Encoding ML Models

Encoding ML Models

We need to embed our ML model into an optimization model

The basic approach is based on two observations:

- A neural network is a collection of connected neurons
- So we just need to encode each neuron using a given optimization method

Let's consider for example a ReLU neuron

This corresponds to the relation:

$$y = \max\left(0, w^T x + \theta\right)$$

Where w is the (row) vector of weights and b is the bias. It can be encoded by:

- Introducing a variable for each input
- Introducing a variable for the output
- Modeling (e.g. in MILP, or SMT, or CP) the sum and max operators

Encoding ML Models

The type of encoding depends on the considered optimization technology

- In CP, we may have a global constraint per neuron or for a the whole network
- In SMT, we could use ITE (If Then Else) predicates to model the max
- In MILP, we would use linear constraints and both numeric/integer variables

In this case, we will adopt a MILP encoding

The relation $y = max(0, wx + \theta)$ can be translated to:

$$\begin{aligned}
&y - s = wx + \theta \\
&z = 1 \Rightarrow s \leq 0 \\
&z = 0 \Rightarrow y \leq 0 \\
&y, s \geq 0, x \in \mathbb{R}^n, z \in \{0, 1\}
\end{aligned}$$

Encoding ML Models

Let's have a better look at the encoding:

$$
\begin{aligned}
& y - s = wx + \theta \\
& z = 1 \Rightarrow s \leq 0 \\
& z = 0 \Rightarrow y \leq 0 \\
& y, s \geq 0, x \in \mathbb{R}^n, z \in \{0, 1\}
\end{aligned}
$$

If $z = 1$, it means that the neuron is active

- In this case s is forced to 0, we have: $y = wx + \theta$
- ...And $wx + \theta$ is non-negative

If $z = 0$, it means that the neuron is inactive

- In this case y (the neuron output) is 0
- We have $s = wx + \theta$ (note that s does not contribute to the neuron output)
- ...And $wx + \theta$ is negative

Loading the Network

We will handle the encoding via the EMLlib

It's a small (and still rough) library for the EML approach. It allows to:

- Load models from ML libraries (currently NNs from keras, DTs from sklearn)
- Convert them into an internal format
- ...And translate such format into an encoding for a target technique

As a first step, let's load both our trained models

In [38]:
```
knn0 = util.load_ml_model('nn0')
knn1 = util.load_ml_model('nn1')
```

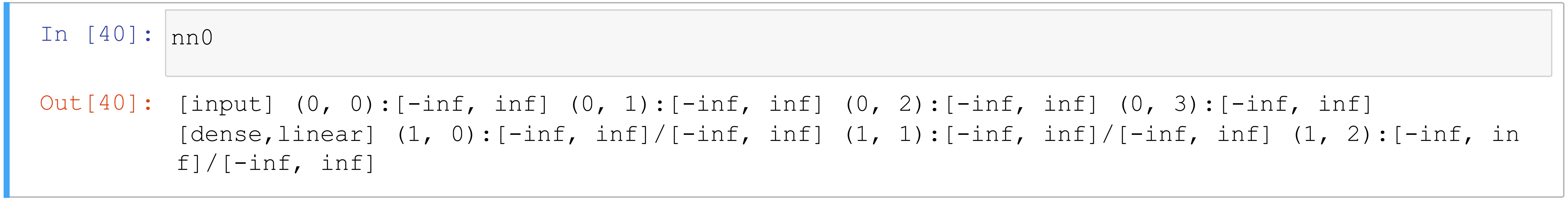
...And then convert the in the EMLlib internal format:

In [39]:
```
nn0 = keras_reader.read_keras_sequential(knn0)
nn1 = keras_reader.read_keras_sequential(knn1)
```

Loading the Network

Printing the loaded network shows "bounds" for each neuron

This is easier to parse for the Linear Regression model:



```
In [40]: nn0

Out[40]: [input] (0, 0):[-inf, inf] (0, 1):[-inf, inf] (0, 2):[-inf, inf] (0, 3):[-inf, inf]
         [dense,linear] (1, 0):[-inf, inf]/[-inf, inf] (1, 1):[-inf, inf]/[-inf, inf] (1, 2):[-inf, in
         f]/[-inf, inf]
```

The bounds represent the domain of output of each neuron

- Currently, most output have an infinite range
- ...Since we have not specified a finite range for the network input

This is a problem since our MILP encoding for each neuron...

