Overview of my research and related software packages

Khalil Al Handawi, PhD

Technical presentation

June 13, 2022

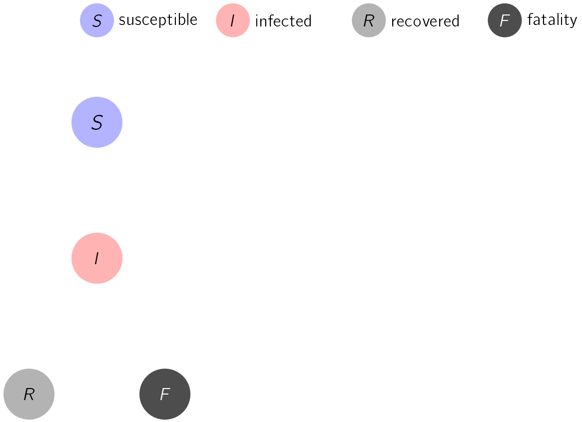
About me

- Khalil Al Handawi (*he/him/il*)
  - Experience with simulation based design
  - Experience with scientific computing
  - Experience with optimization and simulation research
- Born and raised in Abu Dhabi, United Arab Emirates
- Originally from Aleppo, Syria
- Moved to Montréal in 2017

Optimization of public health models using artificial life models

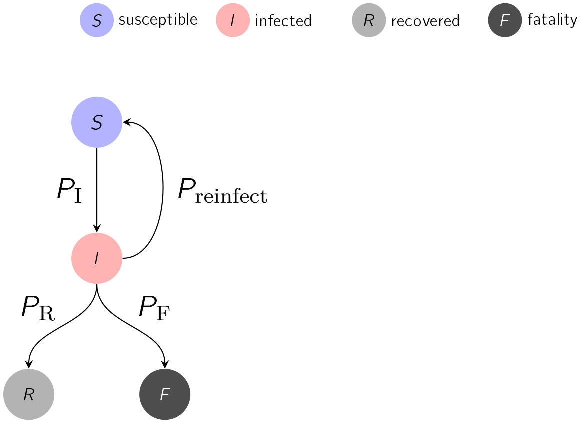
Background: epidemiological models

What are compartmental epidemiological models?



What are compartmental epidemiological models?

- Described by a *stochastic* process



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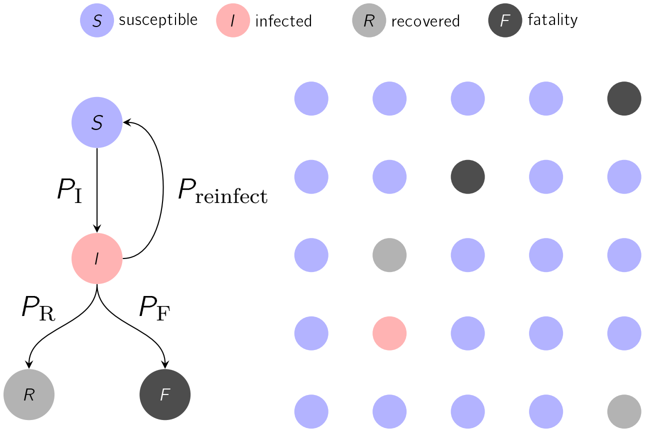

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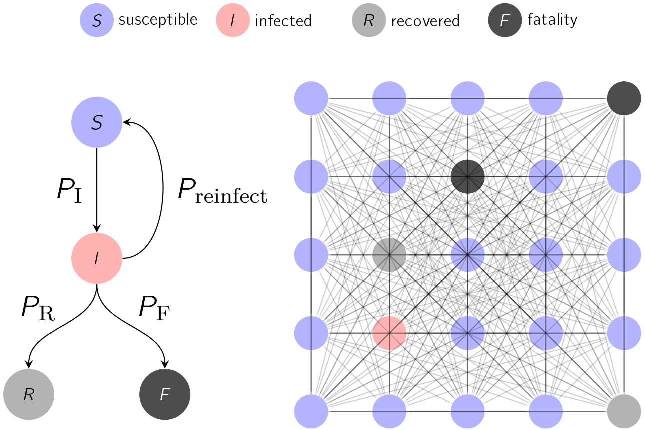
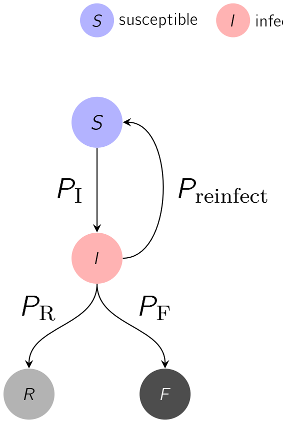
- Assumes *homogenous* interaction

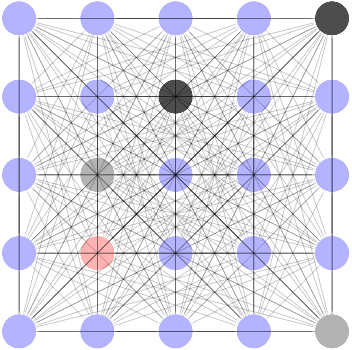


Background: epidemiological models

What are compartmental epidemiological models?

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





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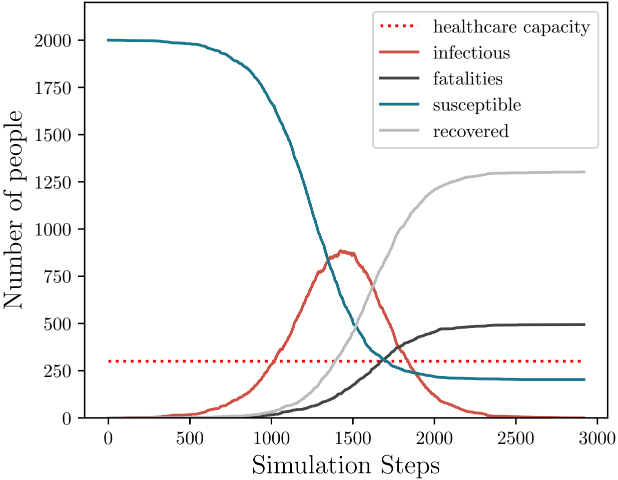
$$\frac{dS}{dt} = -\frac{\beta IS}{N},$$

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

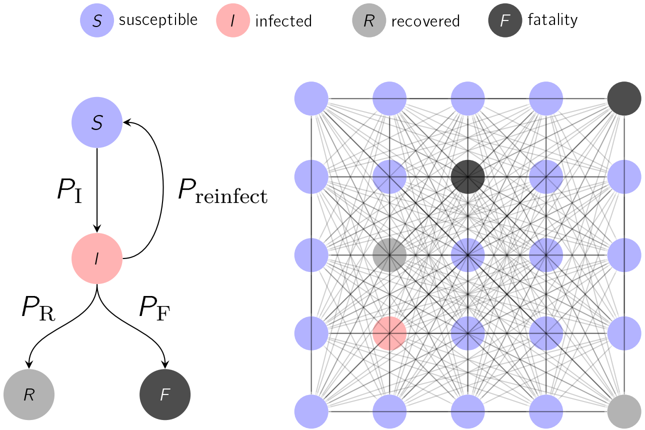
$$\frac{dR}{dt} = \gamma I,$$

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



What are compartmental epidemiological models?

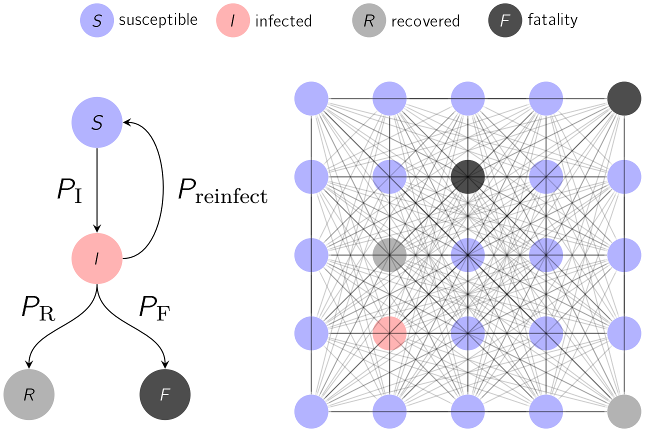
✓ Analytical solutions are available



Background: epidemiological models

What are compartmental epidemiological models?

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



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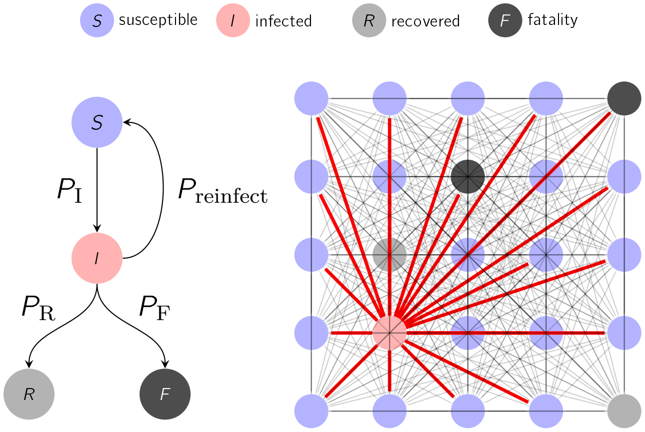
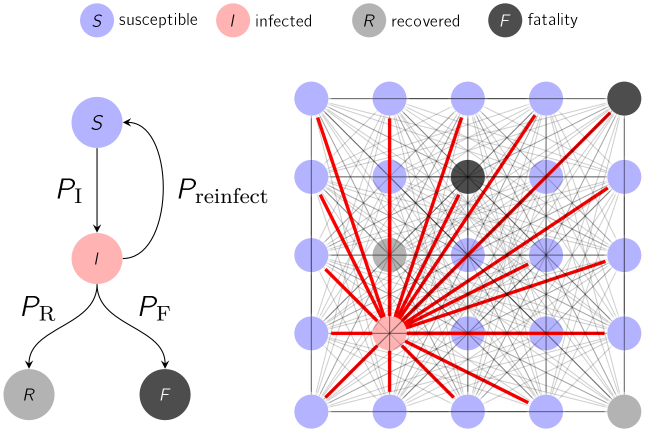
- ✘ Does not account for *geography*



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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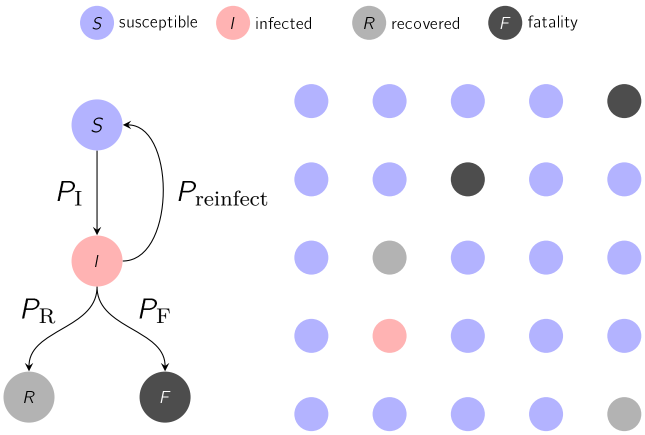
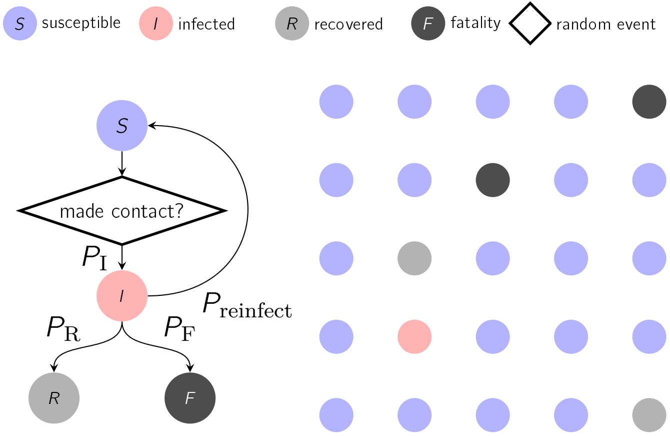


What are agent-based epidemiological models?

- *Stochastic* process



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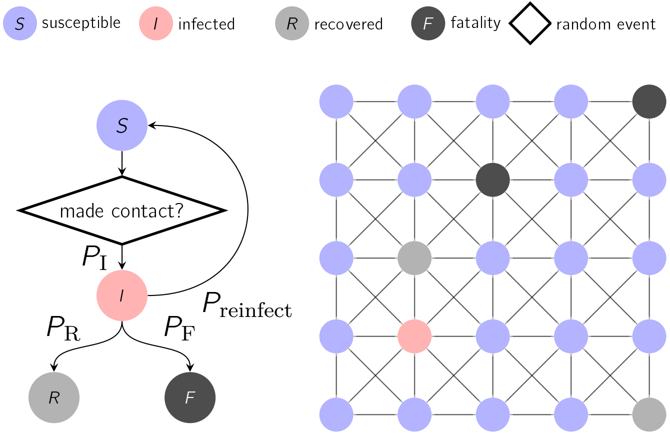

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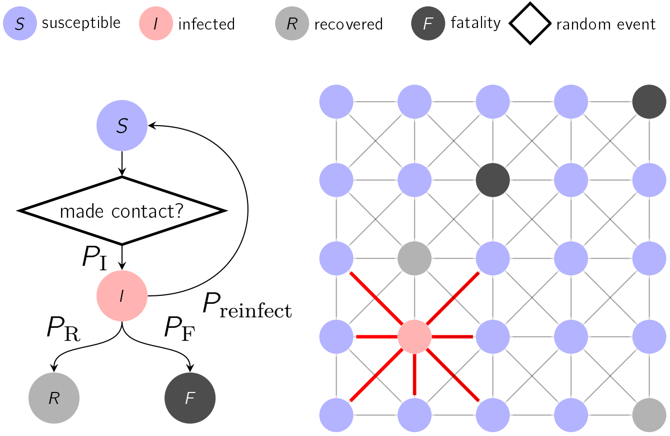

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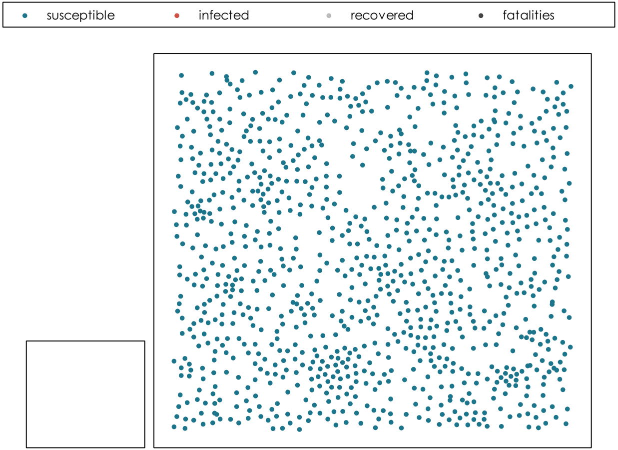
Realization 1



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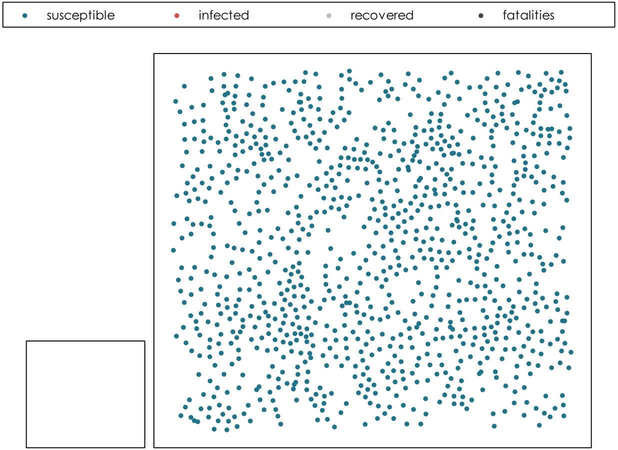
Realization 2



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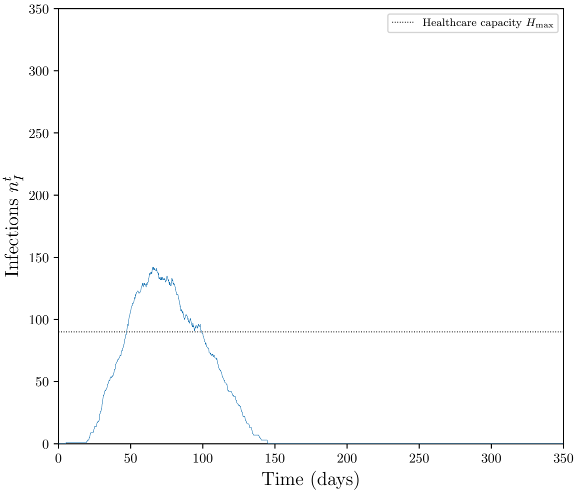

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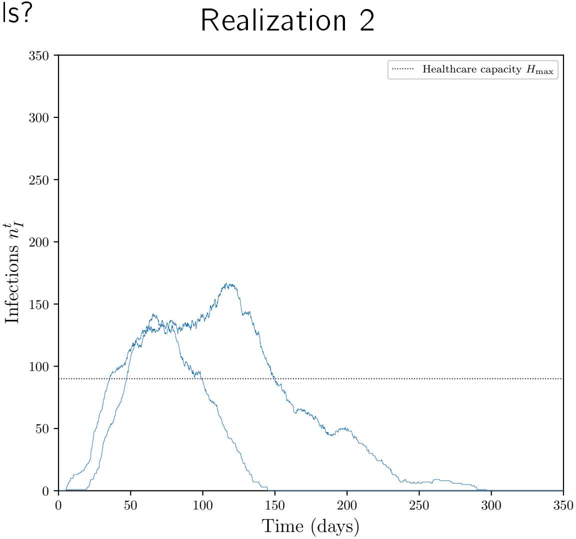

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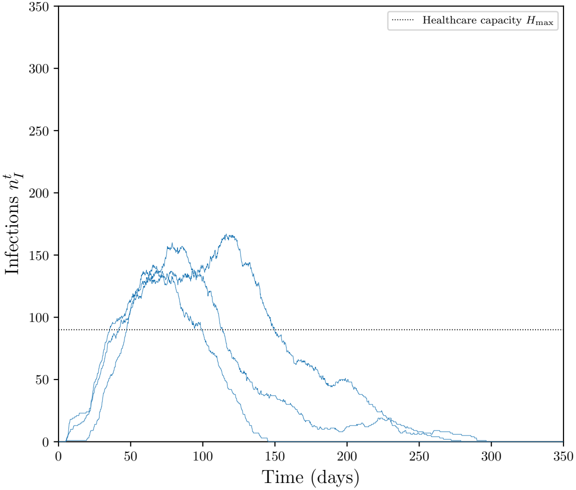

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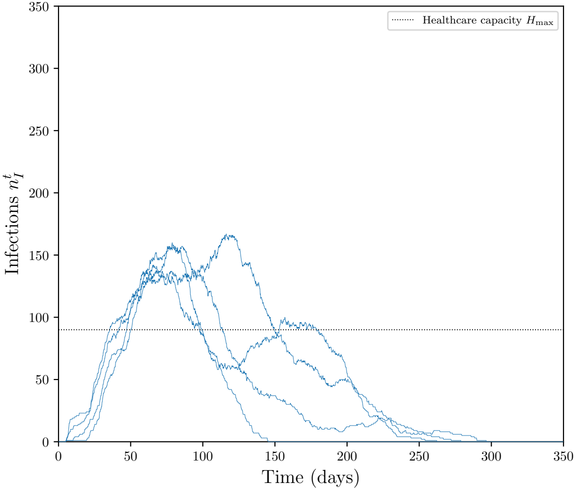

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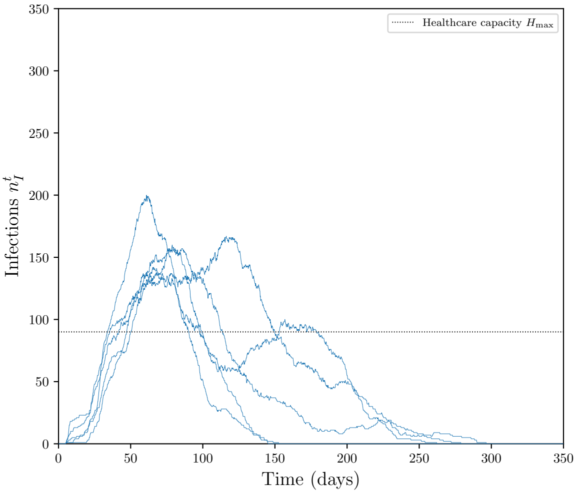

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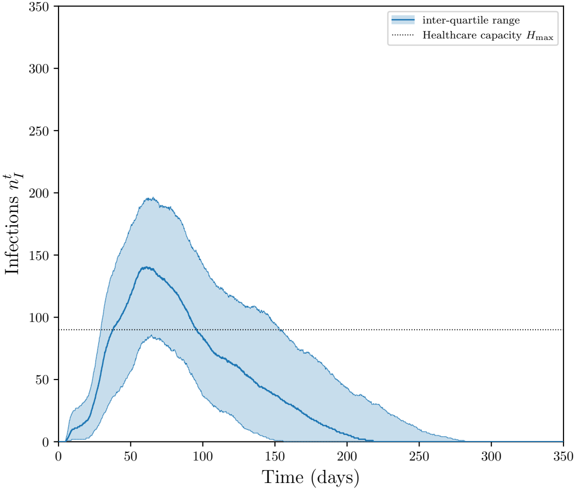

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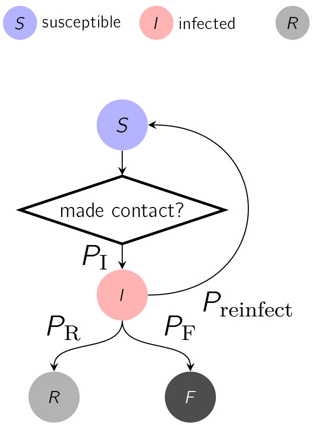
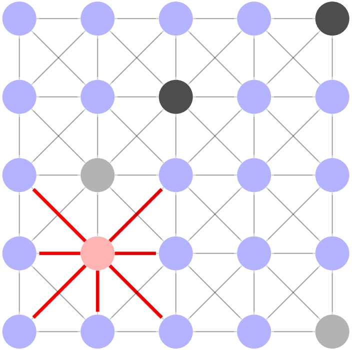
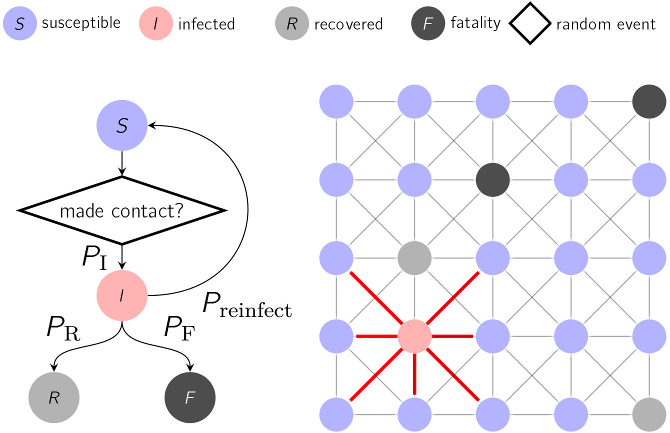
✓ Account for *geography* and *demographics*





What are agent-based epidemiological models?

