

DiseaseModelPINN_notebook_simpleModel

December 17, 2022

```
[ ]: import deepxde as dde
from deepxde.backend import pytorch
import torch
import matplotlib.pyplot as plt
import numpy as np

from SIRD_deepxde_DiseaseModel import SIRD_deepxde_net
from DiseaseModel import SIR,SIRD,SIRDIm,SIRDImRel, SIRDImRelSimple, SIRD2Var, SIRD2VarRelSimple, GeneralModelSolver
from Plot import Plot

# %matplotlib widget

seed = 2
np.random.seed(seed)
dde.config.set_random_seed(seed)
```

Using backend: pytorch

default Torch device: cpu

```
[ ]: time_delta = [0,365] # use three values here for intro time of second variant

# initial_conditions = {
#     "S": 1000000,
#     "I": 1,
#     "R": 0,
# }
# static_parameters = {
#     "alpha": (0.15),
#     "beta": (0.07),
# }
# sird_model = SIR(initial_conditions, static_parameters, time_delta)

# initial_conditions = {
#     "S": 1000000,
#     "I": 1,
```

```

#     "R": 0,
#     "D": 0,
#     }
# static_parameters = {
#     "alpha": (0.2),
#     "beta": (0.05),
#     "gamma": (0.001),
#     }
# sird_model = SIRD(initial_conditions, static_parameters, time_delta)

# initial_conditions = {
#     "S": 1000000,
#     "I": 15,
#     "R": 0,
#     "D": 0,
#     "Im": 0, # should be between 0 and 1
#     }
# static_parameters = {
#     "alpha": 0.12,
#     "beta": 0.07,
#     "gamma": 0.02,
#     "kappa": 0.2,
#     }
# sird_model = SIRDIm(initial_conditions, static_parameters, time_delta)
# initial_conditions = {
#     "S": 1000000,
#     "I": 15,
#     "R": 0,
#     "D": 0,
#     "Im": 0, # should be between 0 and 1
#     }
# static_parameters = {
#     "lambda_": 1.5,
#     "gamma": 0.000,
#     "kappa": 0.2,
#     }
# sird_model = SIRDImRel(initial_conditions, static_parameters, time_delta)
# initial_conditions = {
#     "S": 1000000,
#     "I": 15,
#     "R": 0,
#     "Im": 0, # should be between 0 and 1
#     }
# static_parameters = {
#     "lambda_": 1.5,
#     "kappa": 0.2,
#     }

```

```

# sird_model = SIRDImRelSimple(initial_conditions, static_parameters,
    ↪time_delta)

# initial_conditions = {
#     "S": 1000000,
#     "Ia": 1,
#     "Ib": 0,
#     "Ra": 0,
#     "Rb": 0,
#     "D": 0,
#     "Im_a": 0, # should be between 0 and 1
#     "Im_b": 0, # should be between 0 and 1
# }
# static_parameters = {
#     "alpha_a": 0.23 ,
#     "alpha_b": 0.18,
#     "beta_a": 0.1,
#     "beta_b": 0.08,
#     "gamma_a": 0.00,
#     "gamma_b": 0.00,
#     "kappa_a": 0.8,
#     "kappa_b": 0.5,
# }
# static_parameters = {
#     "alpha_a": 0.11,
#     "alpha_b": 0.12,
#     "beta_a": 0.08,
#     "beta_b": 0.08,
#     "gamma_a": 0.00,
#     "gamma_b": 0.00,
#     "kappa_a": 0.1,
#     "kappa_b": 0.2,
# }
# sird_model = SIRD2Var(initial_conditions, static_parameters, time_delta)

initial_conditions = {
    "S": 1000000,
    "Ia": 1,
    "Ib": 0,
    "Ra": 0,
    "Rb": 0,
    "Im_a": 0,
    "Im_b": 0,
}
static_parameters = {
    "lambda_a": 2.2 ,
    "lambda_b": 1.9,

