# Missile 2feats plusMaxRange

### January 17, 2023

```
[1]: write_images = False
     wirte_output_txt = False
     # Specify everytime Simulation is called
     # WARNING --> Set to False when running more then 10 simulations
                  (otherwise it will be super slow and might crash)
[2]: import numpy as np
[3]: from emukit.core import ContinuousParameter, ParameterSpace
     from emukit.core.initial_designs import RandomDesign
     import GPy
     from GPy.models import GPRegression
     from emukit.model_wrappers import GPyModelWrapper
     from emukit.sensitivity.monte_carlo import MonteCarloSensitivity
     import matplotlib.pyplot as plt
     import mlai.plot as plot
[4]: %run Missile_utils.ipynb
[]:
[5]: simulation_output = 'range'
     # We divide by 1000 to avoid dealing with too large numbers
[6]: run_grid_simulation = True # If true takes much longer and does 3D plots and so on for_
      \hookrightarrow MODEL with 2 FEATS
[]:
    We consider missiles with only 1 stage
[7]: basic_param_spaces = {
         'payload': [10, 2410],
         'missilediam': [0.1, 9.9],
         'rvdiam': [0.1, 9.9],
         'estrange': [100, 4900],
         'fuelmass': [500, 6000], # [500, 6000],
         'drymass': [1000, 3000],
         'Isp0': [100, 800],# [100, 800],
```

```
'thrust0': [10000, 69000],
}

[8]: from sklearn.metrics import mean_squared_error
import math

def compute_rmse(y_actual, y_predicted):
    MSE = mean_squared_error(y_actual, y_predicted)
    RMSE = math.sqrt(MSE)

    return RMSE

def evaluate_prediction(y_actual, y_predicted):
    return compute_rmse(y_actual, y_predicted)
```

# 1 1. Two params

```
[10]: def run_missile_sim(custom_params):
          Recives in input an array of custom parameters.
          Each row represents a set of different parameters
          Each column is a different parameter (#cols = len(custom_param_names))
          default_params_IRAQ = {
               'payload':500,
               'missilediam':0.88,
               'rvdiam':0,
               'estrange':600,
               'numstages':1,
               'fuelmass':[0,5600],
               'drymass':[0,1200],
               'Isp0': [0,226],
               'thrust0': [0,9177.4]
          }
          y = np.zeros((custom_params.shape[0], 1))
```

```
for i in range(custom_params.shape[0]):
        params_to_use = default_params_IRAQ
        # Overwrite default param variables
        for j in range(custom_params.shape[1]):
            param_name = custom_param_names[j]
            if param_name in ['fuelmass', 'drymass', 'Isp0', 'thrust0']:
                params_to_use[param_name][1] = custom_params[i,j]
                params_to_use[param_name] = custom_params[i, j]
            if j==0:
                print('\nNew simulation \n')
            str_to_print = param_name + ': ' + str(custom_params[i,j])
            print(str_to_print)
        # Run simulation
        output_path = 'results/results_' + str(i) + '.txt'
        sim_output = run_one_sim(
            numstages=params_to_use["numstages"],
            fuelmass=params_to_use["fuelmass"],
            drymass=params_to_use["drymass"],
            thrust0=params_to_use["thrust0"],
            Isp0=params_to_use["Isp0"],
            payload=params_to_use["payload"],
            missilediam=params_to_use["missilediam"],
            rvdiam=params_to_use["rvdiam"],
            est_range=params_to_use["estrange"],
            output_path=output_path,
            simulation_output=simulation_output,
        )
        y[i, 0] = sim_output
   return y
def neg_run_missile_sim(custom_params):
    return -run_missile_sim(custom_params)
```

#### 1.1 1. Experimental design

#### 1.1.1 Use model-free experimental design to start

(RandomDesign or Latin Design)

```
[11]: wirte_output_txt = True

# from emukit.core.initial_designs.latin_design import LatinDesign
# design = LatinDesign(parameter_space)

m2_design = RandomDesign(m2_space)
m2_x = m2_design.get_samples(3*2)
```

## m2\_y = neg\_run\_missile\_sim(m2\_x)

#### New simulation

fuelmass: 2461.699830729682
Isp0: 486.9259736726181

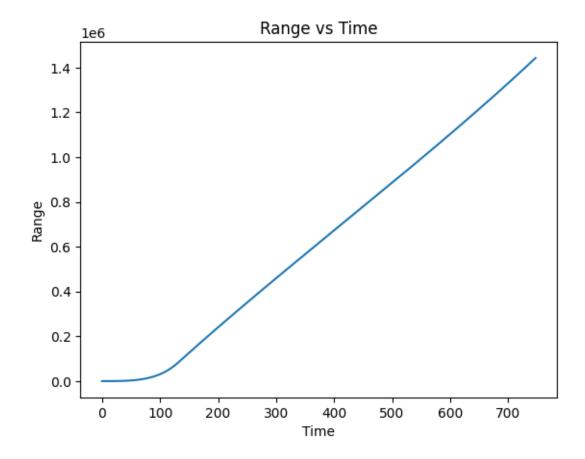
Stage 1 burnout

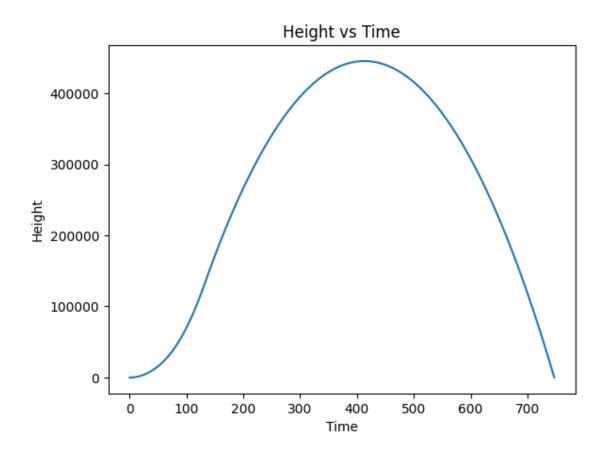
Velocity (km/s): 3.2928421666750873 Angle (deg h): 43.654711759668814 Range (km): 81.70654746630755 Time (sec): 130.5999999999687

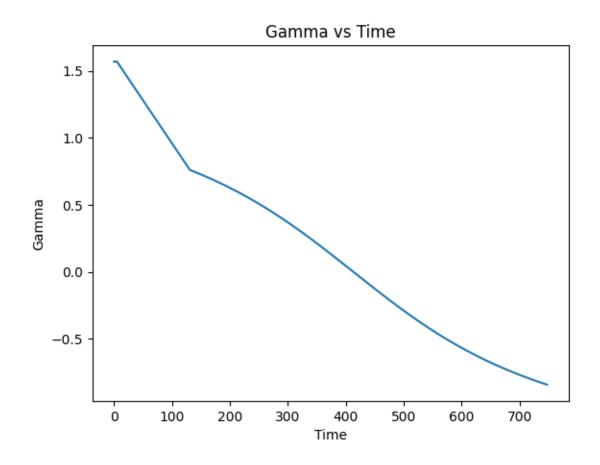
Final results:

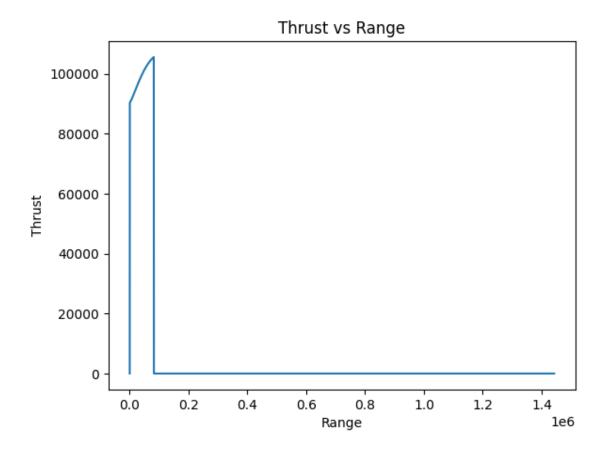
Range (km): 1443.036540282888 Apogee (km): 445.40587370665315

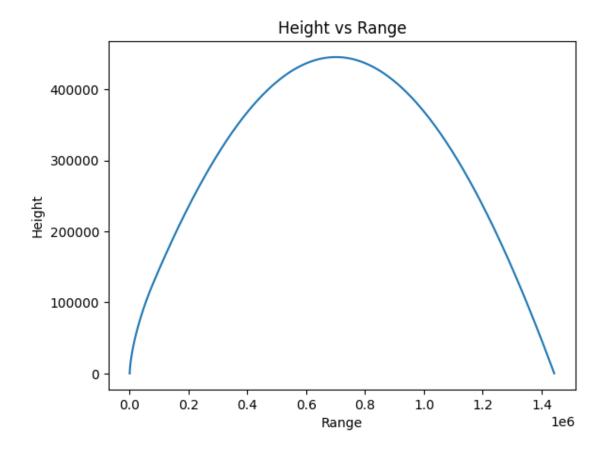
Time to target (sec): 747.300000001014











Data written to 'results/results\_0.txt'