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



Background: epidemiological models

What are agent-based epidemiological models?

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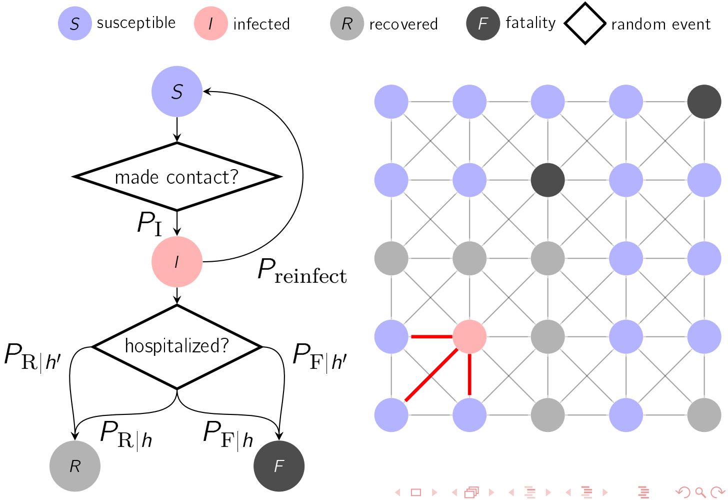

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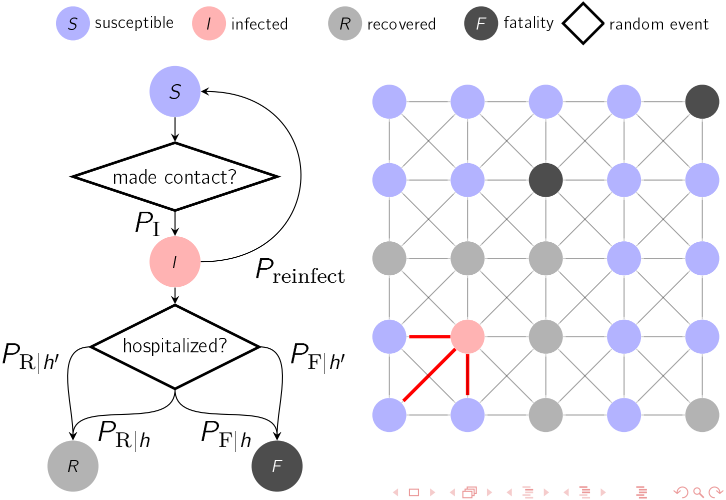

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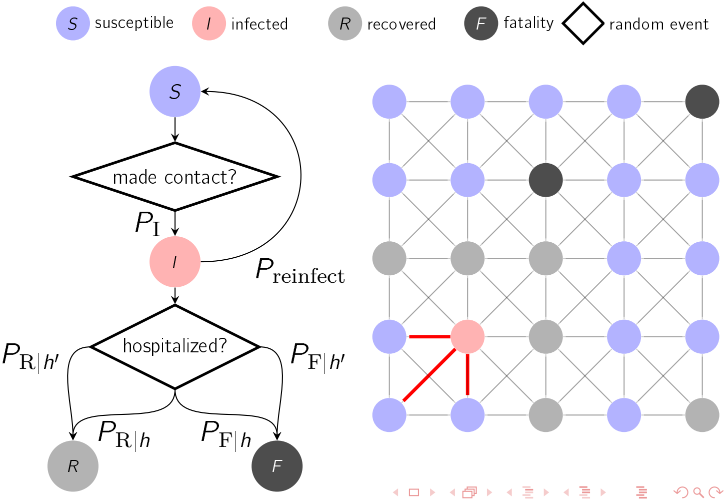
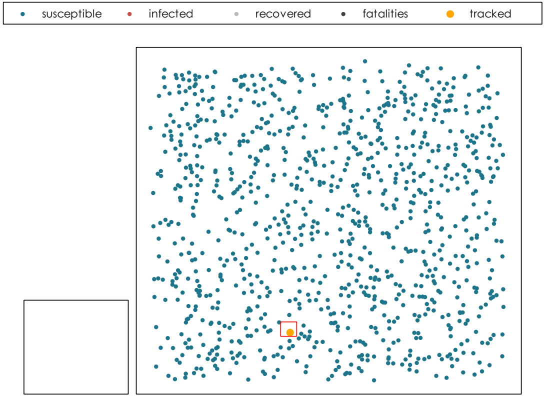
- ✗ Computationally expensive



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

No interventions applied



Public health policy-making problem formulation

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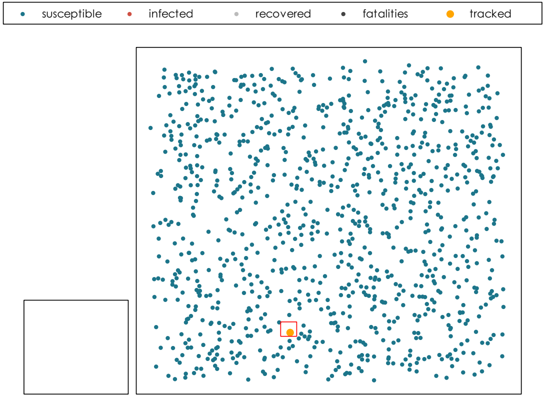

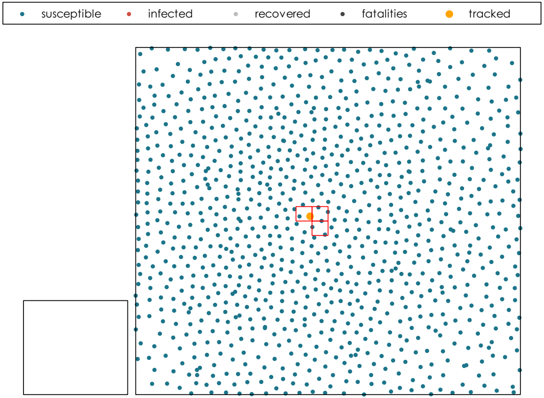

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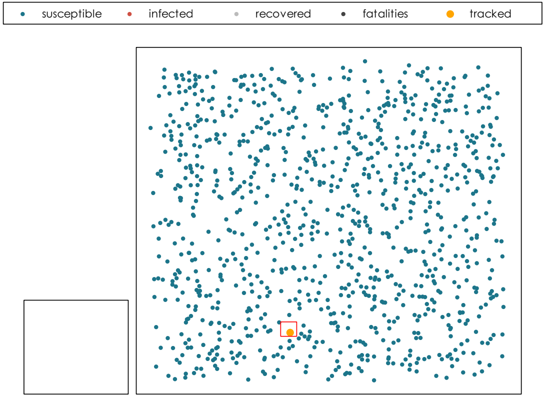

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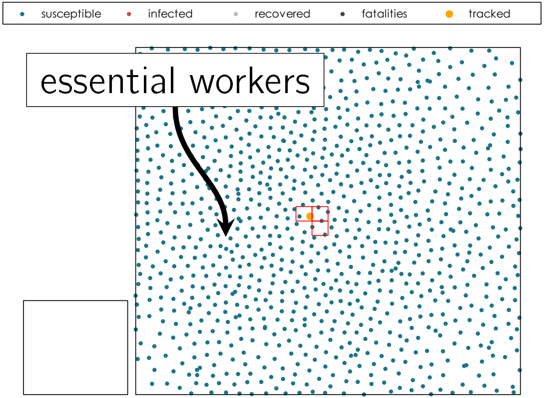

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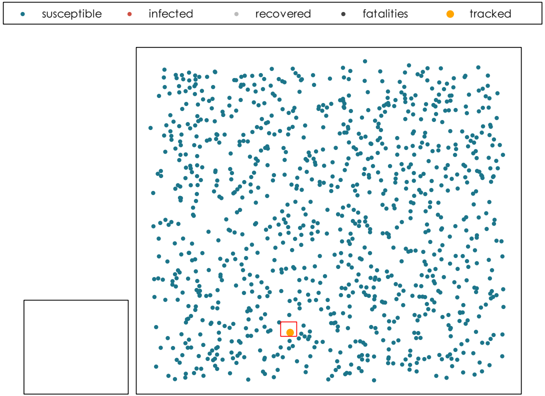

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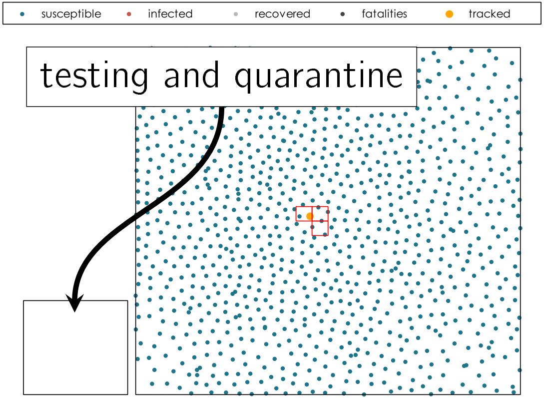

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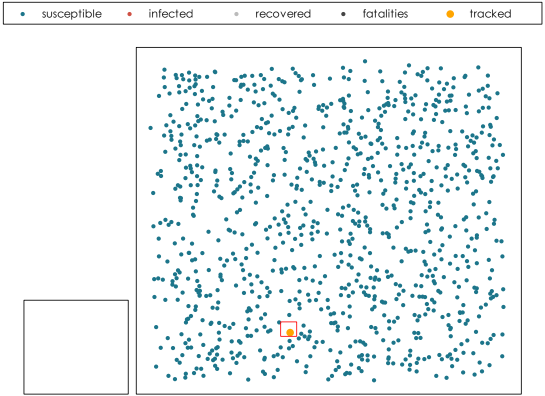

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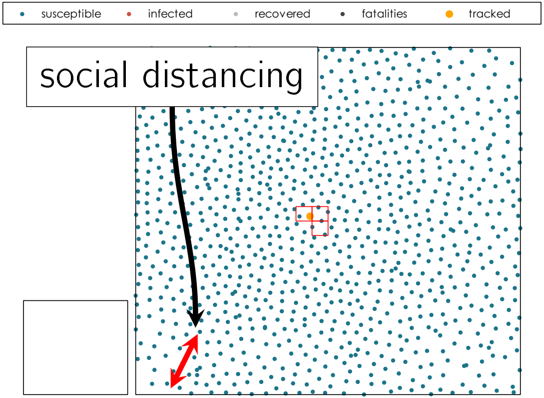

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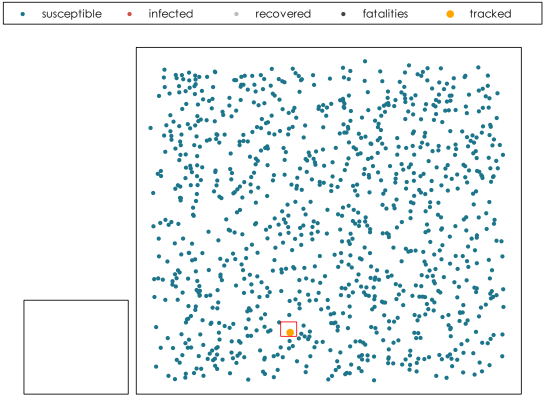

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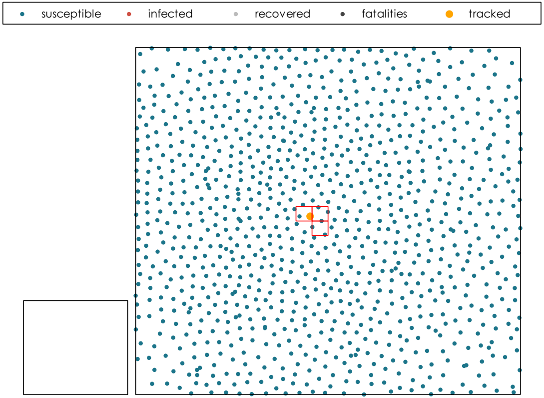

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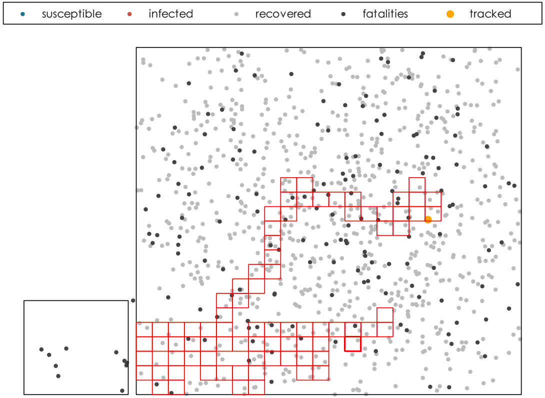

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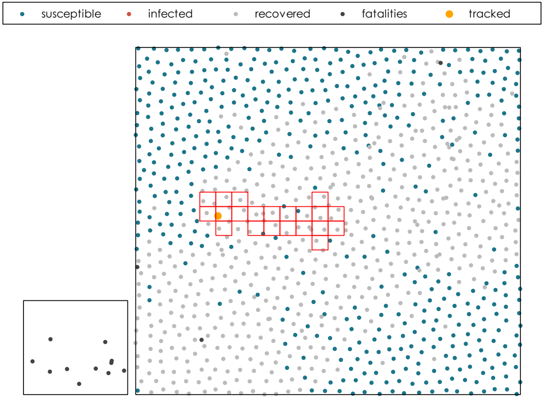

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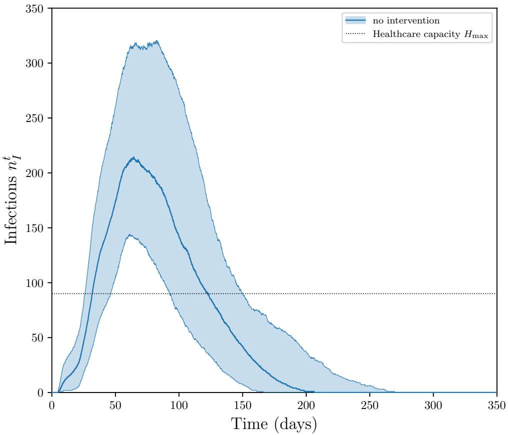
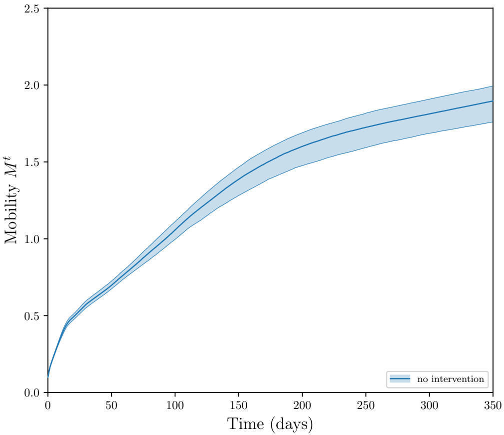
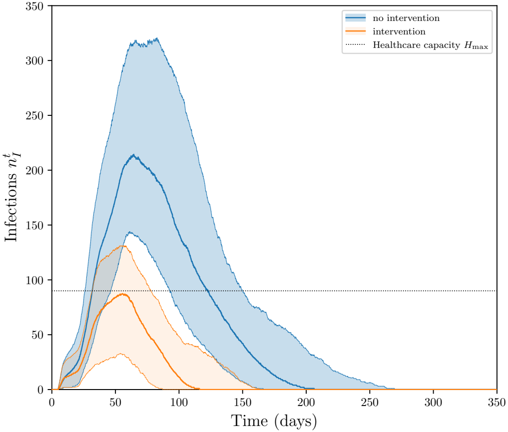


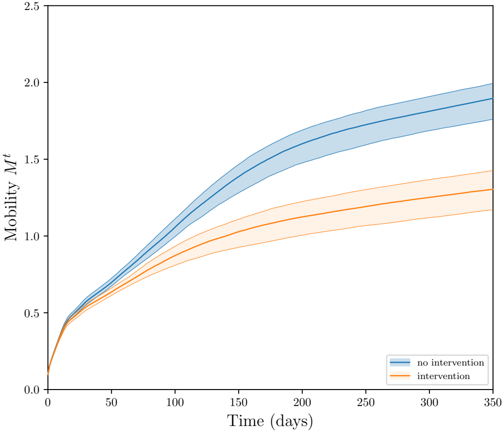


What is the **cost** of public health interventions?

infections ↓



mobility ↓



Optimization problem

Objective and constraints

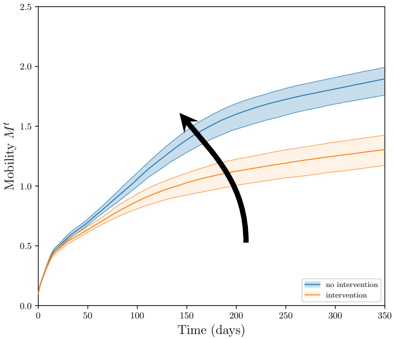
$$\min_{x} \quad f(x) = -M^T$$

subject to

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

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

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

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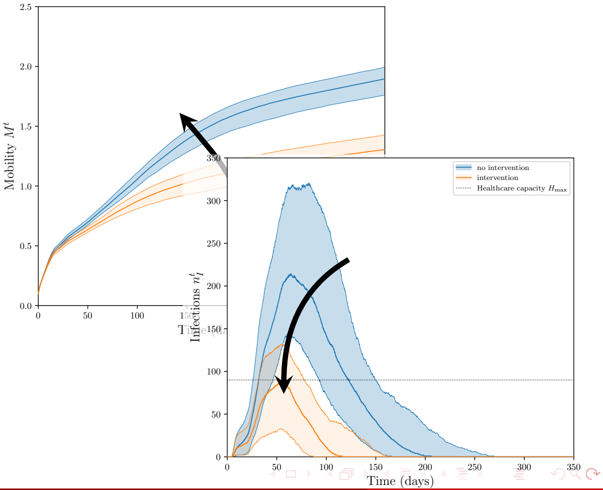