```

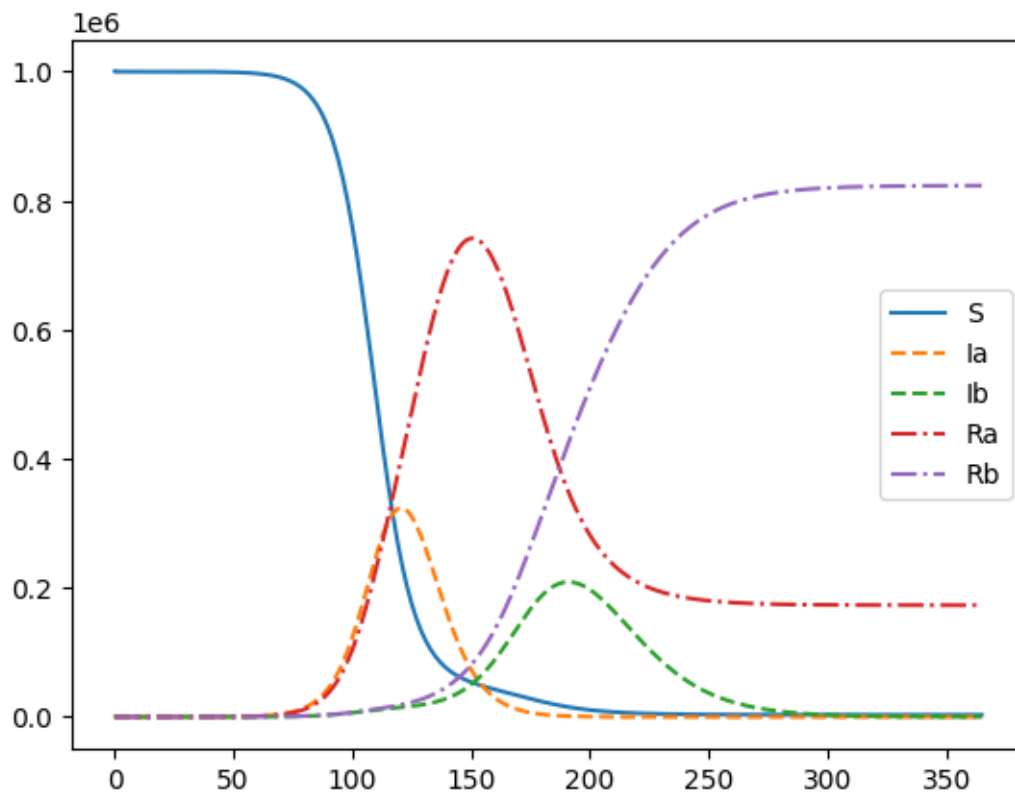
```

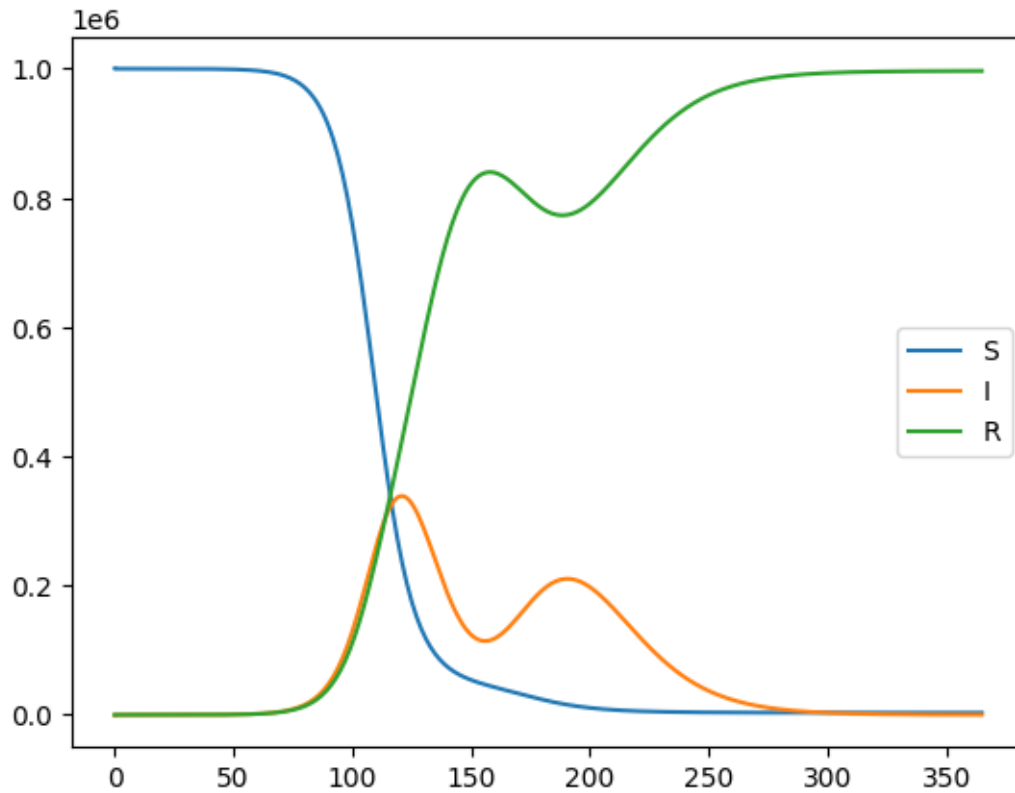
    "kappa_a": 0.8, # should be between 0 and 1
    "kappa_b": 0.5,
}

sird_model = SIRD2VarRelSimple(initial_conditions, static_parameters,
    ↪time_delta)

t_synth, solution_synth_full = sird_model.simulate()
t_synth, solution_synth = sird_model.get_solution_as_sird()
sird_model.plot_solution()
sird_model.plot_sird()

```





```
[ ]: print(sird_model)
```

A Disease Model with description: 'A model that simulates two concurrent diseases and natural herd immunity as a factor of the amount of recovered for each variant':

Parameters:

```
lambda_a = 2.2
lambda_b = 1.9
kappa_a = 0.8
kappa_b = 0.5
```

PDE groups and initial conditions:

```
S = 1000000
Ia = 1
Ib = 0
Ra = 0
Rb = 0
Im_a = 0
Im_b = 0
```