New simulation

fuelmass: 920.1477703768564
Isp0: 599.8626891636919

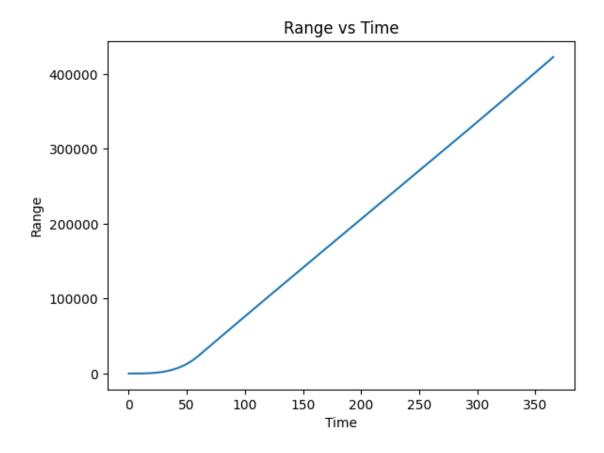
Stage 1 burnout

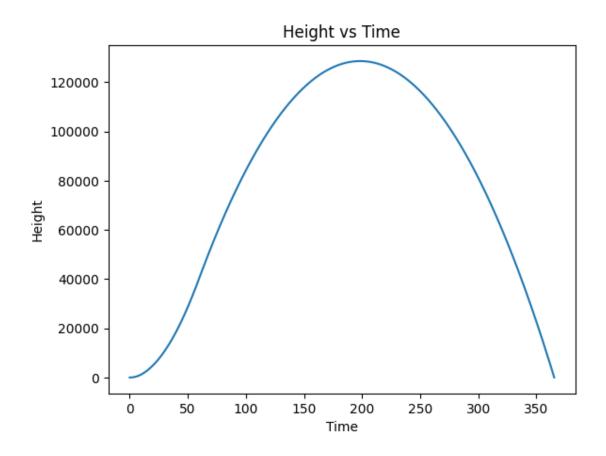
Velocity (km/s): 1.8475465441910104 Angle (deg h): 43.666929694041904 Range (km): 23.859429394146524 Time (sec): 60.20000000000585

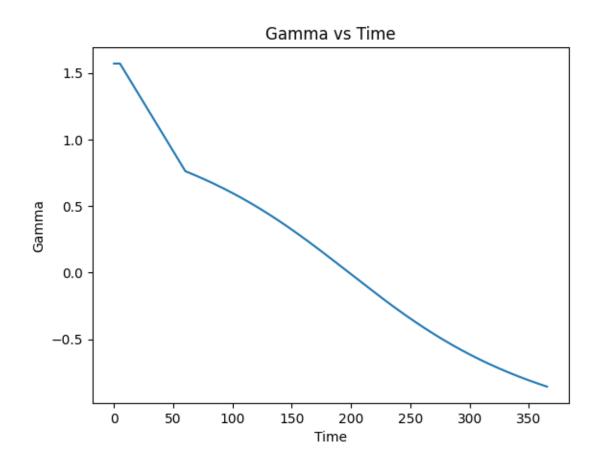
Final results:

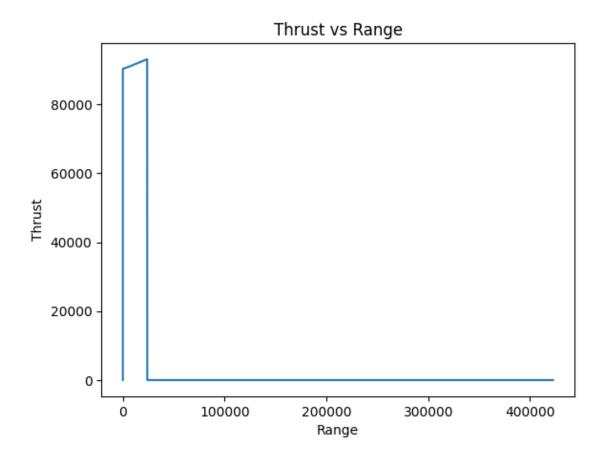
Range (km): 422.7984243339626 Apogee (km): 128.53208806192185

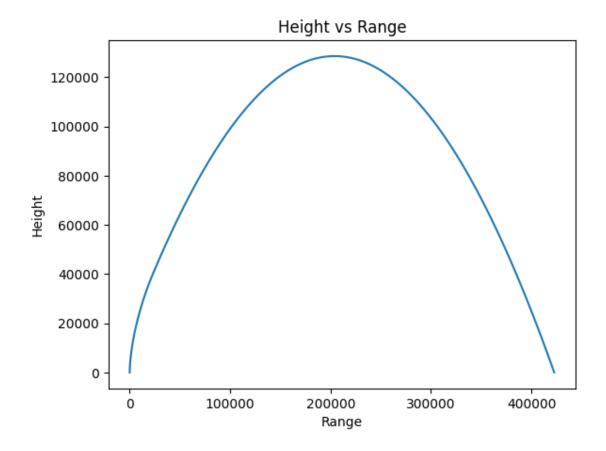
Time to target (sec): 365.400000000146











Data written to 'results/results\_1.txt'

New simulation

fuelmass: 5672.14884132695
Isp0: 167.5983593012405

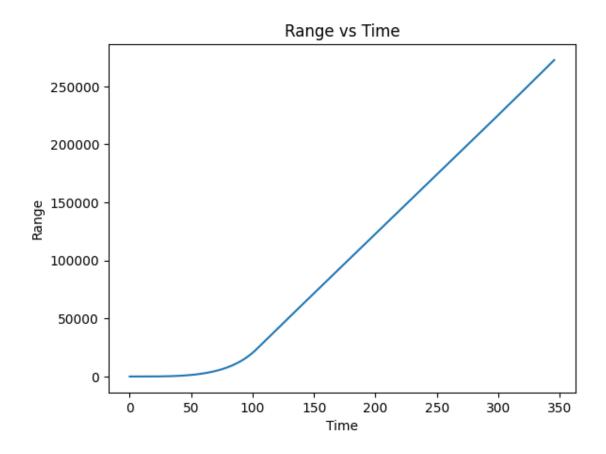
Stage 1 burnout

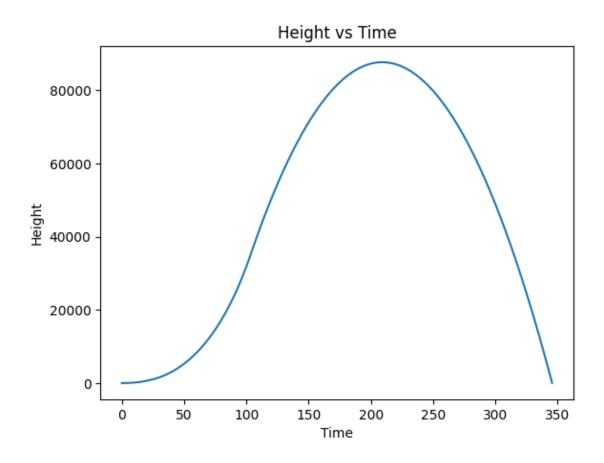
Velocity (km/s): 1.4417597535653883 Angle (deg h): 43.66386706640104 Range (km): 23.8802344333796 Time (sec): 103.5999999999839

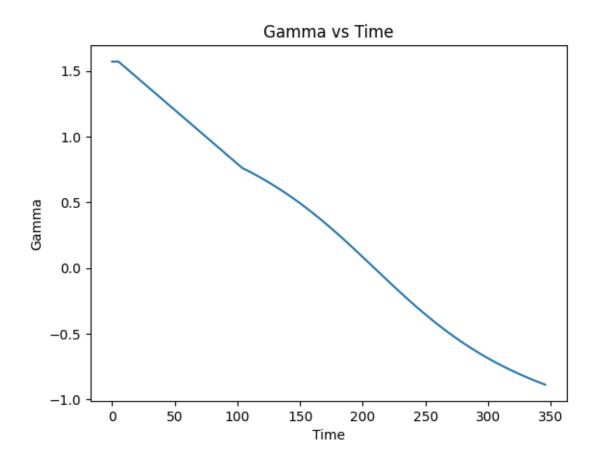
Final results:

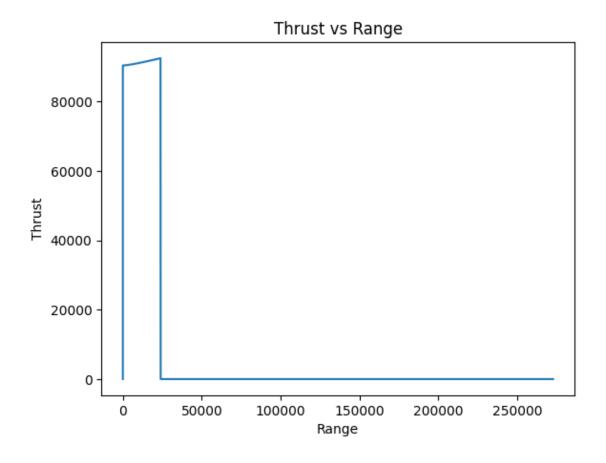
Range (km): 272.7963038431324 Apogee (km): 87.67103398367681

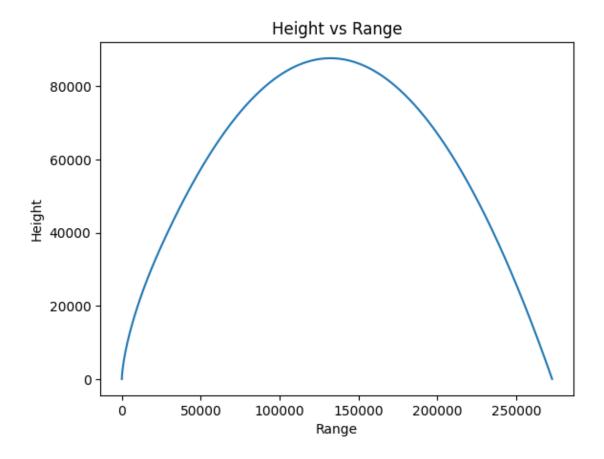
Time to target (sec): 345.700000000101











Data written to 'results/results\_2.txt'

New simulation

fuelmass: 1289.4787352316134
Isp0: 666.2904956492962

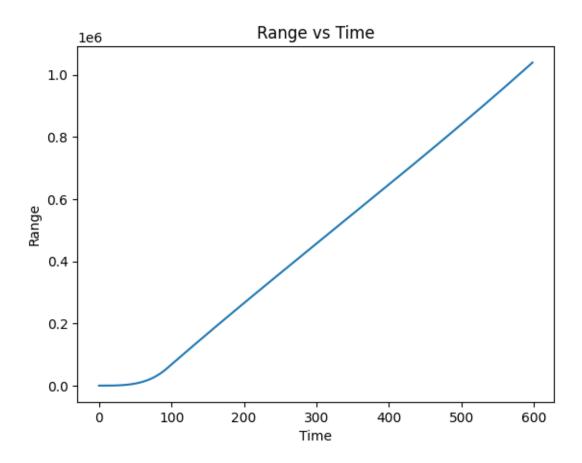
Stage 1 burnout

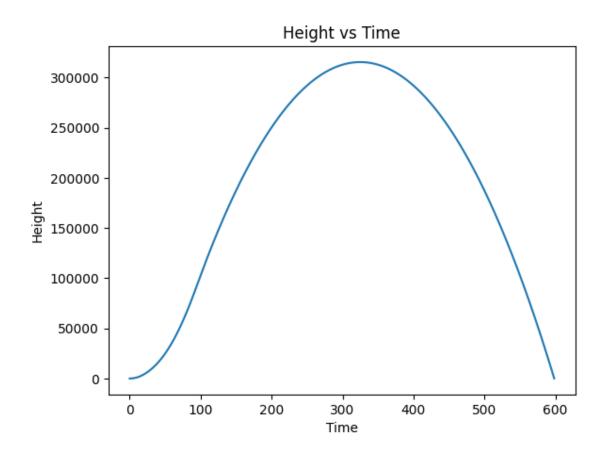
Velocity (km/s): 2.846157313086886 Angle (deg h): 43.660083041406125 Range (km): 55.14622505917165 Time (sec): 93.59999999999896

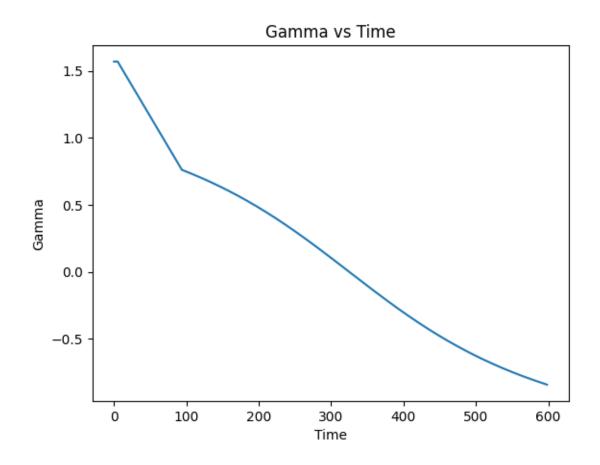
Final results:

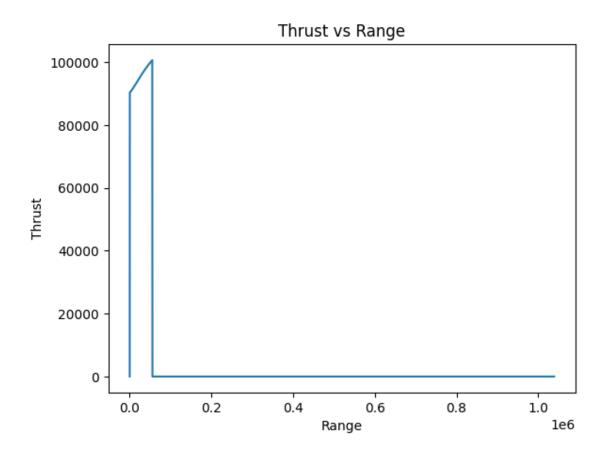
Range (km): 1039.241717666173 Apogee (km): 315.47440889796735

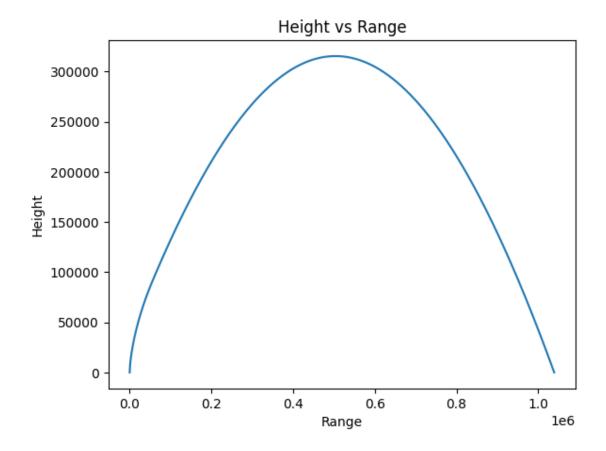
Time to target (sec): 598.400000000675











Data written to 'results/results\_3.txt'

New simulation

fuelmass: 5884.749310520711 Isp0: 614.8107619645466

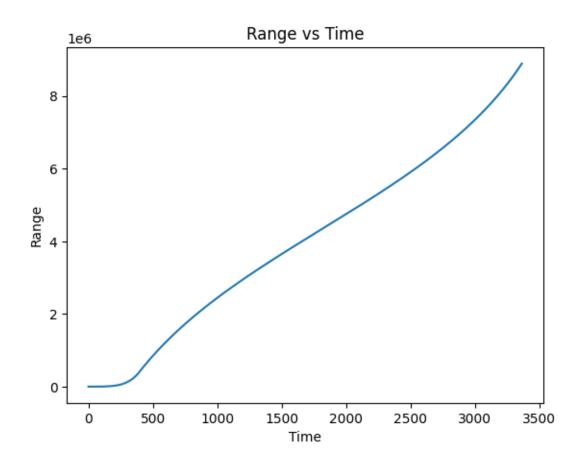
Stage 1 burnout

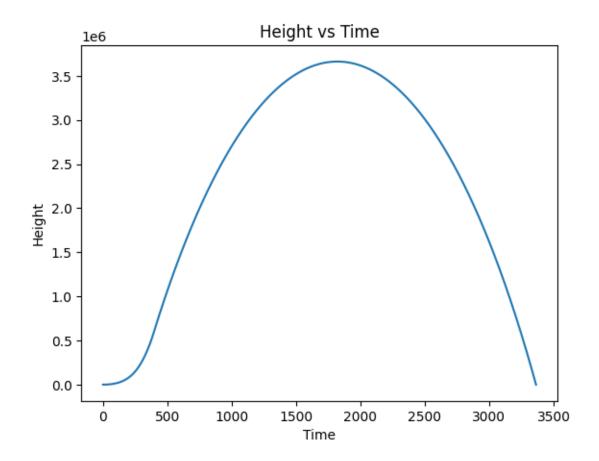
Velocity (km/s): 6.840928406755898 Angle (deg h): 43.65348191761386 Range (km): 400.33202594915537 Time (sec): 394.3000000002116

