DiseaseModelPINN_notebook1

December 16, 2022

```python
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,
  ↪GeneralModelSolver
from Plot import Plot

# %matplotlib widget

seed = 1
np.random.seed(seed)
dde.config.set_random_seed(seed)
```

Using backend: pytorch

default Torch device: cpu

```python
time_delta = [0,2*350] # 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,
```

```python
#         "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,
#         }
```

```python
# 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": 0.11,
    "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)


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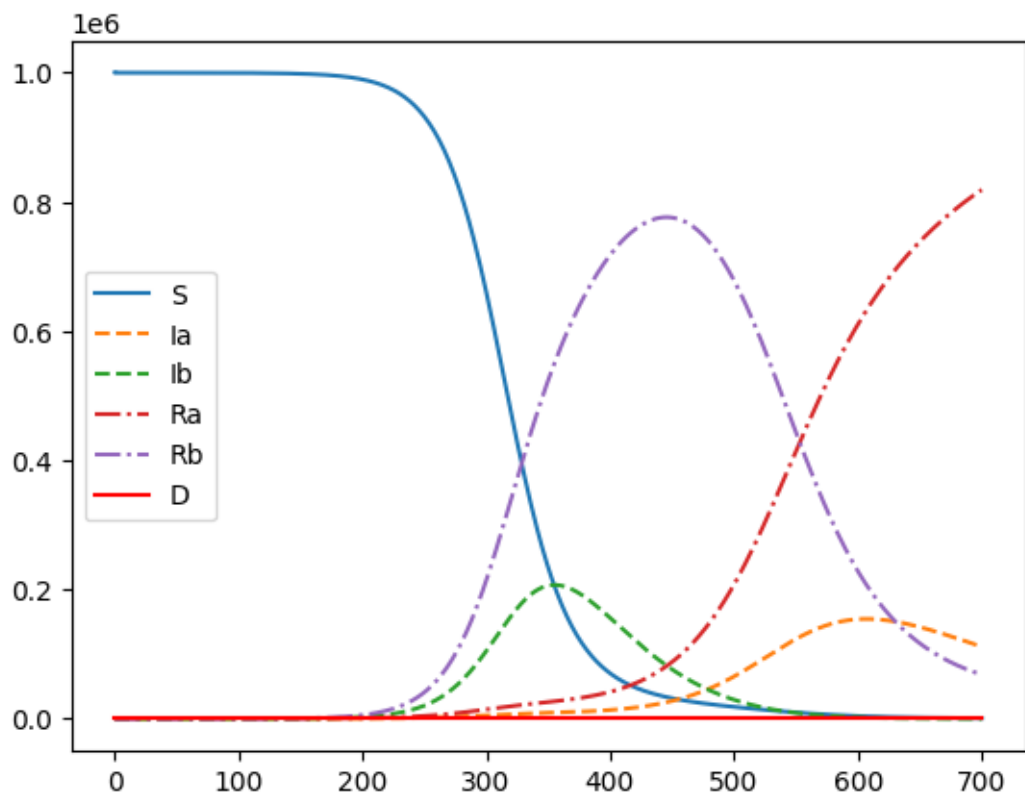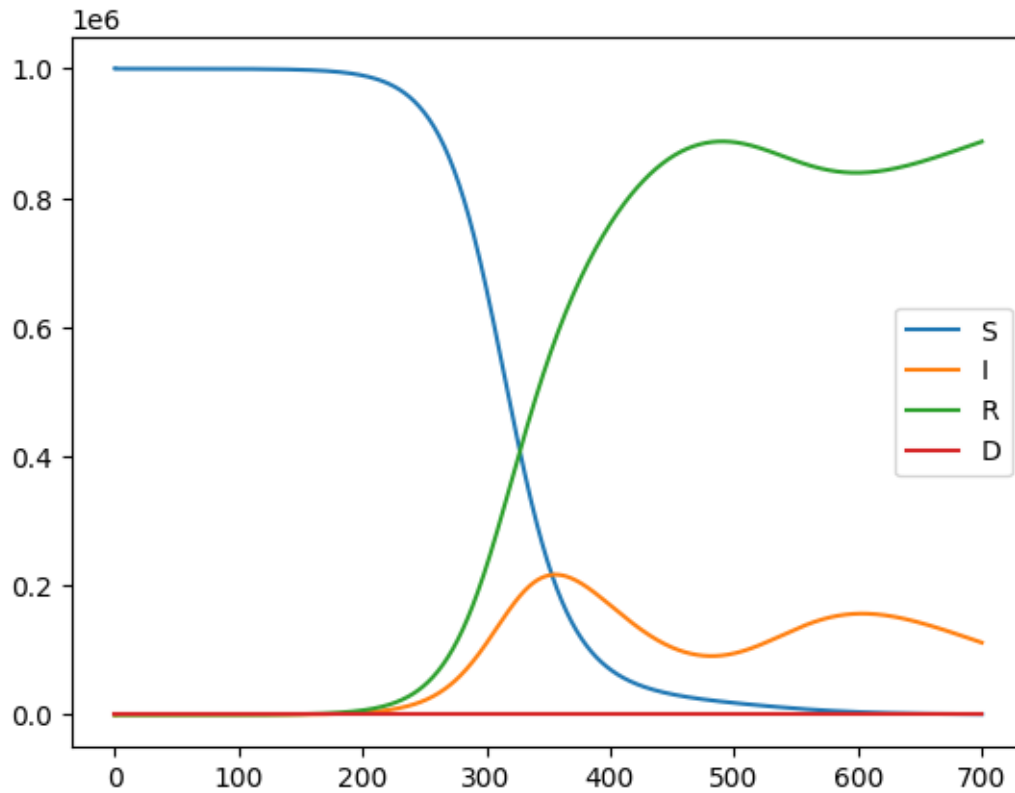
```
[ ]: print(sird_model)
```

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:
        alpha_a = 0.11
        alpha_b = 0.12
        beta_a = 0.08
        beta_b = 0.08
        gamma_a = 0.0
        gamma_b = 0.0
        kappa_a = 0.1
        kappa_b = 0.2

PDE groups and initial conditions:
        S = 1000000
        Ia = 1
        Ib = 0
        Ra = 0
        Rb = 0