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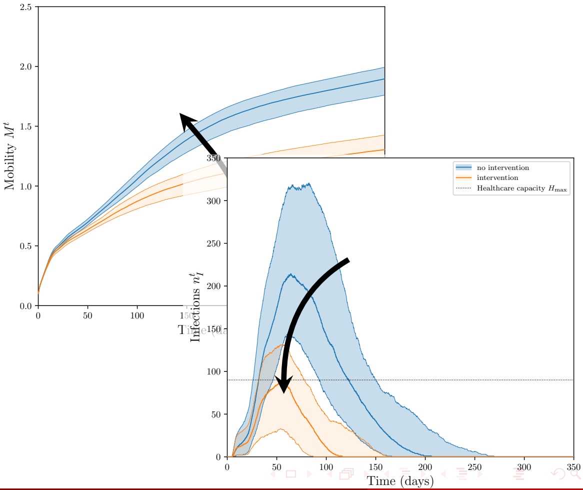

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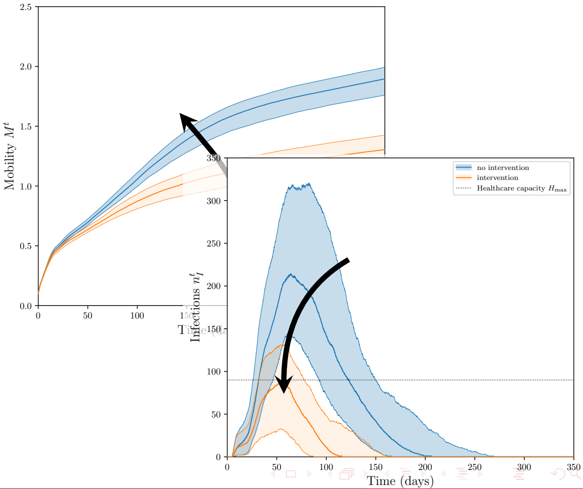

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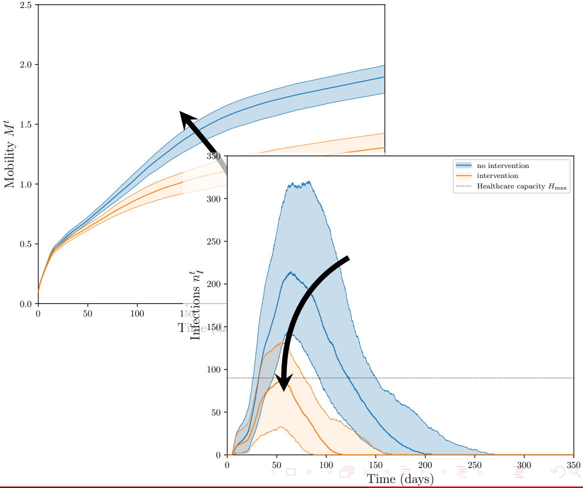
Randomly seeded parameters

- Initial conditions
- Interactions, demographics



Optimization results

StoMADS, `NOMAD`[1], and genetic algorithms were used to solve the problem[2]

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[1] S. Le Digabel et al., 2018 , *https://www.gerad.ca/nomad/Downloads/user_guide.pdf*
[2] K. Al Handawi and M. Kokkolaras, 2021 , *IEEE Transactions on Emerging Topics in Computational Intelligence*

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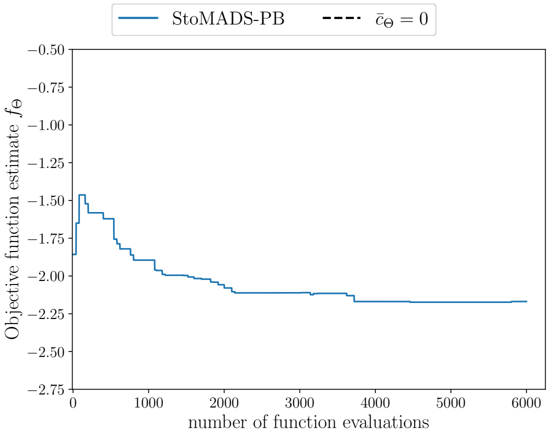
sampling rate $n^k = 4$



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Randomly seeded parameters

- Initial conditions
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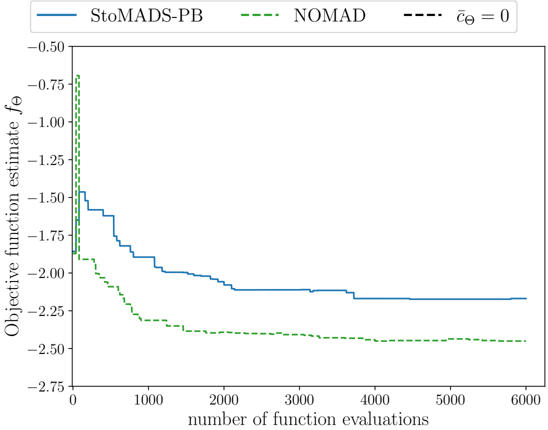

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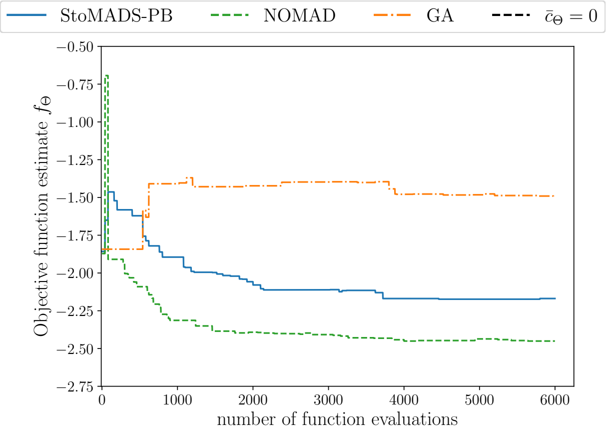

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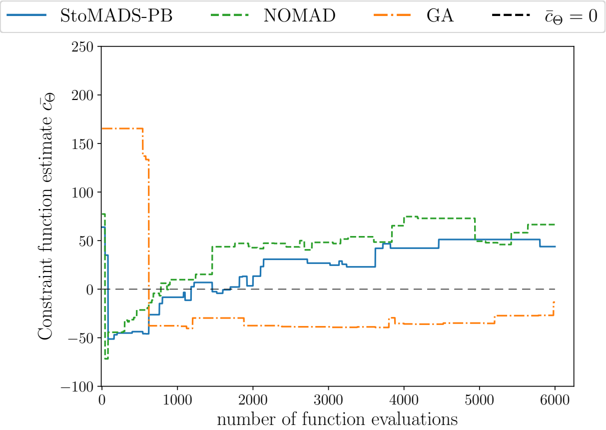

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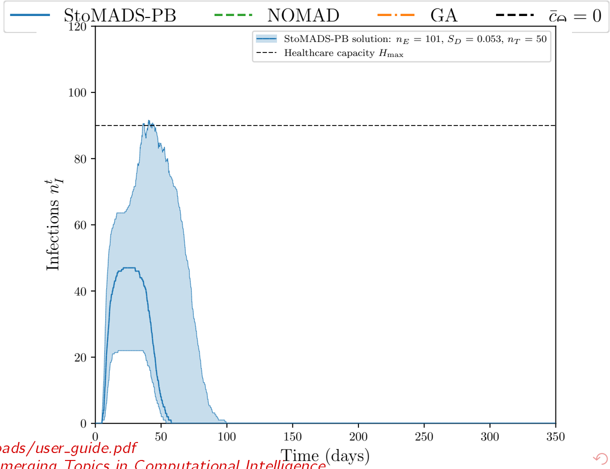

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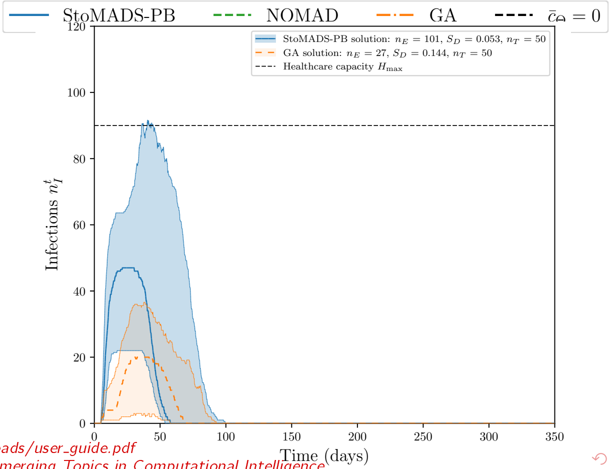

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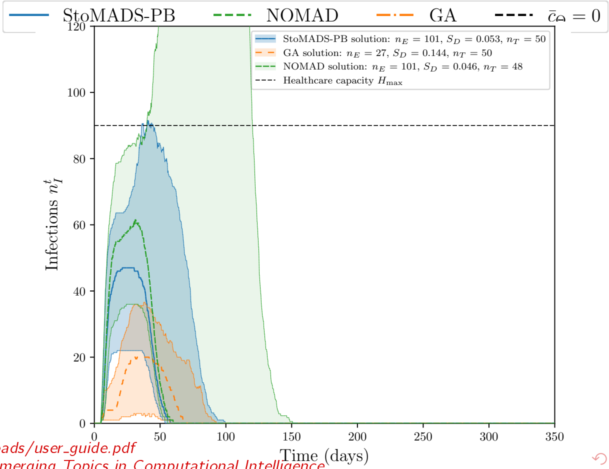

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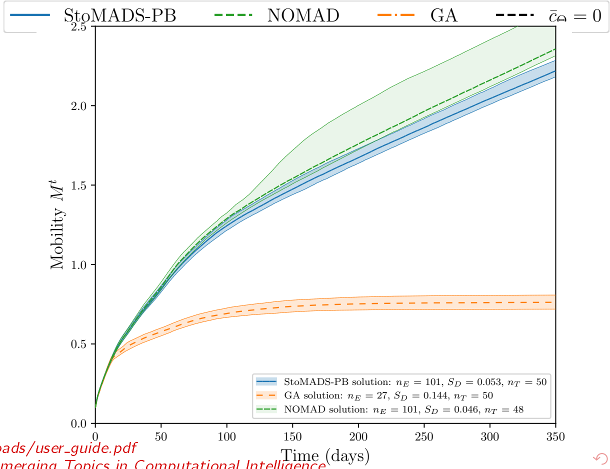

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Pseudo-code of ABM

Input: model parameters, demographics, random seed
Output: n_F^T, $n_{I,\max}$, M^T

[0] Initialization

  set time frame $t \leftarrow 0$, initialize traits A^0, initialize mobility $\mathrm{G}^0 = 0$

[1] Update ABM

  if $t = 50$, then set patient-zero as infected and seed the disease

  loop over agents for $i = 1, 2, \ldots, \bar{n}$ do

    [2] Social interaction

      for $j = 1, 2, \ldots, \bar{n}$ do

        if $j \neq i$ then compute $f_{x,i,j}$, $f_{y,i,j}$

      compute social interaction forces $F_{x,i}^t$, $F_{y,i}^t$

    [3] Update model dynamics update velocities $v_{x,i}^{t+1}$, $v_{y,i}^{t+1}$, update positions $z_{x,i}^{t+1}$, $z_{y,i}^{t+1}$

    [4] Mobility

      for $j_g = 1, 2, \ldots, n_{grids}$ do

        compute grid bounds $l_{x,jg} = \frac{jg \mod ng}{ng}$, $l_{y,jg} = \frac{jg/ng}{ng}$, $u_{x,jg} = \frac{jg \mod ng+1}{ng}$, and $u_{y,jg} = \frac{jg/ng+1}{ng}$

        if $l_{x,jg} < z_{x,i}^{t+1} \leq u_{x,jg}$ *and* $l_{y,jg} < z_{y,i}^{t+1} \leq u_{y,jg}$ then $g_{i,jg}^{t+1} = 1$

        else $g_{i,jg}^{t+1} = g_{i,jg}^t$

      compute mobility of agent i $\mu_i^t = \frac{1}{n_{\text{grids}}} \sum_{jg=1}^{n_{\text{grids}}} g_{i,jg}^t$

    [6] Disease model determine infections, fatalities, and hospitalizations

[7] Termination

if $t < T_{max}$ then

  set $t \leftarrow t + 1$, go to [1]

  otherwise stop

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```
    __global__ void CUDA_GPU::calc_force_m(float* diffs_x, float* diffs_y,
        float* atoms_x, float* atoms_y, float SD_factor, int N)
    {
        int i(threadIdx.x + blockIdx.x * blockDim.x);
        int j(threadIdx.y + blockIdx.y * blockDim.y);

        if (i >= N || j >= N) {
            return;
        }

        float distance = ((atoms_x[i] - atoms_x[j]) * (atoms_x[i] - atoms_x[j])
     +
            (atoms_y[i] - atoms_y[j]) * (atoms_y[i] - atoms_y[j]));
        float distance3 = distance * distance * distance + 1e-15;

        diffs_x[i + N * j] = -SD_factor * (atoms_x[i] - atoms_x[j]) / distance3;

        diffs_y[i + N * j] = -SD_factor * (atoms_y[i] - atoms_y[j]) / distance3;
    }
```

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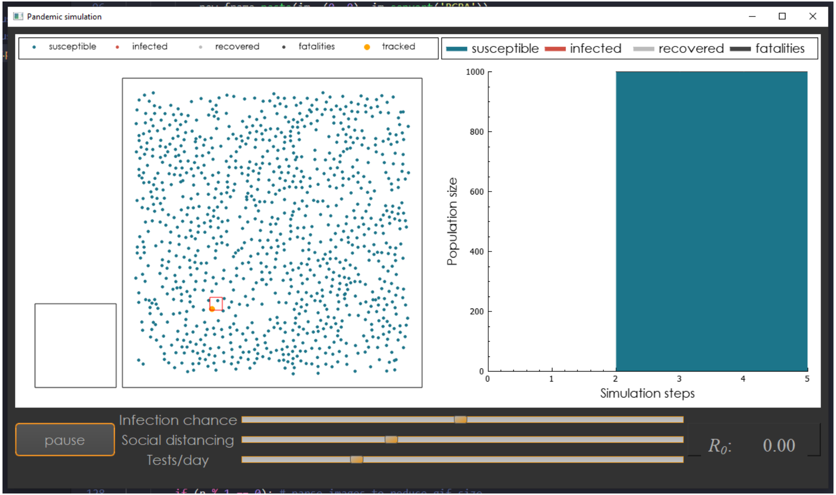
```
__global__ void CUDA_GPU::calc_tracking_matrix(float* G, float* G_track,
    float* atoms_x, float* atoms_y, int n_grids, int N_rows, int N_cols)
{
    int i(threadIdx.x + blockIdx.x * blockDim.x);
    int j(threadIdx.y + blockIdx.y * blockDim.y);

    if (i >= N_rows || j >= N_cols)
    {
        return;
    }

    float g1 = (float)(j % n_grids) / float(n_grids);
    float g2 = (float)(j / n_grids) / float(n_grids);
    float g3 = (float)((j % n_grids) + 1) / float(n_grids);
    float g4 = (float)((j / n_grids) + 1) / float(n_grids);

    bool check = (atoms_x[i] > g1) && (atoms_y[i] > g2) && (atoms_x[i] <= g3
) && (atoms_y[i] <= g4);

    float t = (check) ? 1 : 0;
    G[i + j * N_rows] += t; // update tracing matrix

    float track = (check) ? 1 : G_track[i + j * N_rows];
    G_track[i + j * N_rows] = track; // update tracking matrix

