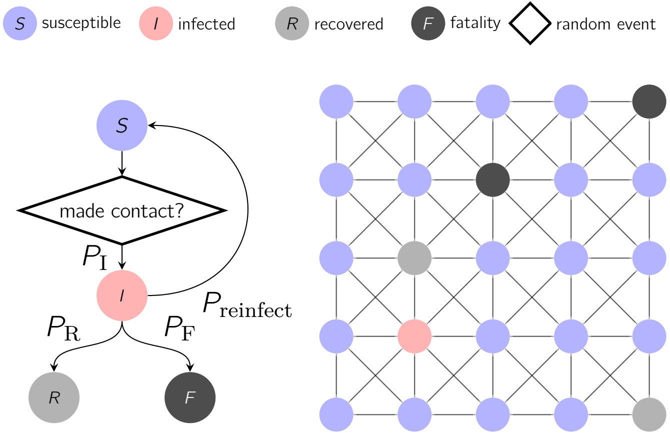

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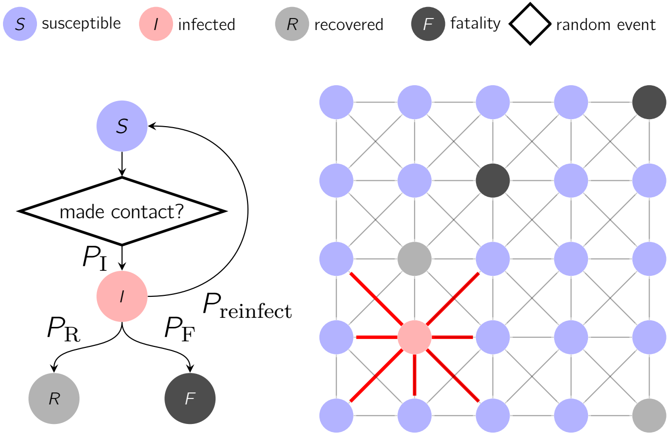

What are agent-based epidemiological models?

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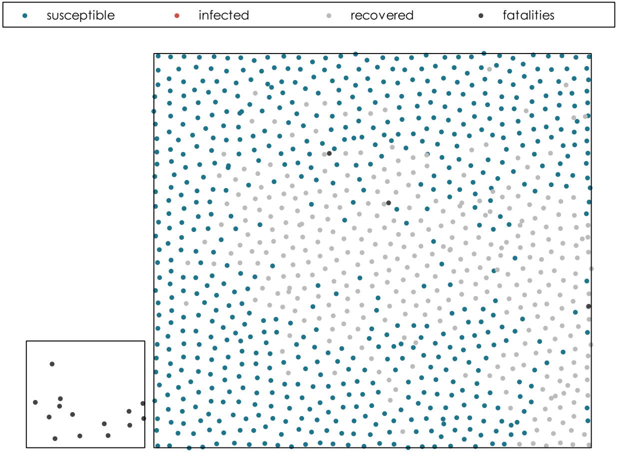
- Stochastic response

Realization 1



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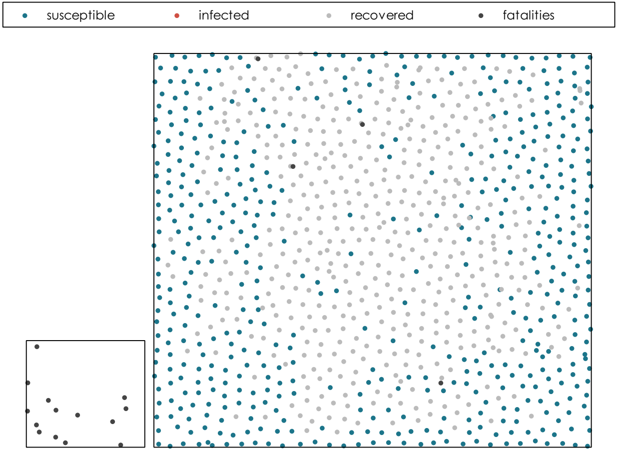
Realization 2



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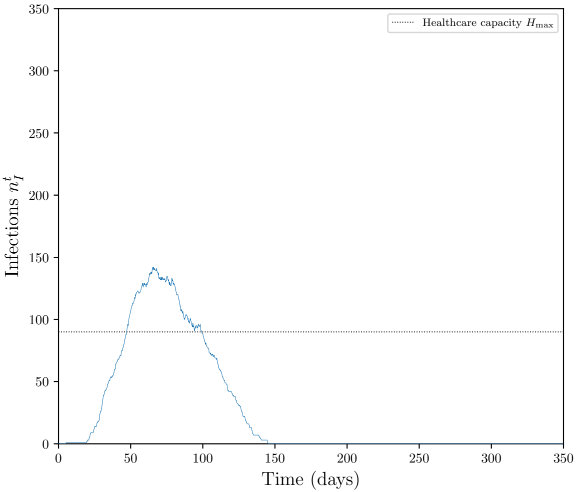

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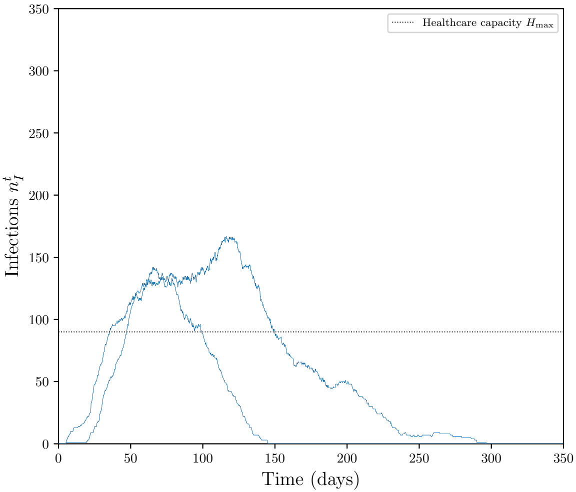

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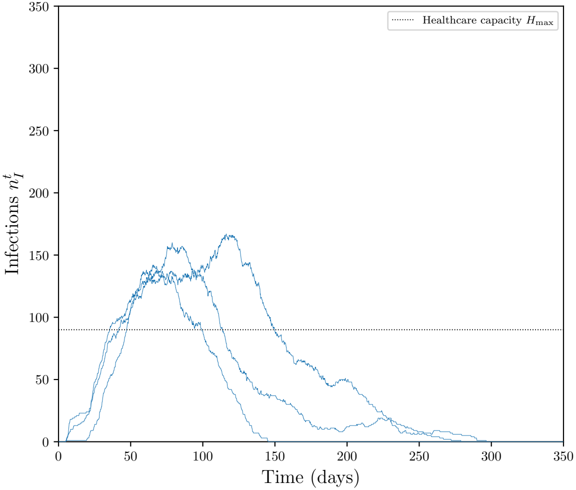

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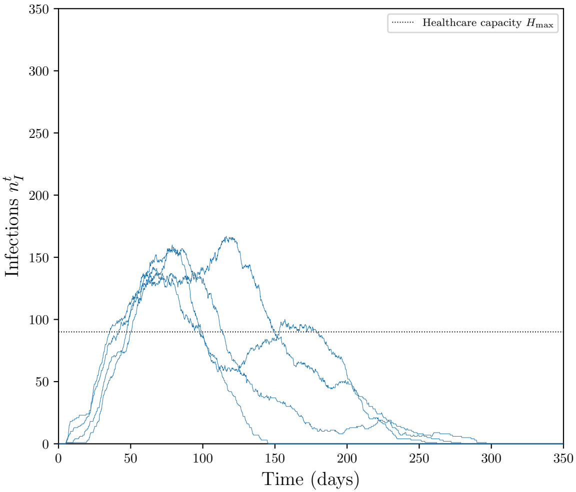

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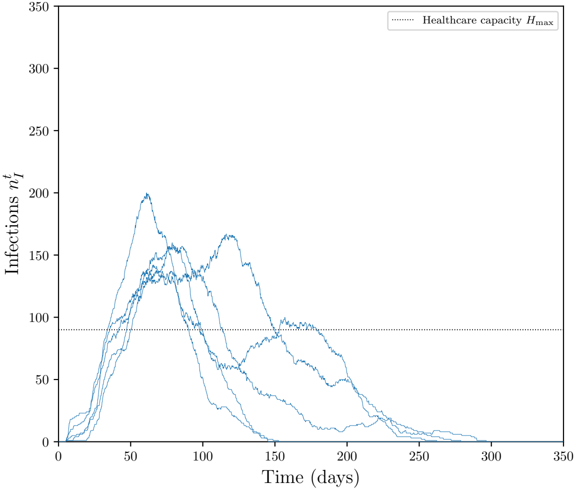

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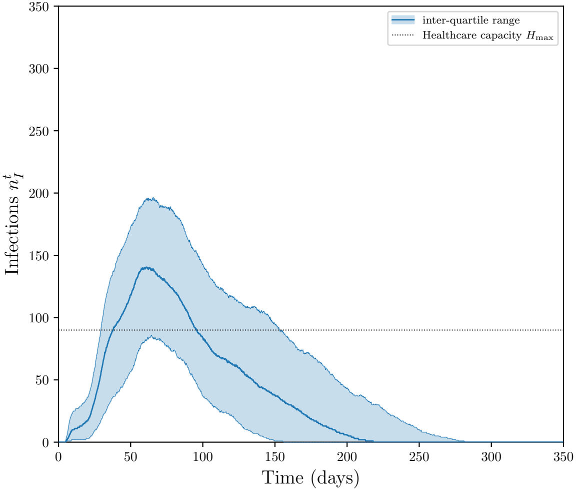
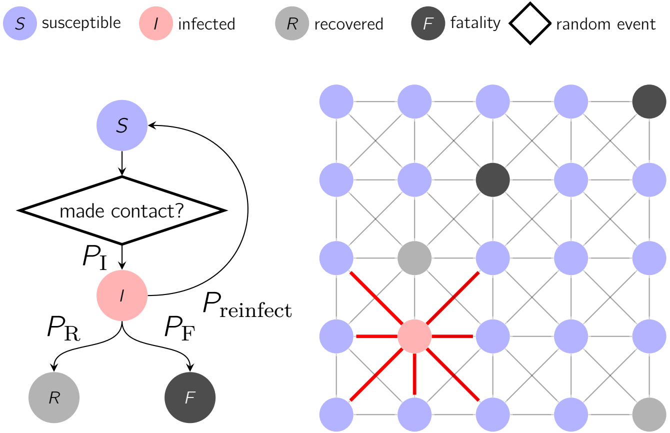


Background: epidemiological models

What are agent-based epidemiological models?

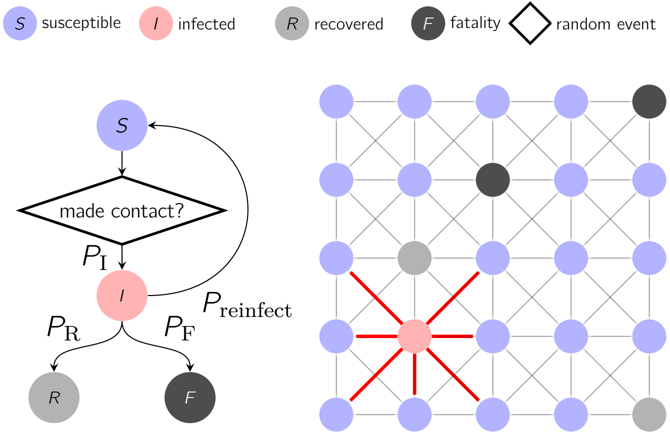
✓ Account for *geography* and *demographics*



Background: epidemiological models

What are agent-based epidemiological models?