```
        D = 0
        Im_a = 0
        Im_b = 0


    PDE equations:
        dS/dt = -(alpha_a/N)*Ia*S  -(alpha_b/N)*Ib*S
        dIa/dt = (alpha_a/N)*S*Ia + (alpha_a/N)*(1 - Im_a)*(Ra + Rb - D)*Ia -
    beta_a*Ia - gamma_a*Ia
        dIb/dt = (alpha_b/N)*S*Ib + (alpha_b/N)*(1 - Im_b)*(Ra + Rb - D)*Ib -
    beta_b*Ib - gamma_b*Ib
        dRa/dt = beta_a*Ia - (alpha_a/N)*(1 - (Im_a))*(Ra)*(Ia) - (alpha_b/N)*(1
    - (Im_b))*(Ra)*(Ib)
        dRb/dt = beta_b*Ib - (alpha_a/N)*(1 - (Im_a))*(Rb)*(Ia) - (alpha_b/N)*(1
    - (Im_b))*(Rb)*(Ib)
        dD/dt = gamma_a*Ia + gamma_b*Ib
        dIm_a/dt = kappa_a*beta_a*Ia/N
        dIm_b/dt = kappa_b*beta_b*Ib/N
    PINN PDE loss equations:
        dS_t - (-(alpha_a/N)*Ia*S  -(alpha_b/N)*Ib*S)
        dIa_t - ((alpha_a/N)*S*Ia + (alpha_a/N)*(1 - Im_a)*(Ra + Rb - D)*Ia -
    beta_a*Ia - gamma_a*Ia)
        dIb_t - ((alpha_b/N)*S*Ib + (alpha_b/N)*(1 - Im_b)*(Ra + Rb - D)*Ib -
    beta_b*Ib - gamma_b*Ib)
        dRa_t - (beta_a*Ia - (alpha_a/N)*(1 - (Im_a))*(Ra)*(Ia) - (alpha_b/N)*(1
    - (Im_b))*(Ra)*(Ib))
        dRb_t - (beta_b*Ib - (alpha_a/N)*(1 - (Im_a))*(Rb)*(Ia) - (alpha_b/N)*(1
    - (Im_b))*(Rb)*(Ib))
        dD_t - (gamma_a*Ia + gamma_b*Ib)
        dIm_a_t - (kappa_a*beta_a*Ia/N)
        dIm_b_t - (kappa_b*beta_b*Ib/N)
```

```python
# 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]
```

```python
model = SIRD_deepxde_net(t, wsol,disease_model=sird_model, with_neumann=False,
    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)
```