}
```

Open source GPU implementation of agent-based modeling[1]

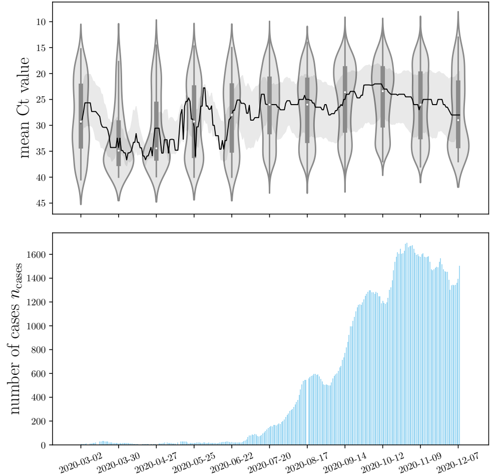


[1] Khalil Al Handawi, 2021 , *https://github.com/khbalhandawi/COVID_SIM_GPU*

COVID-19 incidence now-casting using machine learning

COVID-19 incidence forecasting

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



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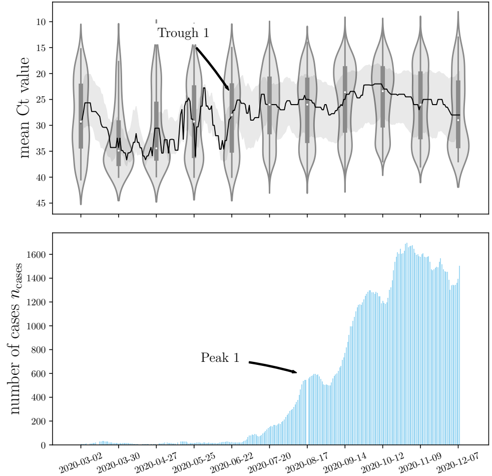

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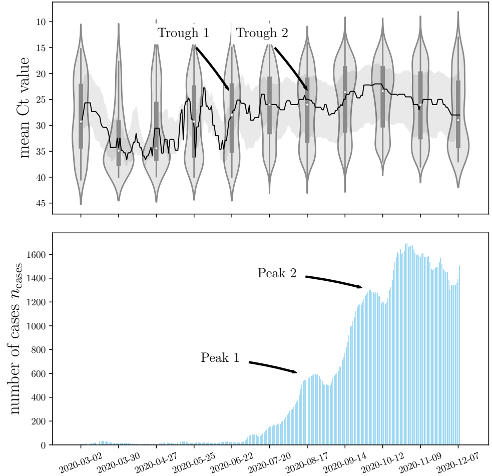

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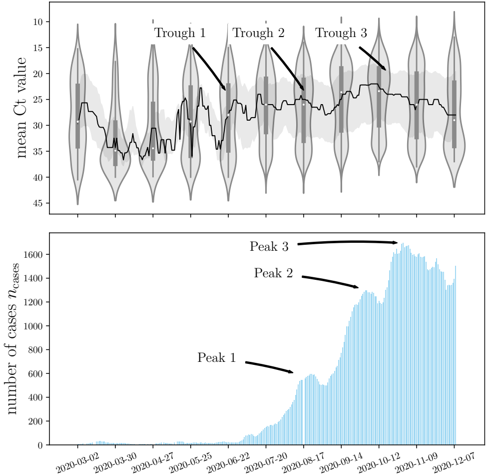

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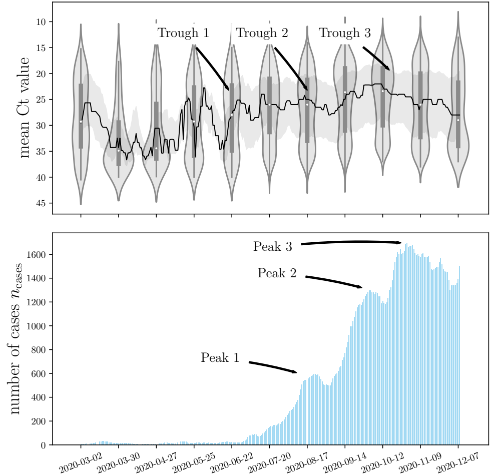

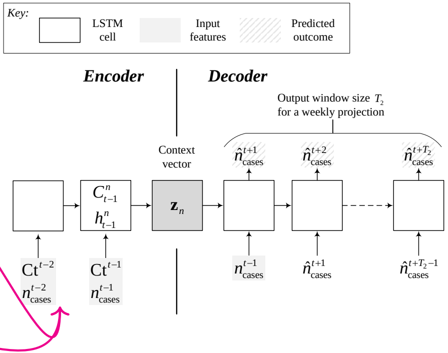

Seq2Seq model

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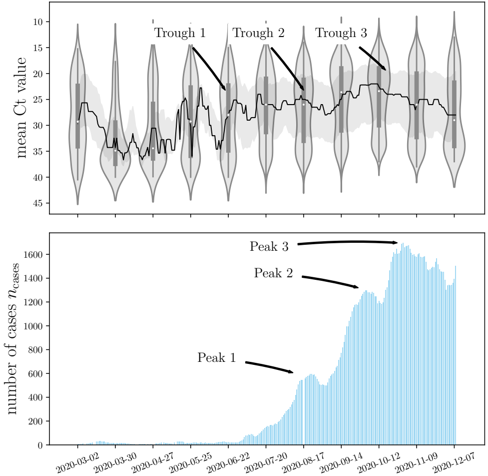

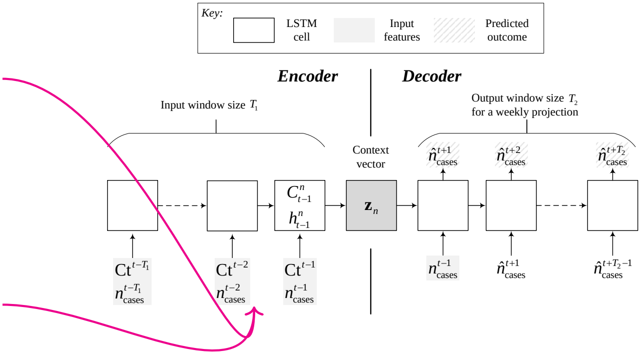

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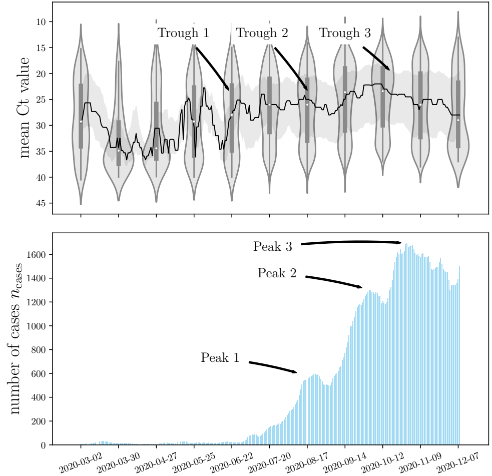

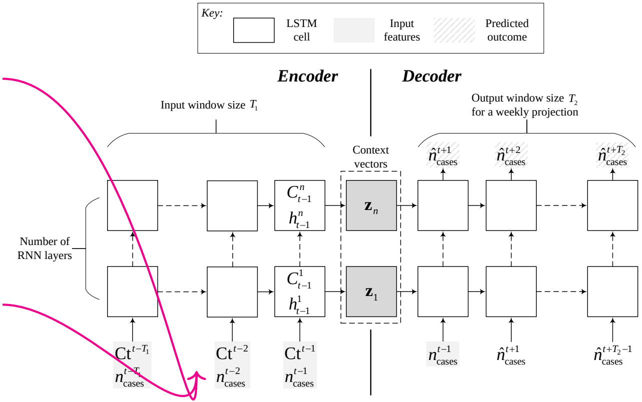

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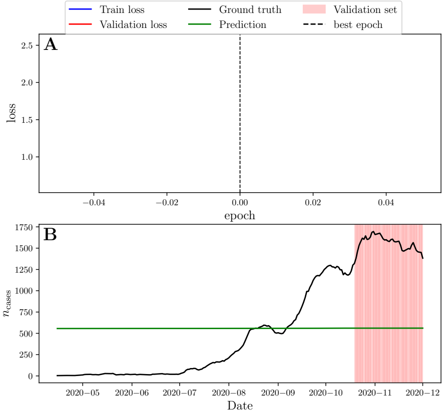
There are several challenges associated with hyperparameter optimization

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



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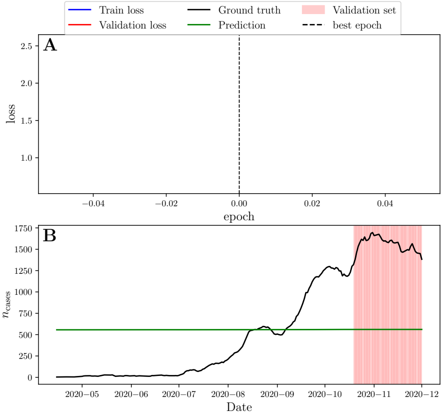

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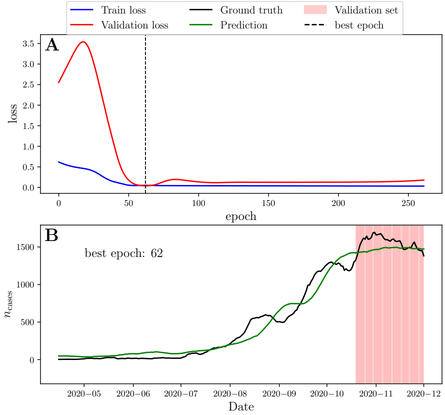

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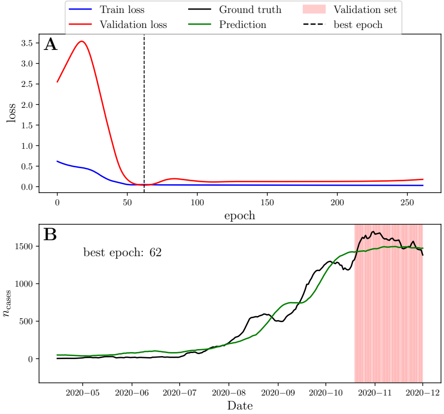

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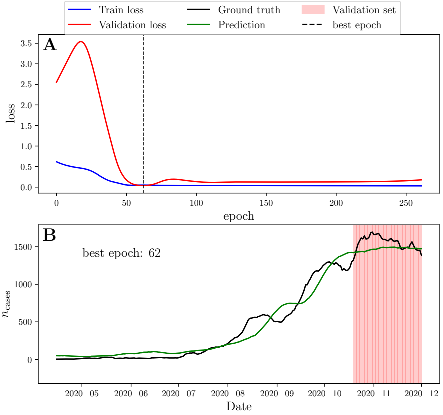

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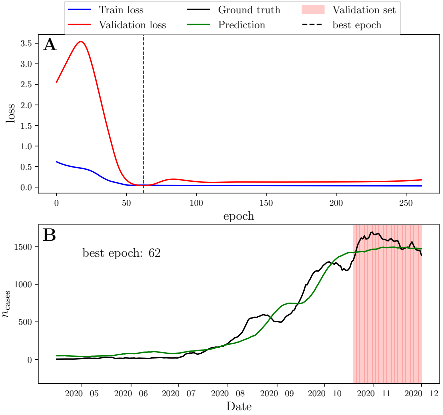

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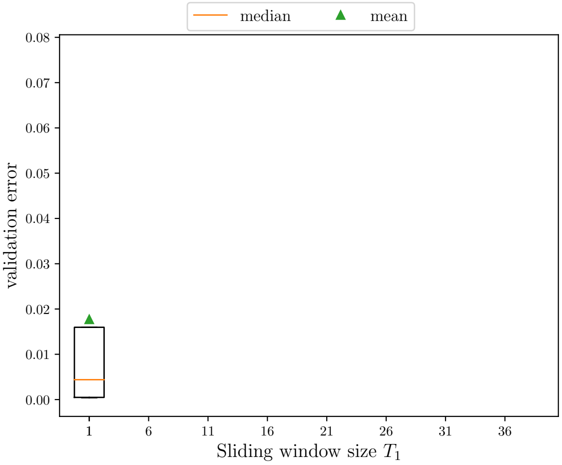

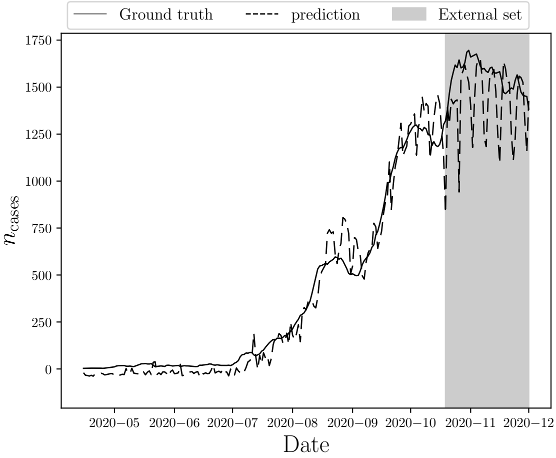

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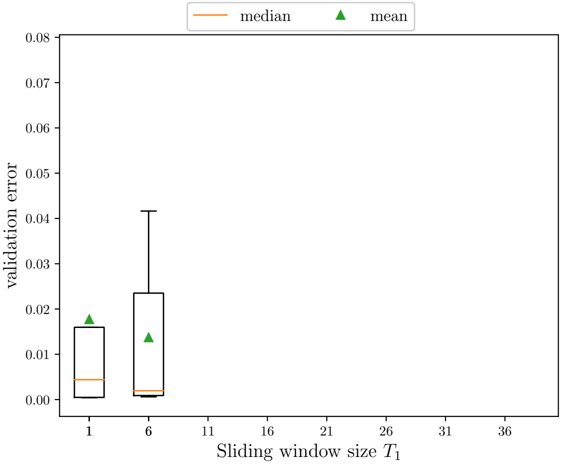

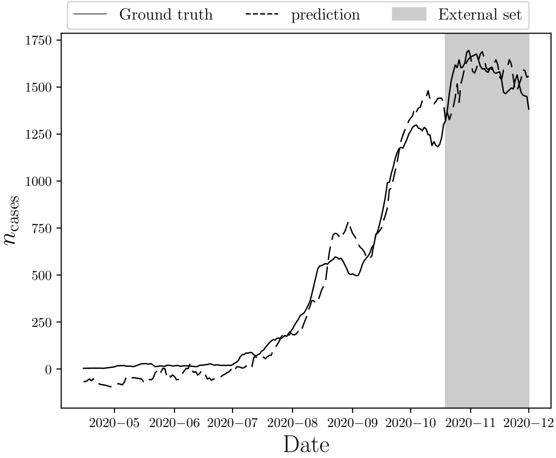

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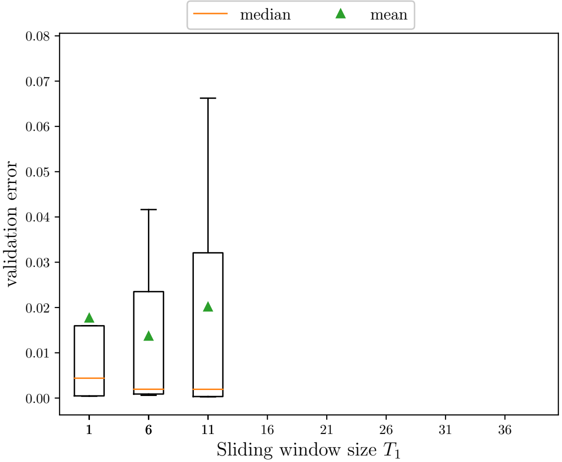

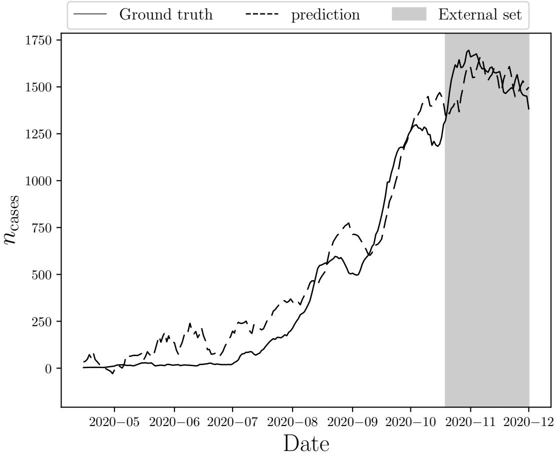

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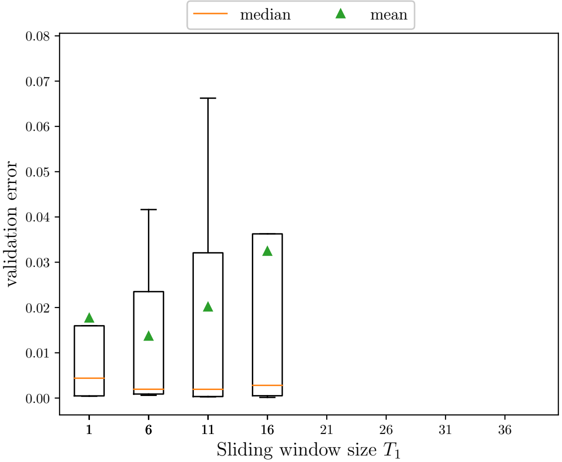

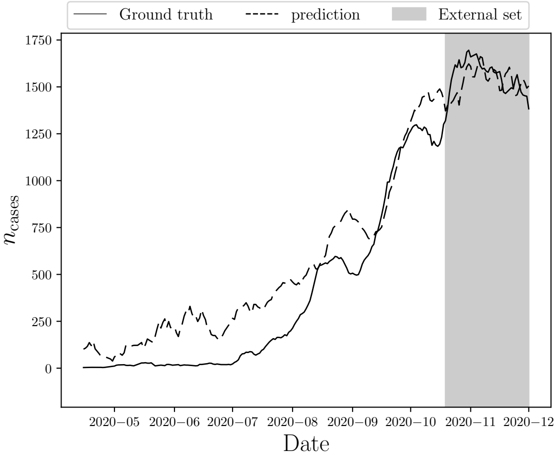

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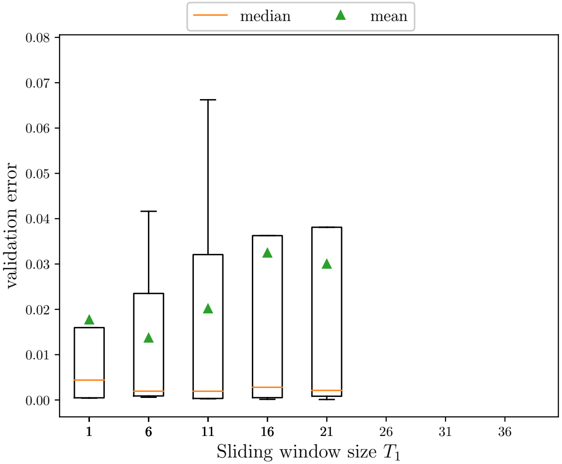

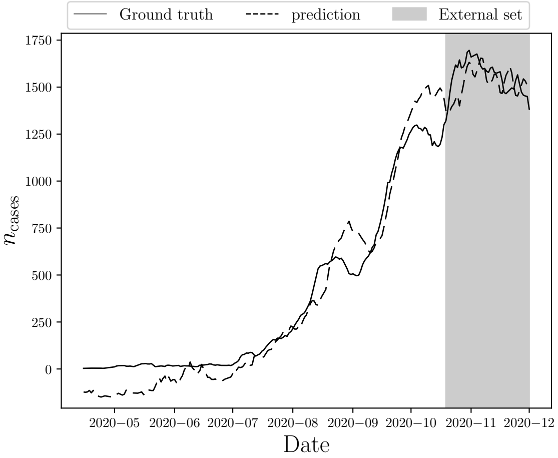

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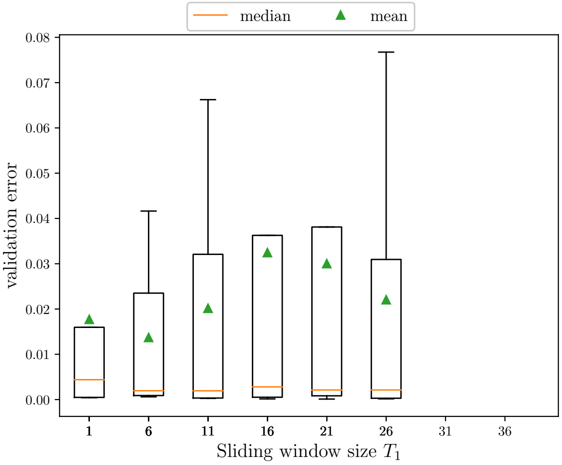
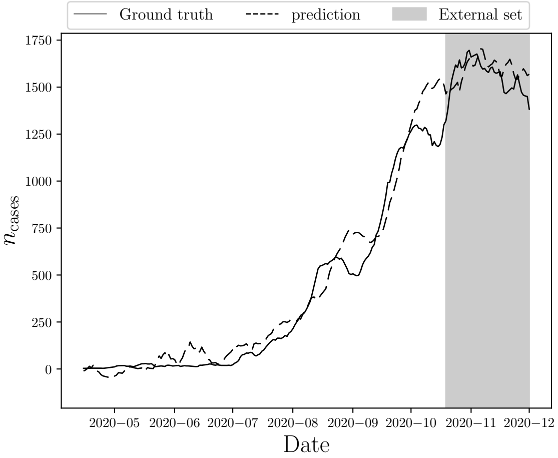
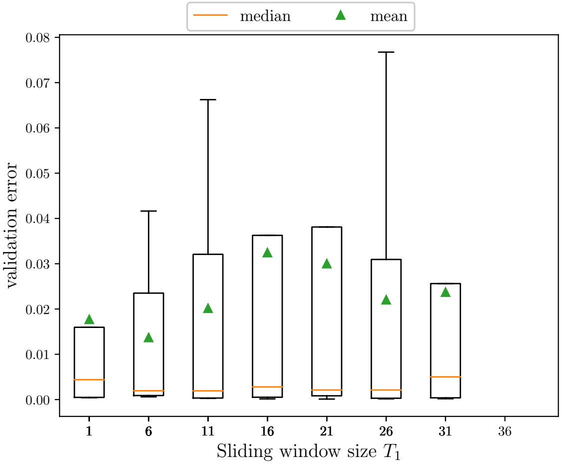


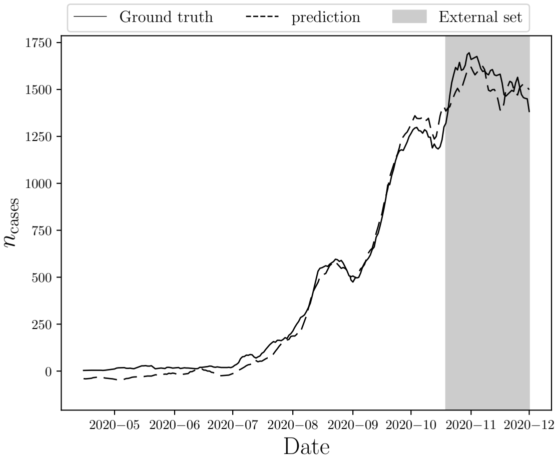


[1] A. Khalil et al., 2021 , *medRxiv*

Hyperparameter tuning

We can use StoMADS to solve such hyperparameter optimization problems[1]





[1] A. Khalil et al., 2021 , *medRxiv*

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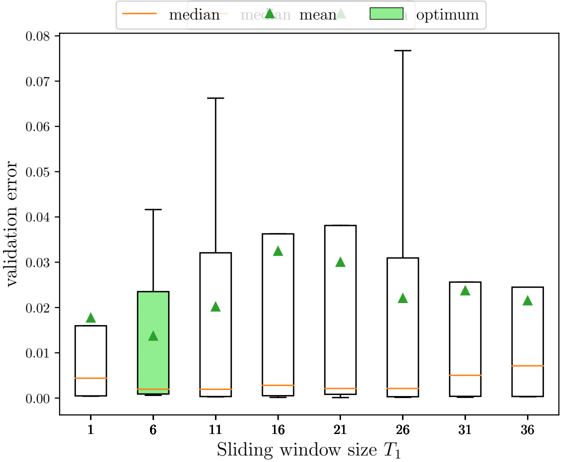

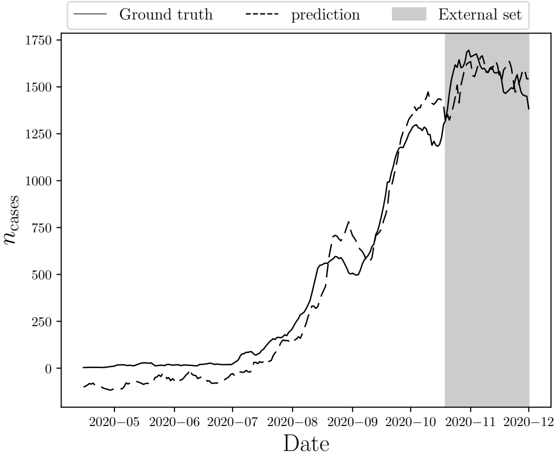

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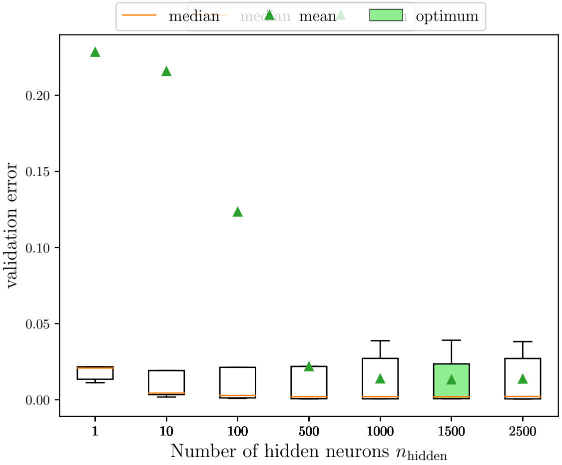

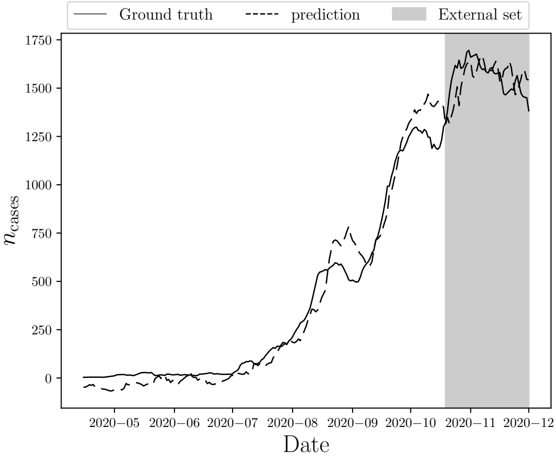

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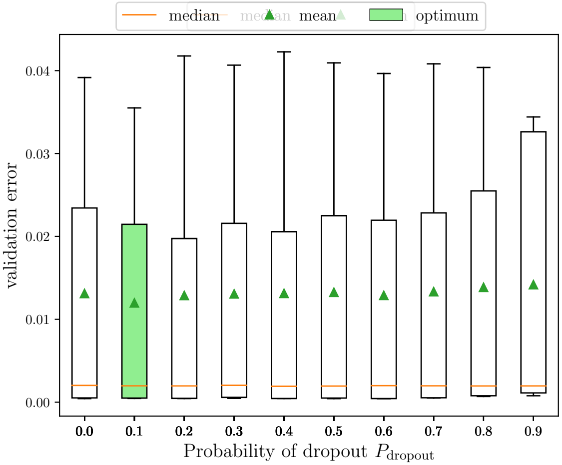
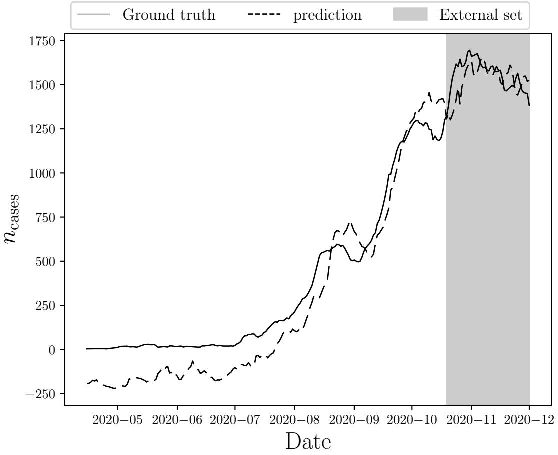




[1] A. Khalil et al., 2021 , *medRxiv*

We can use StoMADS to solve such hyperparameter optimization problems[1]

Objective and constraints

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

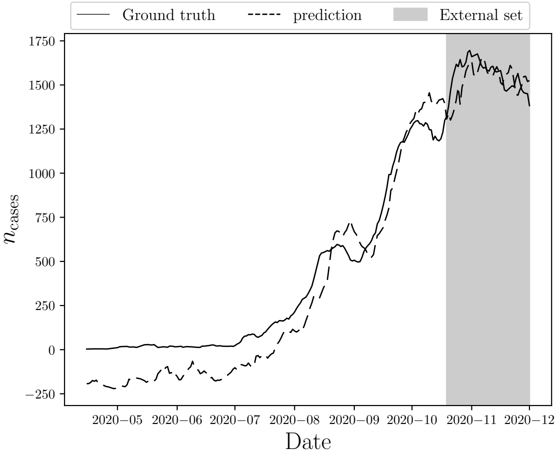
where Θ: realizations

Design variables ($\mathbf{x}$)

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

Randomly seeded parameters

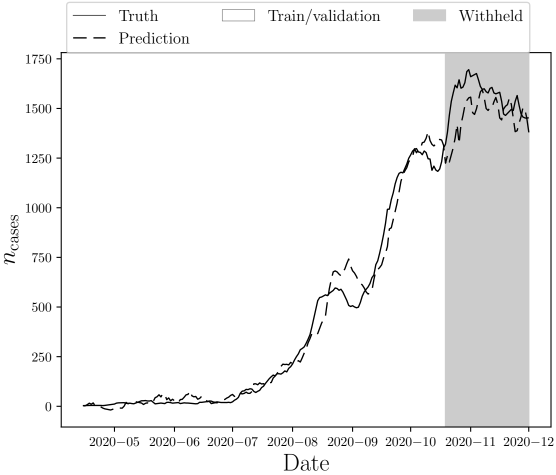
- Initial weights
- Gradient descent steps



[1] A. Khalil et al., 2021 , *medRxiv*

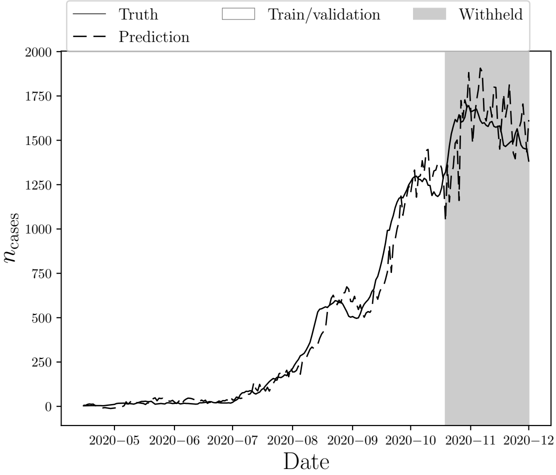
Optimal hyperparameters for the *Seq2Seq* model:

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



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}



Results: Optimal hyperparameters

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

Hyperparameter		**Value**
Sliding window size	T_1	6
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Margin of tolerance	ϵ	1×10^{-2}
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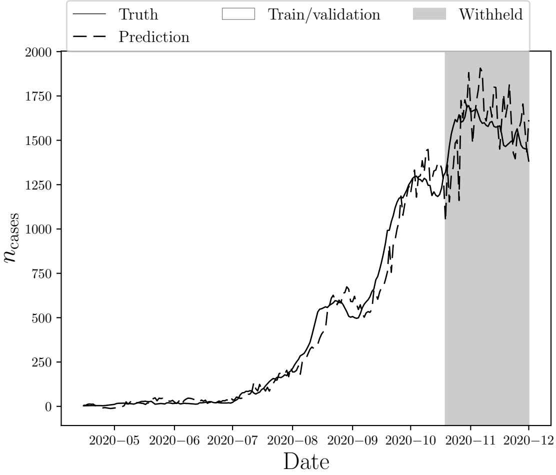
Learning rate	l_{rate}	1×10^{-5}

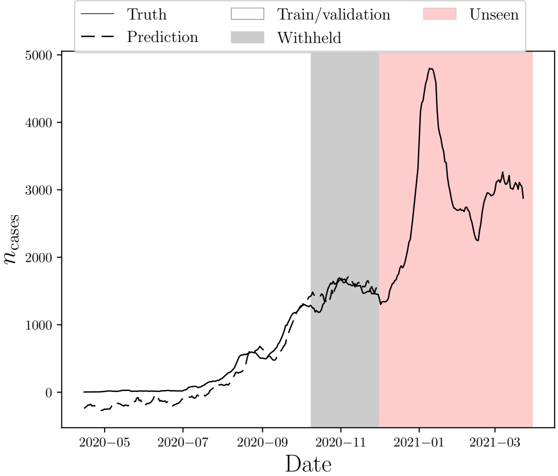
Support vector machine models have **deterministic** performance



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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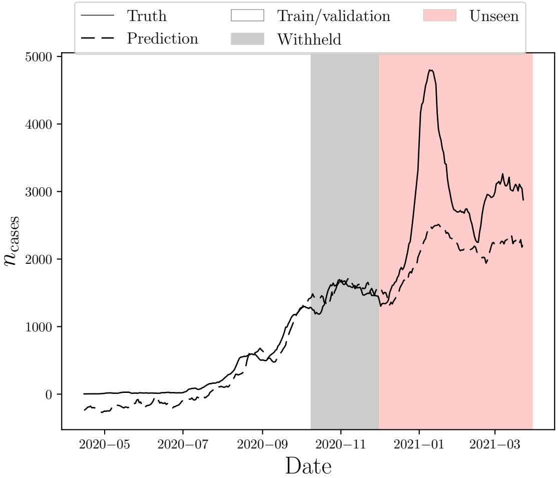

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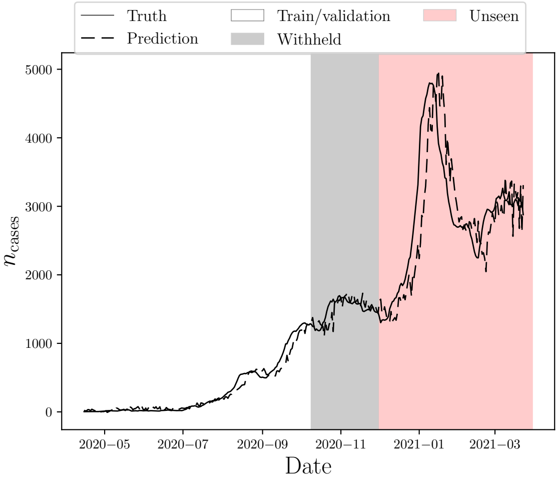

Results: Prospective validation

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

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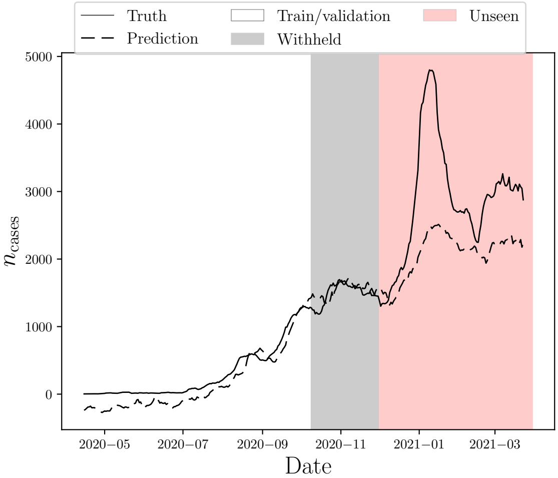
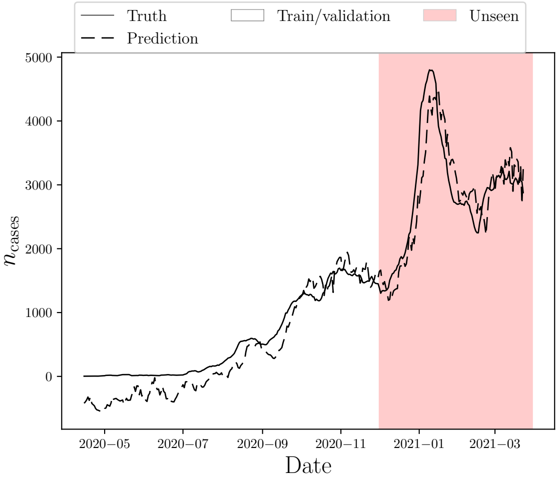


Results: Prospective validation

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

Model	Test error
Seq2Seq	**0.106**
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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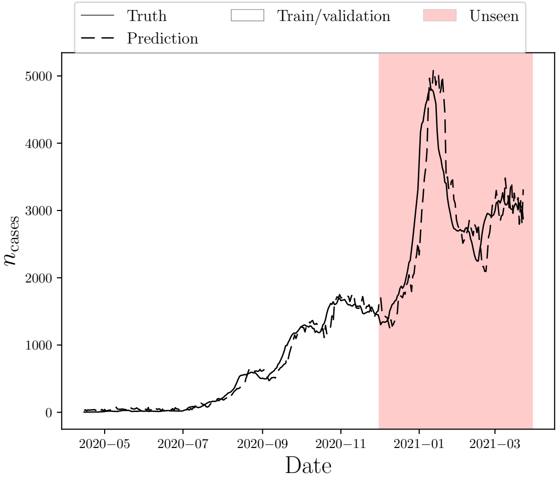
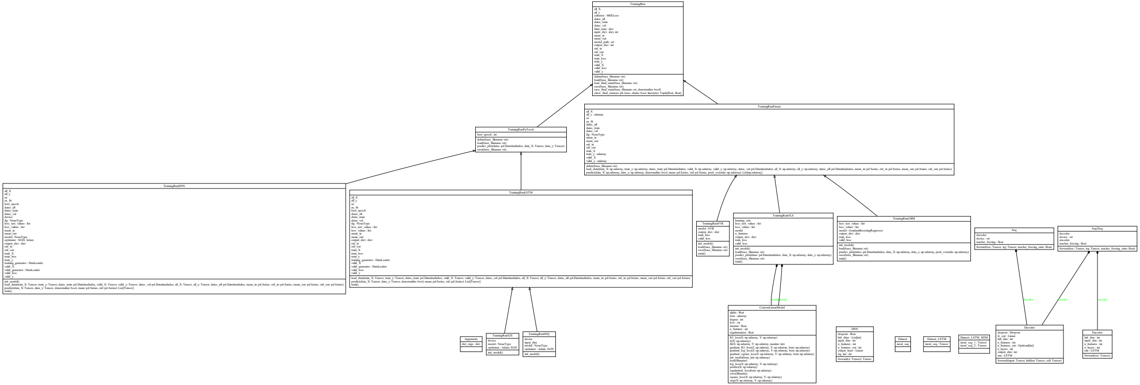


UML diagram of code



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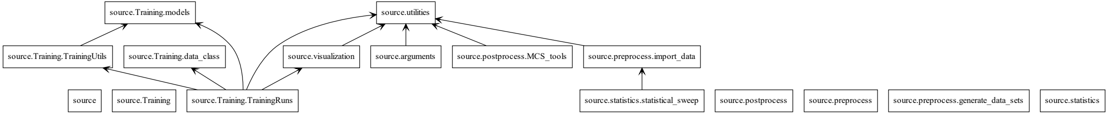
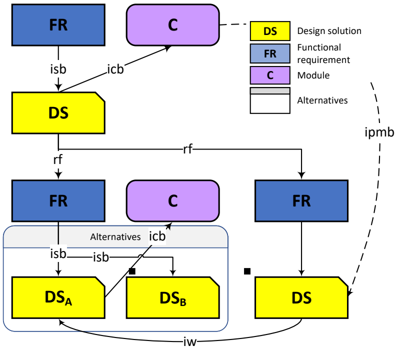


Ongoing work: Design space exploration

Consider a functional model (FM) of a product (conceptual design)

conceptual design

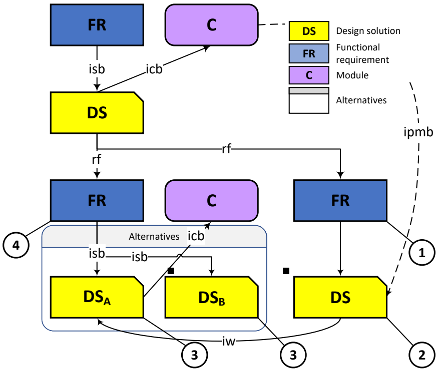


preliminary design

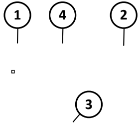
[1] N. Ahmad et al., 2013 , *Research in Engineering Design*
[2] A. Brahma and D. C. Wynn, 2020 , *Research in Engineering Design*

hyperlinks[1] used in multi-domain modelling

conceptual design



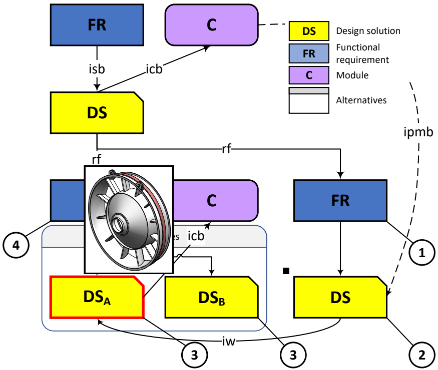
preliminary design



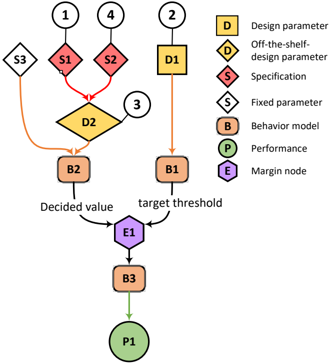
[1] N. Ahmad et al., 2013 , *Research in Engineering Design*
[2] A. Brahma and D. C. Wynn, 2020 , *Research in Engineering Design*

to link FM → margin value analysis[2]

conceptual design



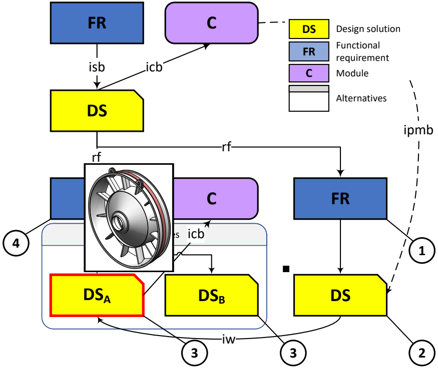
preliminary design



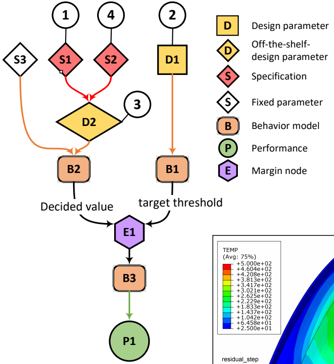
[1] N. Ahmad et al., 2013 , *Research in Engineering Design*
[2] A. Brahma and D. C. Wynn, 2020 , *Research in Engineering Design*

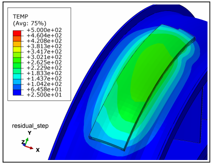
different concepts have different preliminary designs

conceptual design



preliminary design



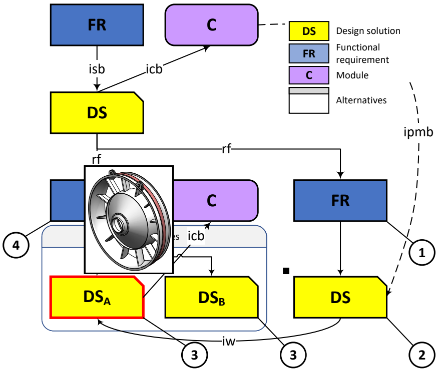


[1] N. Ahmad et al., 2013 , *Research in Engineering Design*