- ✓ Account for *geography* and *demographics*
- ✓ Describe local phenomena



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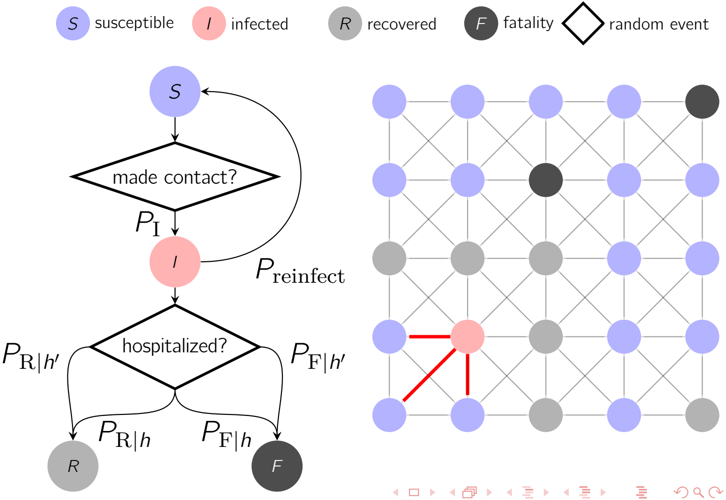

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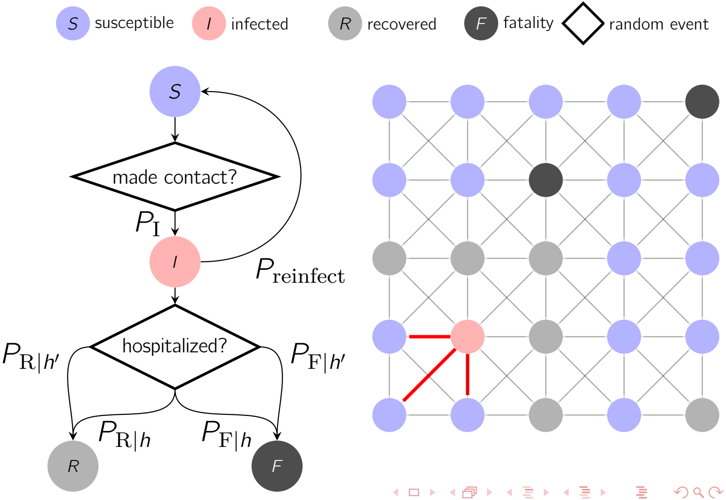

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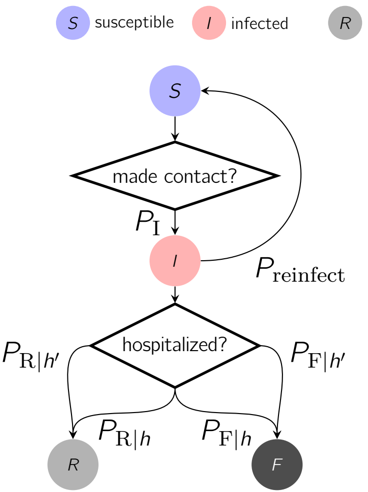
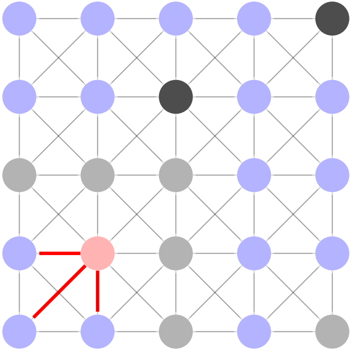
- ✗ Stochastic response makes decision making challenging
- ✗ Computationally expensive

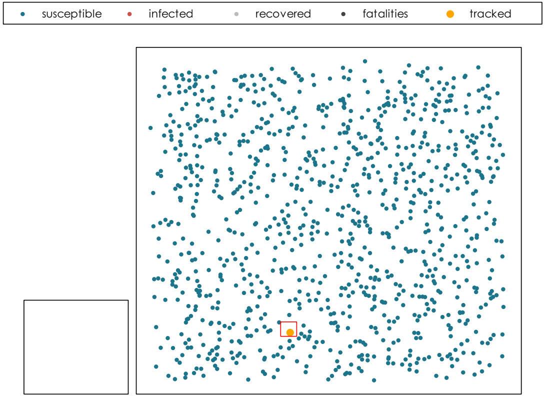




Public health policy-making problem formulation

What is the **cost** of public health interventions?

No interventions applied



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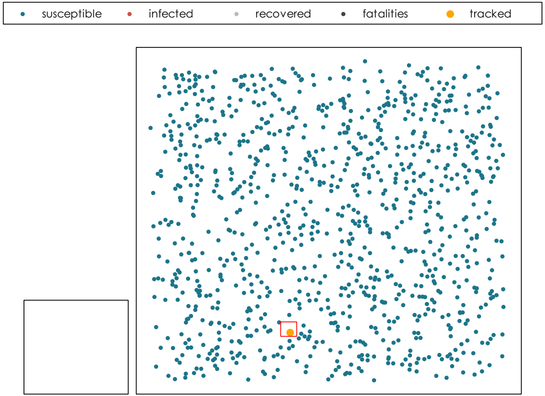

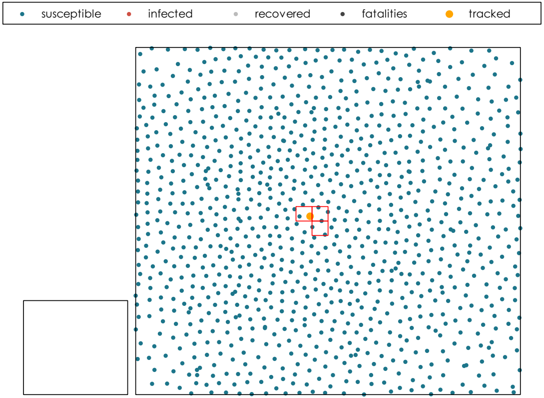

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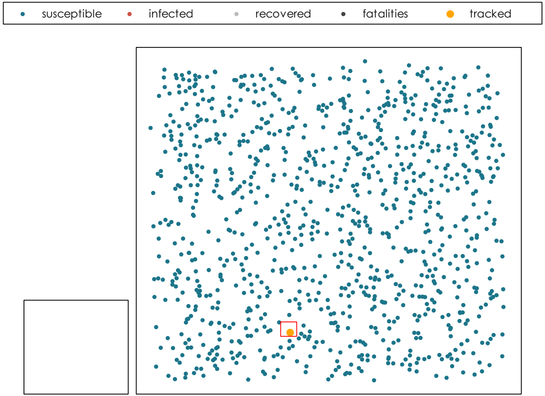

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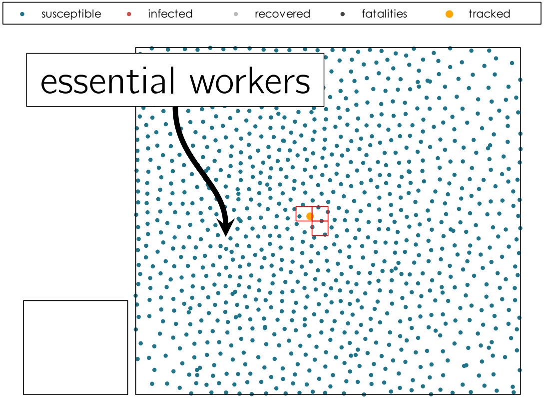

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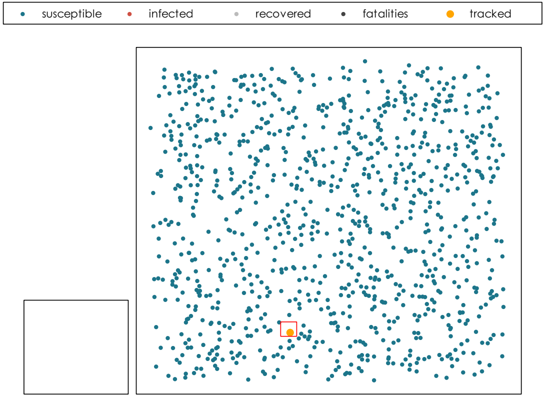

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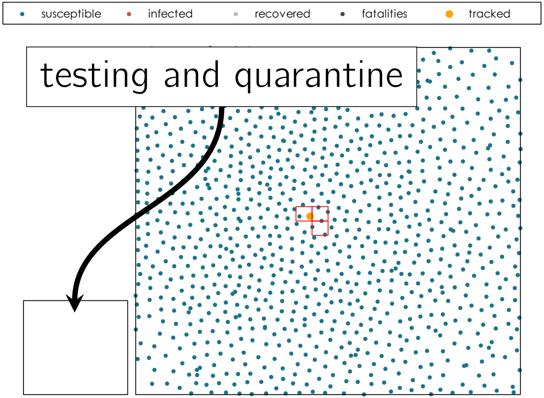

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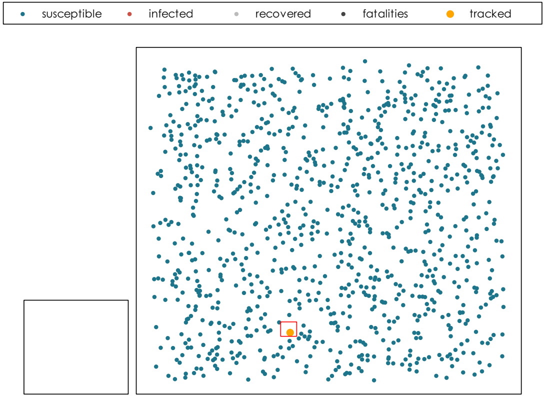

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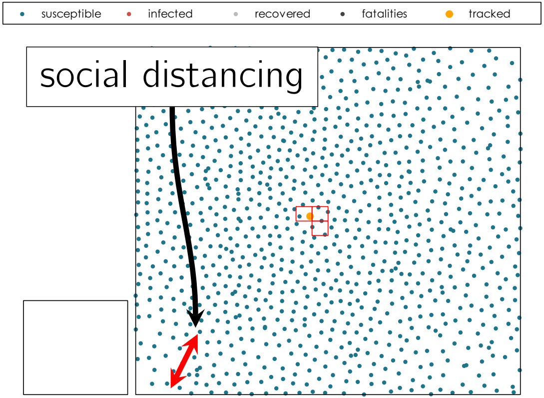

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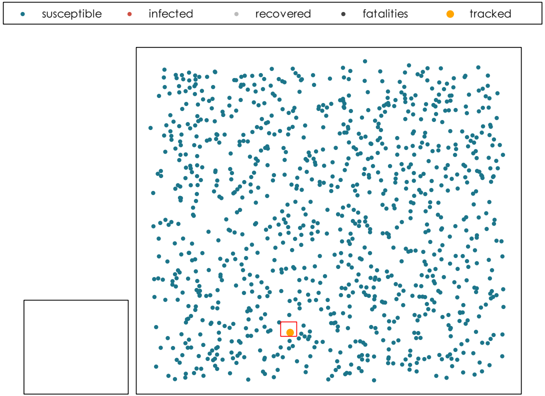

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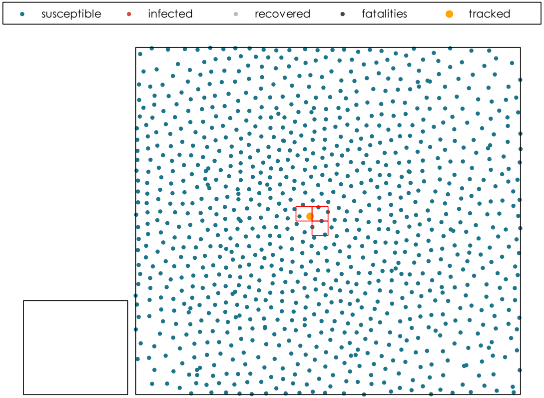

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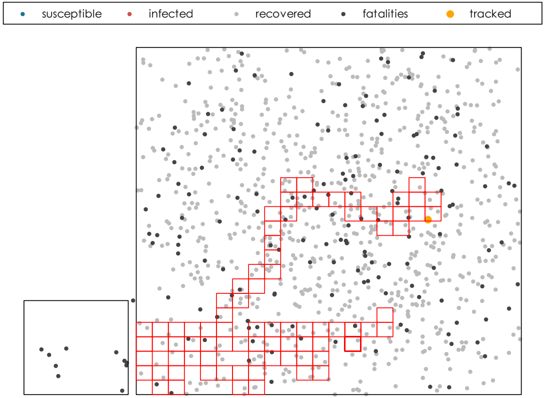

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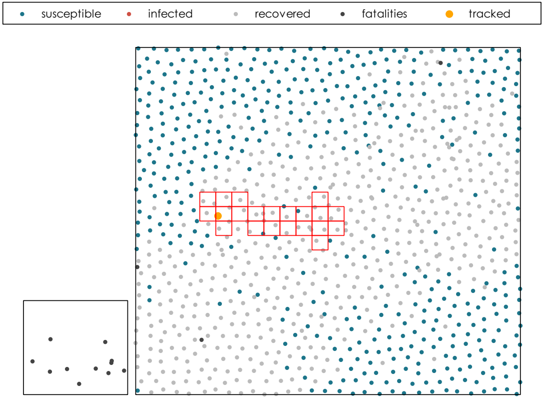

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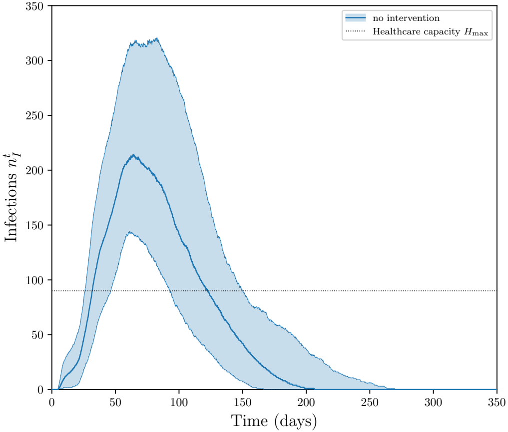
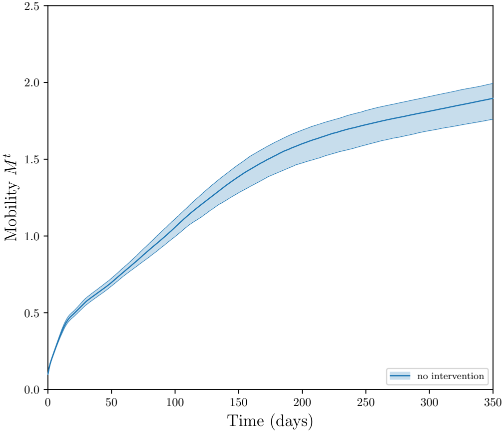
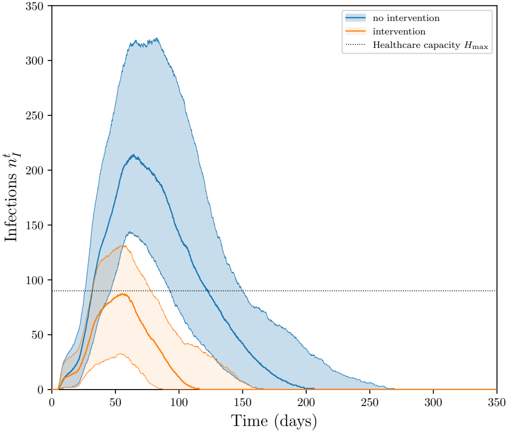