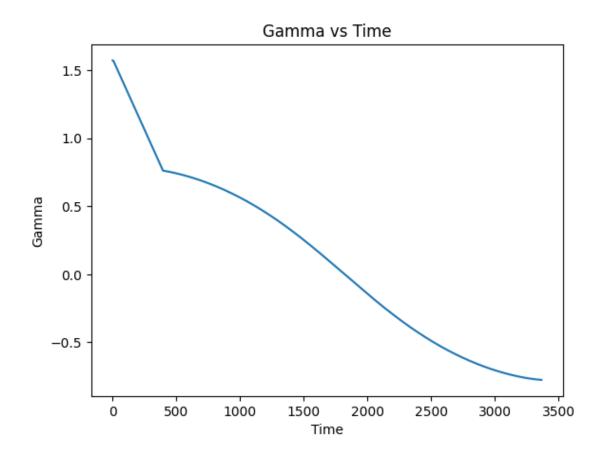
Final results:

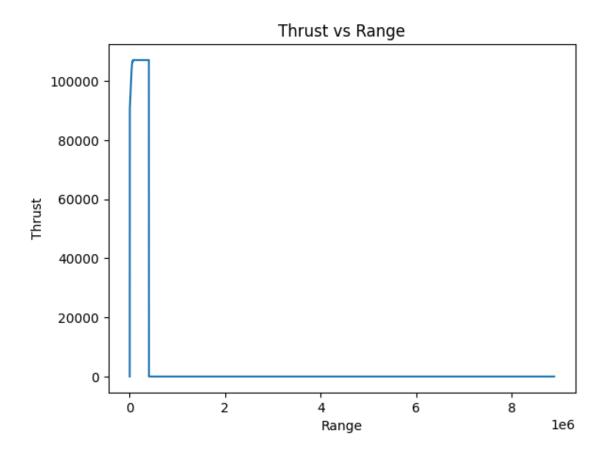
Range (km): 8896.112873729066 Apogee (km): 3662.845779804255

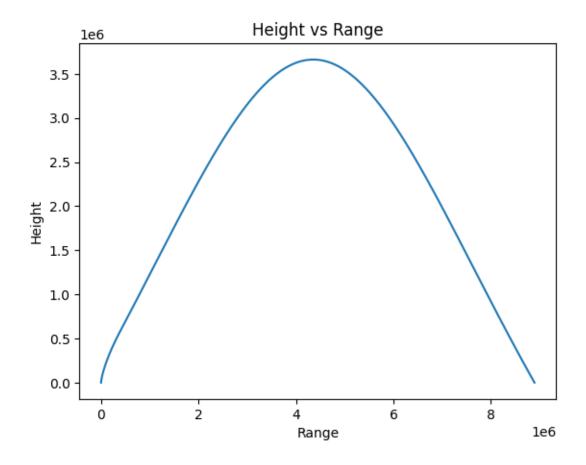
Time to target (sec): 3364.199999980358











Data written to 'results/results\_4.txt'

New simulation

fuelmass: 984.2424643743145
Isp0: 562.9484052008906

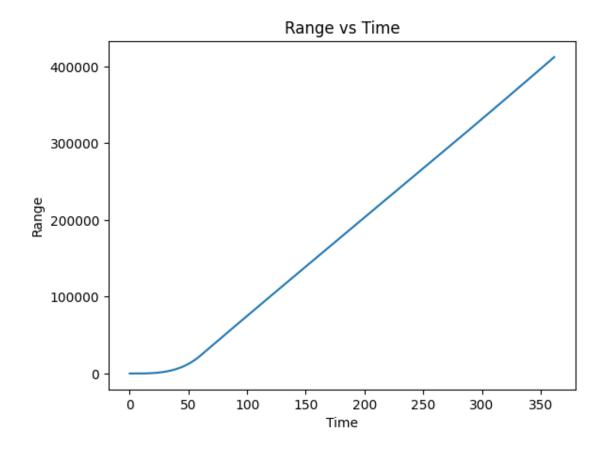
# Stage 1 burnout

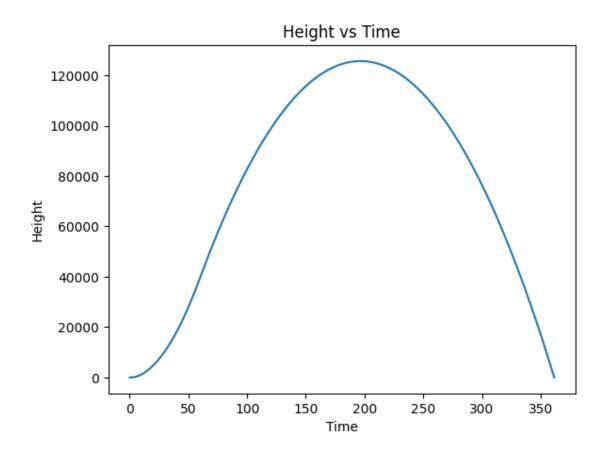
Velocity (km/s): 1.8239142293971027 Angle (deg h): 43.69201511792158 Range (km): 23.533022260837498 Time (sec): 60.4000000000059

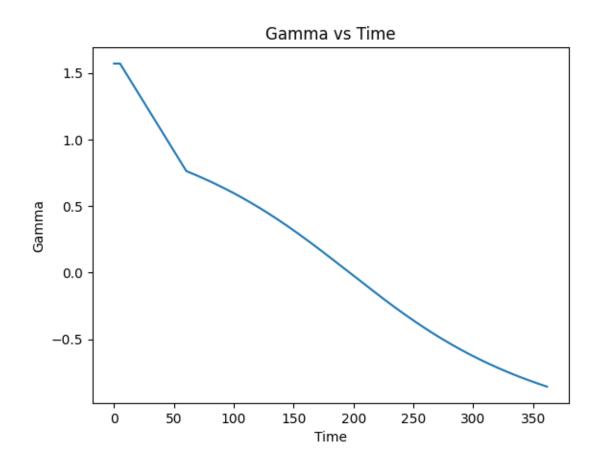
Final results:

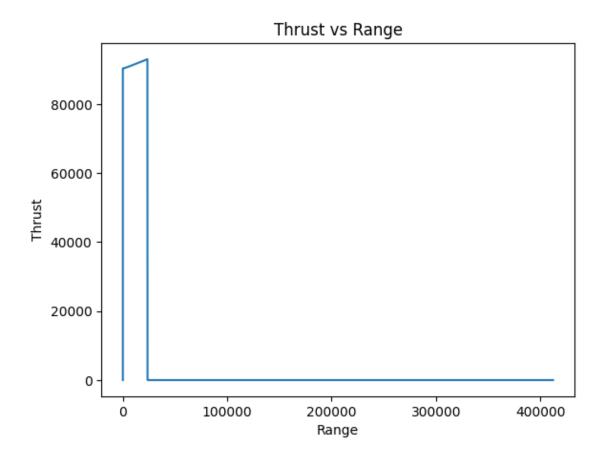
Range (km): 412.37779861564456 Apogee (km): 125.66449326051323