[2] A. Brahma and D. C. Wynn, 2020 , *Research in Engineering Design*

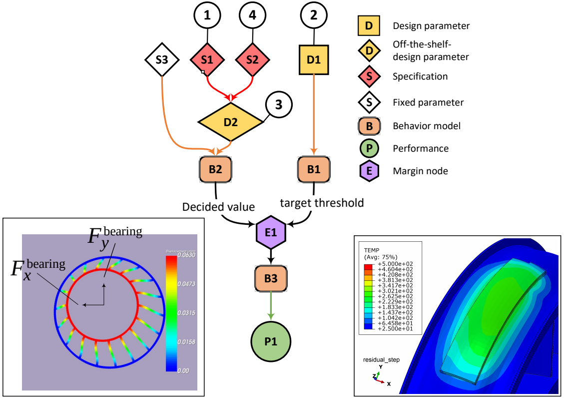
Design space exploration at the conceptual level

different concepts have different preliminary designs

conceptual design



preliminary design



[1] N. Ahmad et al., 2013 , *Research in Engineering Design*
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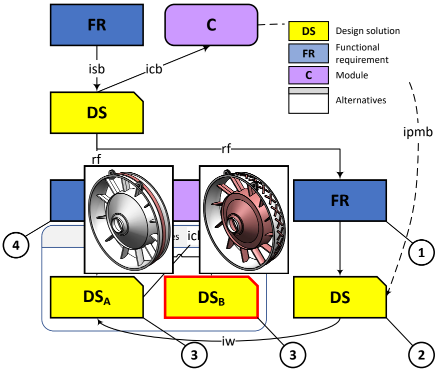
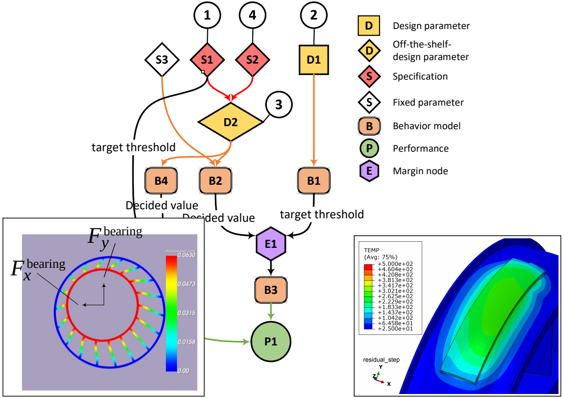
different concepts have different preliminary designs

conceptual design



preliminary design



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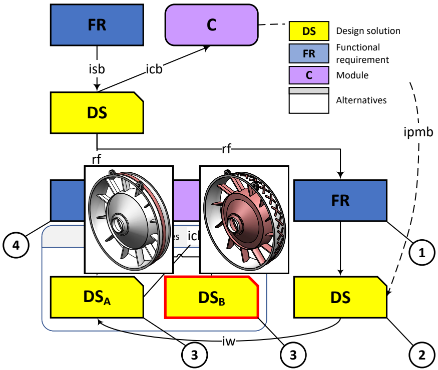
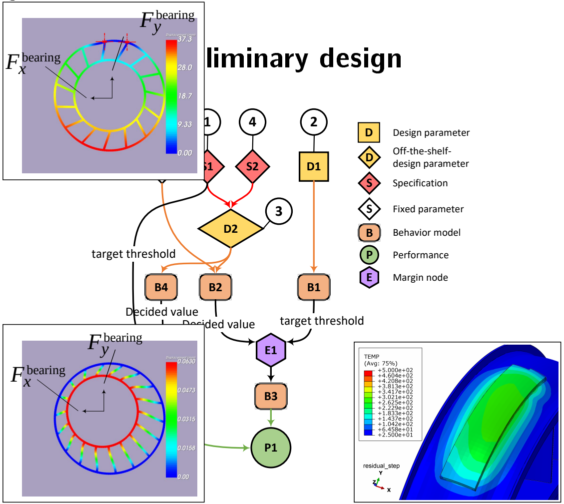
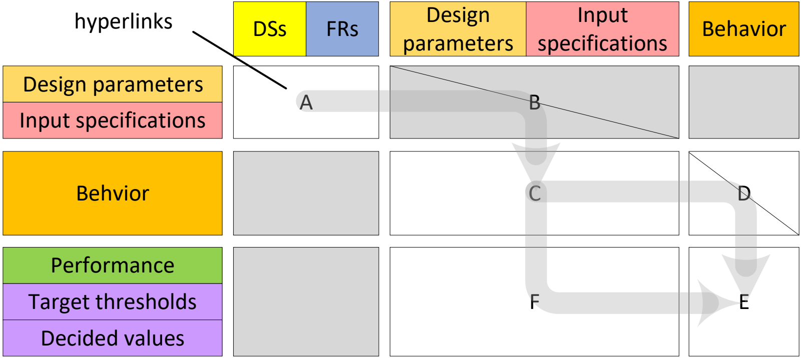


preliminary design



[1] N. Ahmad et al., 2013 , *Research in Engineering Design*
[2] A. Brahma and D. C. Wynn, 2020 , *Research in Engineering Design*

Multi-domain modelling (MDM) matrix for change propagation management can be used to represent hyperlinks [1]



[1] E. C.Y. Koh et al., 2012 , *Research in Engineering Design*

Overview of turbine rear frame design

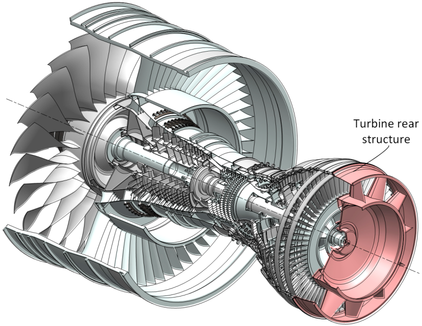
The turbine rear structure (TRS) sits aft of the turbine

Design parameters:

Input Specifications:

Design margins:

Performance parameters:



Trent 900 aeroengine

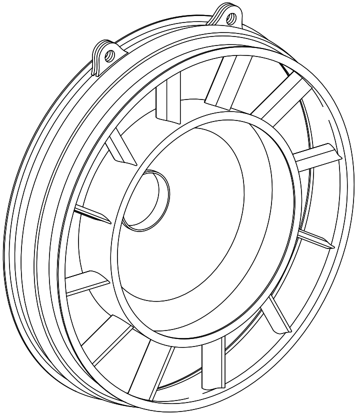
The turbine rear structure (TRS) sits aft of the turbine

Design parameters:

Input Specifications:

Design margins:

Performance parameters:



Turbine rear structure

Overview of turbine rear frame design

We consider the design of a single strut

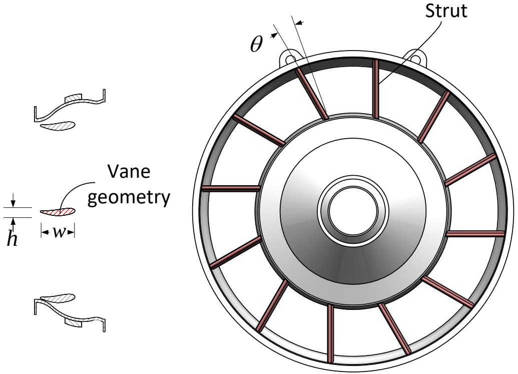
Design parameters:

- vane width w
- vane height h
- lean angle θ
- Material - yield stress σ_y (off-the shelf)

Input Specifications:

Design margins:

Performance parameters:



Turbine rear structure: cross-sectional view

Overview of turbine rear frame design

Variable thermal loads are expected

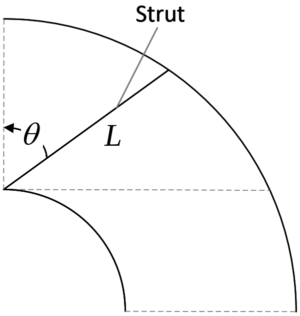
Design parameters:

- vane width w
- vane height h
- lean angle θ
- Material - yield stress σ_y (off-the shelf)

Input Specifications:

Design margins:

Performance parameters:



Thermal expansion

Overview of turbine rear frame design

Which cause thermal expansion

Design parameters:

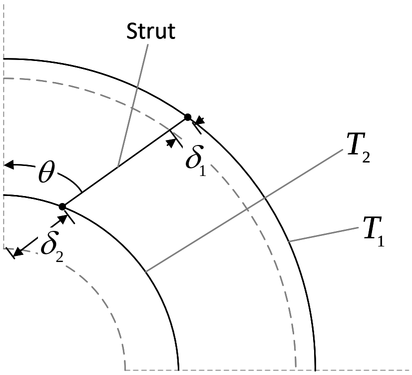
- vane width w
- vane height h
- lean angle θ
- Material - yield stress σ_y (off-the shelf)

Input Specifications:

- Nacelle temperature T_1 ($\downarrow$)
- Gas surface temperature T_2 ($\uparrow$)

Design margins:

Performance parameters:



Thermal expansion

Overview of turbine rear frame design

Which cause thermal expansion and stress on the strut

Design parameters:

- vane width w
- vane height h
- lean angle θ
- Material - yield stress σ_y (off-the shelf)

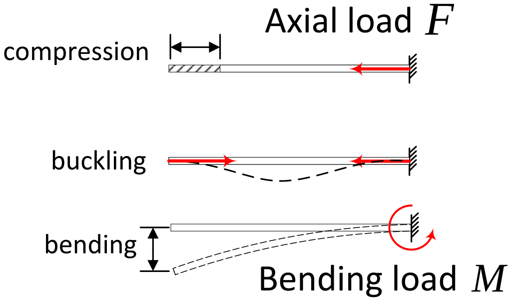
Input Specifications:

- Nacelle temperature T_1 ($\downarrow$)
- Gas surface temperature T_2 ($\uparrow$)

Design margins:

- compression $\sigma_y - \sigma_a \geq 0$
- bending $\sigma_y - \sigma_m \geq 0$
- buckling $F_{\text{buckling}} - F_a \geq 0$

Performance parameters:



Load cases

Which cause thermal expansion and stress on the strut

Design parameters:

- vane width w
- vane height h
- lean angle θ
- Material - yield stress σ_y (off-the shelf)

Input Specifications:

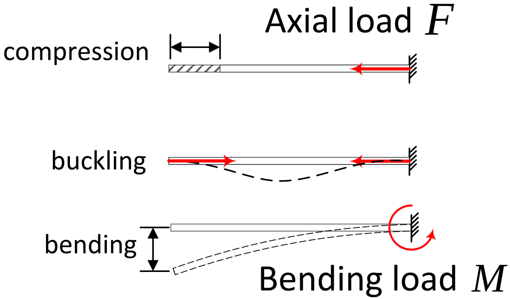
- Nacelle temperature T_1 ($\downarrow$)
- Gas surface temperature T_2 ($\uparrow$)

Design margins:

- compression $\sigma_y - \sigma_a \geq 0$
- bending $\sigma_y - \sigma_m \geq 0$
- buckling $F_{\text{buckling}} - F_a \geq 0$

Performance parameters:

- Weight



Load cases

Overview of turbine rear frame design

The entire problem can be represented compactly as an MDM

Design parameters:

- $D1$ vane width w
- $D2$ vane height h
- $D3$ lean angle θ
- $D4$ Material - yield stress σ_y (off-the shelf)

Input Specifications:

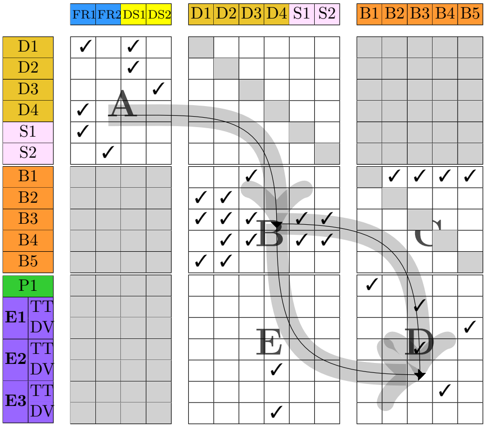
- $S1$ Nacelle temperature T_1 (↓)
- $S2$ Gas surface temperature T_2 (↑)

Design margins:

- $E1$ compression $\sigma_y - \sigma_a \geq 0$
- $E2$ bending $\sigma_y - \sigma_m \geq 0$
- $E3$ buckling $F_{\text{buckling}} - F_a \geq 0$

Performance parameters:

- $P1$ Weight



Calculating impact of excess margin on performance

Need to construct a response surface

Design parameters:

- vane width w
- vane height h
- lean angle θ
- Material - yield stress σ_y (off-the shelf)

Input Specifications:

- Nacelle temperature T_1 ($\downarrow$)
- Gas surface temperature T_2 ($\uparrow$)

Design margins:

- compression $\sigma_y - \sigma_a \geq 0$
- bending $\sigma_y - \sigma_m \geq 0$
- buckling $F_{\text{buckling}} - F_a \geq 0$

Performance parameters:

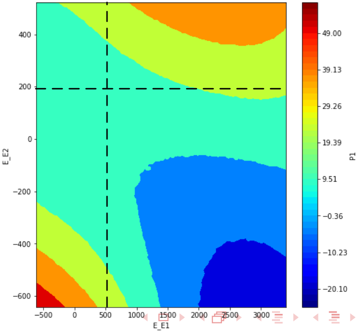
- Weight

Need to find a function f that translates excess to performance

$$\hat{\mathbf{p}} = f(\mathbf{e})$$

$$\mathbf{p} = [p_1, p_2, \cdots, p_j]^T$$

$$\mathbf{e} = [e_1, e_2, \cdots, e_m]^T$$



Calculating impact of excess margin on performance

Need to construct a response surface

Design parameters:

- vane width w
- vane height h
- lean angle θ
- Material - yield stress σ_y (off-the shelf)

Input Specifications:

- Nacelle temperature T_1 ($\downarrow$)
- Gas surface temperature T_2 ($\uparrow$)

Design margins:

- compression $\sigma_y - \sigma_a \geq 0$
- bending $\sigma_y - \sigma_m \geq 0$
- buckling $F_{\text{buckling}} - F_a \geq 0$

Performance parameters:

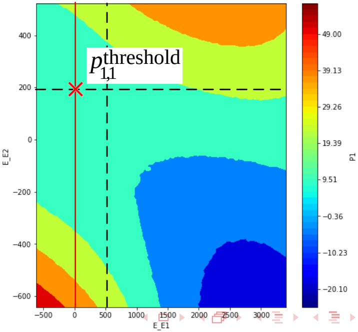
- Weight

Need to find a function f that translates excess to performance

$$\hat{\mathbf{p}} = f(\mathbf{e})$$

$$\mathbf{p}_1^{\text{threshold}} = [p_1, p_2, \cdots, p_j]^T$$

$$\mathbf{e} = [0, e_2, \cdots, e_m]^T$$



Calculating impact of excess margin on performance

Need to construct a response surface

Design parameters:

- vane width w
- vane height h
- lean angle θ
- Material - yield stress σ_y (off-the shelf)

Input Specifications:

- Nacelle temperature T_1 (↓)
- Gas surface temperature T_2 (↑)

Design margins:

- compression $\sigma_y - \sigma_a \geq 0$
- bending $\sigma_y - \sigma_m \geq 0$
- buckling $F_{\text{buckling}} - F_a \geq 0$

Performance parameters:

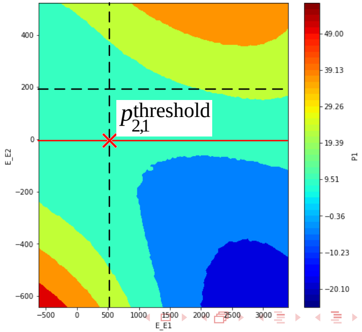
- Weight

Need to find a function f that translates excess to performance

$$\hat{\mathbf{p}} = f(\mathbf{e})$$

$$\mathbf{p}_2^{\text{threshold}} = [p_1, p_2, \cdots, p_j]^T$$

$$\mathbf{e} = [e_1, 0, \cdots, e_m]^T$$



Calculating impact of excess margin on performance

Need to construct a response surface

Design parameters:

- vane width w
- vane height h
- lean angle θ
- Material - yield stress σ_y (off-the shelf)