PDE equations:

```

dS/dt = -(0.1*lambda_a/N)*Ia*S - (0.1*lambda_b/N)*Ib*S
dIa/dt = (0.1*lambda_a/N)*S*Ia + (0.1*lambda_a/N)*(1 - Im_a)*(Ra +
Rb)*Ia - 0.1*Ia
dIb/dt = (0.1*lambda_b/N)*S*Ib + (0.1*lambda_b/N)*(1 - Im_b)*(Ra +
Rb)*Ib - 0.1*Ib
dRa/dt = 0.1*Ia - (0.1*lambda_a/N)*(1 - (Im_a))*(Ra)*(Ia) -
(0.1*lambda_b/N)*(1 - (Im_b))*(Ra)*(Ib)
dRb/dt = 0.1*Ib - (0.1*lambda_a/N)*(1 - (Im_a))*(Rb)*(Ia) -
(0.1*lambda_b/N)*(1 - (Im_b))*(Rb)*(Ib)
dIm_a/dt = kappa_a*0.1*Ia/N
dIm_b/dt = kappa_b*0.1*Ib/N
PINN PDE loss equations:
dS_t - (-(0.1*lambda_a/N)*Ia*S - (0.1*lambda_b/N)*Ib*S)
dIa_t - ((0.1*lambda_a/N)*S*Ia + (0.1*lambda_a/N)*(1 - Im_a)*(Ra +
Rb)*Ia - 0.1*Ia)
dIb_t - ((0.1*lambda_b/N)*S*Ib + (0.1*lambda_b/N)*(1 - Im_b)*(Ra +
Rb)*Ib - 0.1*Ib )
dRa_t - (0.1*Ia - (0.1*lambda_a/N)*(1 - (Im_a))*(Ra)*(Ia) -
(0.1*lambda_b/N)*(1 - (Im_b))*(Ra)*(Ib))
dRb_t - (0.1*Ib - (0.1*lambda_a/N)*(1 - (Im_a))*(Rb)*(Ia) -
(0.1*lambda_b/N)*(1 - (Im_b))*(Rb)*(Ib))
dIm_a_t - (kappa_a*0.1*Ia/N)
dIm_b_t - (kappa_b*0.1*Ib/N)

```

```
[ ]: # keep this even if not subsetting
```

```
t = t_synth
```

```
wsol = solution_synth
```

```
solver = GeneralModelSolver(sird_model)
```

```
# subset
```

```
# max_timestep = 300
```

```
# t_bool = t_synth < max_timestep
```

```
# t = t_synth[t_bool]
```

```
# wsol = wsol_synth[t_bool]
```

```
[ ]: model = SIRD_deepxde_net(t, wsol,disease_model=sird_model, with_neumann=True,␣
```

```
    ↪model_name="diseasemodel_test", with_softadapt=True)
```

```
print(model)
```

```
hyper_print_every = 100
```

```
model.init_model(lr=0.01, print_every=hyper_print_every, activation="tanh",␣
```

```
    ↪nn_layers=2, nn_layer_width=32)
```

PINN model:

Parameters: ['lambda_a', 'lambda_b', 'kappa_a', 'kappa_b']

Loss measures: ['dS_t', 'dIa_t', 'dIb_t', 'dRa_t', 'dRb_t', 'dIm_a_t',
'dIm_b_t', 'ic_Ia', 'ic_Ib', 'ic_Ra', 'ic_Rb', 'ic_Im_a', 'ic_Im_b', 'ic_S',
'observe_S', 'observe_I', 'observe_R', 'observe_SUM', 'sign_Ia', 'sign_Ib',
'sign_Ra', 'sign_Rb', 'sign_Im_a', 'sign_Im_b', 'L1_norm_Ia', 'L1_norm_Ib',

```
'L1_norm_Ra', 'L1_norm_Rb', 'L1_norm_Im_a', 'L1_norm_Im_b', 'ic_neumann_S',
'ic_neumann_Ia', 'ic_neumann_Ib', 'ic_neumann_Ra', 'ic_neumann_Rb',
'ic_neumann_Im_a', 'ic_neumann_Im_b']
```

Compiling model...

'compile' took 0.000061 s

```
[ ]: prev_best_step = 0
      iters = 0
      plot_every=2000

[ ]: TOTAL_ITER = 100_000
      try:
          while True:
              # for n in range(TOTAL_ITER//plot_every):
              model.train_model(iterations=plot_every, print_every=hyper_print_every,
          ↪ use_LBFGSB=False)
              params_nn, best_step = model.get_best_params(out_func=np.exp) #
          ↪ parameters need to be extracted with the exponential function as they have
          ↪ been modelled in logspace
              if best_step > prev_best_step:
                  prev_best_step = best_step
                  break
              elif iters >= TOTAL_ITER:
                  break
          except KeyboardInterrupt:
              print("Training ended prematurely")

      params_nn, best_step = model.get_best_params(out_func=np.exp) # parameters need
          ↪ to be extracted with the exponential function as they have been modelled in
          ↪ logspace
      print(static_parameters, sep="\n")
      t_nn_param, wsol_nn_param, wsol_sird_nn_param = solver(*params_nn)
      # params_nn= tuple(np.exp([*params_nn]))
      # print(*params_nn)
      model.set_synthetic_data(t_synth, solution_synth_full)
      model.set_nn_synthetic_data(t_nn_param, wsol_nn_param, wsol_sird_nn_param)
      plot = Plot(model, values_to_plot=sird_model.initial_conditions_keys) # class
          ↪ that contains plotting functions
      plot.show_known_and_prediction()
      # plot.plot_param_history()
      # plot.plot_loss_history()
```