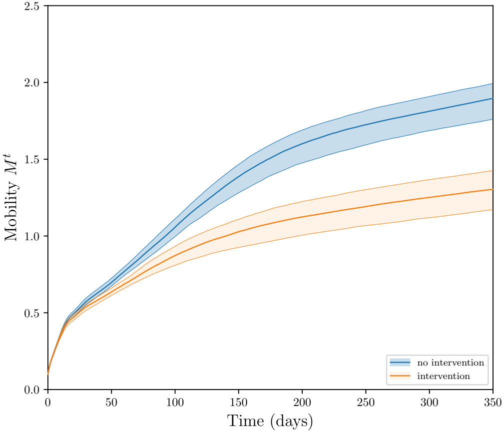


What is the **cost** of public health interventions?

infections ↓



mobility ↓



Optimization problem

Objective and constraints

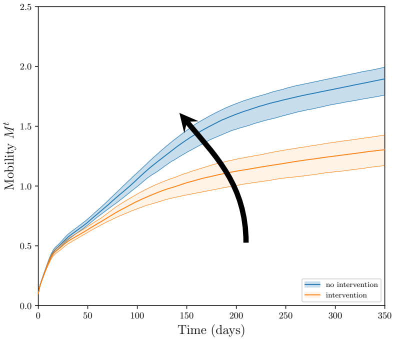
$$\min_{\mathrm{x}} \quad f(\mathrm{x}) = -M^T$$

subject to

where $\quad \mathrm{x} = [n_E, S_D, n_T]^T$

Design variables

- n_E : Number of essential workers
- S_D : Social distancing factor
- n_T : Number of tests daily



Optimization problem

No gradient information available, blackbox is expensive and noisy

Objective and constraints

$$\begin{array}{ll} \min\limits_{x} & f(x) = -M^T \\ \text{subject to} & c(x) \equiv n_{I,\max} - H_{\max} \leq 0 \\ \text{where} & x = [n_E, S_D, n_T]^T \end{array}$$

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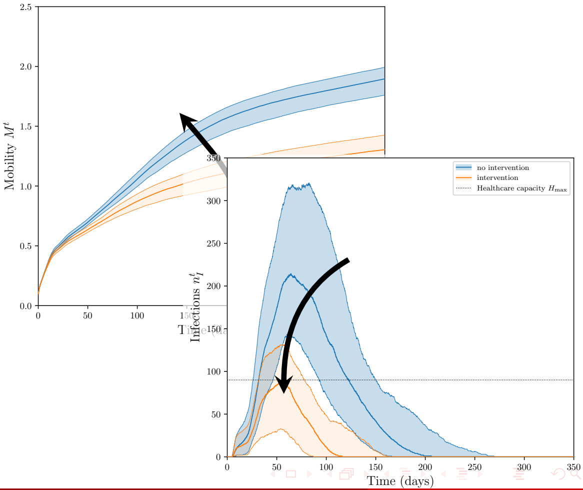

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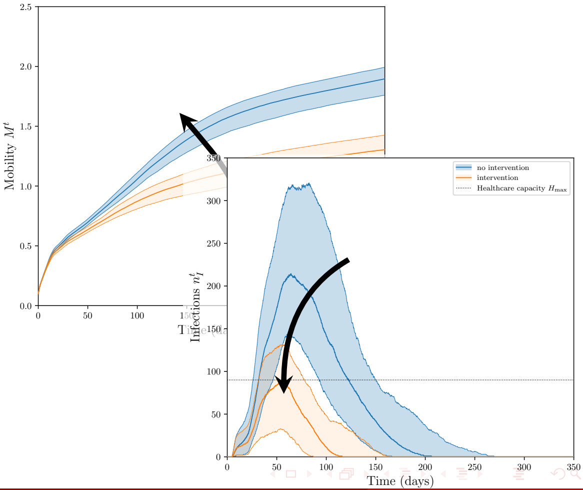

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$$\text{subject to} \quad c(x) = \mathbb{E}_\Theta\left[c_\Theta(x) \equiv n_{I,\max} - H_{\max}\right] \leq 0$$

$$\text{where} \quad x = [n_E, S_D, n_T]^T, \ \Theta\text{: realizations}$$

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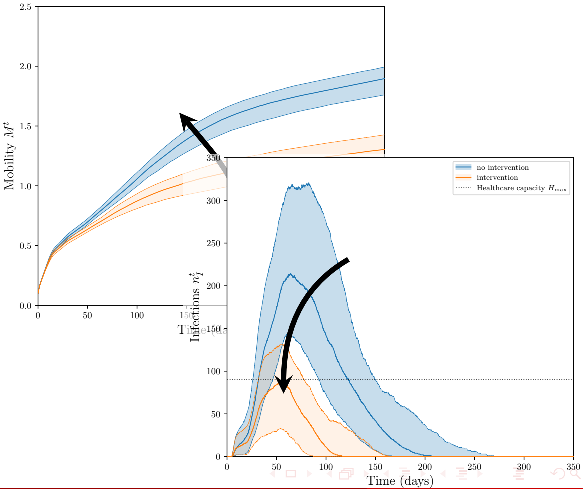

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$$\min_{x} \quad f(x) = \mathbb{E}_{\Theta}\left[f_{\Theta}(x) = -M^T\right]$$

$$\text{subject to} \quad c(x) = \mathbb{E}_{\Theta}\left[c_{\Theta}(x) \equiv n_{I,\max} - H_{\max}\right] \leq 0$$

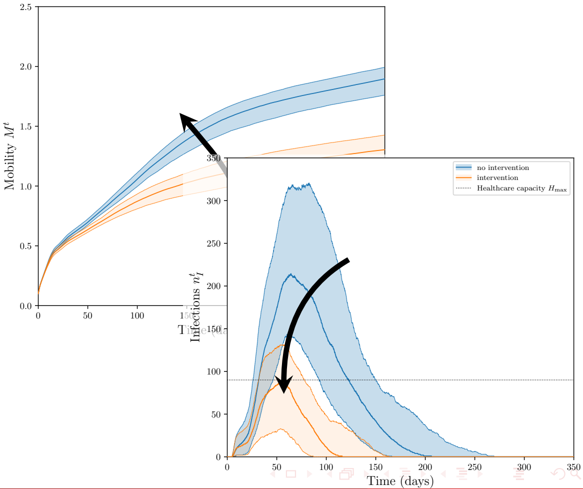
$$\text{where} \quad x = [n_E, S_D, n_T]^T, \ \Theta\text{: realizations}$$

Design variables

- n_E : Number of essential workers
- S_D : Social distancing factor
- n_T : Number of tests daily

Randomly seeded parameters

- Initial conditions
- Interactions, demographics



Optimization results

StoMADS, `NOMAD`, and genetic algorithms were used to solve the problem

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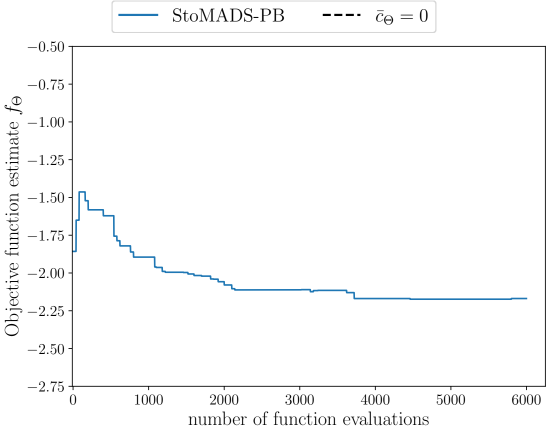
sampling rate $n^k = 4$



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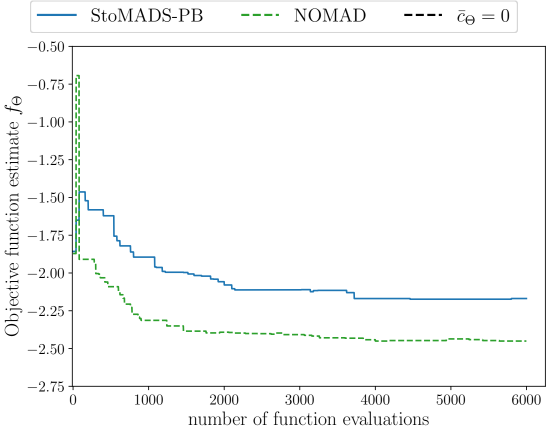

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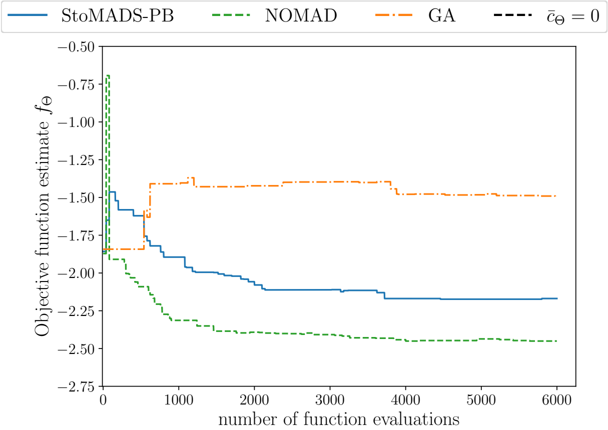

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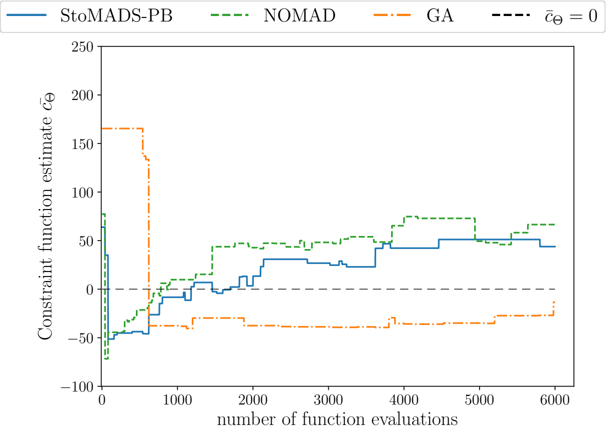

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best known solution

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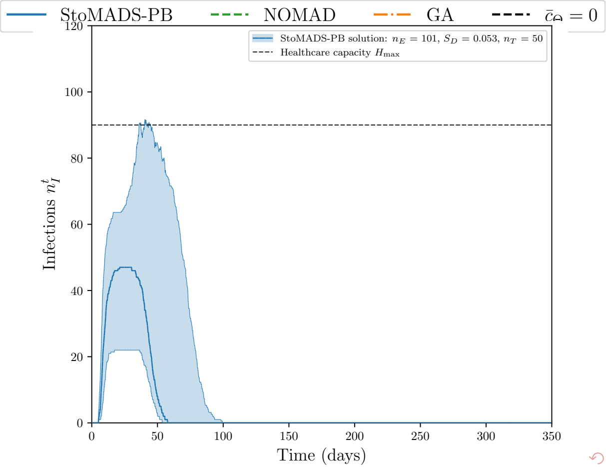

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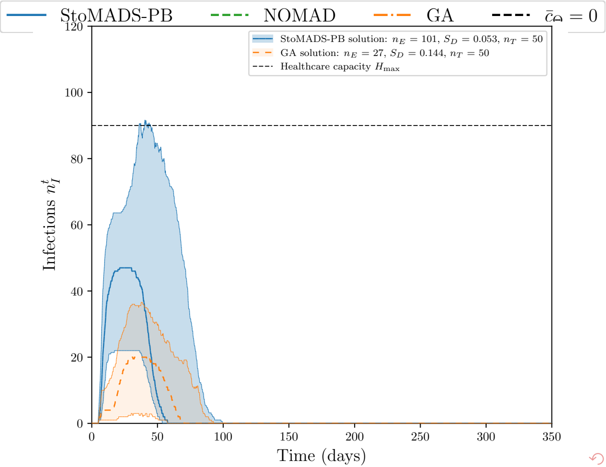

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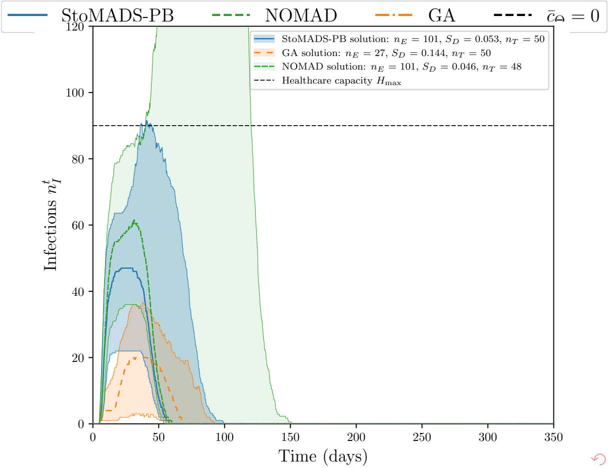