Input Specifications:

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- Gas surface temperature T_2 ($\uparrow$)

Design margins:

- compression $\sigma_y - \sigma_a \geq 0$
- bending $\sigma_y - \sigma_m \geq 0$
- buckling $F_{\text{buckling}} - F_a \geq 0$

Performance parameters:

- Weight

Need to find a function f that translates excess to performance

$$\text{Impact} = \begin{array}{c c} & \text{weight} \\ \begin{array}{c} \text{buckling} \\ \text{compression} \\ \text{bending} \end{array} & \begin{bmatrix} 0.545 \\ 0.111 \\ -1.011 \end{bmatrix} \end{array}$$

Calculating deterioration (allowable change in specifications)

We calculate the maximum allowable deterioration in the specifications

Design parameters:

- vane width w
- vane height h
- lean angle θ
- Material - yield stress σ_y (off-the shelf)

Input Specifications:

- Nacelle temperature T_1 ($\uparrow$)
- Gas surface temperature T_2 ($\downarrow$)

Design margins:

- compression $\sigma_y - \sigma_a \geq 0$
- bending $\sigma_y - \sigma_m \geq 0$
- buckling $F_{\text{buckling}} - F_a \geq 0$

Performance parameters:

- Weight

Gradually change each input specifications until any margin is consumed

$$\mathbf{s} = \begin{array}{c} T_1 \\ T_2 \end{array} \begin{bmatrix} 450 \\ 425 \end{bmatrix}$$

$$\mathbf{e} = \begin{array}{c} \text{buckling} \\ \text{compression} \\ \text{bending} \end{array} \begin{bmatrix} 597.440 \\ 72.6904696 \\ 451.9918707 \end{bmatrix}$$

Calculating deterioration (allowable change in specifications)

We calculate the maximum allowable deterioration in the specifications

Design parameters:

- vane width w
- vane height h
- lean angle θ
- Material - yield stress σ_y (off-the shelf)

Input Specifications:

- Nacelle temperature T_1 ($\uparrow$)
- Gas surface temperature T_2 ($\downarrow$)

Design margins:

- compression $\sigma_y - \sigma_a \geq 0$
- bending $\sigma_y - \sigma_m \geq 0$
- buckling $F_{\text{buckling}} - F_a \geq 0$

Performance parameters:

- Weight

Gradually change each input specifications until any margin is consumed

$$\mathbf{s} = \begin{array}{c} T_1\uparrow \\ T_2 \end{array} \begin{bmatrix} 454.5 \\ 425 \end{bmatrix}$$

$$\mathbf{e} = \begin{array}{c} \text{buckling} \\ \text{compression} \\ \text{bending} \end{array} \begin{bmatrix} 488.404 \\ 0 \\ 450.4889005 \end{bmatrix}$$

Calculating deterioration (allowable change in specifications)

We calculate the maximum allowable deterioration in the specifications

Design parameters:

- vane width w
- vane height h
- lean angle θ
- Material - yield stress σ_y (off-the shelf)

Input Specifications:

- Nacelle temperature T_1 ($\uparrow$)
- Gas surface temperature T_2 ($\downarrow$)

Design margins:

- compression $\sigma_y - \sigma_a \geq 0$
- bending $\sigma_y - \sigma_m \geq 0$
- buckling $F_{\text{buckling}} - F_a \geq 0$

Performance parameters:

- Weight

Gradually change each input specifications until any margin is consumed

$$\mathbf{s} = \begin{array}{c} T_1 \\ T_2\downarrow \end{array} \begin{bmatrix} 450 \\ 420.75 \end{bmatrix}$$

$$\mathbf{e} = \begin{array}{c} \text{buckling} \\ \text{compression} \\ \text{bending} \end{array} \begin{bmatrix} 488.404 \\ 0 \\ 450.4889005 \end{bmatrix}$$

Calculating deterioration (allowable change in specifications)

We calculate the maximum allowable deterioration in the specifications

Design parameters:

- vane width w
- vane height h
- lean angle θ
- Material - yield stress σ_y (off-the shelf)

Input Specifications:

- Nacelle temperature T_1 ($\uparrow$)
- Gas surface temperature T_2 ($\downarrow$)

Design margins:

- compression $\sigma_y - \sigma_a \geq 0$
- bending $\sigma_y - \sigma_m \geq 0$
- buckling $F_{\text{buckling}} - F_a \geq 0$

Performance parameters:

- Weight

Gradually change each input specifications until any margin is consumed

$$\mathbf{s}^{\max} = \begin{array}{c} T_1\uparrow \\ T_2\downarrow \end{array} \begin{bmatrix} 454.5 \\ 420.75 \end{bmatrix}$$

Calculating deterioration (allowable change in specifications)

We calculate the maximum allowable deterioration in the specifications

Design parameters:

- vane width w
- vane height h
- lean angle θ
- Material - yield stress σ_y (off-the shelf)

Input Specifications:

- Nacelle temperature T_1 ($\uparrow$)
- Gas surface temperature T_2 ($\downarrow$)

Design margins:

- compression $\sigma_y - \sigma_a \geq 0$
- bending $\sigma_y - \sigma_m \geq 0$
- buckling $F_{\text{buckling}} - F_a \geq 0$

Performance parameters:

- Weight

Gradually change each input specifications until any margin is consumed

$$\text{deterioration} = \begin{array}{c} T_1 \\ T_2 \end{array} \begin{bmatrix} 0.01 \\ 0.01 \end{bmatrix}$$

We calculate the change absorption capability as a function of deterioration

Design parameters:

- vane width w
- vane height h
- lean angle θ
- Material - yield stress σ_y (off-the shelf)

Input Specifications:

- Nacelle temperature T_1 ($\downarrow$)
- Gas surface temperature T_2 ($\uparrow$)

Design margins:

- compression $\sigma_y - \sigma_a \geq 0$
- bending $\sigma_y - \sigma_m \geq 0$
- buckling $F_{\text{buckling}} - F_a \geq 0$

Performance parameters:

- Weight

Change absorption is calculated using the following equation:

$$\text{absorption}_{mi} = \frac{t_{mi}^{\text{new}} - t_{mi}^{\text{nominal}}}{t_{mi}^{\text{nominal}} \times \text{deterioration}_i}$$

for each margin node m and specification i

$$\text{absorption} = \begin{array}{r c} & \begin{array}{cc} T_1 & T_2 \end{array} \\ \begin{array}{r} \text{buckling} \\ \text{compression} \\ \text{bending} \end{array} & \begin{bmatrix} 2.79 & 3.87 \\ 1.98 & 3.04 \\ 2.58 & 3.66 \end{bmatrix} \end{array}$$

Constructing the margin value plot (MVP)

Using "impact" and "absorption" we can construct a tradespace (MVP)

Design parameters:

- vane width
- vane height
- lean angle
- Material - yield stress σ_y (off-the shelf)

Input Specifications:

- Nacelle temperature T_1 ($\downarrow$)
- Gas surface temperature T_2 ($\uparrow$)

Design margins:

- compression $\sigma_y - \sigma_a \geq 0$
- bending $\sigma_y - \sigma_m \geq 0$
- buckling $F_{\text{buckling}} - F_a \geq 0$

Performance parameters:

- Weight

$$\text{Impact} = \begin{array}{r} \\ \text{buckling} \\ \text{compression} \\ \text{bending} \end{array} \begin{array}{c} \text{weight} \\ \begin{bmatrix} 0.545 \\ 0.111 \\ -1.011 \end{bmatrix} \end{array}$$

$$\text{absorption} = \begin{array}{r} \\ \text{buckling} \\ \text{compression} \\ \text{bending} \end{array} \begin{array}{c} \begin{array}{cc} T_1 & T_2 \end{array} \\ \begin{bmatrix} 2.79 & 3.87 \\ 1.98 & 3.04 \\ 2.58 & 3.66 \end{bmatrix} \end{array}$$