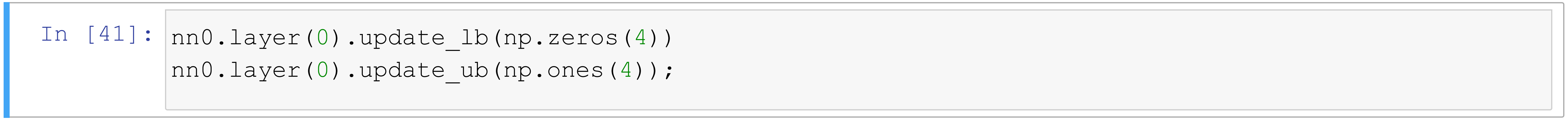
...Requires finite bounds to linearize the indicator constraints

- Actually, the tighter the bounds, the better the MILP encoding will work

Loading the Network

We can use 0 and 1 as bounds for all our inputs

...Since the population is normalized and β is typically a low value

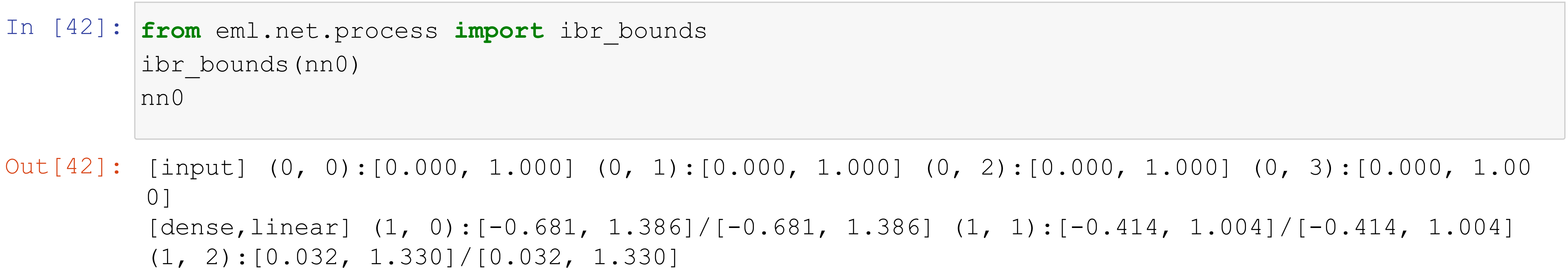


```
In [41]: nn0.layer(0).update_lb(np.zeros(4))
         nn0.layer(0).update_ub(np.ones(4));
```

Internal bounds can be inferred with one round of constraint propagation

- This needs to be done for the weighted sum in each neuron
- ...And for the ReLU, when actually present

The process is implemented in the `ibr_bounds` function:



```
In [42]: from eml.net.process import ibr_bounds
         ibr_bounds(nn0)
         nn0

Out[42]: [input] (0, 0):[0.000, 1.000] (0, 1):[0.000, 1.000] (0, 2):[0.000, 1.000] (0, 3):[0.000, 1.00
         0]
         [dense,linear] (1, 0):[-0.681, 1.386]/[-0.681, 1.386] (1, 1):[-0.414, 1.004]/[-0.414, 1.004]
         (1, 2):[0.032, 1.330]/[0.032, 1.330]
```

Network and I/O Variables

We will consider a planning problem over eoh weeks

So, we will create eoh distinct encodings of the same network

- Each will connect variables representing S, I, R, β for week t
- ...With variables representing S, I, R for week $t + 1$, i.e.:

$$
\begin{aligned}
&(S_{t+1}, I_{t+1}, R_{t+1}) = NN(S_t, I_t, R_t, \beta_t) && \forall t = 0..eoh - 1 \\
&\beta_t \in [0, 1] && \forall t = 0..eoh - 1 \\
&S_t, I_t, R_t \in [0, 1] && \forall t = 0..eoh
\end{aligned}
$$

Where $NN(\ldots)$ represents the network encoding

- We need extra S, I, R variables to represent the final state
- The S_0, I_0, R_0 will be fixed to the values from the initial state

Our objective will be to maximize S_{eoh}

Network ad I/O Variables

The code for the planning problem is in `solve_sir_planning`

We use the CBC solver via Google Or-tools:

```
slv = pywraplp.Solver.CreateSolver('CBC')
```