Training model...

```
Step      Train loss
Test loss
```

Test metric

30000 [5.98e-04, 1.95e-04, 1.48e-05, 9.66e-05, 2.63e-04, 1.32e-04, 2.13e-04, 6.49e-02, 1.41e-02, 1.15e-03, 2.87e-02, 1.81e-02, 3.43e-02, 1.33e-02, 3.35e-01, 8.49e-02, 5.03e-01, 2.11e-01, 1.03e-02, 9.59e-03, 0.00e+00, 0.00e+00, 2.93e-04, 1.03e-03, 1.71e-02, 1.04e-02, 6.69e-04, 1.73e-03, 1.43e-03, 3.60e-03, 2.44e-02, 2.44e-02, 2.44e-02, 2.44e-02, 2.44e-02, 2.44e-02] [5.98e-04, 1.95e-04, 1.48e-05, 9.66e-05, 2.63e-04, 1.32e-04, 2.13e-04, 6.49e-02, 1.41e-02, 1.15e-03, 2.87e-02, 1.81e-02, 3.43e-02, 1.33e-02, 3.35e-01, 8.49e-02, 5.03e-01, 2.11e-01, 1.03e-02, 9.59e-03, 0.00e+00, 0.00e+00, 2.93e-04, 1.03e-03, 1.71e-02, 1.04e-02, 6.69e-04, 1.73e-03, 1.43e-03, 3.60e-03, 2.44e-02, 2.44e-02, 2.44e-02, 2.44e-02] []

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 2.61e-04, 5.15e-06, 3.68e-06, 1.30e-06, 1.35e-05, 3.51e-05, 1.39e-05, 1.42e-04,
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Best model at step 28867:

train loss: 1.03e-04

test loss: 1.03e-04

test metric: []

'train' took 46.255551 s

Best train step: 28867

lambda_a: 1.5008877759545223

lambda_b: 1.6943118629846954

kappa_a: 0.11167805260458141

kappa_b: 0.3695164855562565

Training model...

Step Train loss

Test loss

Test metric

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Best model at step 28867:

train loss: 1.03e-04

test loss: 1.03e-04

test metric: []

'train' took 47.423085 s

Best train step: 28867

lambda_a: 1.5008877759545223

lambda_b: 1.6943118629846954

kappa_a: 0.11167805260458141

kappa_b: 0.3695164855562565

Training model...

Step Train loss

Test loss

Test metric

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Best model at step 28867:

train loss: 1.03e-04
 test loss: 1.03e-04
 test metric: []

'train' took 44.281615 s

Best train step: 28867
lambda_a: 1.5008877759545223
lambda_b: 1.6943118629846954
kappa_a: 0.11167805260458141
kappa_b: 0.3695164855562565
Training model...

Step	Train loss	Test loss	Test metric
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Best model at step 28867:

train loss: 1.03e-04

test loss: 1.03e-04

test metric: []

'train' took 40.082856 s

Best train step: 28867

lambda_a: 1.5008877759545223

lambda_b: 1.6943118629846954

kappa_a: 0.11167805260458141

kappa_b: 0.3695164855562565

Training model...

Step Train loss

Test loss

Test metric

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Best model at step 28867:

train loss: 1.03e-04

test loss: 1.03e-04

test metric: []

'train' took 42.610279 s

Best train step: 28867

lambda_a: 1.5008877759545223

lambda_b: 1.6943118629846954

kappa_a: 0.11167805260458141

kappa_b: 0.3695164855562565

Training model...

Step Train loss

Test loss

Test metric

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Best model at step 28867:

train loss: 1.03e-04

test loss: 1.03e-04

test metric: []

'train' took 48.690258 s

Best train step: 28867

lambda_a: 1.5008877759545223

lambda_b: 1.6943118629846954

kappa_a: 0.11167805260458141

kappa_b: 0.3695164855562565

Training model...

Step Train loss

Test loss

Test metric

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Best model at step 28867:

train loss: 1.03e-04
 test loss: 1.03e-04
 test metric: []

'train' took 51.012227 s

Best train step: 28867
lambda_a: 1.5008877759545223
lambda_b: 1.6943118629846954
kappa_a: 0.11167805260458141
kappa_b: 0.3695164855562565
Training model...

Step Train loss

Test loss

Test metric

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```

Best model at step 28867:

```

train loss: 1.03e-04
test loss: 1.03e-04
test metric: []

```

'train' took 45.719898 s

```

Best train step: 28867
lambda_a: 1.5008877759545223
lambda_b: 1.6943118629846954
kappa_a: 0.11167805260458141
kappa_b: 0.3695164855562565
Training model...