Constructing the margin value plot (MVP)

Using "impact" and "absorption" we can construct a tradespace (MVP)

Design parameters:

- vane width
- vane height
- lean angle
- Material - yield stress σ_y (off-the shelf)

Input Specifications:

- Nacelle temperature T_1 ($\downarrow$)
- Gas surface temperature T_2 ($\uparrow$)

Design margins:

- compression $\sigma_y - \sigma_a \geq 0$
- bending $\sigma_y - \sigma_m \geq 0$
- buckling $F_{\text{buckling}} - F_a \geq 0$

Performance parameters:

- Weight

We aggregate across each performance and specification

$$\text{Impact} = \begin{array}{c} \text{buckling} \\ \text{compression} \\ \text{bending} \end{array} \begin{bmatrix} 0.545 \\ 0.111 \\ -1.011 \end{bmatrix}$$

$$\text{absorption} = \begin{array}{c} \text{buckling} \\ \text{compression} \\ \text{bending} \end{array} \begin{bmatrix} 3.33 \\ 2.51 \\ 3.12 \end{bmatrix}$$

Using "impact" and "absorption" we can construct a tradespace (MVP)

Design parameters:

- vane width $w = 6.78$
- vane height $h = 125.60$
- lean angle $\theta = 14.6$
- Material - yield stress σ_y (off-the shelf)

Input Specifications:

- Nacelle temperature T_1 ($\downarrow$)
- Gas surface temperature T_2 ($\uparrow$)

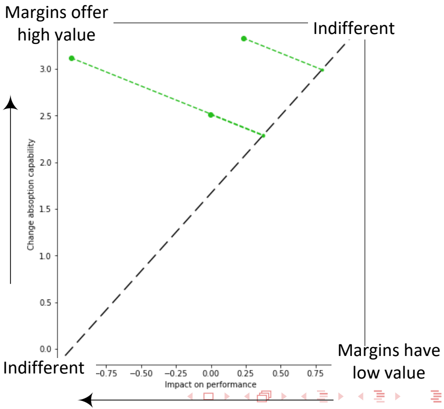
Design margins:

- compression $\sigma_y - \sigma_a \geq 0$
- bending $\sigma_y - \sigma_m \geq 0$
- buckling $F_{\text{buckling}} - F_a \geq 0$

Performance parameters:

- Weight

Design A: $d = 2.70$



Constructing the margin value plot (MVP)

Using "impact" and "absorption" we can construct a tradespace (MVP)

Design A: $d = 2.70$

Design B: $d = 3.13$

Design parameters:

- vane width $w = 11.5$
- vane height $h = 113.33$
- lean angle $\theta = 18.0$
- Material - yield stress σ_y (off-the shelf)

Input Specifications:

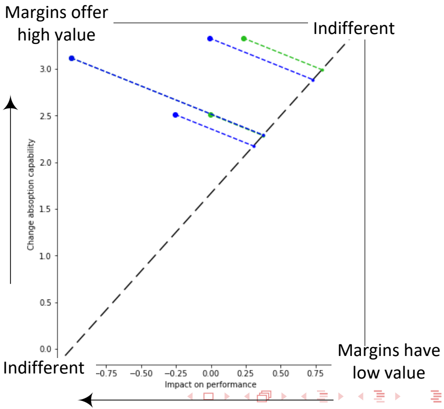
- Nacelle temperature T_1 ($\downarrow$)
- Gas surface temperature T_2 ($\uparrow$)

Design margins:

- compression $\sigma_y - \sigma_a \geq 0$
- bending $\sigma_y - \sigma_m \geq 0$
- buckling $F_{\text{buckling}} - F_a \geq 0$

Performance parameters:

- Weight



Constructing the margin value plot (MVP)

Using "impact" and "absorption" we can construct a tradespace (MVP)

Design parameters:

- vane width $w = 5.42$
- vane height $h = 106.14$
- lean angle $\theta = 15.7$
- Material - yield stress σ_y (off-the shelf)

Input Specifications:

- Nacelle temperature T_1 ($\downarrow$)
- Gas surface temperature T_2 ($\uparrow$)

Design margins:

- compression $\sigma_y - \sigma_a \geq 0$
- bending $\sigma_y - \sigma_m \geq 0$
- buckling $F_{\text{buckling}} - F_a \geq 0$

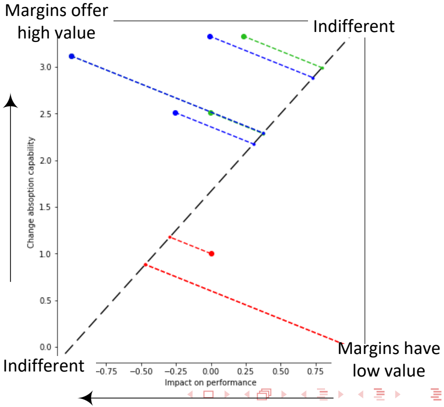
Performance parameters:

- Weight

Design A: $d = 2.70$

Design B: $d = 3.13$

Design C: $d = -3.77$



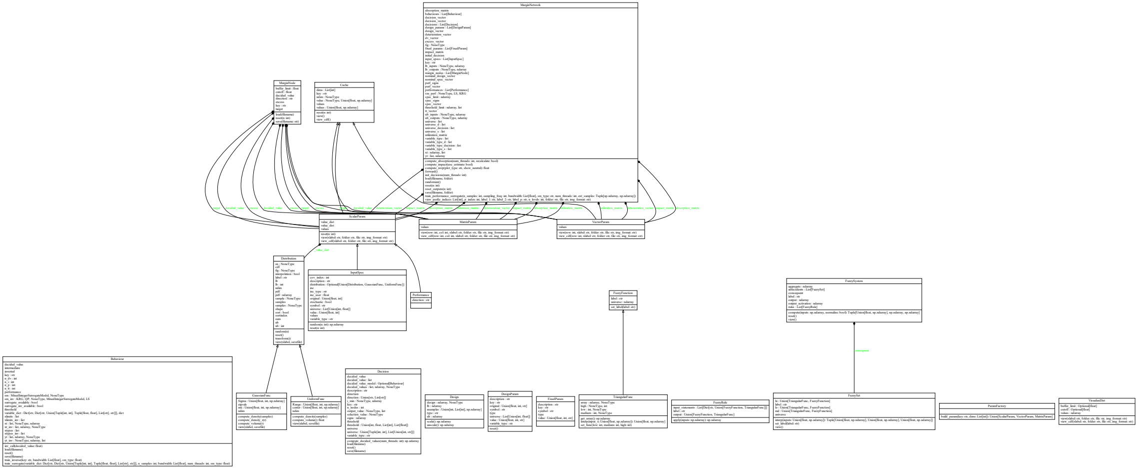
Pseudo-code of MVM

Input: set of possible choices $\mathcal{D}$, chosen design $\mathrm{c} \in \mathcal{D}$, the MAN given by analytic functions, models, and surrogates, n_{samples}, Joint PDF $F_{\mathrm{S}}(\mathrm{s})$

Output: estimated mean impact and change absorption $\bar{\bar{\mathrm{a}}}$, $\bar{\bar{\mathrm{i}}}$

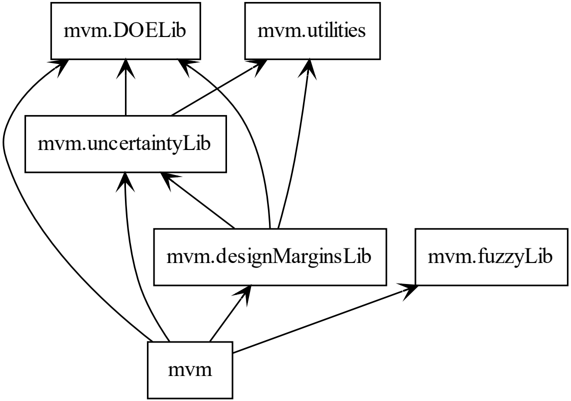
```
[0] Initialization: set counter i_sample ← 0, initialize aggregate absorption and impact ā̄ ∈ ℝ^e and ī̄ ∈ ℝ^e
[1] Monte-carlo simulation: draw sample input specifications S ∈ ℝ^n ~ F_S(s)
[2] Calculate threshold, decided, excess, and performance values: t = f(S, c), d = g(c), e = (t − d) i^{excess T}, p = h(S, c)
[3] Calculate allowable deterioration
    loop over input specifications for k = 1, 2, ..., n do
        perform a line search along the kth direction to identify the root of: min((f(x, c) − d) i^{excess T}) = 0, s'_k ← x*, s_k^limit ← s'_k
[4] Calculate margin value metrics
    initialization tensors and vectors, I ∈ ℝ^{m×e} ← 0 and A ∈ ℝ^{n×e} ← 0, v ∈ ℝ^n ← 0, ā ∈ ℝ^e ← 0, and ī ∈ ℝ^e ← 0
    loop over margin nodes for i = 1, 2, ..., e do
        [a] Calculate impact on performance
        d^threshold ← d, d_i^threshold ← t_i, c_i^threshold = g^{-1}(d^threshold), p_i^threshold = h(S, c_i^threshold)
        loop over performance parameters for j = 1, 2, ..., m do
            i_{i,j} ← (p_j − p_{j,i}^threshold) i_j^p / p_{j,i}^threshold
        [b] Calculate change absorption capability
        loop over input specifications for k = 1, 2, ..., n do
            calculate deterioration v_k = (s_k^limit − s_k)/s_k
            a_{i,k} ← (f_i(s_k^limit, c) − f_i(S, c))/(f_i(S, c) v_k)
        [c] Aggregate metrics: ā_i ← (1/n) Σ_{k=1}^{n} a_{i,k}, ī_i ← (1/m) Σ_{k=1}^{m} i_{i,j}
[5] sum of monte-carlo samples: ā̄ ← ā̄ + ā, ī̄ ← ī̄ + ī
[6] Termination, if i_sample < n_samples then
    set i_sample ← i_sample + 1, go to [1]
    otherwise ā̄ ← ā̄/n_samples and ī̄ ← ī̄/n_samples, stop
```

UML diagram of mvmlib[1]



[1] Khalil Al Handawi, 2022 , *https://github.com/sed-group/mvmlib*

UML diagram of `mvmlib`[1]



[1] Khalil Al Handawi, 2022, https://github.com/sed-group/mvmlib

Thank you for your time

Overview of mesh adaptive direct search

No gradient information available, blackbox is expensive[1]

Objective and constraints

$$
\begin{array}{ll}
\min\limits_{x} & f(x) \\
\text{subject to} & c(x) \leq 0 \\
\text{where} & x: \ \text{variables}
\end{array}
$$

- SEARCH step and POLL step

[1] C. Audet and W. Hare, 2017 , *Derivative-Free and Blackbox Optimization*

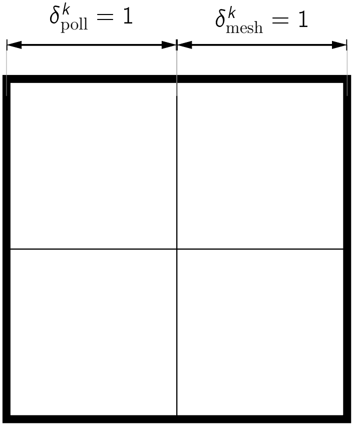
Overview of mesh adaptive direct search

No gradient information available, blackbox is expensive[1]

Objective and constraints

$$\begin{aligned} \min_{x} \quad & f(x) \\ \text{subject to} \quad & c(x) \leq 0 \\ \text{where} \quad & x: \ \text{variables} \end{aligned}$$

- SEARCH step and POLL step
- we focus on the POLL step



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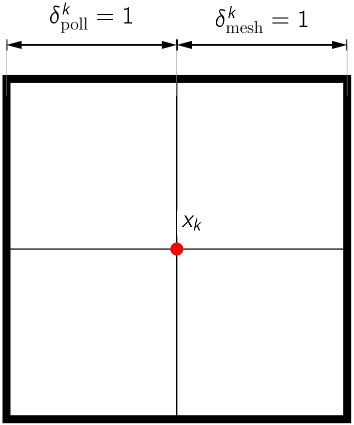
- SEARCH step and POLL step
- we focus on the POLL step
- incumbent solution: x_k



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Overview of mesh adaptive direct search

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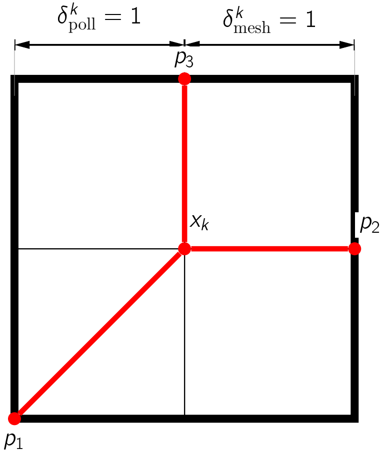
Objective and constraints

$$\begin{array}{lll} \min\limits_{x} & f(x) & \\ \text{subject to} & c(x) \leq 0 & \\ \text{where} & x: & \text{variables} \end{array}$$

- SEARCH step and POLL step
- we focus on the POLL step
- incumbent solution: x_k
- trail points: $\{p_1, p_2, \cdots, p_k\}$



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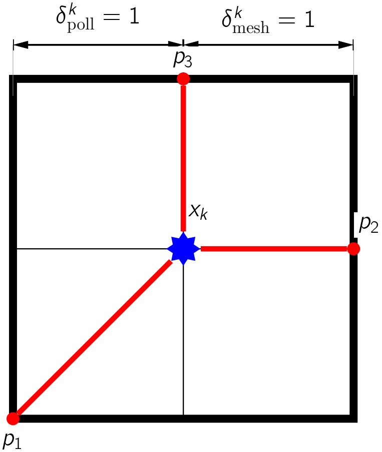