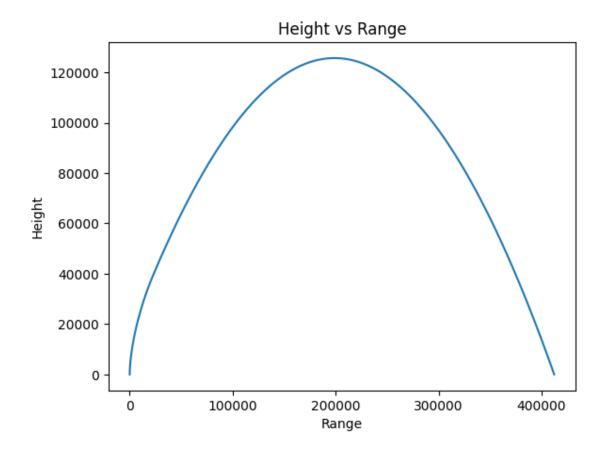
Time to target (sec): 361.7000000001374











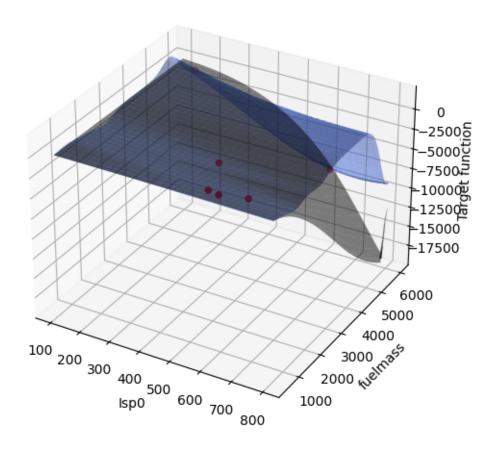
Data written to 'results/results\_5.txt'

```
[12]: # Build model
      m2\_var\_kernel = (100)**2
      m2_lengthscale = 100 # 100 # 1
      m2_var_noise = 1e-5 # small value
      #kern = GPy.kern.RBF(input_dim=2, lengthscale=lengthscale, variance =var_kernel) # ,u
      → lengthscale=0.08, variance=20
      # kern = GPy.kern.Matern32(input_dim=1)
      # kern = GPy.kern.Linear(input_dim=1)
      constrain_lengthscale = True
      m2_rbf_kern = GPy.kern.RBF(input_dim=2, lengthscale=m2_lengthscale)
      if constrain_lengthscale:
          \verb|m2_rbf_kern.lengthscale.constrain_bounded(m2_lengthscale, m2_lengthscale*1e12)|
      # m2_kern = m2_rbf_kern + \
            GPy.kern.Linear(input_dim=2)
      m2_kern = (GPy.kern.RBF(input_dim=2, lengthscale=500) * \
                 GPy.kern.RBF(input_dim=2, lengthscale=100)) * \
          GPy.kern.Linear(input_dim=2)
      \# m2\_kern = m2\_rbf\_kern
```

```
m2_model_gpy = GPRegression(m2_x,m2_y, kernel=m2_kern)
      m2_model_gpy.kern.variance = m2_var_kernel
      m2_model_gpy.likelihood.variance.fix(m2_var_noise)
      display(m2_model_gpy)
     reconstraining parameters rbf.lengthscale
     <GPy.models.gp_regression.GPRegression at 0x7fba29a8d2d0>
[13]: \# m2\_model\_qpy\_opt = m2\_model\_qpy
      # m2_model_gpy_opt.optimize()
      # m2_model_gpy_opt.plot()
[14]: m2_model_emukit = GPyModelWrapper(m2_model_gpy)
      m2_model_emukit.optimize()
[15]: display(m2_model_gpy)
     <GPy.models.gp_regression.GPRegression at 0x7fba29a8d2d0>
[16]: # Create data for plot
      wirte_output_txt = False
      nr_points_plot = 101
      m2_param_1_x_plot = np.linspace(m2_space.parameters[0].min, m2_space.parameters[0].
      →max, nr_points_plot)[:, None]
      m2_param_2_x_plot = np.linspace(m2_space.parameters[1].min, m2_space.parameters[1].
      →max, nr_points_plot)[:, None]
      m2_x_plot_mesh, m2_y_plot_mesh = np.meshgrid(m2_param_1_x_plot, m2_param_2_x_plot)
      m2_x_plot = np.array([m2_x_plot_mesh, m2_y_plot_mesh]).T.reshape(-1,2)
      # TEMP read data from txt
      # np.savetxt('test1.txt', a, fmt='%f')
      \# m2\_y\_plot = np.loadtxt('m2\_y\_plot\_neg.txt', dtype=float)[:,None]
      if run_grid_simulation:
          m2_y_plot = neg_run_missile_sim(m2_x_plot) # TAKES LONG TIME
          m2_Z = m2_y_plot.reshape(m2_x_plot_mesh.shape)
[17]: m2_x
[17]: array([[2461.69983073, 486.92597367],
             [ 920.14777038, 599.86268916],
             [5672.14884133, 167.5983593],
             [1289.47873523, 666.29049565],
             [5884.74931052, 614.81076196],
             [ 984.24246437, 562.9484052 ]])
[18]: # Compute current prediction
      m2_mu_plot_grid_pred1, var_plot_grid_pred1 = m2_model_emukit.predict(m2_x_plot)
      m2_mu_plot_pred1 = m2_mu_plot_grid_pred1.reshape(m2_x_plot_mesh.shape)
      m2_var_plot_pred1 = var_plot_grid_pred1.reshape(m2_x_plot_mesh.shape)
```

RMSE m2 (before experiment design loop): 3903.7185215433874

```
[19]: if run_grid_simulation:
          # 3D Plot
          add_bands = False
          # REVERSE
          fig = plt.figure()
          ax = fig.add_subplot(projection='3d')
          # True surface
          surf = ax.plot_surface(m2_y_plot_mesh, m2_x_plot_mesh, (m2_Z).transpose(),
                                 alpha = .5,
                                 label='target function',
                                 color='black'
          # Mean predicted
          surf = ax.plot_surface(m2_y_plot_mesh, m2_x_plot_mesh, (m2_mu_plot_pred1).
       →transpose(),
                                 alpha = .5,
                                 label='model', # Mean
                                 color='royalblue'
          # True points observed
          ax.scatter(m2_x[:,1], m2_x[:,0], m2_y, marker='o', color='red')
          ax.set_xlabel(m2_param_2)
          ax.set_ylabel(m2_param_1)
          ax.set_zlabel('Target function')
          plt.tight_layout()
```



```
[20]: if run_grid_simulation:
          from matplotlib import colors
          divnorm=colors.TwoSlopeNorm(vcenter=0.) # vmin=-5., vcenter=0., vmax=10
          ## Heatmaps
          extents = [m2_space.parameters[1].min, m2_space.parameters[1].max,
                     m2_space.parameters[0].min, m2_space.parameters[0].max]
          # True values
          fig, ax = plt.subplots()
          im = ax.imshow(m2_Z, extent=extents, aspect='auto', origin='lower')
          ax.set_title('Target function')
          ax.set_xlabel(m2_param_2)
          ax.set_ylabel(m2_param_1)
          fig.colorbar(im, ax=ax)
          fig.show()
          # Model
          fig, ax = plt.subplots()
          im = ax.imshow(m2_mu_plot_pred1, extent=extents, aspect='auto', origin='lower')
          ax.set_title('Model (mean)')
```

```
ax.set_xlabel(m2_param_2)
   ax.set_ylabel(m2_param_1)
   fig.colorbar(im, ax=ax)
   fig.show()
   # Difference
   fig, ax = plt.subplots()
   vmin = (m2_mu_plot_pred1-m2_Z).min()
   vmax = (m2_mu_plot_pred1-m2_Z).max()
   vmin_max = max(abs(vmin), abs(vmax))
   divnorm=colors.TwoSlopeNorm(vcenter=0., vmin=-vmin_max, vmax=vmin_max) # vmin=-5.,u
\rightarrow vcenter=0., vmax=10
   im = ax.imshow(m2_mu_plot_pred1-m2_Z, extent=extents, aspect='auto', cmap="bwr",_
→norm=divnorm, origin='lower')
   ax.set_title('Difference between model and target function')
   ax.set_xlabel(m2_param_2)
   ax.set_ylabel(m2_param_1)
   # Add points where simulation evaluated
   ax.plot(m2_x[:,1], m2_x[:,0], 'ro')
   fig.colorbar(im, ax=ax)
   fig.show()
```

/var/folders/98/fv11ygzs4p51c21s8jln0jzc0000gn/T/ipykernel\_12821/375354680.py:1
6: UserWarning:Matplotlib is currently using
module://matplotlib\_inline.backend\_inline, which is a non-GUI backend, so cannot

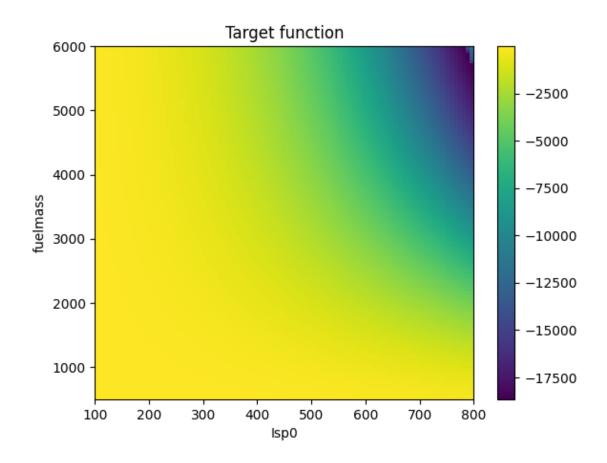
module://matplotlib\_inline.backend\_inline, which is a non-GUI backend, so cannot show the figure.