We start by building the network I/O variables:

```
for t in range(nweeks+1):
    X['S', t] = slv.NumVar(0, 1, f'S_{t}')
    X['I', t] = slv.NumVar(0, 1, f'I_{t}')
    X['R', t] = slv.NumVar(0, 1, f'R_{t}')
    if t < nweeks: X['b', t] = slv.NumVar(0, 1, f'b_{t}')
```

- The network will be embedded as an encoding
- ...Which cannot be defined unless we have the variables first

Network Encodings

The EMLlib handles multiple target solver via "backend" objects

Therefore we need to build a backend for Or-tools:

```
bkd = ortools_backend.OrtoolsBackend()
```

- The backend defines the primitives to build the NN constraints

The encoding themselves are built using the `encode` function:

```
for t in range(1, nweeks+1):
    vin = [X['S',t-1], X['I',t-1], X['R',t-1], X['b',t-1]]
    vout = [X['S',t], X['I',t], X['R',t]]
    encode(bkd, nn, slv, vin, vout, f'nn_{t}')
```

- Neurons are processed one by one
- Intermediate variables are built as needed

Non-Pharmaceutical Intervention

Now we need to setup the rest of the optimization model

...Since we delayed this even too much to focus on the NN encoding

- At each week we can choose to apply a number of NPIs
- ...Which stands for "Non-Pharmaceutical Interventions"

Each NPI i has a (socio-economical) cost c_i

- ...And can reduce the current β value by a factor r_i
- β has a "base value", which depends on the disease itself

So, if we apply NPIs 1, 3, and 4:

- We pay a cost equal to $c_1 + c_3 + c_4$
- And we have $\beta = r_1 r_3 r_4 \beta_{base}$

We assume the total cost cannot exceed a maximum budget

Non-Pharmaceutical Intervention

This part of the problem can be formalized as follows:

We introduce a binary variable x_{it} for each NPI and week (except the last)

$$x_{it} \in \{0, 1\} \qquad \forall i = 1...n_{npi}, \forall t = 0...eoh - 1$$

- $x_{it} = 1$ iff we apply NPI i at week t

The budget constraint can then be stated as:

$$\sum_{t=0}^{eoh-1} \sum_{i=1}^{n_{npi}} c_i x_{it} \leq C$$

- Where C is the budget value

Non-Pharmaceutical Intervention

The effect on β is non-linear and trickier to handle

We linearize it by introducing multiple variables for β at each week

- β_{0t} represents the "base" β value
- β_{it} represents β as affected by the i-th NPI
- Therefore $\beta_{n_{npi},t}$ is the same as the variable connected to the NN for week t

For each intermediate variable we have:

$$\begin{aligned} \beta_{it} &\geq r_i \beta_{i-1,t} - 1 + x_{it} && \forall i = 1..n_{npi}, \forall t = 0..eoh - 1 \\ \beta_{it} &\geq \beta_{i-1,t} - x_{it} && \forall i = 1..n_{npi}, \forall t = 0..eoh - 1 \end{aligned}$$

- If $x_{it} = 1$, the first constraint is active and the second is trivialized
- If $x_{it} = 0$, the opposite is true

Non-Pharmaceutical Intervention

An analogous set of constraints handles the upper bounds

$$\begin{aligned} \beta_{it} &\leq r_i \beta_{i-1,t} + 1 - x_{it} && \forall i = 1..n_{npi}, \forall t = 0..eoh - 1 \\ \beta_{it} &\leq \beta_{i-1,t} + x_{it} && \forall i = 1..n_{npi}, \forall t = 0..eoh - 1 \end{aligned}$$

Together with the previous set:

$$\begin{aligned} \beta_{it} &\geq r_i \beta_{i-1,t} - 1 + x_{it} && \forall i = 1..n_{npi}, \forall t = 0..eoh - 1 \\ \beta_{it} &\geq \beta_{i-1,t} - x_{it} && \forall i = 1..n_{npi}, \forall t = 0..eoh - 1 \end{aligned}$$

...We obtain the desired behavior, e.g.:

- If $x_{1t} = x_{3t} = x_{4t} = 1$
- ...Then $\beta_{n_{npi}t} = r_1 r_3 r_4 \beta_{0,t}$