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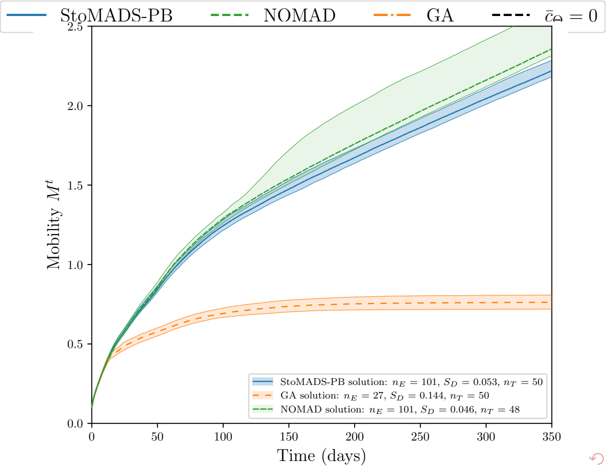

Conclusion

Formulated and solved public health policy-making problems

- Identified a public health policy that favored

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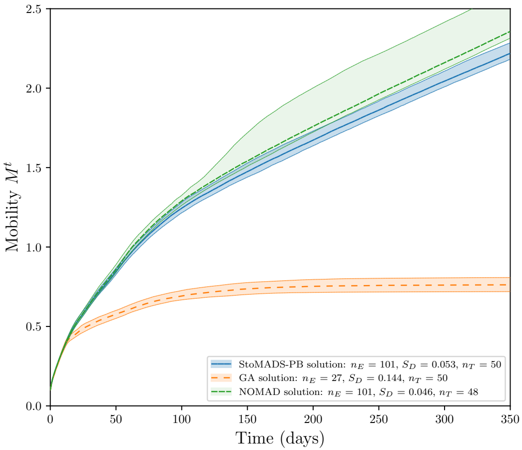

Conclusion

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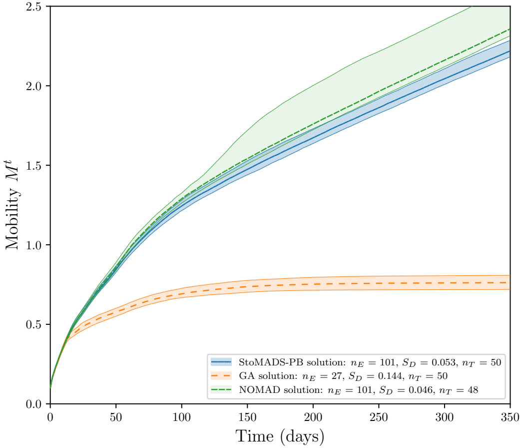

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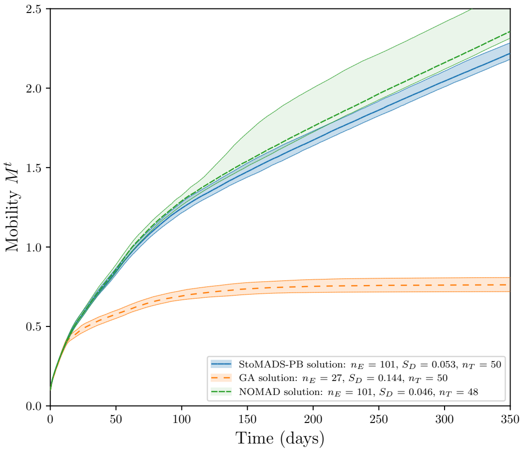

Conclusion

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  - High testing capacity n_T
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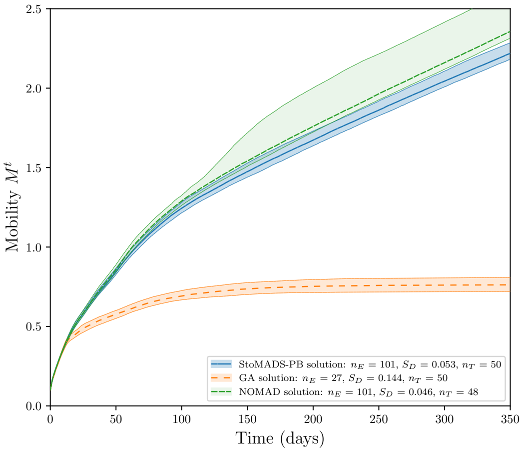

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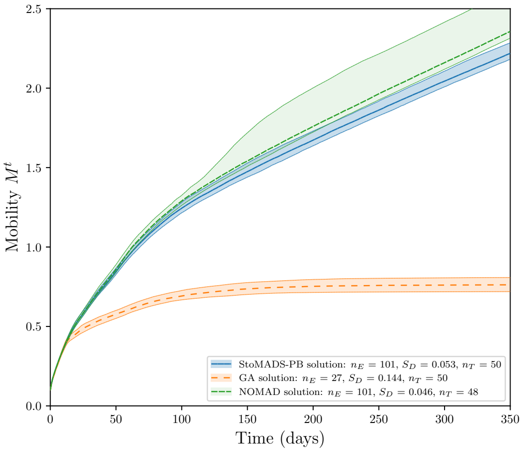

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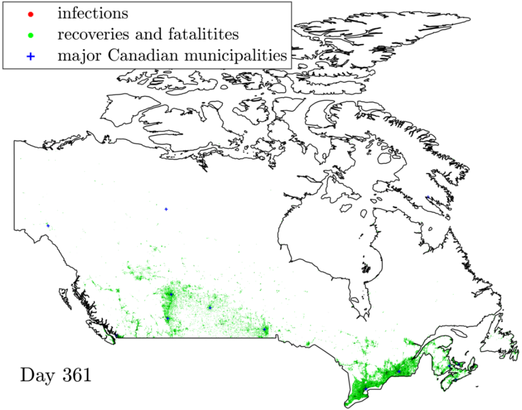

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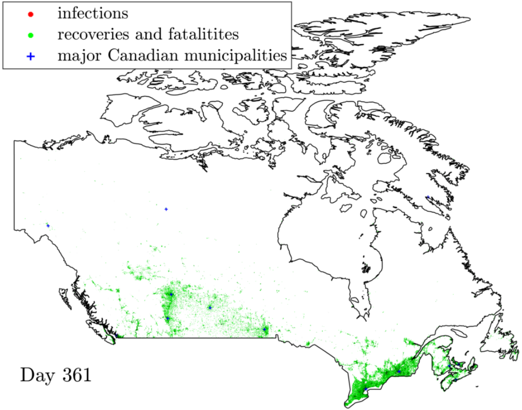
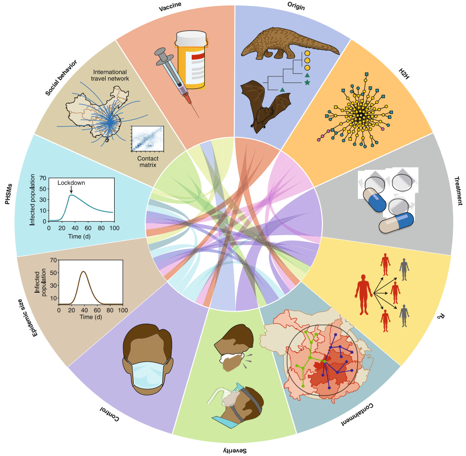


Research displinces in epidemiology

Forecasting novel epidemics is a multidisciplinary field involving multiple *targets*

Inputs for forecasting **epidemic size:**



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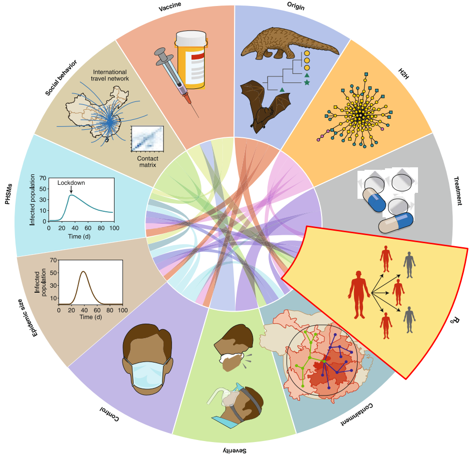

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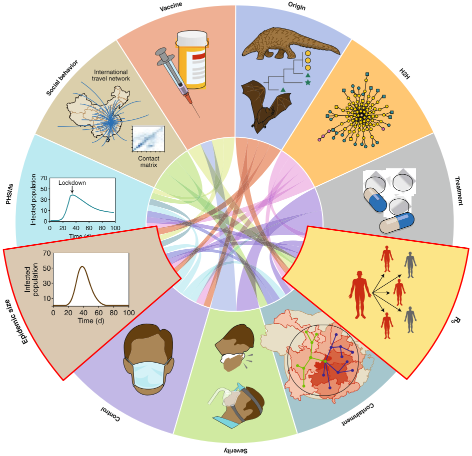

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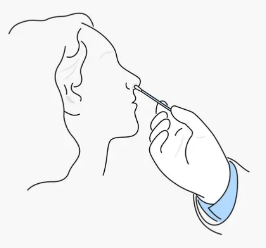

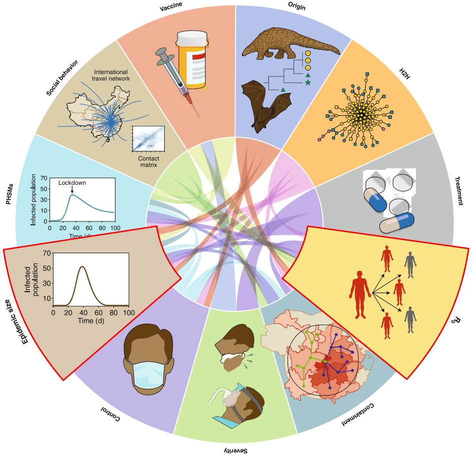

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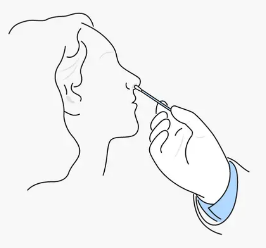
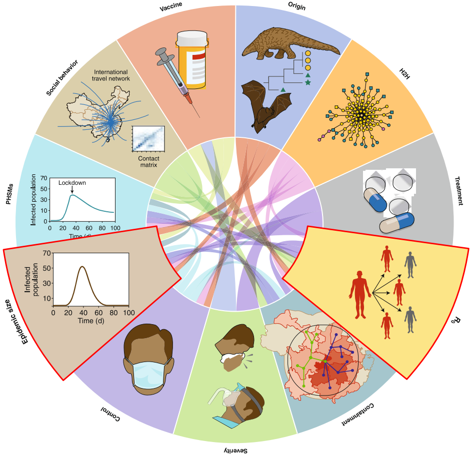
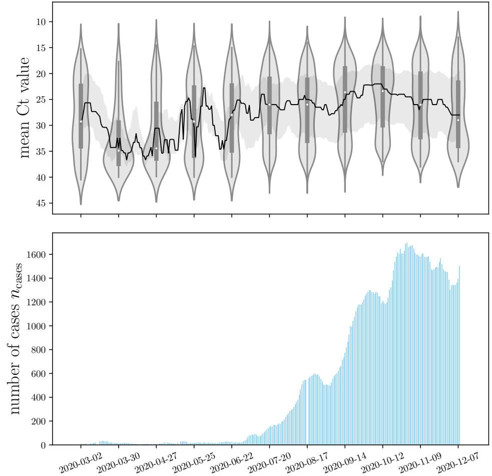




Nowcasting epidemic trajectory using statistical models

Joint work with: Dr. Ibrahim Chamseddine, Dr. Athar Khalil, and Prof. Michael Kokkolaras

How to *design* a machine learning model for forecasting a time-series?