```

```

Step      Train loss
Test loss

```

Test metric

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Best model at step 28867:

train loss: 1.03e-04

test loss: 1.03e-04

test metric: []

'train' took 48.978525 s

Best train step: 28867

lambda_a: 1.5008877759545223

lambda_b: 1.6943118629846954

kappa_a: 0.11167805260458141

kappa_b: 0.3695164855562565

Training model...

Step Train loss

Test loss

Test metric

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Best model at step 28867:

train loss: 1.03e-04

test loss: 1.03e-04

test metric: []

'train' took 43.183387 s

Best train step: 28867

lambda_a: 1.5008877759545223

lambda_b: 1.6943118629846954

kappa_a: 0.11167805260458141

kappa_b: 0.3695164855562565

Training model...

Step Train loss

Test loss

Test metric

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Best model at step 28867:

train loss: 1.03e-04
 test loss: 1.03e-04
 test metric: []

'train' took 43.103287 s

Best train step: 28867
lambda_a: 1.5008877759545223
lambda_b: 1.6943118629846954
kappa_a: 0.11167805260458141
kappa_b: 0.3695164855562565
Training model...

Step	Train loss
Test loss	
Test metric	
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```

Best model at step 28867:

```

train loss: 1.03e-04
test loss: 1.03e-04
test metric: []

```

'train' took 49.360314 s

```

Best train step: 28867
lambda_a: 1.5008877759545223
lambda_b: 1.6943118629846954
kappa_a: 0.11167805260458141
kappa_b: 0.3695164855562565
Training model...

```

```

Step      Train loss
Test loss

```


Test metric

54000 [9.50e-06, 1.96e-06, 5.20e-06, 6.34e-06, 4.24e-06, 1.52e-06, 3.34e-06, 9.92e-06, 1.71e-04, 7.08e-07, 5.24e-07, 7.79e-08, 9.07e-08, 1.62e-05, 1.51e-04, 2.60e-03, 2.78e-03, 1.36e-05, 2.50e-06, 0.00e+00, 1.38e-08, 6.92e-09, 0.00e+00, 0.00e+00, 1.09e-05, 1.61e-04, 1.88e-07, 9.54e-08, 9.51e-08, 1.19e-07, 2.84e-11, 2.84e-11, 2.84e-11, 2.84e-11, 2.84e-11, 2.84e-11] [9.50e-06, 1.96e-06, 5.20e-06, 6.34e-06, 4.24e-06, 1.52e-06, 3.34e-06, 9.92e-06, 1.71e-04, 7.08e-07, 5.24e-07, 7.79e-08, 9.07e-08, 1.62e-05, 1.51e-04, 2.60e-03, 2.78e-03, 1.36e-05, 2.50e-06, 0.00e+00, 1.38e-08, 6.92e-09, 0.00e+00, 0.00e+00, 1.09e-05, 1.61e-04, 1.88e-07, 9.54e-08, 9.51e-08, 1.19e-07, 2.84e-11, 2.84e-11, 2.84e-11, 2.84e-11, 2.84e-11, 2.84e-11] []

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Best model at step 28867:

train loss: 1.03e-04

test loss: 1.03e-04

test metric: []

'train' took 43.516946 s

Best train step: 28867

lambda_a: 1.5008877759545223

lambda_b: 1.6943118629846954

kappa_a: 0.11167805260458141

kappa_b: 0.3695164855562565

Training model...

Step Train loss

Test loss

Test metric

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Best model at step 28867:

train loss: 1.03e-04

test loss: 1.03e-04

test metric: []

'train' took 45.731935 s

Best train step: 28867

lambda_a: 1.5008877759545223

lambda_b: 1.6943118629846954

kappa_a: 0.11167805260458141

kappa_b: 0.3695164855562565

Training model...

Step Train loss

Test loss

Test metric

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 1.15e-04, 9.40e-05, 6.07e-05, 5.11e-07, 3.59e-07, 1.15e-08, 1.81e-07, 4.11e-07,
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 1.64e-06, 3.12e-06, 3.33e-07, 1.06e-06, 4.34e-07, 1.72e-07, 1.72e-07, 1.72e-07,
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 5.20e-07, 2.25e-08, 3.46e-07, 4.80e-12, 2.99e-07, 8.94e-05, 5.16e-05, 6.40e-05,
 3.87e-05, 4.48e-07, 2.77e-07, 7.27e-09, 8.89e-08, 4.45e-07, 3.56e-07, 5.13e-07,
 1.55e-06, 2.06e-06, 2.31e-07, 3.64e-07, 2.55e-07, 2.29e-08, 2.29e-08, 2.29e-08,
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Best model at step 28867:

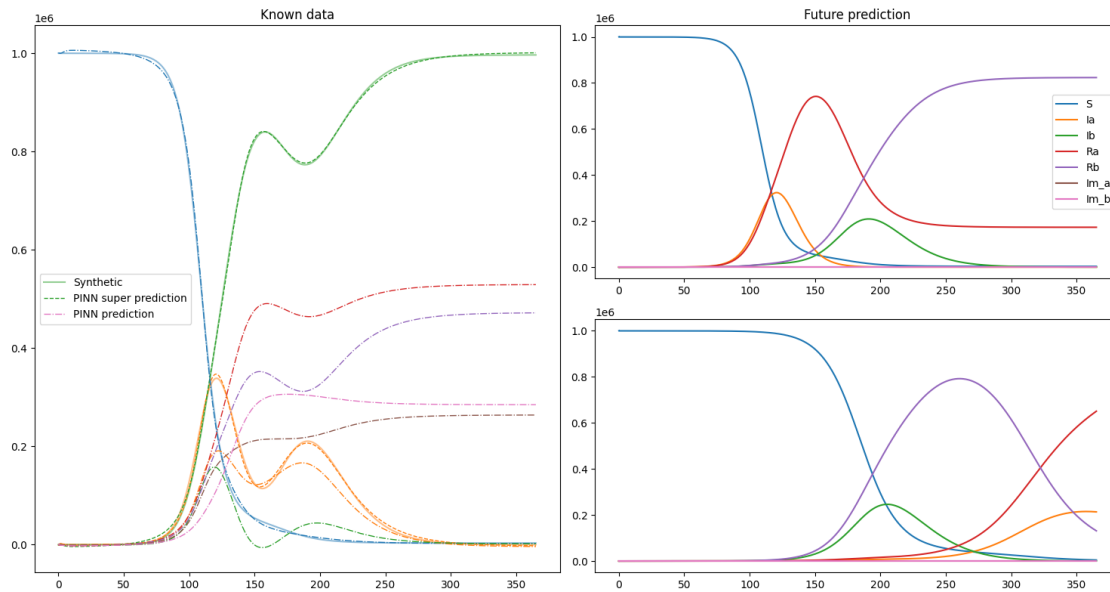
train loss: 1.03e-04
 test loss: 1.03e-04
 test metric: []

'train' took 43.086333 s

Best train step: 28867
lambda_a: 1.5008877759545223
lambda_b: 1.6943118629846954
kappa_a: 0.11167805260458141
kappa_b: 0.3695164855562565
Training model...

Step	Train loss	Test loss	Test metric
60000	[1.17e-06, 8.31e-06, 1.90e-06, 9.31e-06, 8.79e-06, 3.88e-06, 1.93e-06, 2.81e-07, 9.33e-12, 5.20e-07, 2.25e-08, 3.46e-07, 4.80e-12, 2.99e-07, 8.94e-05, 5.16e-05, 6.40e-05, 3.87e-05, 4.48e-07, 2.77e-07, 7.27e-09, 8.89e-08, 4.45e-07, 3.56e-07, 5.13e-07, 1.55e-06, 2.06e-06, 2.31e-07, 3.64e-07, 2.55e-07, 2.29e-08, 2.29e-08, 2.29e-08, 2.29e-08, 2.29e-08, 2.29e-08]	[1.17e-06, 8.31e-06, 1.90e-06, 9.31e-06, 8.79e-06, 3.88e-06, 1.93e-06, 2.81e-07, 9.33e-12, 5.20e-07, 2.25e-08, 3.46e-07, 4.80e-12, 2.99e-07, 8.94e-05, 5.16e-05, 6.40e-05, 3.87e-05, 4.48e-07, 2.77e-07, 7.27e-09, 8.89e-08, 4.45e-07, 3.56e-07, 5.13e-07, 1.55e-06, 2.06e-06, 2.31e-07, 3.64e-07, 2.55e-07, 2.29e-08, 2.29e-08, 2.29e-08, 2.29e-08]	[]
60100	[9.43e-07, 8.51e-06, 2.04e-06, 9.23e-06, 8.77e-06, 4.13e-06, 1.90e-06, 1.98e-07, 6.67e-11, 3.74e-07, 1.05e-07, 6.36e-08, 3.59e-07, 2.32e-07, 6.72e-05, 3.58e-05, 5.27e-05, 3.12e-05, 5.65e-07, 4.01e-07, 6.64e-09, 8.87e-08, 4.60e-07, 1.33e-07, 5.82e-07, 1.48e-06, 1.60e-06, 2.52e-07, 2.42e-07, 2.36e-07, 1.94e-10, 1.94e-10, 1.94e-10, 1.94e-10, 1.94e-10, 1.94e-10]	[9.43e-07, 8.51e-06, 2.04e-06, 9.23e-06, 8.77e-06, 4.13e-06, 1.90e-06, 1.98e-07, 6.67e-11, 3.74e-07, 1.05e-07, 6.36e-08, 3.59e-07, 2.32e-07, 6.72e-05, 3.58e-05, 5.27e-05, 3.12e-05, 5.65e-07, 4.01e-07, 6.64e-09, 8.87e-08, 4.60e-07, 1.33e-07, 5.82e-07, 1.48e-06, 1.60e-06, 2.52e-07, 2.42e-07, 2.36e-07, 1.94e-10, 1.94e-10, 1.94e-10, 1.94e-10]	[]