The details of the code can be found in the `solve_sir_planning`

Solving the NPI Planning Problem

We will consider the following set of NPIs

```
In [43]: npis = [
             util.NPI('masks-indoor', effect=0.75, cost=1),
             util.NPI('masks-outdoor', effect=0.9, cost=1),
             util.NPI('dad', effect=0.7, cost=3),
             util.NPI('bar-rest', effect=0.6, cost=3),
             util.NPI('transport', effect=0.6, cost=4)
         ]
```

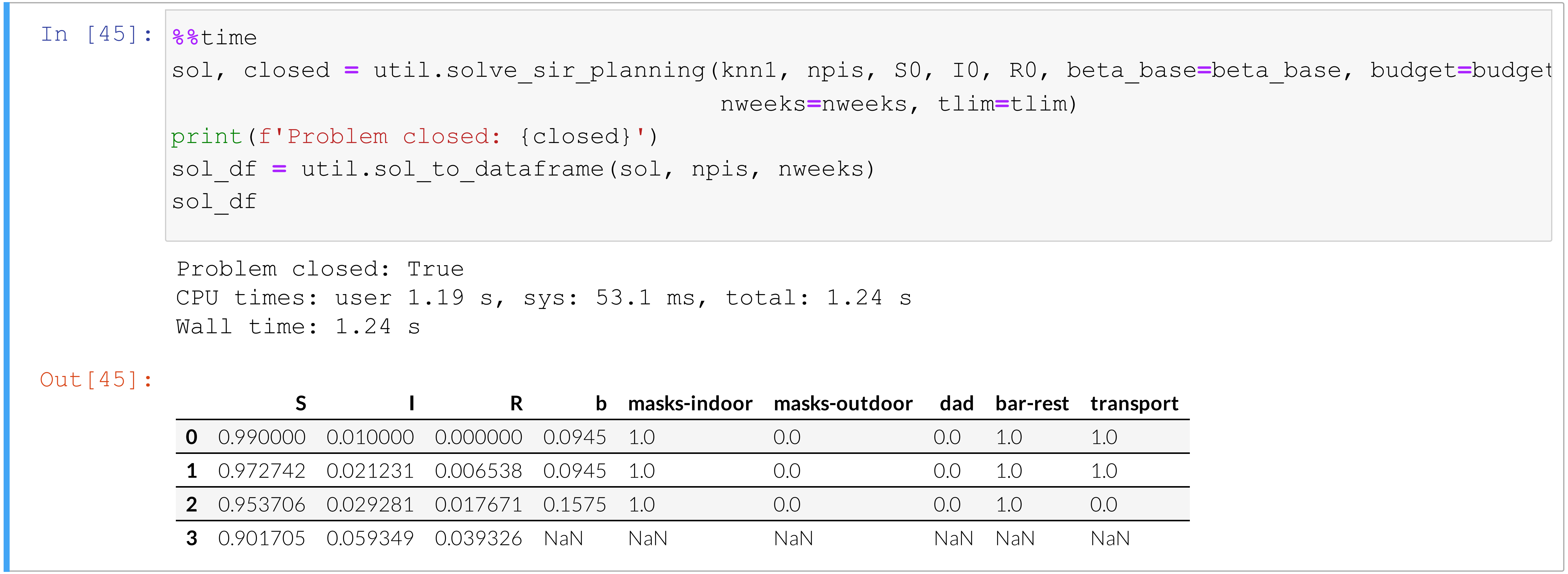
We will consider a horizon of 3 weeks and the following parameters:

```
In [44]: S0, I0, R0 = 0.99, 0.01, 0.00
         nweeks = 3
         tlim = 30
         beta_base = 0.35
         budget = 20
         gamma = 1/14
```

- β has a very high value (to better see the impact of our decisions)

Solution and Evalution

Let's start by using the (much more accurate) NN model



In [45]:

```
%%time
sol, closed = util.solve_sir_planning(knn1, npis, S0, I0, R0, beta_base=beta_base, budget=budget
                                      nweeks=nweeks, tlim=tlim)
print(f'Problem closed: {closed}')
sol_df = util.sol_to_dataframe(sol, npis, nweeks)
sol_df
```

```
Problem closed: True
CPU times: user 1.19 s, sys: 53.1 ms, total: 1.24 s
Wall time: 1.24 s
```

Out[45]:

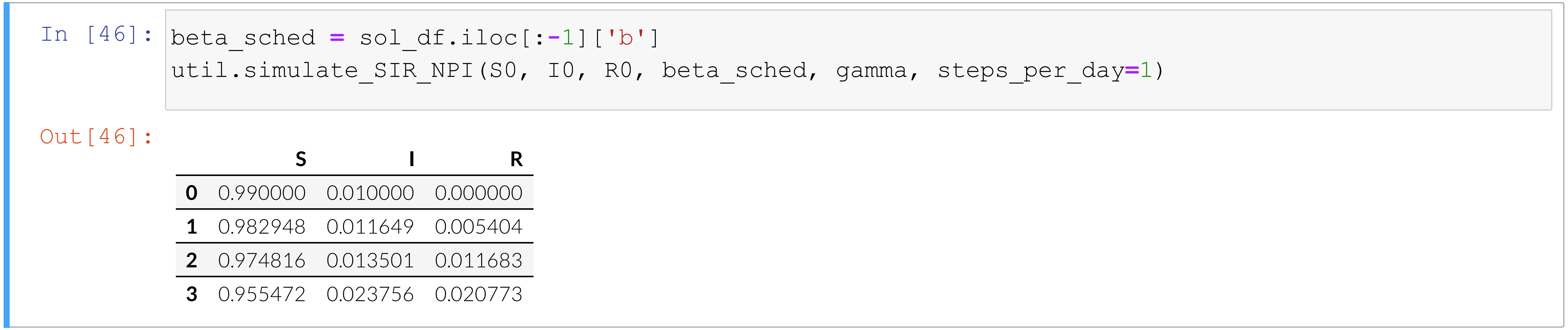
	S	I	R	b	masks-indoor	masks-outdoor	dad	bar-rest	transport
0	0.990000	0.010000	0.000000	0.0945	1.0	0.0	0.0	1.0	1.0
1	0.972742	0.021231	0.006538	0.0945	1.0	0.0	0.0	1.0	1.0
2	0.953706	0.029281	0.017671	0.1575	1.0	0.0	0.0	1.0	0.0
3	0.901705	0.059349	0.039326	NaN	NaN	NaN	NaN	NaN	NaN

- The result seem pretty good
- ...But are we sure about that?

Solution and Evalution

Our optimization model relies on predictions

We need to test their quality on the simulator:



In [46]:
```python
beta_sched = sol_df.iloc[:-1]['b']
util.simulate_SIR_NPI(S0, I0, R0, beta_sched, gamma, steps_per_day=1)
```

Out[46]:

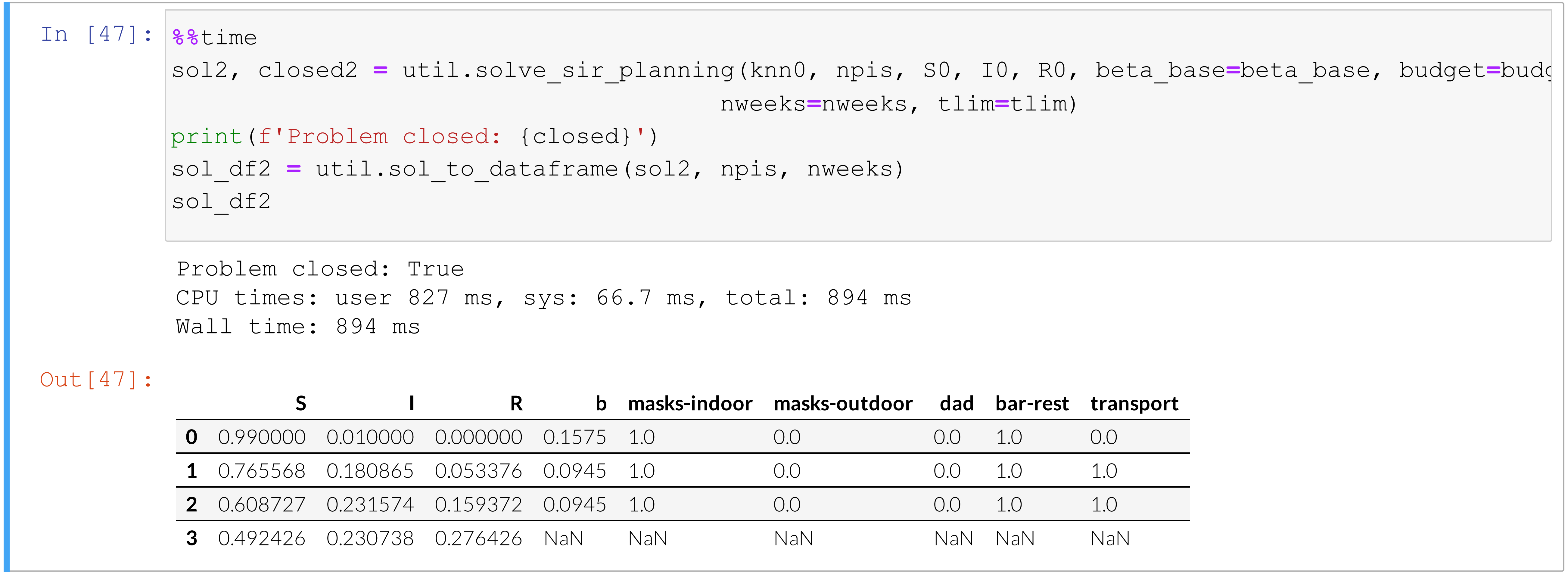
	S	I	R
0	0.990000	0.010000	0.000000
1	0.982948	0.011649	0.005404
2	0.974816	0.013501	0.011683
3	0.955472	0.023756	0.020773