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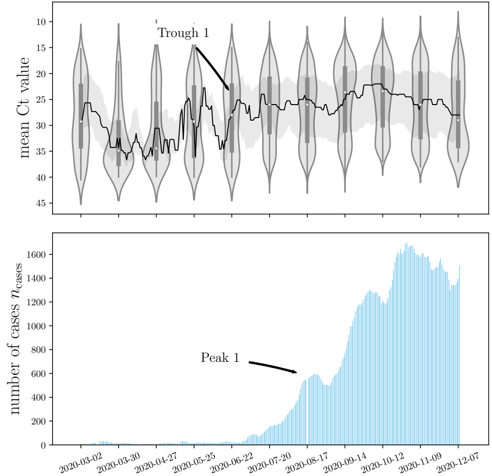

COVID-19 incidence forecasting

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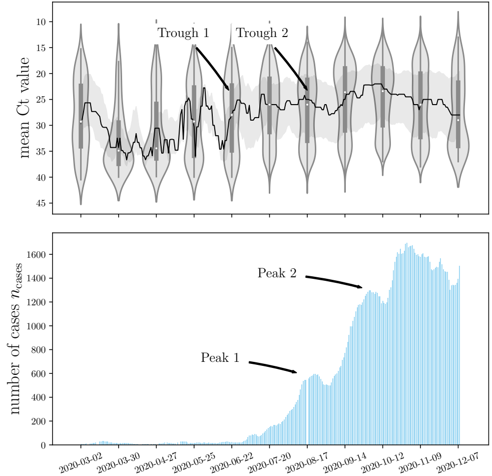

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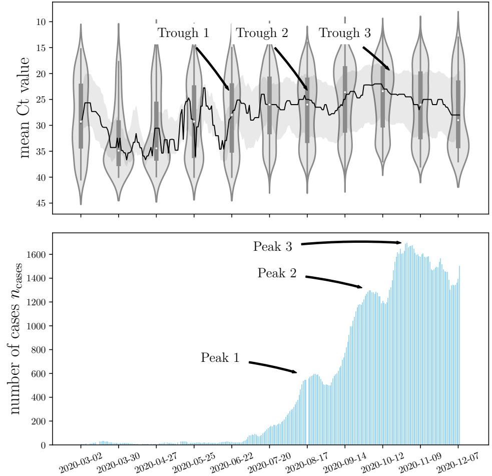

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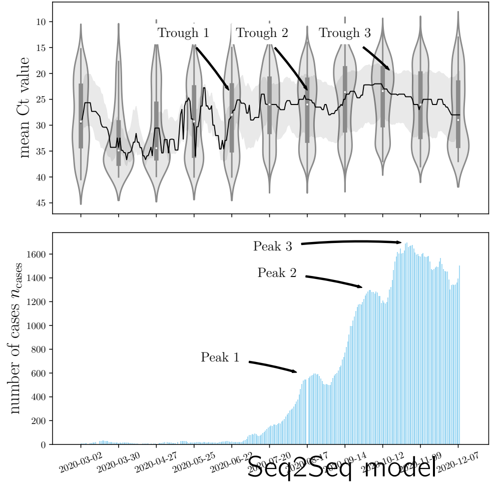

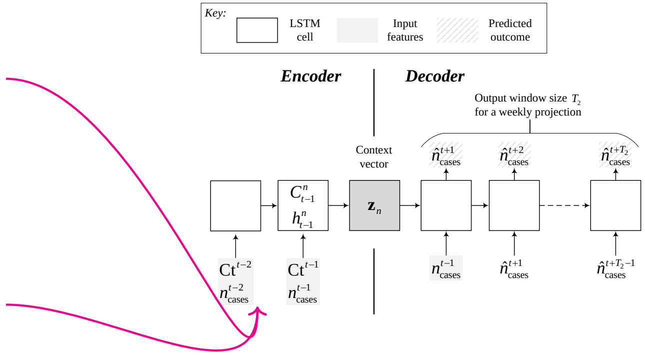

Seq2Seq model

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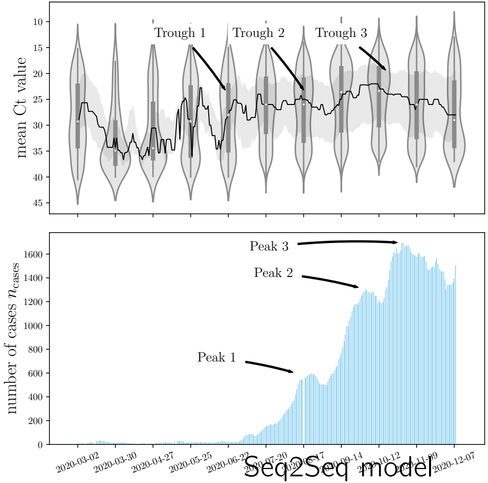

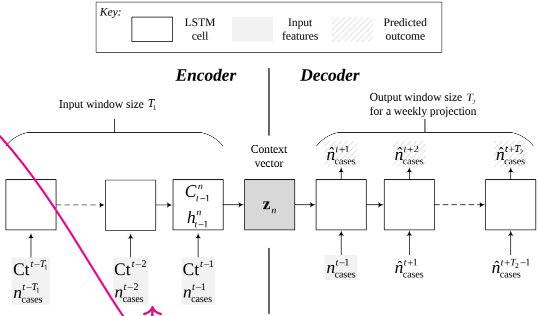

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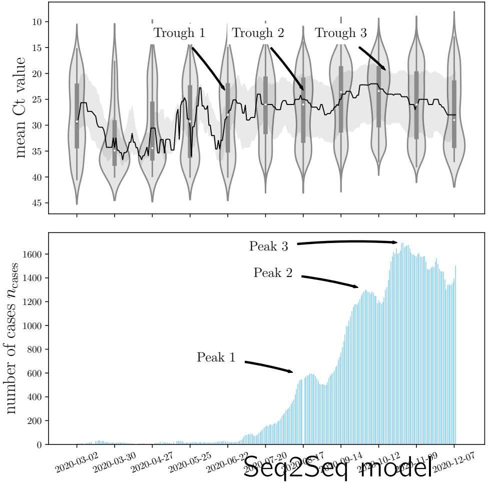
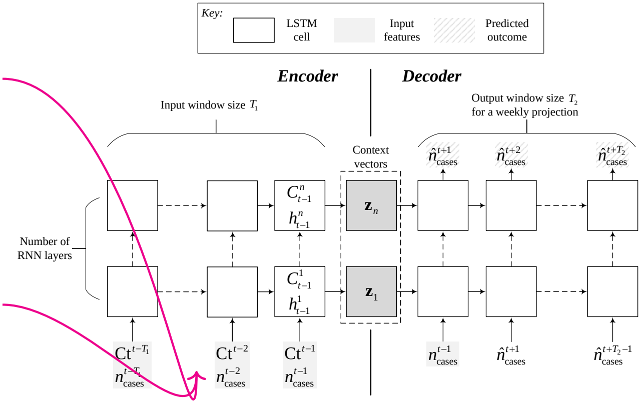


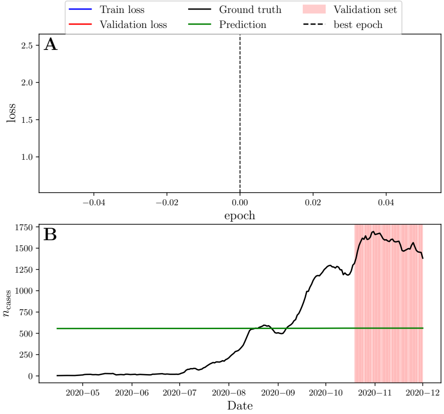


Seq2Seq model

Training the model

There are several challenges associated with hyperparameter optimization

- The number of epochs can be tuned using *early stopping*
- This is a form of *regularization* to reduce over-fitting



Effect of number of epochs on testing loss

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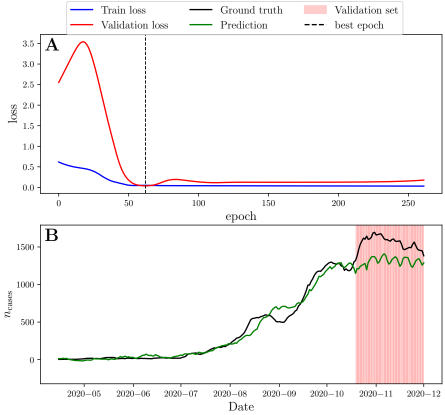

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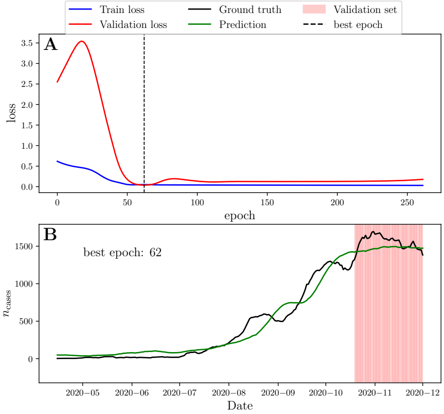

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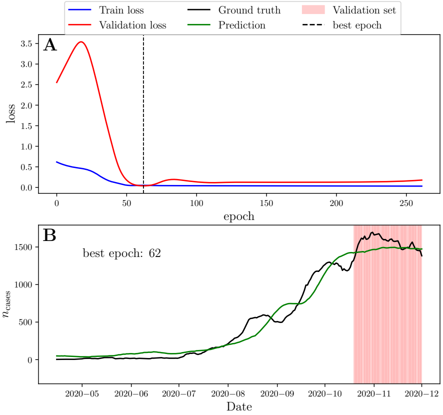

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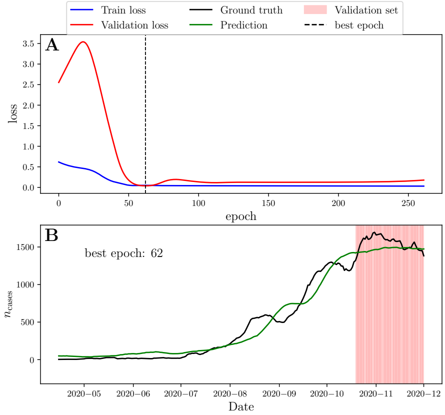

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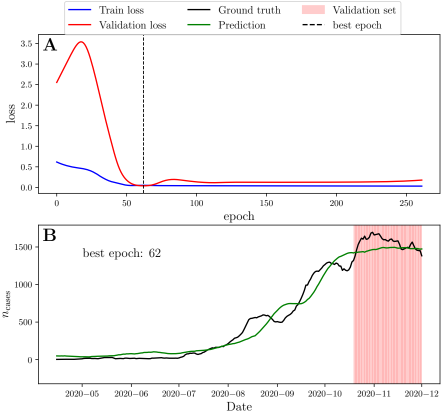
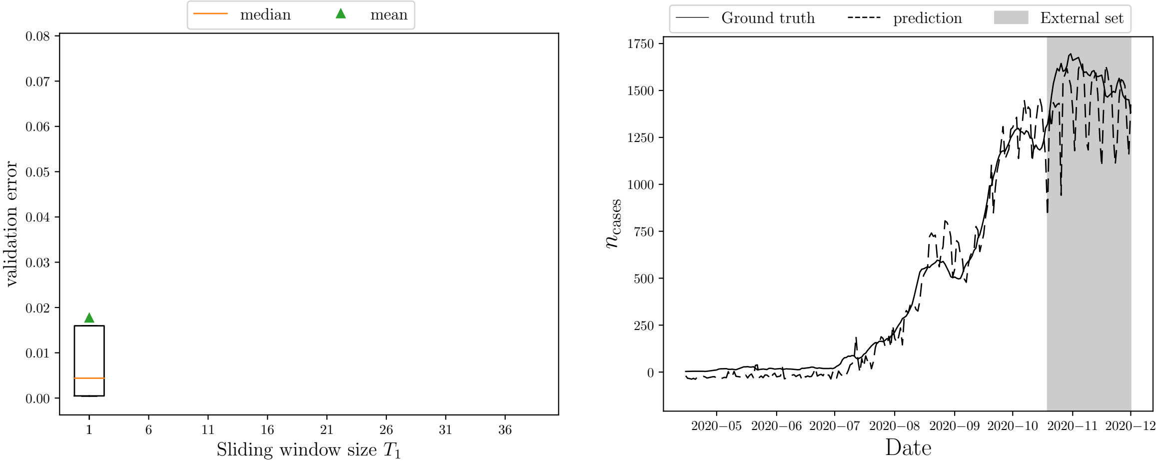


Effect of number of epochs on testing loss

Hyperparameter tuning

We can use StoMADS to solve such hyperparameter optimization problems



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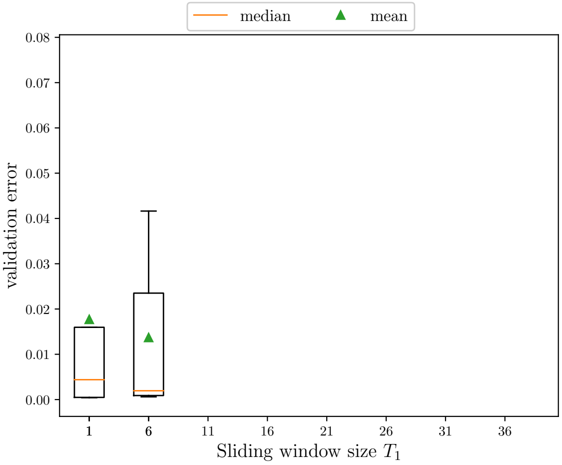