```
PINN model:
Parameters: ['alpha_a', 'alpha_b', 'beta_a', 'beta_b', 'gamma_a', 'gamma_b',
'kappa_a', 'kappa_b']
Loss measures: ['dS_t', 'dIa_t', 'dIb_t', 'dRa_t', 'dRb_t', 'dD_t', 'dIm_a_t',
'dIm_b_t', 'ic_Ia', 'ic_Ib', 'ic_Ra', 'ic_Rb', 'ic_D', 'ic_Im_a', 'ic_Im_b',
'ic_S', 'observe_S', 'observe_I', 'observe_R', 'observe_D', 'observe_SUM',
'sign_Ia', 'sign_Ib', 'sign_Ra', 'sign_Rb', 'sign_D', 'sign_Im_a', 'sign_Im_b']
Compiling model…
'compile' took 0.000064 s
```

```
[ ]: TOTAL_ITER = 2000
    plot_every=500
    # for n in range(TOTAL_ITER//plot_every):
    model.train_model(iterations=TOTAL_ITER, print_every=hyper_print_every,␣
     ↪use_LBFGSB=False)
    # params_nn = model.get_best_params()
    # params_nn= tuple(np.exp([*params_nn]))
    # print(*params_nn)
    # t_nn_param, wsol_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)
    # 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
28000     [1.56e-05, 4.49e-06, 2.44e-05, 8.76e-06, 3.27e-05, 3.28e-06, 4.46e-07,
2.60e-06, 1.94e-07, 5.68e-06, 2.09e-05, 2.08e-05, 1.53e-08, 3.92e-07, 4.92e-06,
5.81e-06, 6.64e-04, 5.49e-04, 7.39e-04, 1.09e-05, 9.22e-07, 1.10e-05, 4.95e-05,
6.30e-08, 3.02e-05, 1.09e-05, 9.17e-06, 2.05e-05]    [1.56e-05, 4.49e-06,
2.44e-05, 8.76e-06, 3.27e-05, 3.28e-06, 4.46e-07, 2.60e-06, 1.94e-07, 5.68e-06,
2.09e-05, 2.08e-05, 1.53e-08, 3.92e-07, 4.92e-06, 5.81e-06, 6.64e-04, 5.49e-04,
7.39e-04, 1.09e-05, 9.22e-07, 1.10e-05, 4.95e-05, 6.30e-08, 3.02e-05, 1.09e-05,
9.17e-06, 2.05e-05]    []
28100     [1.07e-05, 3.54e-06, 1.47e-05, 6.12e-06, 2.69e-05, 3.79e-06, 2.67e-07,
1.13e-06, 3.00e-06, 6.10e-05, 2.05e-04, 3.83e-04, 8.31e-07, 1.53e-06, 9.19e-06,
```

```
4.74e-05, 4.59e-03, 5.82e-04, 7.36e-03, 9.51e-06, 1.66e-04, 3.78e-06, 2.80e-06,
6.35e-06, 1.71e-04, 8.90e-06, 8.28e-06, 3.77e-05]    [1.07e-05, 3.54e-06,
1.47e-05, 6.12e-06, 2.69e-05, 3.79e-06, 2.67e-07, 1.13e-06, 3.00e-06, 6.10e-05,
2.05e-04, 3.83e-04, 8.31e-07, 1.53e-06, 9.19e-06, 4.74e-05, 4.59e-03, 5.82e-04,
7.36e-03, 9.51e-06, 1.66e-04, 3.78e-06, 2.80e-06, 6.35e-06, 1.71e-04, 8.90e-06,
8.28e-06, 3.77e-05]    []
Unexpected exception formatting exception. Falling back to standard exception