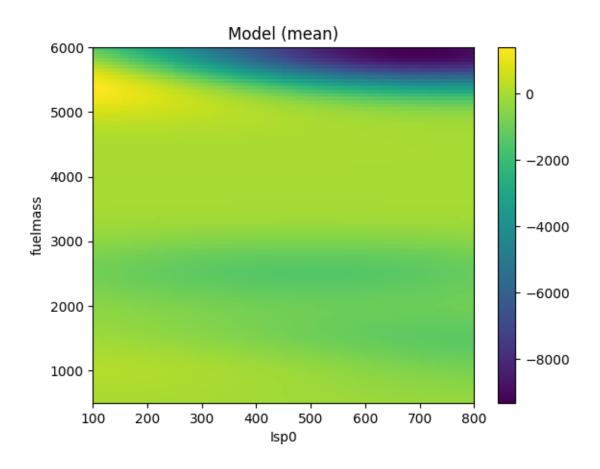
/var/folders/98/fv11ygzs4p51c21s8jln0jzc0000gn/T/ipykernel\_12821/375354680.py:2
5: UserWarning:Matplotlib is currently using

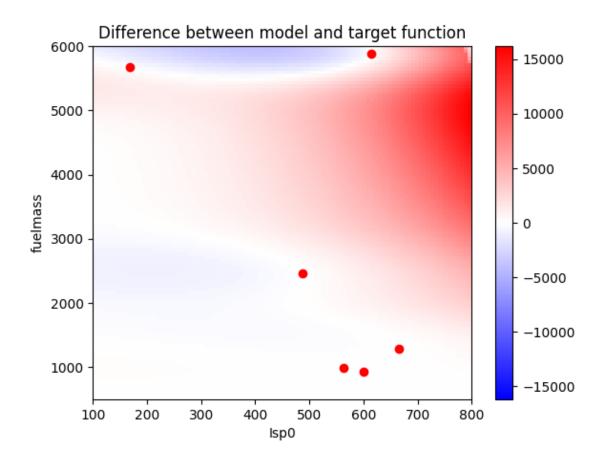
module://matplotlib\_inline.backend\_inline, which is a non-GUI backend, so cannot show the figure.

/var/folders/98/fv11ygzs4p51c21s8jln0jzc0000gn/T/ipykernel\_12821/375354680.py:4
1: UserWarning:Matplotlib is currently using
module://matplotlib\_inline.backend\_inline, which is a non-GUI backend, so cannot

show the figure.







# 1.1.2 Use the model created for model-based experimental design

use the model to decide which are the best points to collect using some data collection criteria (acquisition function).

```
[22]: from emukit.experimental_design.experimental_design_loop import ExperimentalDesignLoop from emukit.experimental_design.acquisitions import IntegratedVarianceReduction, 

→ ModelVariance

[23]: # help(ExperimentalDesignLoop)

[24]: m2_2_model_emukit = m2_model_emukit
```

# 

### New simulation

fuelmass: 4878.682066574241
Isp0: 461.4762727822375

Stage 1 burnout

Velocity (km/s): 4.60441860679277 Angle (deg h): 43.654584270916445 Range (km): 180.9857845303747 Time (sec): 245.299999999935

Final results:

Range (km): 3158.6045364931383 Apogee (km): 1024.5547134484984

Time to target (sec): 1305.59999999998

# New simulation

fuelmass: 4063.558783485642
Isp0: 453.93151760855153

Stage 1 burnout

Velocity (km/s): 4.148526147315459 Angle (deg h): 43.6658239525756 Range (km): 141.29851062716125 Time (sec): 200.9999999999287

Final results:

Range (km): 2455.4076192902166 Apogee (km): 780.1861276418522

Time to target (sec): 1080.500000001128

### New simulation

fuelmass: 3359.559699489315
Isp0: 454.40837486922806

Stage 1 burnout

Velocity (km/s): 3.7347111955387606 Angle (deg h): 43.65568417600361 Range (km): 110.61947219954926 Time (sec): 166.3999999999483

Final results:

Range (km): 1921.834343633677 Apogee (km): 601.3264485166641

Time to target (sec): 908.800000001381

#### New simulation

fuelmass: 5294.398743759096
Isp0: 539.4919760902346

Stage 1 burnout

Velocity (km/s): 5.695852002695544 Angle (deg h): 43.652577078192486 Range (km): 275.74542902940306 Time (sec): 311.300000000023

Final results:

Range (km): 5391.4508728134 Apogee (km): 1883.2069889190313

Time to target (sec): 1993.699999992822

# New simulation

fuelmass: 3408.998763550249
Isp0: 415.6613997100321

Stage 1 burnout

Velocity (km/s): 3.3727624303170067 Angle (deg h): 43.67239006023836 Range (km): 92.78530499827153 Time (sec): 154.3999999999552

Final results:

Range (km): 1536.594448949843 Apogee (km): 478.9712769531256

Time to target (sec): 796.400000001125

/Users/ilariasartori/opt/anaconda3/envs/mlphysical/lib/python3.10/site-packages/paramz/transformations.py:111: RuntimeWarning:overflow encountered in expm1

New simulation

fuelmass: 2896.2379759805713 Isp0: 331.12115826598097

Stage 1 burnout

Velocity (km/s): 2.302811097766833 Angle (deg h): 43.67993464313428 Range (km): 45.242701936516895 Time (sec): 104.4999999999834

Final results:

Range (km): 683.8659833643062 Apogee (km): 212.4717865973708

Time to target (sec): 502.0000000004565

New simulation

fuelmass: 4302.336283094621
Isp0: 109.29918212473977

Stage 1 burnout

Velocity (km/s): 0.8040715537876274 Angle (deg h): 43.64002781579093 Range (km): 7.515094916182927 Time (sec): 51.30000000000046

Final results:

Range (km): 84.6779995910292 Apogee (km): 27.832012844593667

Time to target (sec): 184.499999999988

New simulation

fuelmass: 5477.659772906554
Isp0: 572.3713751105622

Stage 1 burnout

Velocity (km/s): 6.165465906582221 Angle (deg h): 43.652665713593436 Range (km): 322.98278611907114 Time (sec): 341.700000000092

Final results:

Range (km): 6665.66385236041 Apogee (km): 2454.426413741662

Time to target (sec): 2435.2999999988806

/Users/ilariasartori/opt/anaconda3/envs/mlphysical/lib/python3.10/site-packages/GPy/kern/src/stationary.py:168: RuntimeWarning:overflow encountered in

### divide

/Users/ilariasartori/opt/anaconda3/envs/mlphysical/lib/python3.10/site-packages/GPy/kern/src/rbf.py:76: RuntimeWarning:invalid value encountered in multiply

### New simulation

fuelmass: 2260.443240465954 Isp0: 163.12095340257792

Stage 1 burnout

Velocity (km/s): 0.8696399980272381 Angle (deg h): 43.70693234408902 Range (km): 7.148694549839851 Time (sec): 40.200000000003

Final results:

Range (km): 96.08810747152313 Apogee (km): 30.95470331963349

Time to target (sec): 182.399999999992

# New simulation

fuelmass: 4858.534711073726
Isp0: 690.8678746429392

Stage 1 burnout

Velocity (km/s): 7.282476943800215 Angle (deg h): 43.65652882926793 Range (km): 423.61641898494685 Time (sec): 365.8000000000147

Final results:

Range (km): 10508.38724670863 Apogee (km): 4779.527743628276

Time to target (sec): 4161.69999997609

## New simulation

fuelmass: 5201.95186360266 Isp0: 182.18562042460977

Stage 1 burnout

Velocity (km/s): 1.543963902919711 Angle (deg h): 43.657267408173055 Range (km): 26.244727751061593 Time (sec): 103.299999999984

Range (km): 311.52260811939465 Apogee (km): 99.66079834232968

Time to target (sec): 362.90000000014

#### New simulation

fuelmass: 4382.367256166273 Isp0: 583.5270161047214

Stage 1 burnout

Velocity (km/s): 5.759430979309827 Angle (deg h): 43.65557522375997 Range (km): 265.62123014250244 Time (sec): 278.6999999999999

Final results:

Range (km): 5508.384487262774 Apogee (km): 1928.2628851721356

Time to target (sec): 1997.499999992788

#### New simulation

fuelmass: 3798.4939118156003
Isp0: 669.0055434316113

Stage 1 burnout

Velocity (km/s): 6.269029188826729 Angle (deg h): 43.665853106098794 Range (km): 297.9843220169598 Time (sec): 276.8999999999446

Final results:

Range (km): 6867.107278116062 Apogee (km): 2542.7983191009175

Time to target (sec): 2442.69999998874

# New simulation

fuelmass: 1663.9494898800779
Isp0: 321.15414775099043

Stage 1 burnout

Velocity (km/s): 1.4861658425338886 Angle (deg h): 43.649248537620174 Range (km): 17.901050240157193 Time (sec): 58.3000000000056