Objective and constraints

$$\begin{aligned} \min_{x} \quad & f(x) \\ \text{subject to} \quad & c(x) \le 0 \\ \text{where} \quad & x: \text{ variables} \end{aligned}$$

- SEARCH step and POLL step
- we focus on the POLL step
- incumbent solution: x_k
- trail points: $\{p_1, p_2, \cdots, p_k\}$

Poll **failure**



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Objective and constraints

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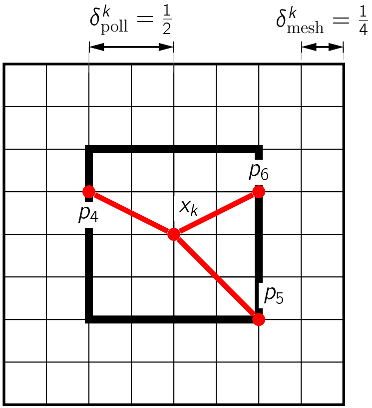
- SEARCH step and POLL step
- we focus on the POLL step
- incumbent solution: x_k
- trail points: $\{p_1, p_2, \cdots, p_k\}$



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Objective and constraints

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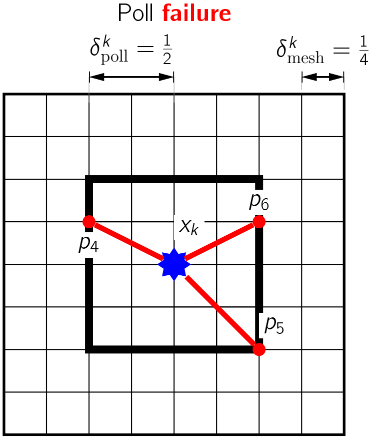
- SEARCH step and POLL step
- we focus on the POLL step
- incumbent solution: x_k
- trail points: $\{p_1, p_2, \cdots, p_k\}$



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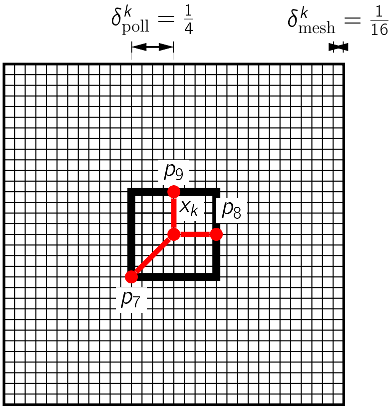

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Objective and constraints

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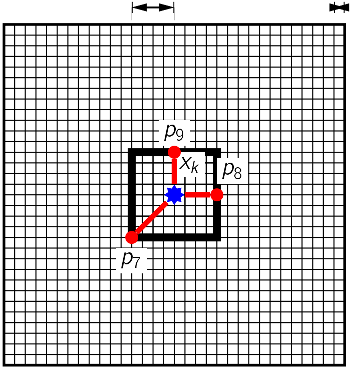
- SEARCH step and POLL step
- we focus on the POLL step
- incumbent solution: x_k
- trail points: $\{p_1, p_2, \cdots, p_k\}$

Poll **failure**

$\delta^k_{\text{poll}} = \frac{1}{4}$ $\delta^k_{\text{mesh}} = \frac{1}{16}$



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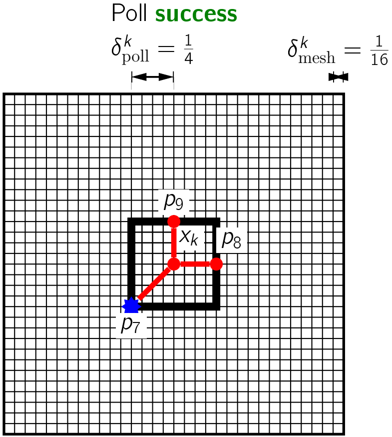
Overview of mesh adaptive direct search

No gradient information available, blackbox is expensive[1]

Objective and constraints

$$\begin{array}{ll} \min_{x} & f(x) \\ \text{subject to} & c(x) \leq 0 \\ \text{where} & x: \ \text{variables} \end{array}$$

- SEARCH step and POLL step
- we focus on the POLL step
- incumbent solution: x_k
- trail points: $\{p_1, p_2, \cdots, p_k\}$
- successful trail point p_7



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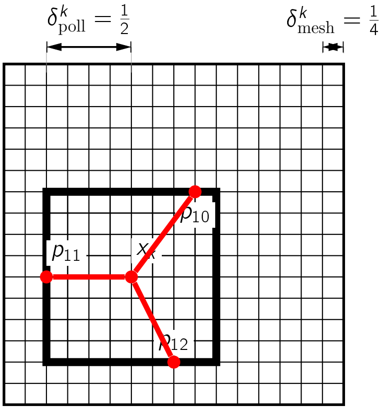
No gradient information available, blackbox is expensive[1]

Objective and constraints

$$\begin{array}{ll} \min_{x} & f(x) \\ \text{subject to} & c(x) \leq 0 \\ \text{where} & x: \text{ variables} \end{array}$$

- SEARCH step and POLL step
- we focus on the POLL step
- incumbent solution: x_k
- trail points: $\{p_1, p_2, \cdots, p_k\}$
- successful trail point p_7



[1] C. Audet and W. Hare, 2017 , *Derivative-Free and Blackbox Optimization*

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$$\begin{array}{ll} \min_{x} & f(x) \\ \text{subject to} & c(x) \leq 0 \\ \text{where} & x: \ \text{variables} \end{array}$$

- SEARCH step and POLL step
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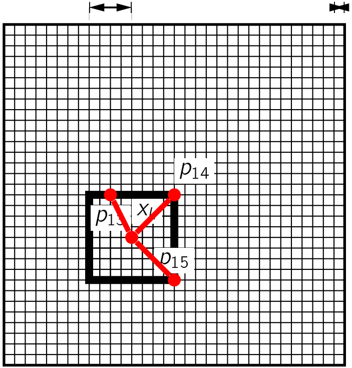
Poll **failure**

$\delta^k_{\text{poll}} = \frac{1}{4}$ $\delta^k_{\text{mesh}} = \frac{1}{16}$



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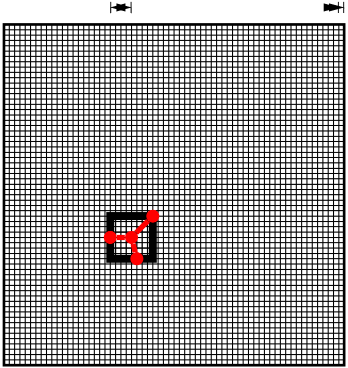
Poll **failure**

$\delta^k_{\text{poll}} = \frac{1}{8}$ $\delta^k_{\text{mesh}} = \frac{1}{64}$



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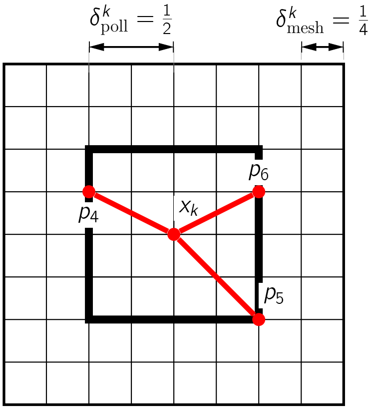

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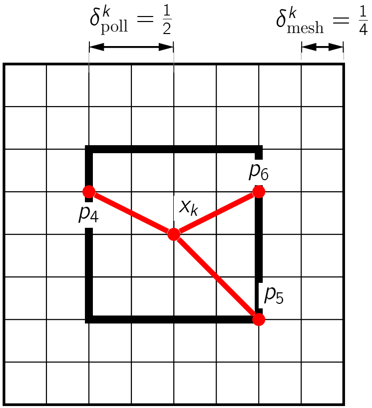

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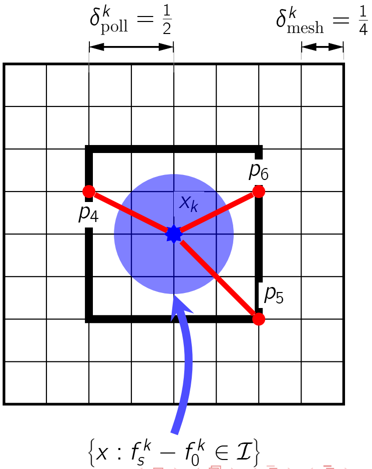
Poll **certain failure**



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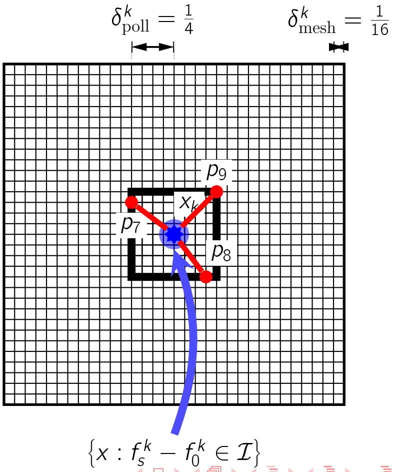

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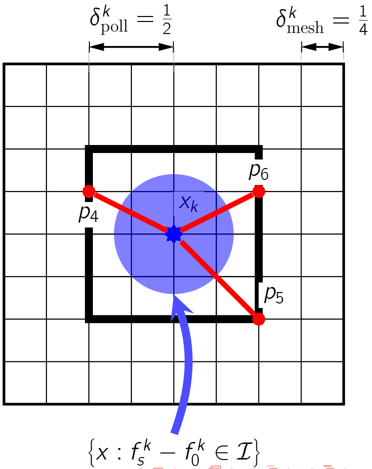

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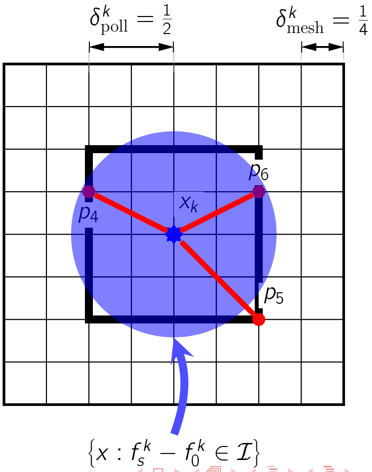

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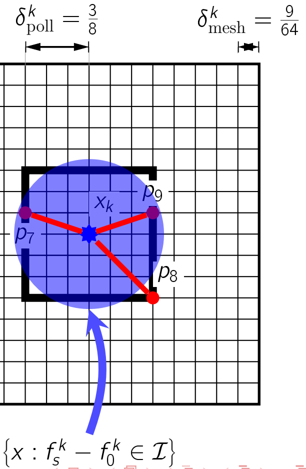

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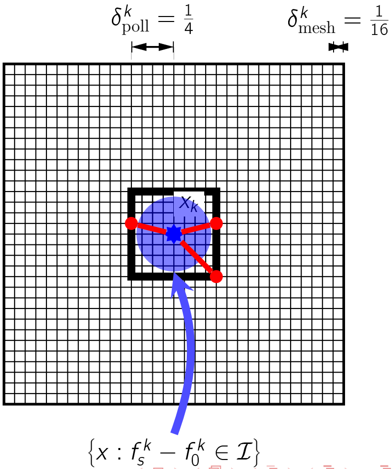

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Constraint handling using the *progressive barrier* approach [2]

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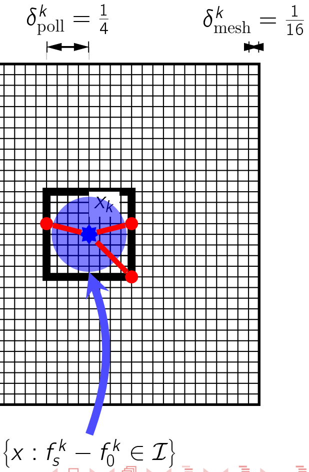


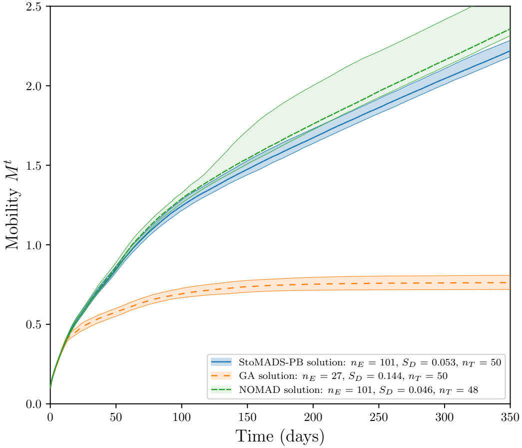
[1] C. Audet et al., 2021 , *Computational Optimization and Applications*
[2] K. J. Dzahini et al., 2022 , *Mathematical Programming*

Conclusion

Formulated and solved public health policy-making problems

- Identified a public health policy that favored

best known solution



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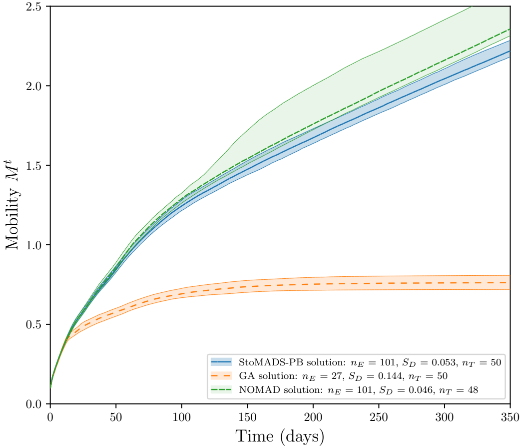

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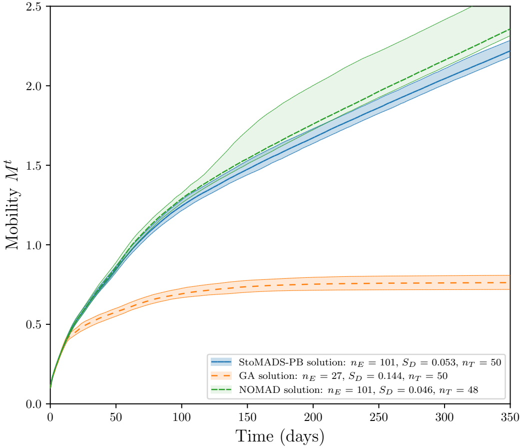

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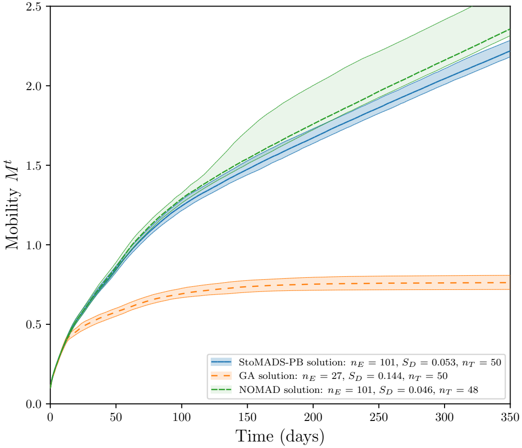

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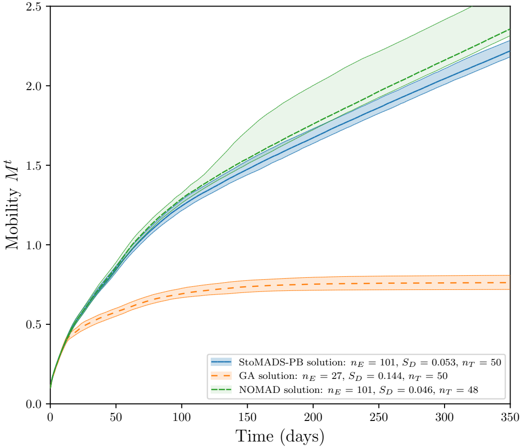

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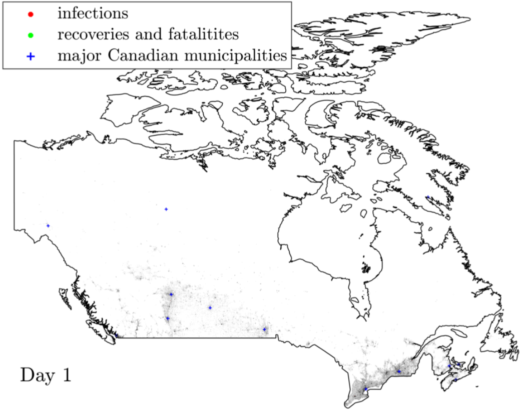

[1] N. Ferguson et al., 2020 , *Imperial College COVID-19 Response Team*

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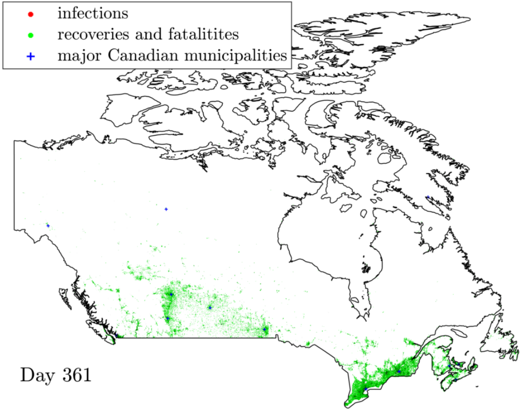

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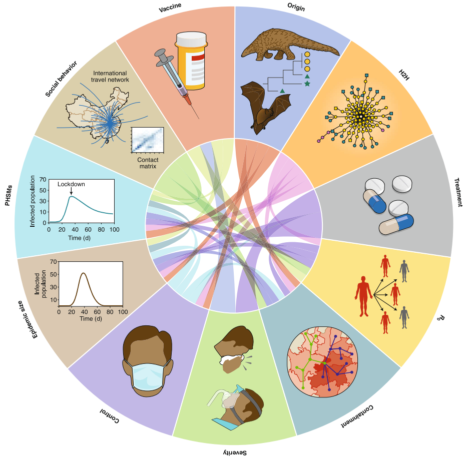

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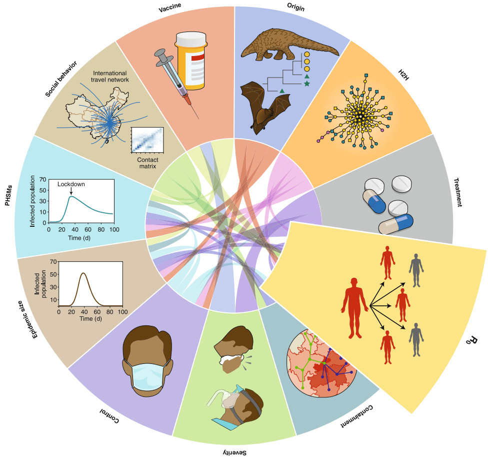

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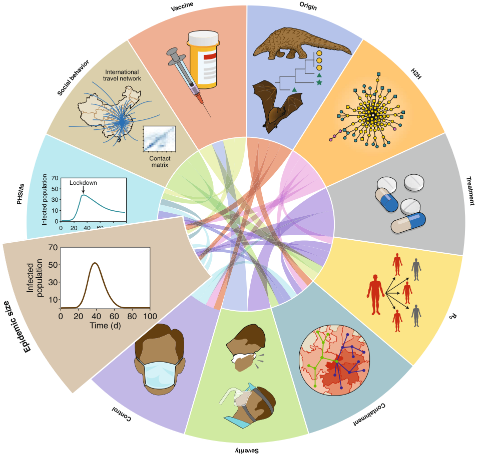

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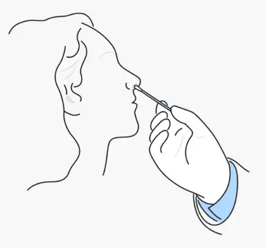

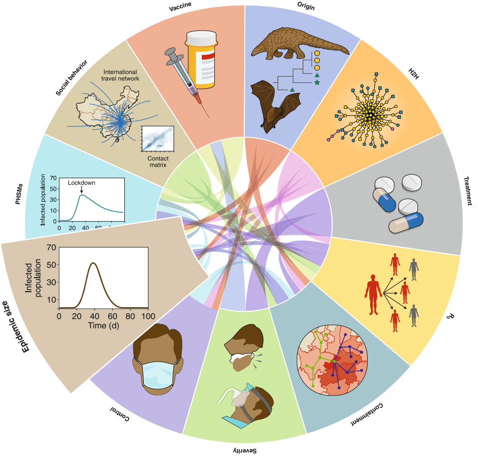

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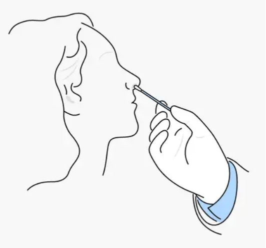

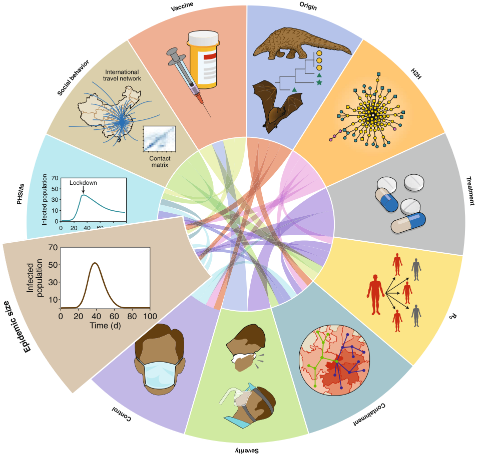

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Conclusion and future directions

Model discovery and development facilitated by hyperparameter optimization

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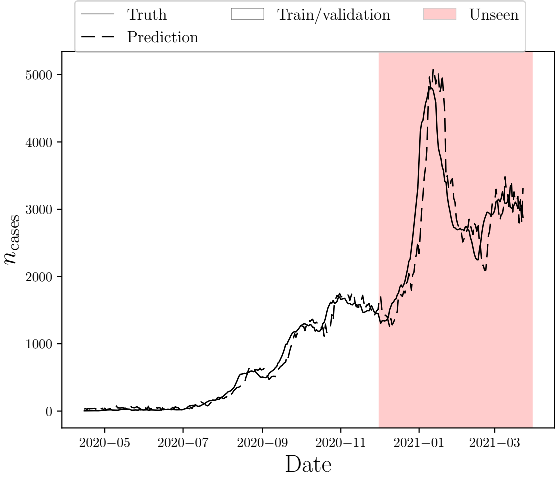

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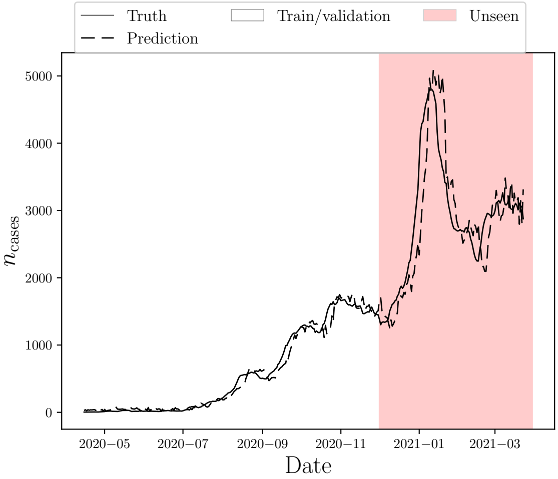

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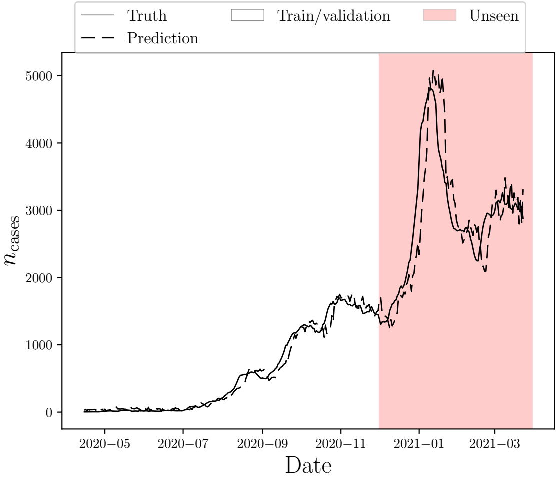
- Simpler models perform well when historical data is limited
- Works well on other datasets[1]



[1] J. A. Hay et al., 2021 , *Science*

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

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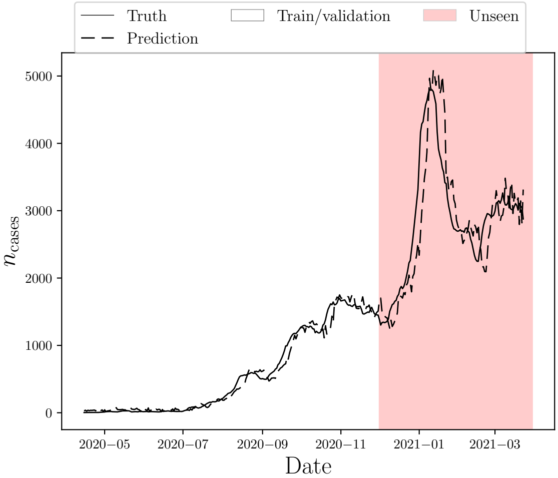

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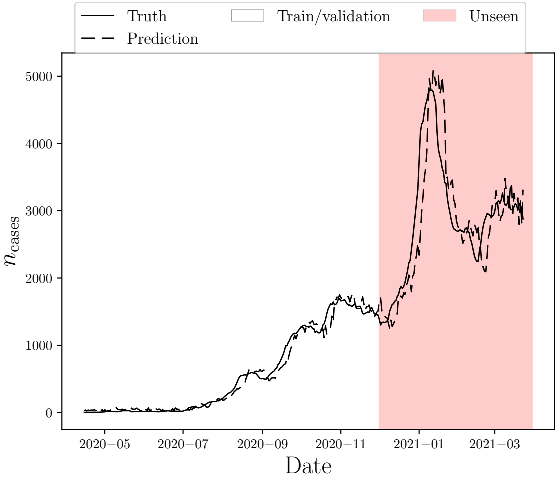

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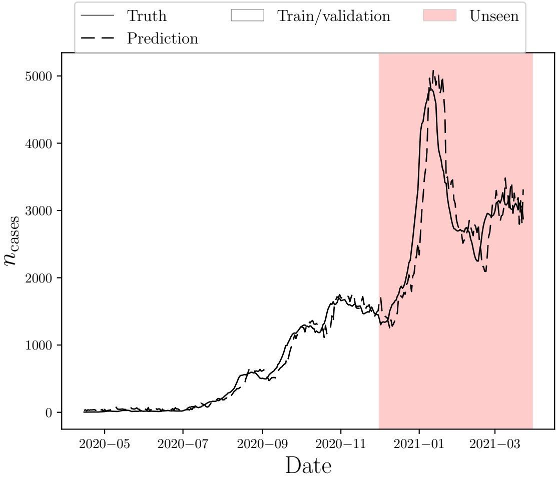

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