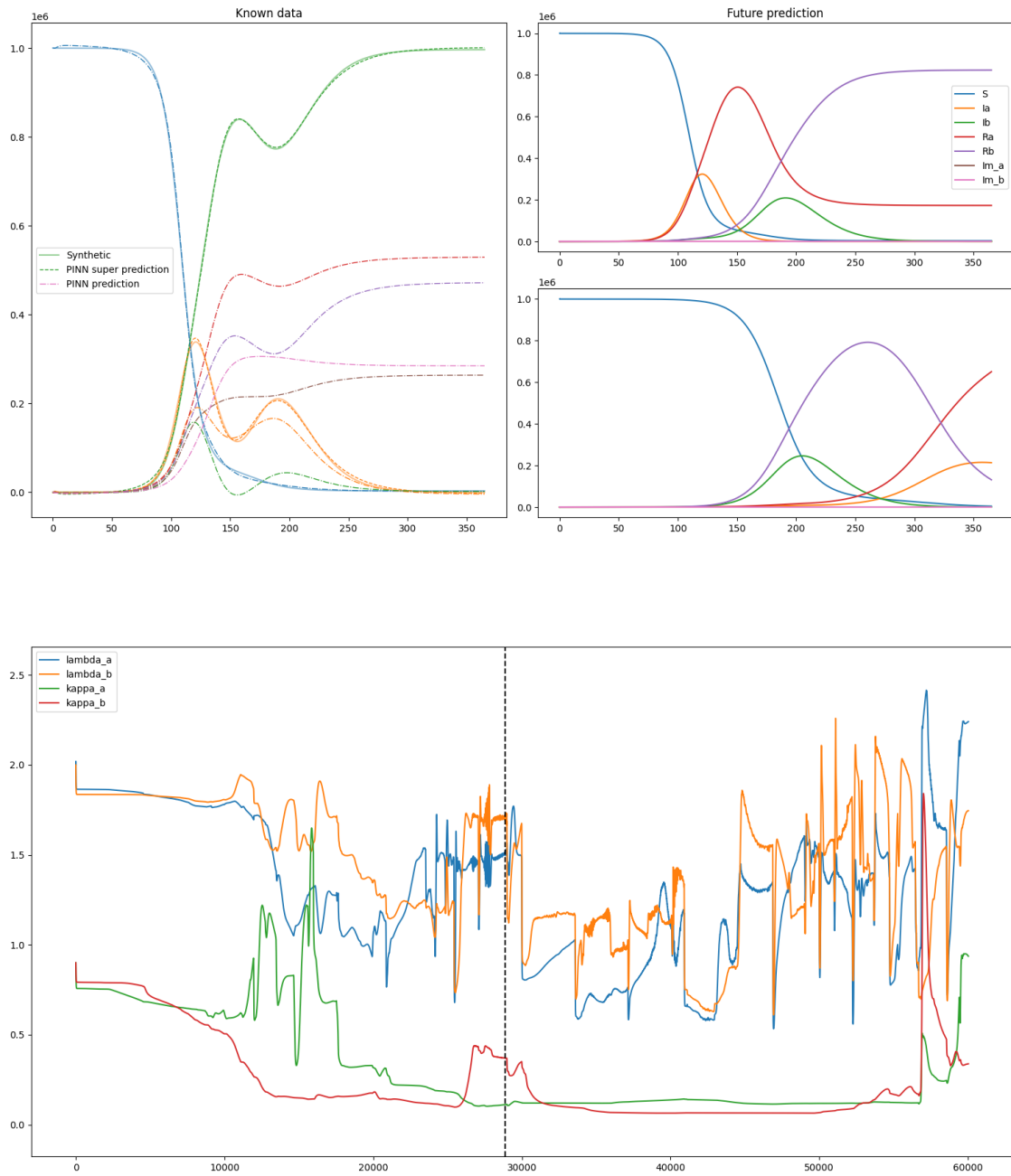
Training ended prematurely
Best train step: 28867
lambda_a: 1.5008877759545223
lambda_b: 1.6943118629846954
kappa_a: 0.11167805260458141
kappa_b: 0.3695164855562565
{'lambda_a': 2.2, 'lambda_b': 1.9, 'kappa_a': 0.8, 'kappa_b': 0.5}