Range (km): 276.50437057575783 Apogee (km): 85.86155110888325

Time to target (sec): 302.3000000000024

#### New simulation

fuelmass: 2829.5869516857406 Isp0: 769.6565317945232

Stage 1 burnout

Velocity (km/s): 6.215772159933899 Angle (deg h): 43.651089743905366 Range (km): 269.7946874779557 Time (sec): 237.299999999998

Final results:

Range (km): 6631.344926032913 Apogee (km): 2416.697072218072

Time to target (sec): 2319.399999998986

#### New simulation

fuelmass: 1961.3797131591502
Isp0: 697.6850215516242

Stage 1 burnout

Velocity (km/s): 4.306158919270915 Angle (deg h): 43.65343099905379 Range (km): 124.9228096064081 Time (sec): 149.0999999999582

Final results:

Range (km): 2612.527347830653 Apogee (km): 818.6171338226619

Time to target (sec): 1067.800000001243

# New simulation

fuelmass: 5881.813300113165
Isp0: 503.30838012419605

Stage 1 burnout

Velocity (km/s): 5.448519541845869 Angle (deg h): 43.65790950484454 Range (km): 262.1433621509185 Time (sec): 322.60000000000485

Range (km): 4823.478410005139 Apogee (km): 1651.7654218953978

Time to target (sec): 1836.299999994254

#### New simulation

fuelmass: 1007.2053326384988 Isp0: 198.50752896674112

Stage 1 burnout

Velocity (km/s): 0.6209856645291464 Angle (deg h): 43.82293544970517 Range (km): 2.8409097063050073 Time (sec): 21.80000000000043

Final results:

Range (km): 47.441415598430595 Apogee (km): 15.043319913360616

Time to target (sec): 121.599999999737

#### New simulation

fuelmass: 5830.769420256684
Isp0: 183.36895827670898

Stage 1 burnout

Velocity (km/s): 1.6151947273442484 Angle (deg h): 43.65148588966079 Range (km): 29.552128447297665 Time (sec): 116.4999999999766

Final results:

Range (km): 342.6933346377176 Apogee (km): 109.58406795928896

Time to target (sec): 389.30000000002

# New simulation

fuelmass: 770.2349778825693
Isp0: 251.91851421042284

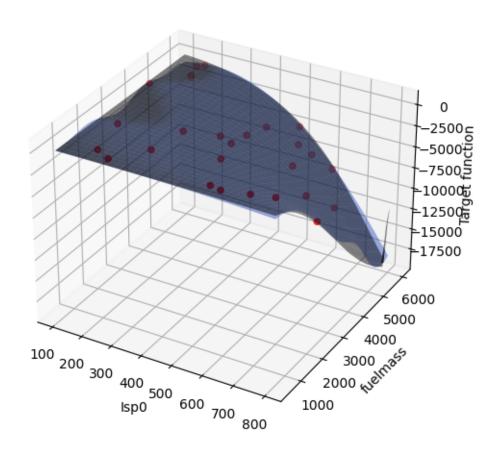
Stage 1 burnout

Velocity (km/s): 0.6388740947266406 Angle (deg h): 43.710547909155665 Range (km): 2.8761548020949204 Time (sec): 21.20000000000035

```
[26]: m2_2_model_emukit.X.shape
[26]: (26, 2)
[27]: m2_2_model_emukit.__dict__
[27]: {'model': <GPy.models.gp_regression.GPRegression at 0x7fba29a8d2d0>,
       'n_restarts': 1}
[28]: m2_ed.__dict__
[28]: {'candidate_point_calculator':
      <emukit.core.loop.candidate_point_calculators.SequentialPointCalculator at</pre>
      0x7fba588c0040>,
       'model_updaters': [<emukit.core.loop.model_updaters.FixedIntervalUpdater at
      0x7fba48e45ea0>],
       'loop_state': <emukit.core.loop.loop_state.LoopState at 0x7fba48e45db0>,
       'loop_start_event': Event([]),
       'iteration_end_event': Event([]),
       'model': <emukit.model_wrappers.gpy_model_wrappers.GPyModelWrapper at
      0x7fba29a8c3d0>}
[29]: if run_grid_simulation:
          # Compute new prediction
          m2_mu_plot_grid_pred2, var_plot_grid_pred2 = m2_2_model_emukit.predict(m2_x_plot)
          m2_mu_plot_pred2 = m2_mu_plot_grid_pred2.reshape(m2_x_plot_mesh.shape)
          m2_var_plot_pred2 = var_plot_grid_pred2.reshape(m2_x_plot_mesh.shape)
          m2_2_rmse = evaluate_prediction(y_actual=m2_y_plot,__
       →y_predicted=m2_mu_plot_grid_pred2)
          print("RMSE m2 (post experiment design loop): ", m2_2_rmse)
     RMSE m2 (post experiment design loop): 295.0875402186592
[30]: if run_grid_simulation:
          # 3D Plot
          add_bands = False
          # REVERSE
          fig = plt.figure()
          ax = fig.add_subplot(projection='3d')
          # True surface
          surf = ax.plot_surface(m2_y_plot_mesh, m2_x_plot_mesh, (m2_Z).transpose(),
                                 alpha = .5,
                                 label='target function',
                                  color='black'
```

Range (km): 49.94744211562406 Apogee (km): 15.707653805022598

Time to target (sec): 123.3999999999726



```
[31]: if run_grid_simulation:

# REVERSE
```

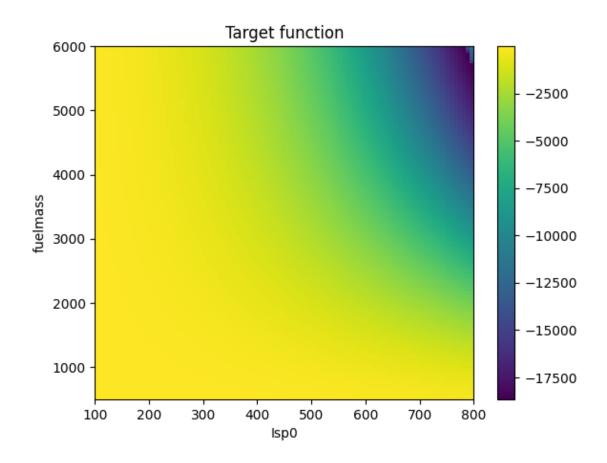
```
## Heatmaps
   extents = [m2_space.parameters[1].min, m2_space.parameters[1].max,
              m2_space.parameters[0].min, m2_space.parameters[0].max]
   # True values
   fig, ax = plt.subplots()
   im = ax.imshow(m2_Z, extent=extents, aspect='auto', origin='lower')
   ax.set_title('Target function')
   ax.set_xlabel(m2_param_2)
   ax.set_ylabel(m2_param_1)
   fig.colorbar(im, ax=ax)
   fig.show()
   # Model
   fig, ax = plt.subplots()
   im = ax.imshow(m2_mu_plot_pred2, extent=extents, aspect='auto', origin='lower')
   ax.set_title('Model (mean)')
   ax.set_xlabel(m2_param_2)
   ax.set_ylabel(m2_param_1)
   fig.colorbar(im, ax=ax)
   fig.show()
   # Difference
   fig, ax = plt.subplots()
   vmin = (m2_mu_plot_pred2-m2_Z).min()
   vmax = (m2_mu_plot_pred2-m2_Z).max()
   vmin_max = max(abs(vmin), abs(vmax))
   divnorm=colors.TwoSlopeNorm(vcenter=0., vmin=-vmin_max, vmax=vmin_max) # vmin=-5.,u
\rightarrow vcenter=0., vmax=10
   im = ax.imshow(m2_mu_plot_pred2-m2_Z, extent=extents, aspect='auto', cmap="bwr", u
→norm=divnorm, origin='lower')
   ax.set_title('Difference between model and target function')
   ax.set_xlabel(m2_param_2)
   ax.set_ylabel(m2_param_1)
   # Add points where simulation evaluated
   ax.plot(np.array(m2_2_model_emukit.X)[:,1], np.array(m2_2_model_emukit.X)[:,0],__

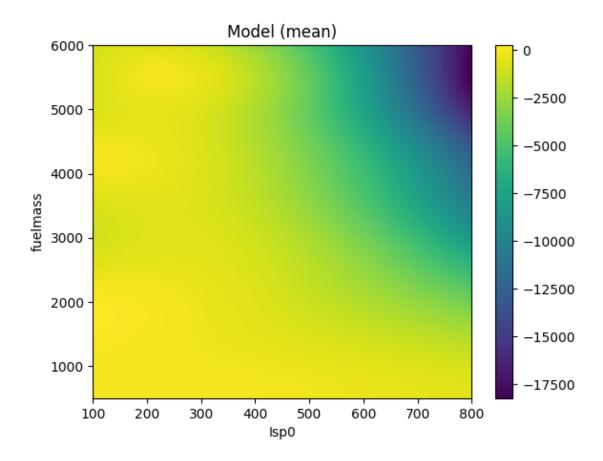
¬'ro')
   fig.colorbar(im, ax=ax)
   fig.show()
```