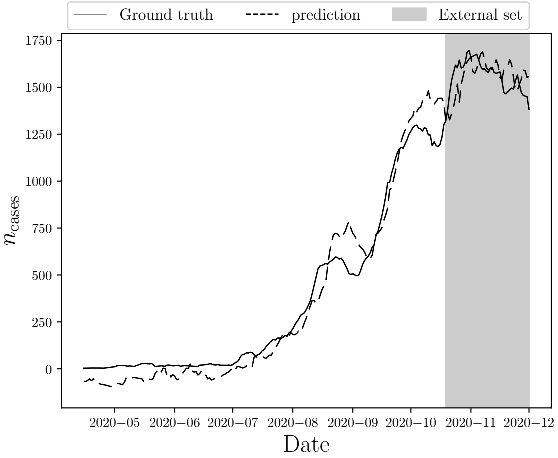

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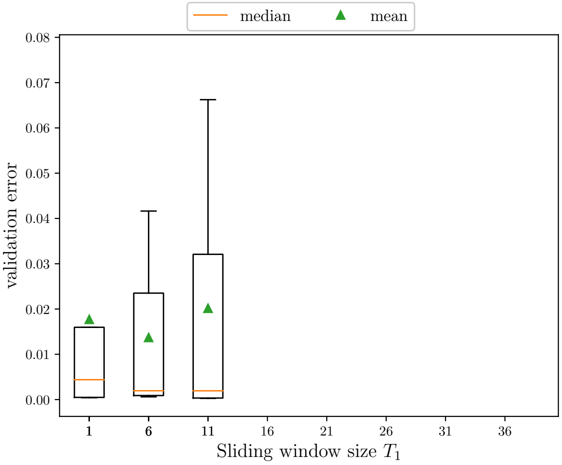

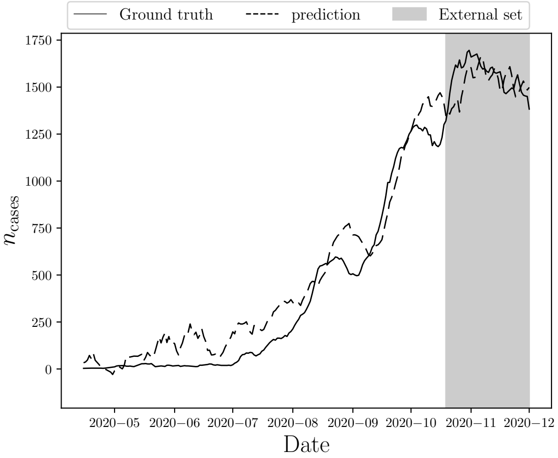

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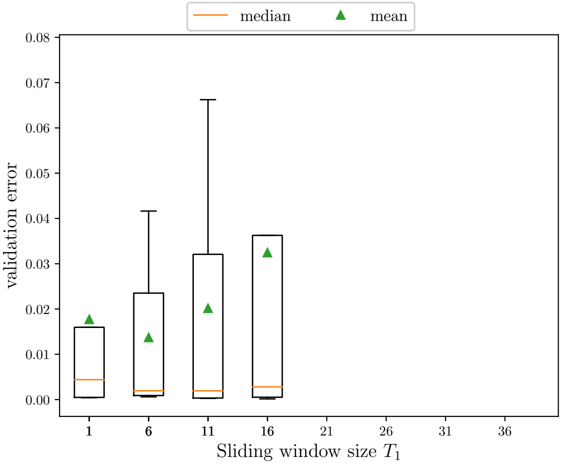

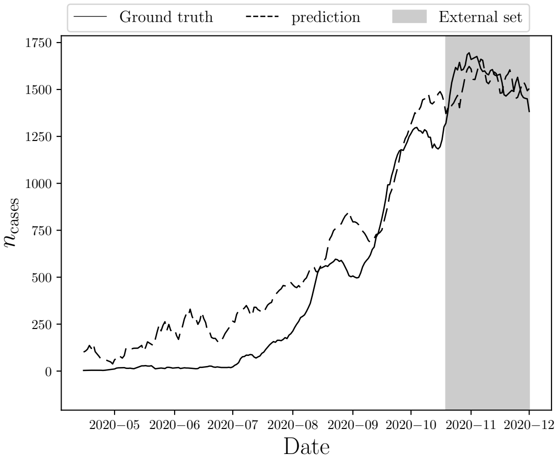

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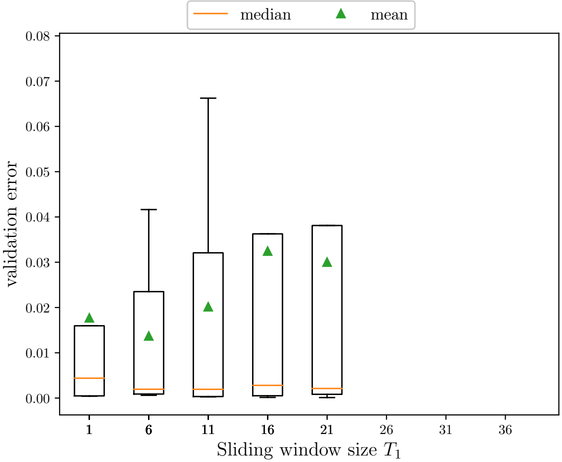

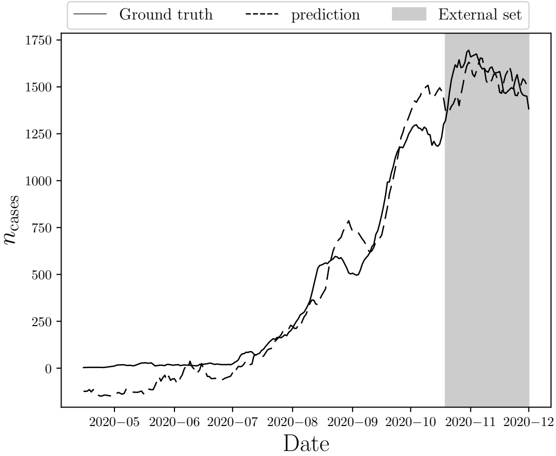

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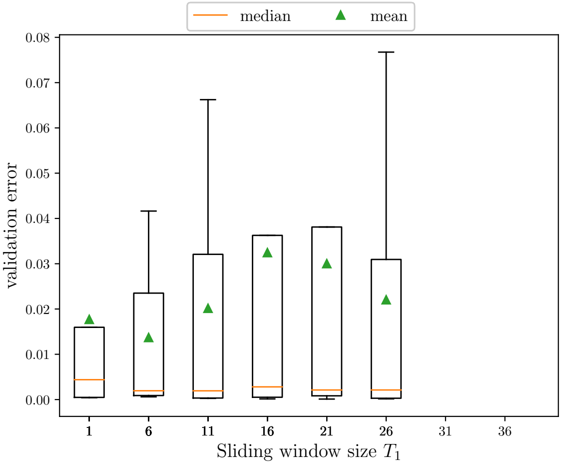

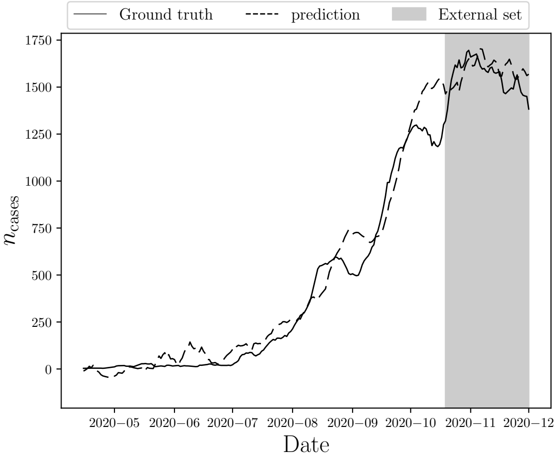

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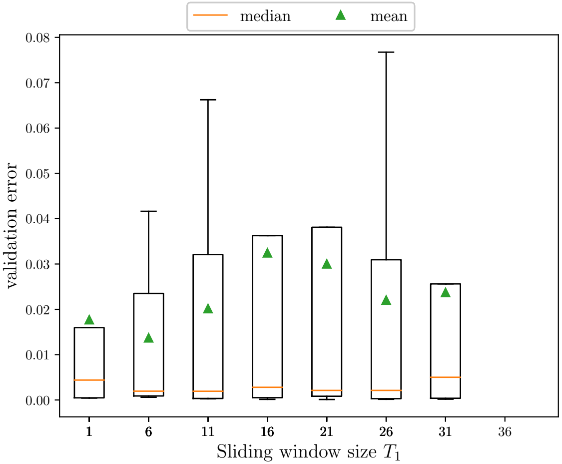

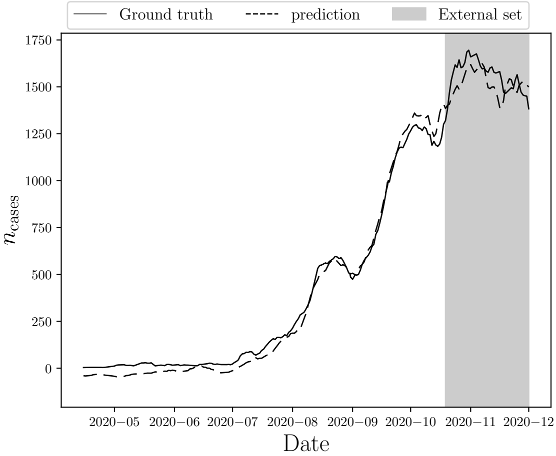

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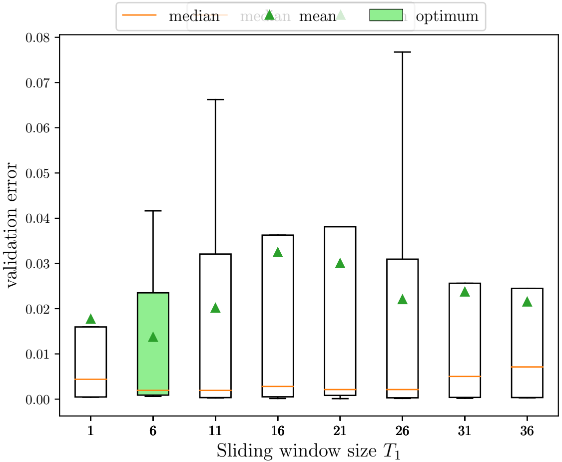

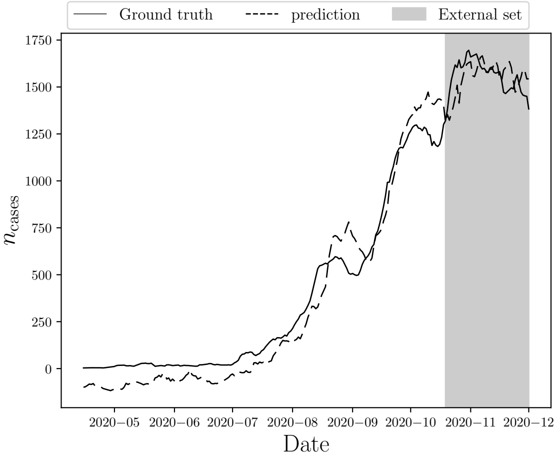

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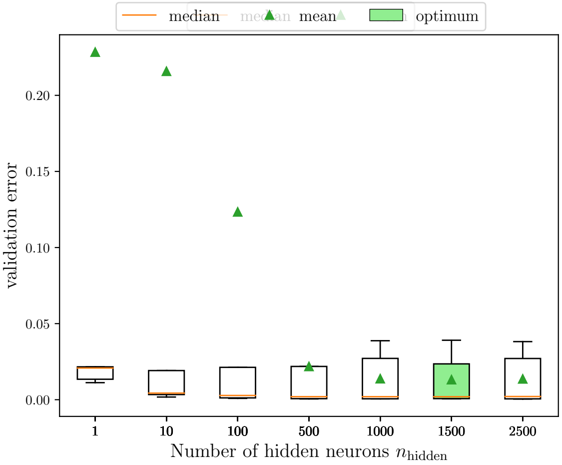

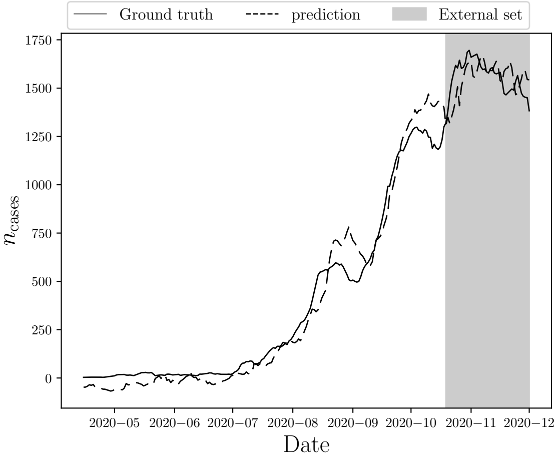

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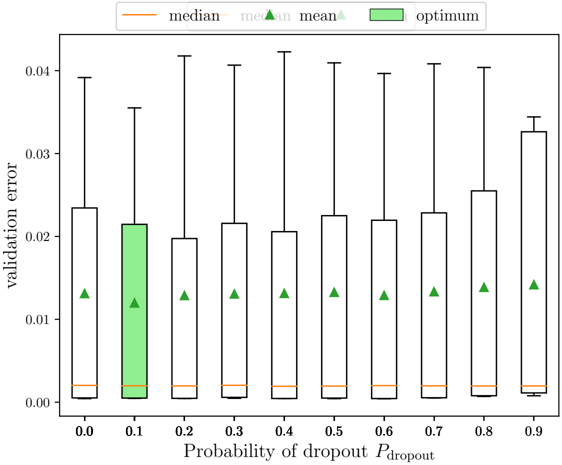

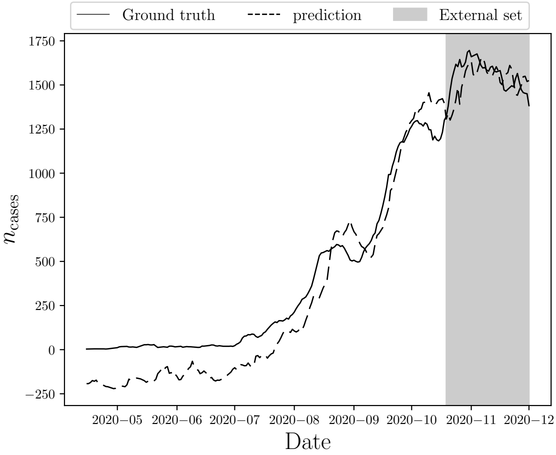

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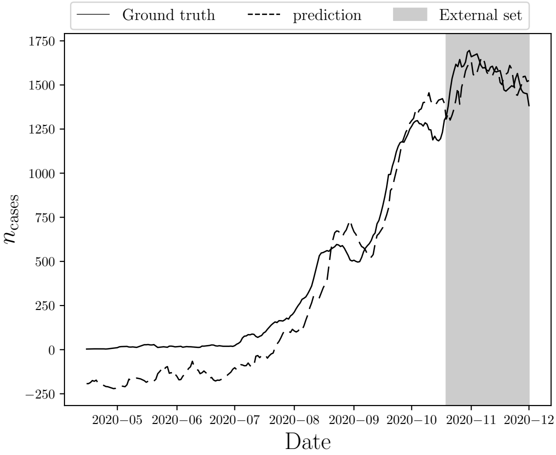
where Θ: realizations

Design variables ($\mathbf{x}$)

- T_1 : Input dimension
- n_{hidden} : Number of hidden neurons
- P_{dropout} : Probability of dropout, etc.