Unless we've been unlucky during training (it's stochastic!)

- The final value for S should be close to 0.95
- ...And possibly quite different from our model predictions!

Solution and Evalution

It's even more clear if we use the Linear Regression model



```
In [47]: %%time
         sol2, closed2 = util.solve_sir_planning(knn0, npis, S0, I0, R0, beta_base=beta_base, budget=budg
                                                 nweeks=nweeks, tlim=tlim)
         print(f'Problem closed: {closed}')
         sol_df2 = util.sol_to_dataframe(sol2, npis, nweeks)
         sol_df2
```

```
Problem closed: True
CPU times: user 827 ms, sys: 66.7 ms, total: 894 ms
Wall time: 894 ms
```

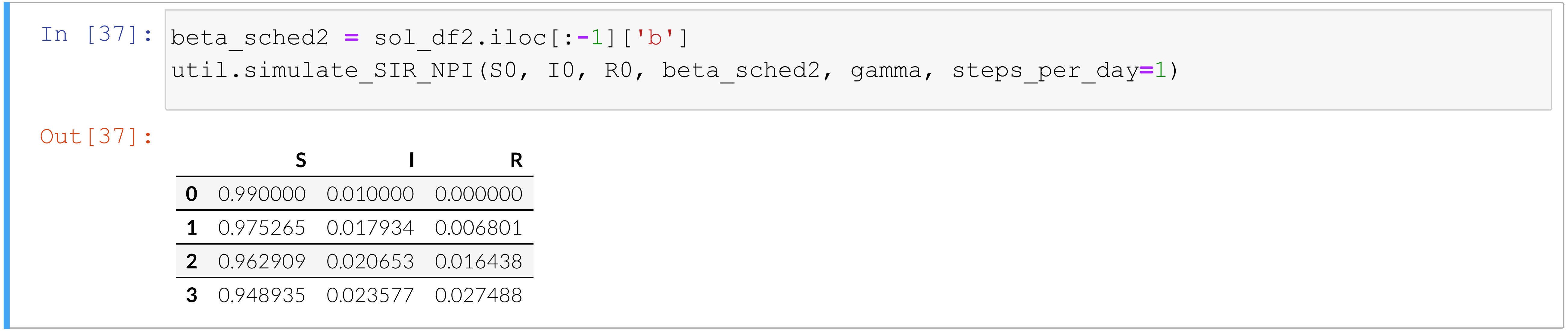
Out[47]:

	S	I	R	b	masks-indoor	masks-outdoor	dad	bar-rest	transport
0	0.990000	0.010000	0.000000	0.1575	1.0	0.0	0.0	1.0	0.0
1	0.765568	0.180865	0.053376	0.0945	1.0	0.0	0.0	1.0	1.0
2	0.608727	0.231574	0.159372	0.0945	1.0	0.0	0.0	1.0	1.0
3	0.492426	0.230738	0.276426	NaN	NaN	NaN	NaN	NaN	NaN

- Now the solution process is very fast
- ...And it looks like a disaster

Solution and Evalution

However, if we evaluate the solutions via the simulator...