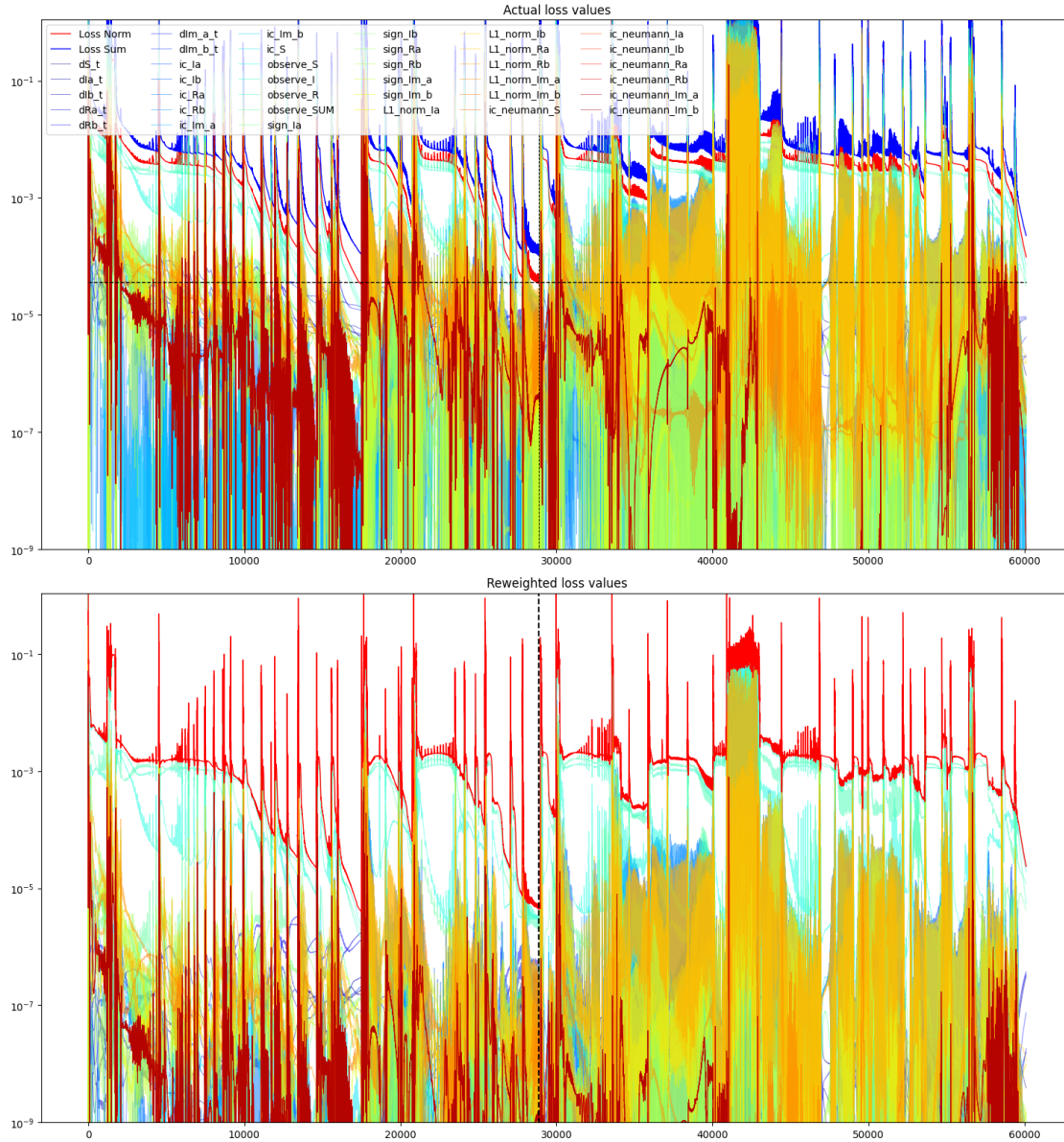


```
[ ]: params_nn, best_step = model.get_best_params(out_func=np.exp) # parameters need
    ↪ to be extracted with the exponential function as they have been modelled in
    ↪ logspace
    print(static_parameters, sep="\n")
    t_nn_param, wsol_nn_param, wsol_sird_nn_param = solver(*params_nn)

    model.set_synthetic_data(t_synth, solution_synth_full)
    model.set_nn_synthetic_data(t_nn_param, wsol_nn_param, wsol_sird_nn_param)
    plot = Plot(model, values_to_plot=sird_model.initial_conditions_keys) # class
    ↪ that contains plotting functions
    plot.show_known_and_prediction()
    plot.plot_param_history()
    plot.plot_loss_history()
```

```
Best train step: 28867
lambda_a: 1.5008877759545223
lambda_b: 1.6943118629846954
kappa_a: 0.11167805260458141
kappa_b: 0.3695164855562565
{'lambda_a': 2.2, 'lambda_b': 1.9, 'kappa_a': 0.8, 'kappa_b': 0.5}
```



```
[ ]: # model.set_synthetic_data(t_synth, solution_synth_full)
# model.set_nn_synthetic_data(t_nn_param, wsol_nn_param, wsol_sird_nn_param)
# plot = Plot(model, values_to_plot=sird_model.initial_conditions_keys) # class
# that contains plotting functions
# plot.show_known_and_prediction()
# plot.plot_param_history()
# plot.plot_loss_history()
```

```
[ ]: # from SIRD_normal_nn import SIRD_net
# max_timestep = 100000
# t_bool = t_synth < max_timestep
```

```
# t = t_synth[t_bool]
# wsol = solution_synth[t_bool]

# net = SIRD_net(t, wsol, init_num_people=1e6)
# net.train()
# net.plot(t_synth, solution_synth)
```

```
[ ]: # fig, ax = plt.subplots()
      # net.plot(ax, t_synth)
```

```
[ ]:
```