Randomly seeded parameters

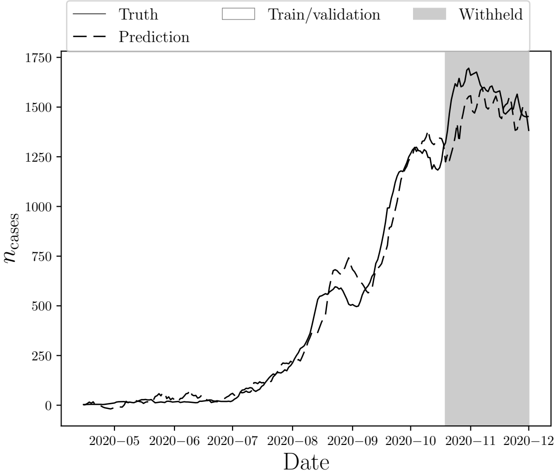
- Initial weights
- Gradient descent steps



Results: Optimal hyperparameters

Optimal hyperparameters for the *Seq2Seq* model:

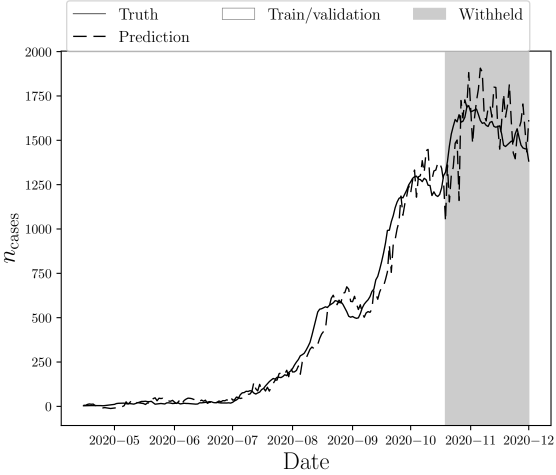
Hyperparameter		**Value**
Sliding window size	T_1	6
Number of hidden neurons	n_{hidden}	1500
Probability of dropout	P_{dropout}	0.8
Number of hidden layers	n_{hidden}	2
Teacher forcing probability	P_{teacher}	0.3
Learning rate	l_{rate}	1×10^{-4}
batch size	b_{size}	32



Results: Optimal hyperparameters

Optimal hyperparameters for the *support vector machine regression (SVR)* model:

Hyperparameter		Value
Sliding window size	T_1	6
Ridge factor	λ	1×10^{-4}
Margin of tolerance	ϵ	1×10^{-2}
Stopping criteria tolerance	ϵ_{tol}	0.1
Learning rate	l_{rate}	1×10^{-5}



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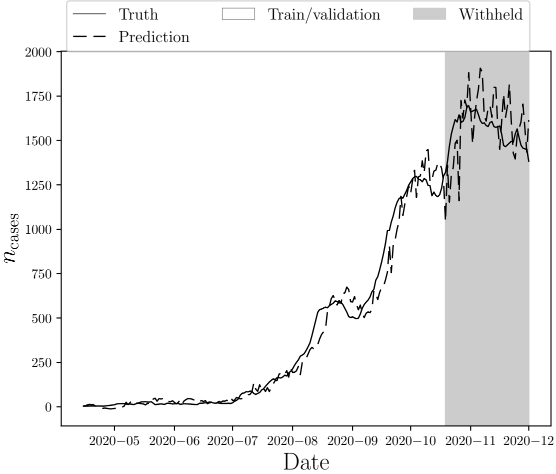
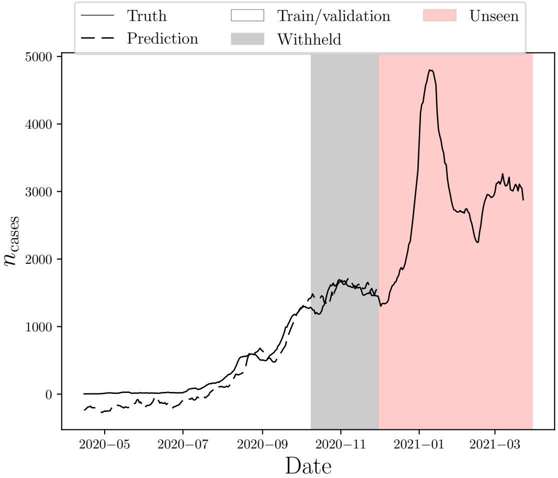
Support vector machine models have **deterministic** performance



Results: Prospective validation

Performance of models on **unseen** data (first 4 months of 2021):

Model	Test error
Seq2Seq	0.571
Long short term memory (LSTM) cell	0.326
feedforward neural network	0.255
Support vector machine	0.168
Gradient boosting	1.444
Linear regression	0.160



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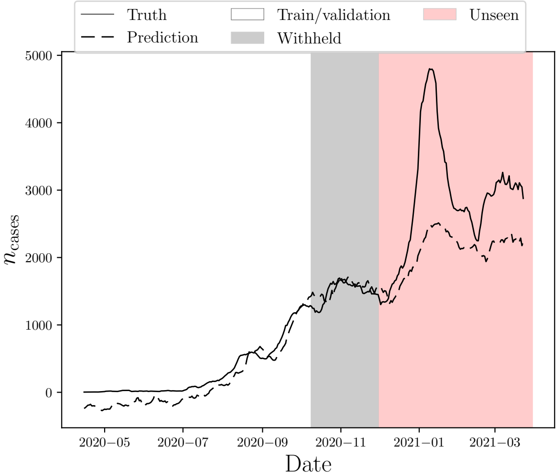

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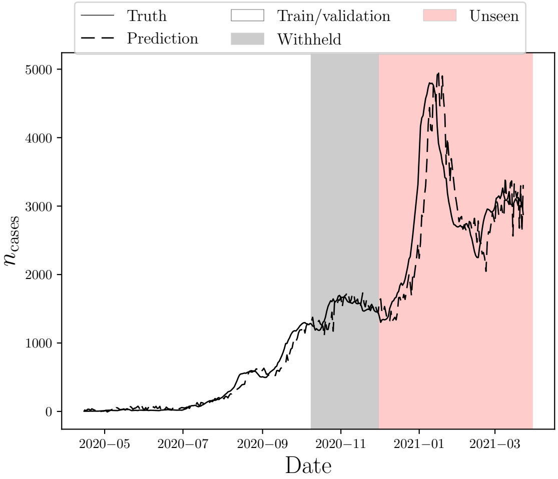

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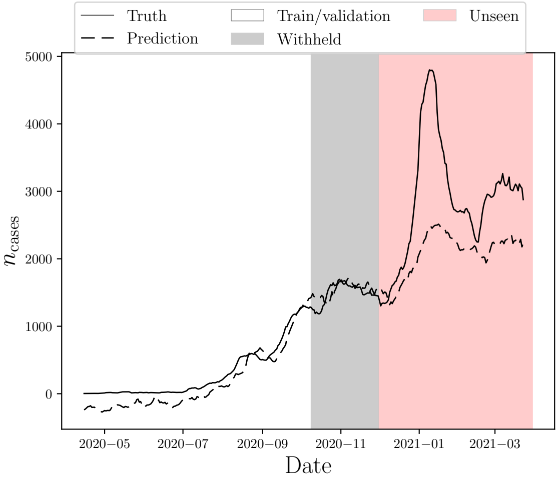

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Effect of increasing number of training days (Adding 1 month of data):

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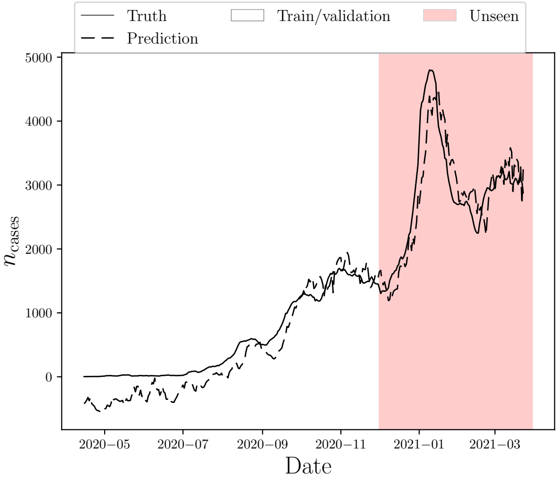

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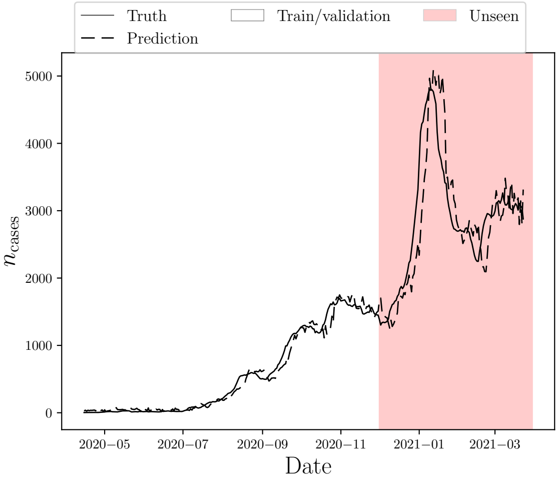

Conclusion and future directions

Model discovery and development facilitated by hyperparameter optimization

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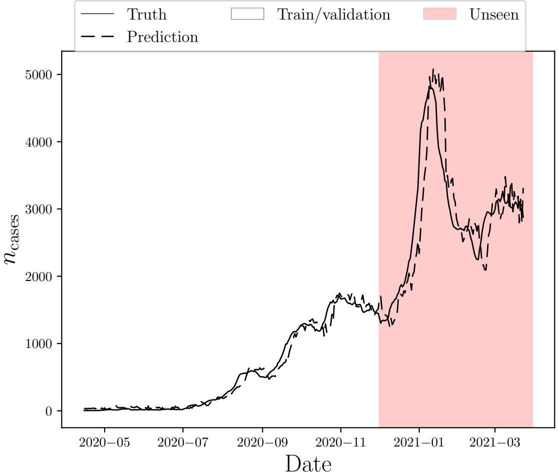

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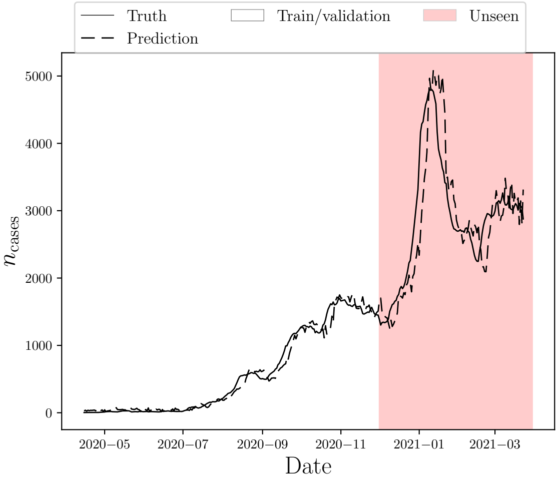
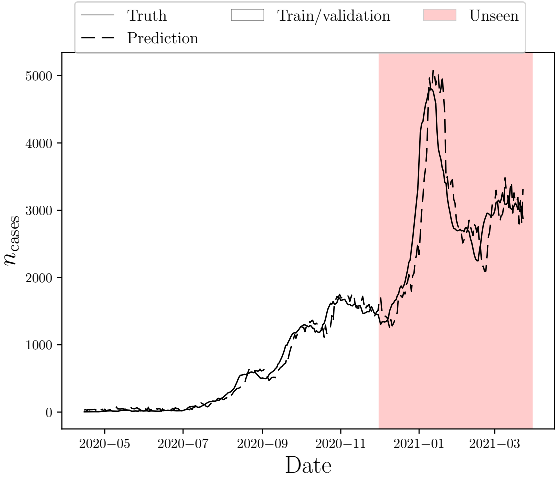