In [37]:

```
beta_sched2 = sol_df2.iloc[:-1]['b']
util.simulate_SIR_NPI(S0, I0, R0, beta_sched2, gamma, steps_per_day=1)
```

Out[37]:

	S	I	R
0	0.990000	0.010000	0.000000
1	0.975265	0.017934	0.006801
2	0.962909	0.020653	0.016438
3	0.948935	0.023577	0.027488

...They are not bad at all!

Our ML models are making mistakes

- For many reasons: bias, compound error, "weak spots"
- ...But as long as they guide the solver in the right place, we get a good solution

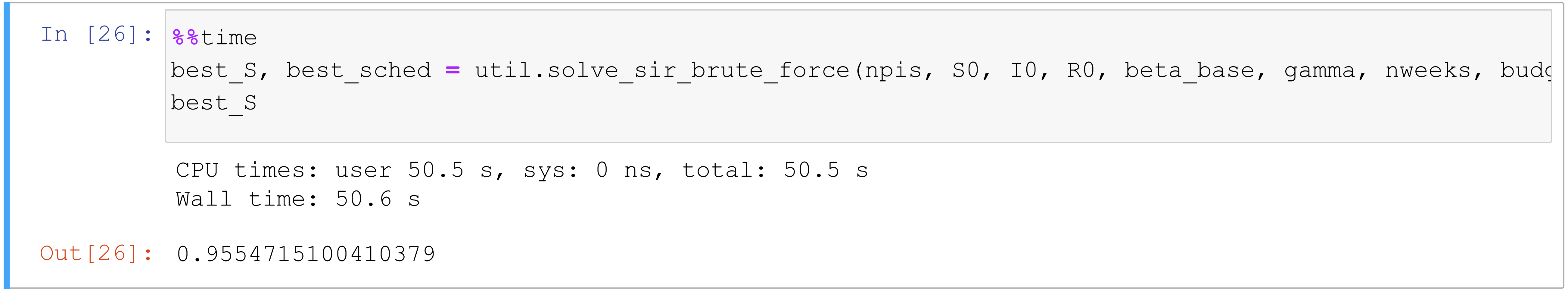
This is good news, but leave some open issues (see later)

Solution and Evaluation

The main issue is: how much can we trust our models?

In our case, it turns out the answer is "a lot"

- Here's what we get by solving the problem via brute force:



In [26]:

```
%%time
best_S, best_sched = util.solve_sir_brute_force(npis, S0, I0, R0, beta_base, gamma, nweeks, budg
best_S
```

```
CPU times: user 50.5 s, sys: 0 ns, total: 50.5 s
Wall time: 50.6 s
```

Out[26]:

```
0.9554715100410379
```

- The NN solution in particular is almost perfect
- ...And we obtain it in a much less time
- As the problem size grows, the gap in computation time becomes larger

A Few Important Technicalities

Handling NNs in MILP is very challenging, for two main reasons:

First, fully connected layers rely on dense matrix products

- Most MILP solvers are designed and optimized for sparse problems
- Dense MILPs are best tackled using different techniques
- There is a tension between the (dense) NN and the (sparse) problem structure

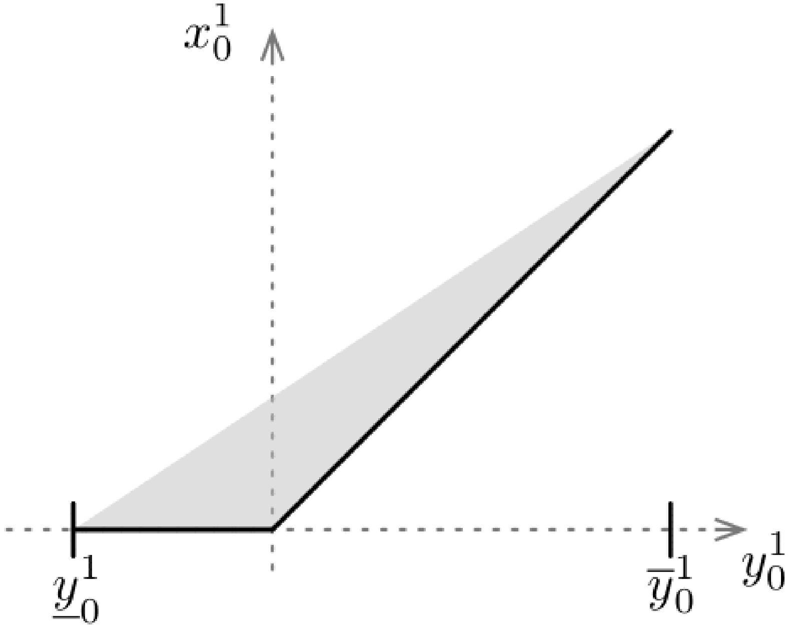
Second, ReLUs are non-linear

- Their linearization may lead to a poor relaxation
- ...Depending on the bounds for the input of the ReLU itself
- I.e. the bounds for the weighted sum $w^T x + \theta$