Traceback (most recent call last):
  File "/Users/jhh/Library/Mobile Documents/com~apple~CloudDocs/DTU/11Semester
Msc/Deep Learning/Deep_Learning_Project_PINN/.venv/lib/python3.9/site-
packages/IPython/core/interactiveshell.py", line 3433, in run_code
    exec(code_obj, self.user_global_ns, self.user_ns)
  File "/var/folders/8b/mml3g7gs5qxgxz__8ll8y5_40000gn/T/ipykernel_67682/4092164
500.py", line 4, in <module>
    model.train_model(iterations=TOTAL_ITER, print_every=hyper_print_every,
use_LBFGSB=False)
  File "/Users/jhh/Library/Mobile Documents/com~apple~CloudDocs/DTU/11Semester
Msc/Deep Learning/Deep_Learning_Project_PINN/exercises_Jakob/SIRD_deepxde_Diseas
eModel.py", line 286, in train_model
  File "/Users/jhh/Library/Mobile Documents/com~apple~CloudDocs/DTU/11Semester
Msc/Deep Learning/Deep_Learning_Project_PINN/.venv/lib/python3.9/site-
packages/deepxde/utils/internal.py", line 22, in wrapper
    result = f(*args, **kwargs)
  File "/Users/jhh/Library/Mobile Documents/com~apple~CloudDocs/DTU/11Semester
Msc/Deep Learning/Deep_Learning_Project_PINN/.venv/lib/python3.9/site-
packages/deepxde/model.py", line 679, in train
    self._train_sgd(iterations, display_every)
  File "/Users/jhh/Library/Mobile Documents/com~apple~CloudDocs/DTU/11Semester
Msc/Deep Learning/Deep_Learning_Project_PINN/.venv/lib/python3.9/site-
packages/deepxde/model.py", line 696, in _train_sgd
    self._train_step(
  File "/Users/jhh/Library/Mobile Documents/com~apple~CloudDocs/DTU/11Semester
Msc/Deep Learning/Deep_Learning_Project_PINN/.venv/lib/python3.9/site-
packages/deepxde/model.py", line 593, in _train_step
    self.train_step(inputs, targets)
  File "/Users/jhh/Library/Mobile Documents/com~apple~CloudDocs/DTU/11Semester
Msc/Deep Learning/Deep_Learning_Project_PINN/.venv/lib/python3.9/site-
packages/deepxde/model.py", line 410, in train_step
    self.opt.step(closure)
  File "/Users/jhh/Library/Mobile Documents/com~apple~CloudDocs/DTU/11Semester
Msc/Deep Learning/Deep_Learning_Project_PINN/.venv/lib/python3.9/site-
packages/torch/optim/optimizer.py", line 198, in wrapper
    out = func(*args, **kwargs)
  File "/Users/jhh/Library/Mobile Documents/com~apple~CloudDocs/DTU/11Semester
Msc/Deep Learning/Deep_Learning_Project_PINN/.venv/lib/python3.9/site-
packages/torch/optim/optimizer.py", line 29, in _use_grad
    ret = func(self, *args, **kwargs)
```

```
File "/Users/jhh/Library/Mobile Documents/com~apple~CloudDocs/DTU/11Semester
Msc/Deep Learning/Deep_Learning_Project_PINN/.venv/lib/python3.9/site-
packages/torch/optim/adam.py", line 237, in step
    loss = closure()
  File "/Users/jhh/Library/Mobile Documents/com~apple~CloudDocs/DTU/11Semester
Msc/Deep Learning/Deep_Learning_Project_PINN/.venv/lib/python3.9/site-
packages/deepxde/model.py", line 407, in closure
    total_loss.backward()
  File "/Users/jhh/Library/Mobile Documents/com~apple~CloudDocs/DTU/11Semester
Msc/Deep Learning/Deep_Learning_Project_PINN/.venv/lib/python3.9/site-
packages/torch/_tensor.py", line 484, in backward
    torch.autograd.backward(
  File "/Users/jhh/Library/Mobile Documents/com~apple~CloudDocs/DTU/11Semester
Msc/Deep Learning/Deep_Learning_Project_PINN/.venv/lib/python3.9/site-
packages/torch/autograd/__init__.py", line 197, in backward
    Variable._execution_engine.run_backward(  # Calls into the C++ engine to run
the backward pass
KeyboardInterrupt

During handling of the above exception, another exception occurred:

Traceback (most recent call last):
  File "/Users/jhh/Library/Mobile Documents/com~apple~CloudDocs/DTU/11Semester
Msc/Deep Learning/Deep_Learning_Project_PINN/.venv/lib/python3.9/site-
packages/IPython/core/interactiveshell.py", line 2052, in showtraceback
    stb = self.InteractiveTB.structured_traceback(
  File "/Users/jhh/Library/Mobile Documents/com~apple~CloudDocs/DTU/11Semester
Msc/Deep Learning/Deep_Learning_Project_PINN/.venv/lib/python3.9/site-
packages/IPython/core/ultratb.py", line 1118, in structured_traceback
    return FormattedTB.structured_traceback(
  File "/Users/jhh/Library/Mobile Documents/com~apple~CloudDocs/DTU/11Semester
Msc/Deep Learning/Deep_Learning_Project_PINN/.venv/lib/python3.9/site-
packages/IPython/core/ultratb.py", line 1012, in structured_traceback
    return VerboseTB.structured_traceback(
  File "/Users/jhh/Library/Mobile Documents/com~apple~CloudDocs/DTU/11Semester
Msc/Deep Learning/Deep_Learning_Project_PINN/.venv/lib/python3.9/site-
packages/IPython/core/ultratb.py", line 865, in structured_traceback
    formatted_exception = self.format_exception_as_a_whole(etype, evalue, etb,
number_of_lines_of_context,
  File "/Users/jhh/Library/Mobile Documents/com~apple~CloudDocs/DTU/11Semester
Msc/Deep Learning/Deep_Learning_Project_PINN/.venv/lib/python3.9/site-
packages/IPython/core/ultratb.py", line 818, in format_exception_as_a_whole
    frames.append(self.format_record(r))
  File "/Users/jhh/Library/Mobile Documents/com~apple~CloudDocs/DTU/11Semester
Msc/Deep Learning/Deep_Learning_Project_PINN/.venv/lib/python3.9/site-
packages/IPython/core/ultratb.py", line 736, in format_record
    result += ''.join(_format_traceback_lines(frame_info.lines, Colors,
self.has_colors, lvals))
```

```
  File "/Users/jhh/Library/Mobile Documents/com~apple~CloudDocs/DTU/11Semester
Msc/Deep Learning/Deep_Learning_Project_PINN/.venv/lib/python3.9/site-
packages/stack_data/utils.py", line 144, in cached_property_wrapper
    value = obj.__dict__[self.func.__name__] = self.func(obj)
  File "/Users/jhh/Library/Mobile Documents/com~apple~CloudDocs/DTU/11Semester
Msc/Deep Learning/Deep_Learning_Project_PINN/.venv/lib/python3.9/site-
packages/stack_data/core.py", line 734, in lines
    pieces = self.included_pieces
  File "/Users/jhh/Library/Mobile Documents/com~apple~CloudDocs/DTU/11Semester
Msc/Deep Learning/Deep_Learning_Project_PINN/.venv/lib/python3.9/site-
packages/stack_data/utils.py", line 144, in cached_property_wrapper
    value = obj.__dict__[self.func.__name__] = self.func(obj)
  File "/Users/jhh/Library/Mobile Documents/com~apple~CloudDocs/DTU/11Semester
Msc/Deep Learning/Deep_Learning_Project_PINN/.venv/lib/python3.9/site-
packages/stack_data/core.py", line 681, in included_pieces
    pos = scope_pieces.index(self.executing_piece)
  File "/Users/jhh/Library/Mobile Documents/com~apple~CloudDocs/DTU/11Semester
Msc/Deep Learning/Deep_Learning_Project_PINN/.venv/lib/python3.9/site-
packages/stack_data/utils.py", line 144, in cached_property_wrapper
    value = obj.__dict__[self.func.__name__] = self.func(obj)
  File "/Users/jhh/Library/Mobile Documents/com~apple~CloudDocs/DTU/11Semester
Msc/Deep Learning/Deep_Learning_Project_PINN/.venv/lib/python3.9/site-
packages/stack_data/core.py", line 660, in executing_piece
    return only(
  File "/Users/jhh/Library/Mobile Documents/com~apple~CloudDocs/DTU/11Semester
Msc/Deep Learning/Deep_Learning_Project_PINN/.venv/lib/python3.9/site-
packages/executing/executing.py", line 190, in only
    raise NotOneValueFound('Expected one value, found 0')
executing.executing.NotOneValueFound: Expected one value, found 0
```

```python
params_nn = model.get_best_params(out_func=np.exp) # parameters need to be
 extracted with the exponential functino as they have been modelled in
 logspace
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)
print(static_parameters, sep="\n")
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: 21450
alpha_a: 0.06304064124819105
alpha_b: 0.24498094528718772
```

```
beta_a: 0.027546424776009944
beta_b: 0.0928990158005352
gamma_a: 0.0003208634032008179
gamma_b: 0.00020575115325401687
kappa_a: 0.2316546651118463
kappa_b: 0.22876587059108575
{'alpha_a': 0.11, 'alpha_b': 0.12, 'beta_a': 0.08, 'beta_b': 0.08, 'gamma_a':
0.0, 'gamma_b': 0.0, 'kappa_a': 0.1, 'kappa_b': 0.2}
```

Actual loss values

Reweighted loss values