Conclusion and future directions

Model discovery and development facilitated by hyperparameter optimization

- Cycle Threshold (Ct) is a useful feature for incidence projection
- Model that generalizes well on unseen data
- Simpler models perform well when historical data is limited
- Works well on other datasets[1]



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StoMADS can be improved to solve a wide variety of HPO problems

- Can be used to meet deployment targets

Objective and constraints

$$\min_{x} \quad f(x) = \mathbb{E}_\Theta\left[f_\Theta(x) = \mathrm{error}_{\mathrm{CV}}\right]$$
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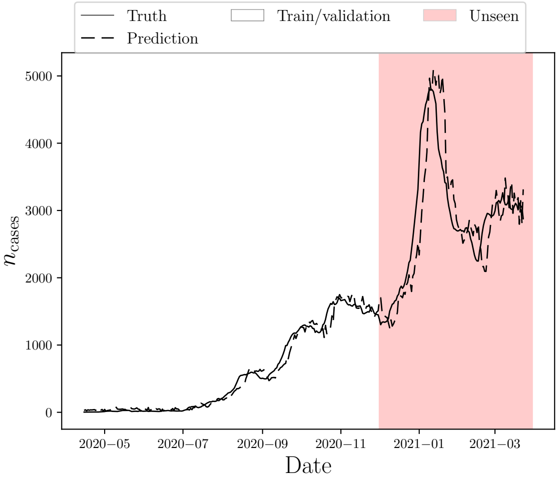

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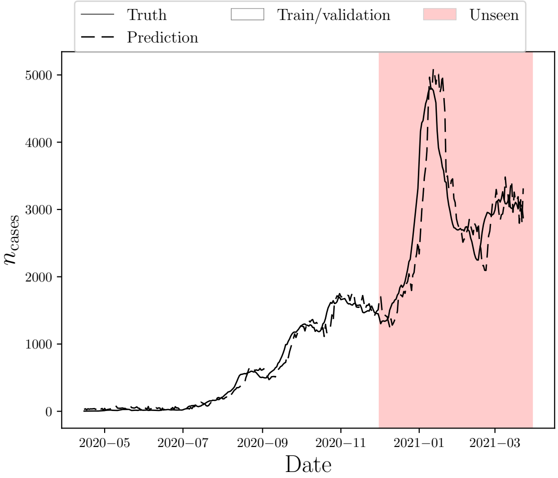

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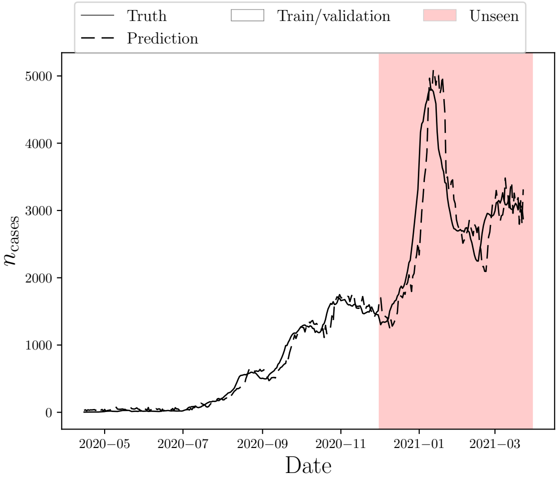

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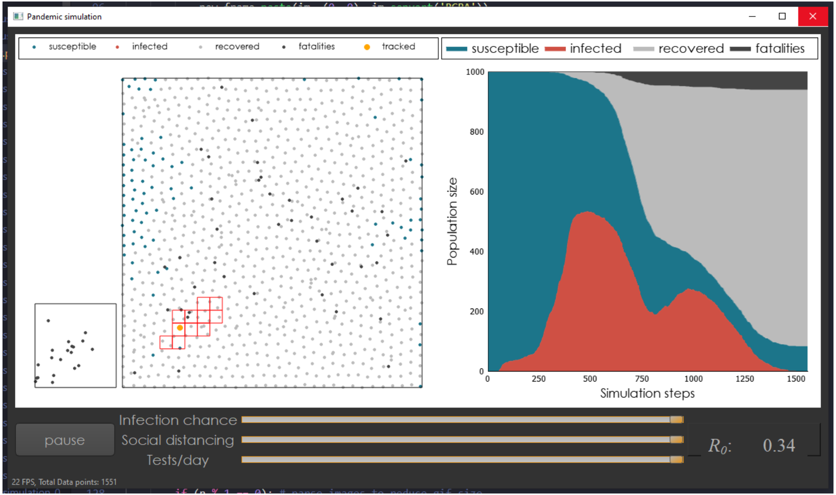
- Mixed variable version is needed

Thank you for your time

Open source GPU implementation of agent-based modeling



No gradient information available, blackbox is expensive and **noisy**

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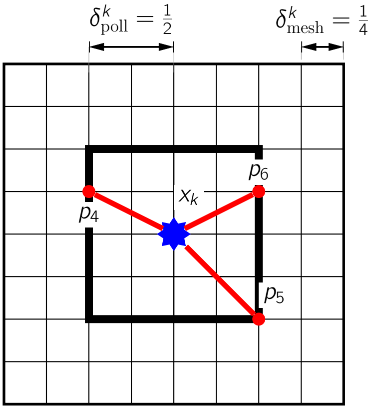
where x : variables Θ: realizations

- Constructs estimates of objective:

$$f^k = \frac{1}{n^k}\sum_{i=1}^{n^k} f_{\Theta_{0,i}}(x_k)$$

- n^k is the sampling rate

Poll **failure**



Overview of stochastic mesh adaptive direct search

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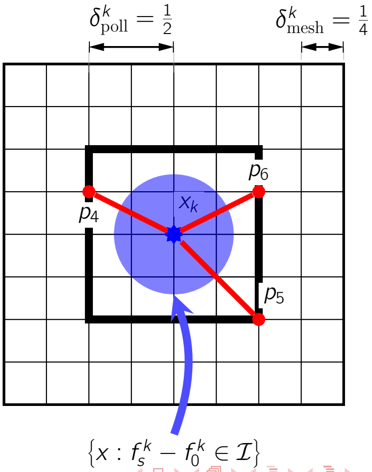
Poll **certain failure**



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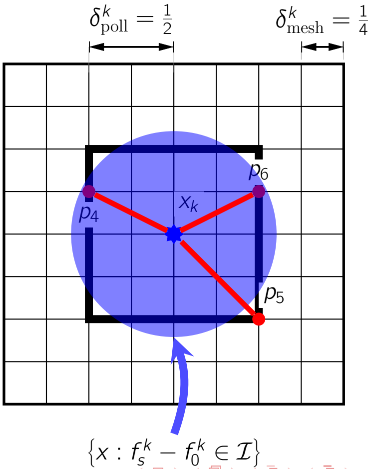

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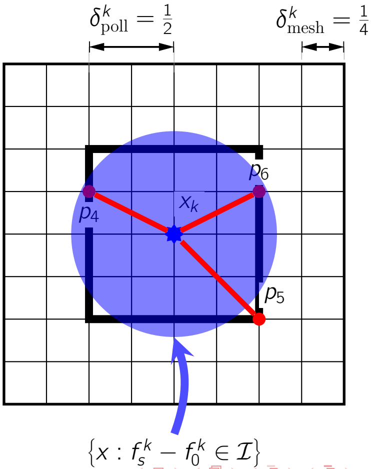
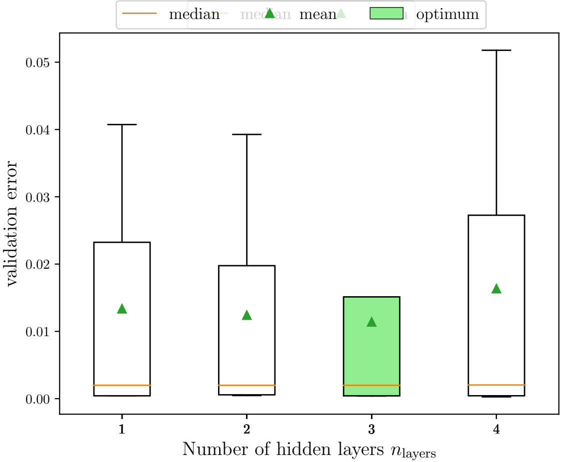
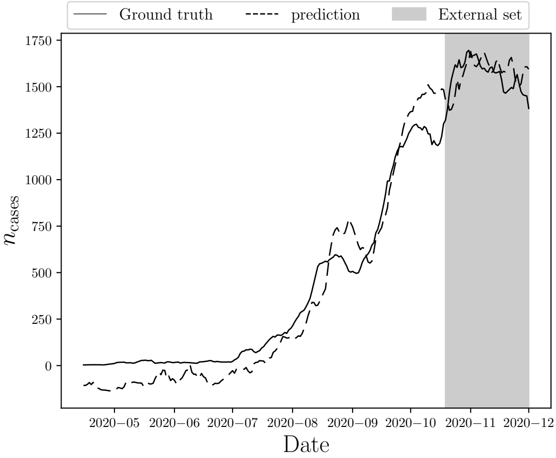
Constraint handling using the *progressive barrier* approach [2]

Poll **uncertain failure**



We can use StoMADS to solve such hyperparameter optimization problems





Hyperparameter tuning: other hyperparamters

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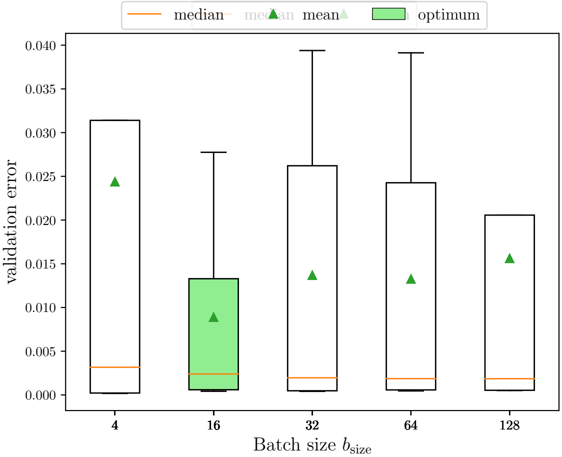

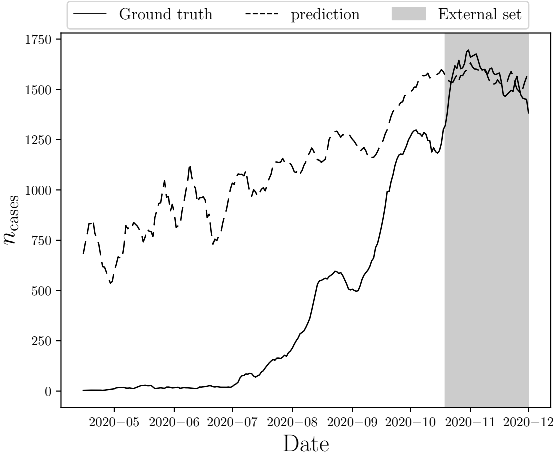

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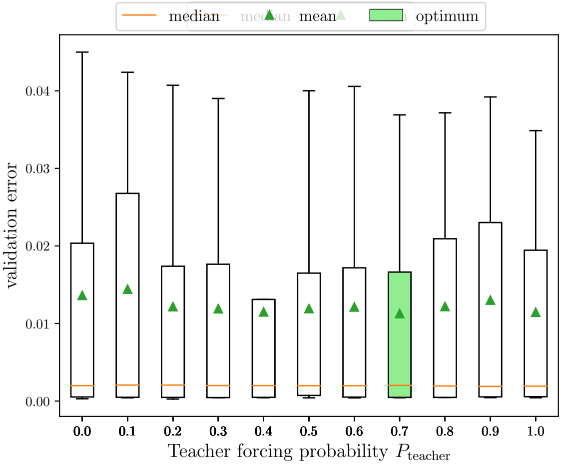

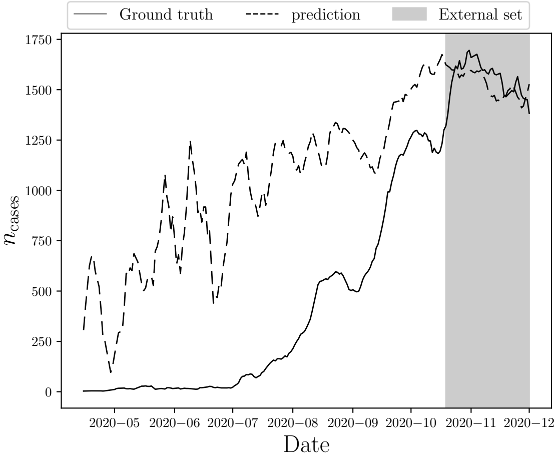

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