A Few Important Technicalities

This is easier to understand with a picture

The true ReLU function is the one depicted with a thick black line

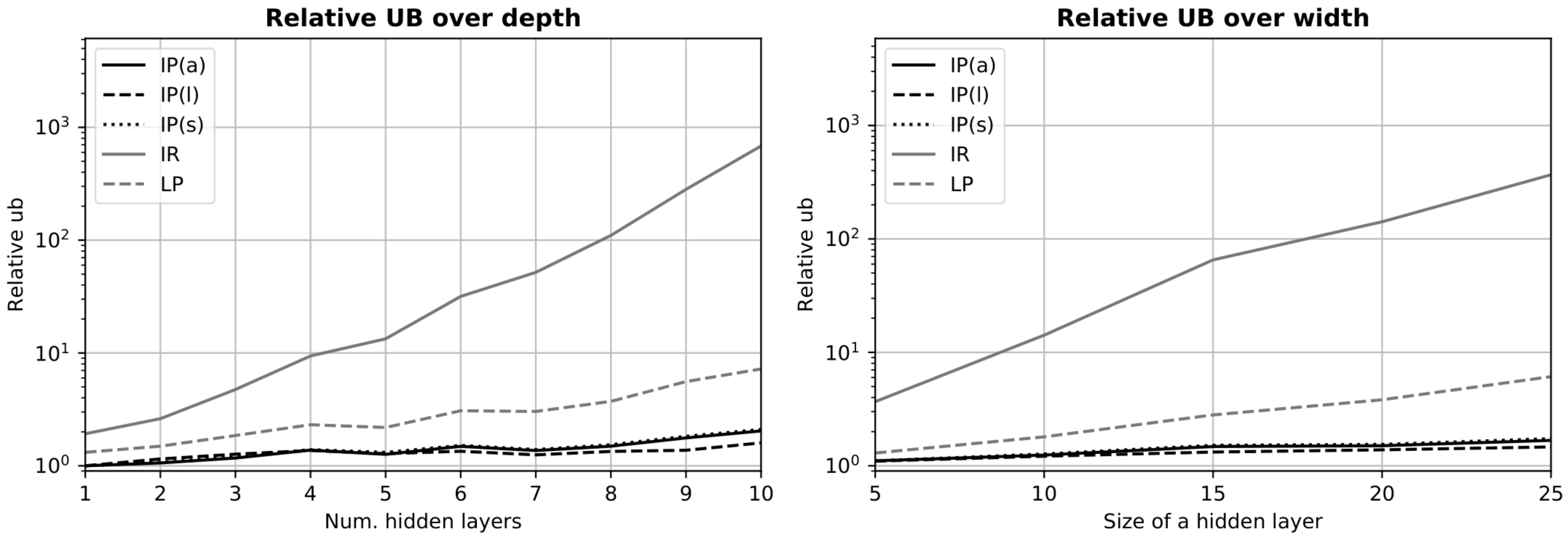


...But it's LP relaxation corresponds to the shaded area

- To make things worse, bounds on the ReLU inputs
- ...Tend to become weaker as the network size grows

A Few Important Technicalities

Here are some results on bound quality for a NN trained on a simple dataset



- As depth and width grow, the bounds become exponentially worse
- We see it happening in our problem when we increase the number of weeks

Currently, this is one of the major challenges for NN verification

The only upside is that bound tightening method tend to work very well in this setup

Some Considerations

This kind of hybrid approach can be complex to build

- But sometimes it's (almost) the only choice!
- It generally worked in our case

EML-like approaches can be used to generate adversarial examples

- It is at the basis of some tools for NN verification

There are several open issues

- The optimizer often ends up finding weaknesses in the ML model
  - Can we bound the error, or define confidence intervals?
  - Can we use re-train the model to fix mistakes?
- The approach scalability is limited
  - Large (even moderately large) ML models are currently out of reach
  - How to improve that?