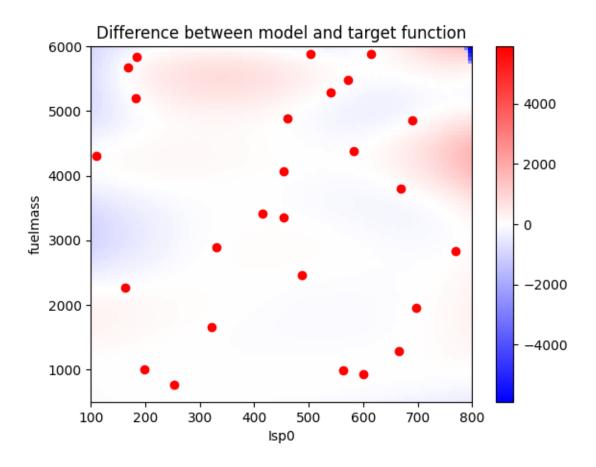
```
/var/folders/98/fv11ygzs4p51c21s8jln0jzc0000gn/T/ipykernel_12821/2861625379.py:
15: UserWarning:Matplotlib is currently using
module://matplotlib_inline.backend_inline, which is a non-GUI backend, so cannot
show the figure.

/var/folders/98/fv11ygzs4p51c21s8jln0jzc0000gn/T/ipykernel_12821/2861625379.py:
24: UserWarning:Matplotlib is currently using
module://matplotlib_inline.backend_inline, which is a non-GUI backend, so cannot
show the figure.

/var/folders/98/fv11ygzs4p51c21s8jln0jzc0000gn/T/ipykernel_12821/2861625379.py:
40: UserWarning:Matplotlib is currently using
module://matplotlib_inline.backend_inline, which is a non-GUI backend, so cannot
show the figure.
```







# 1.2 2. Maximization

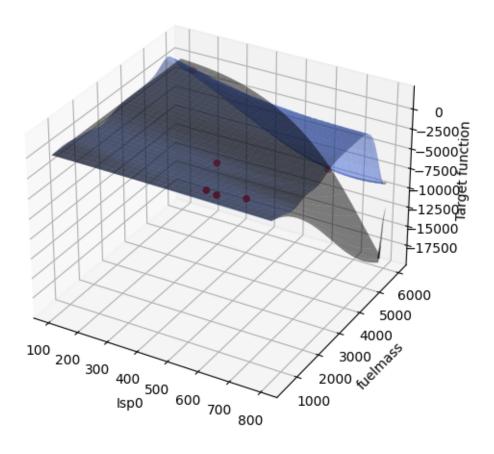
```
[32]: m2_model_gpy = GPRegression(m2_x,m2_y, kernel=m2_kern)
    m2_model_gpy.kern.variance = m2_var_kernel
    m2_model_gpy.likelihood.variance.fix(m2_var_noise)

m2_model_emukit = GPyModelWrapper(m2_model_gpy)
    m2_model_emukit.optimize()
```

/Users/ilariasartori/opt/anaconda3/envs/mlphysical/lib/python3.10/site-packages/paramz/transformations.py:111: RuntimeWarning:overflow encountered in expm1

RMSE m2 (before experiment design loop): 3903.716104090036

```
[34]: if run_grid_simulation:
          # 3D Plot
          add_bands = False
          # REVERSE
          fig = plt.figure()
          ax = fig.add_subplot(projection='3d')
          # True surface
          surf = ax.plot_surface(m2_y_plot_mesh, m2_x_plot_mesh, (m2_Z).transpose(),
                                 alpha = .5,
                                 label='target function',
                                 color='black'
          # Mean predicted
          surf = ax.plot_surface(m2_y_plot_mesh, m2_x_plot_mesh, (m2_mu_plot_pred1).
       →transpose(),
                                 alpha = .5,
                                 label='model', # Mean
                                 color='royalblue'
          # True points observed
          ax.scatter(m2_x[:,1], m2_x[:,0], m2_y, marker='o', color='red')
          ax.set_xlabel(m2_param_2)
          ax.set_ylabel(m2_param_1)
          ax.set_zlabel('Target function')
          plt.tight_layout()
```



```
[35]: if run_grid_simulation:
          from matplotlib import colors
            divnorm=colors.TwoSlopeNorm(vcenter=0.) # vmin=-5., vcenter=0., vmax=10
          # REVERSE
          ## Heatmaps
          extents = [m2_space.parameters[1].min, m2_space.parameters[1].max,
                     m2_space.parameters[0].min, m2_space.parameters[0].max]
          # True values
          fig, ax = plt.subplots()
          im = ax.imshow(m2_Z, extent=extents, aspect='auto', origin='lower')
          ax.set_title('Target function')
          ax.set_xlabel(m2_param_2)
          ax.set_ylabel(m2_param_1)
          fig.colorbar(im, ax=ax)
          fig.show()
          # Model
          fig, ax = plt.subplots()
          im = ax.imshow(m2_mu_plot_pred1, extent=extents, aspect='auto', origin='lower')
```

```
ax.set_title('Model (mean)')
   ax.set_xlabel(m2_param_2)
   ax.set_ylabel(m2_param_1)
   fig.colorbar(im, ax=ax)
   fig.show()
   # Difference
   vmin = (m2_mu_plot_pred1-m2_Z).min()
   vmax = (m2_mu_plot_pred1-m2_Z).max()
   vmin_max = max(abs(vmin), abs(vmax))
   divnorm=colors.TwoSlopeNorm(vcenter=0., vmin=-vmin_max, vmax=vmin_max) # vmin=-5.,u
\rightarrow vcenter=0., vmax=10
   fig, ax = plt.subplots()
   im = ax.imshow(m2_mu_plot_pred1-m2_Z, extent=extents, aspect='auto', cmap="bwr", __
→norm=divnorm, origin='lower')
   ax.set_title('Difference between model and target function')
   ax.set_xlabel(m2_param_2)
   ax.set_ylabel(m2_param_1)
   # Add points where simulation evaluated
   ax.plot(m2_x[:,1], m2_x[:,0], 'ro')
   fig.colorbar(im, ax=ax)
   fig.show()
```

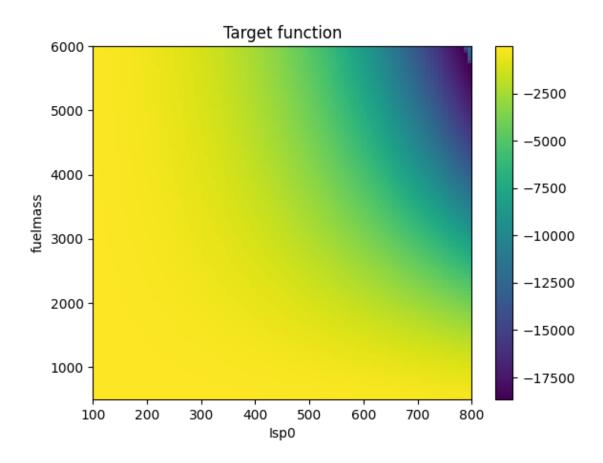
/var/folders/98/fv11ygzs4p51c21s8jln0jzc0000gn/T/ipykernel\_12821/2119566484.py: 17: UserWarning:Matplotlib is currently using module://matplotlib\_inline.backend\_inline, which is a non-GUI backend, so cannot show the figure.

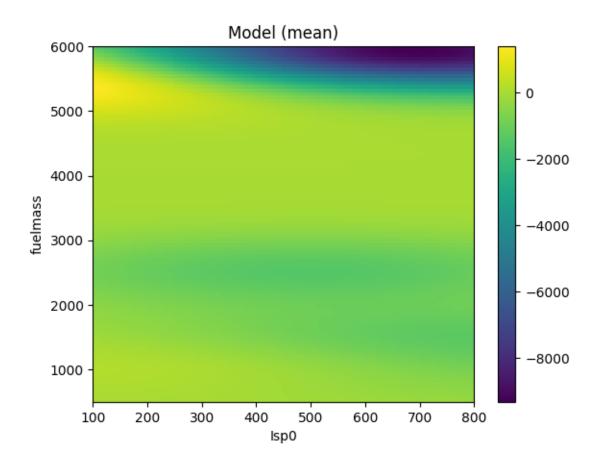
/var/folders/98/fv11ygzs4p51c21s8jln0jzc0000gn/T/ipykernel\_12821/2119566484.py: 26: UserWarning:Matplotlib is currently using

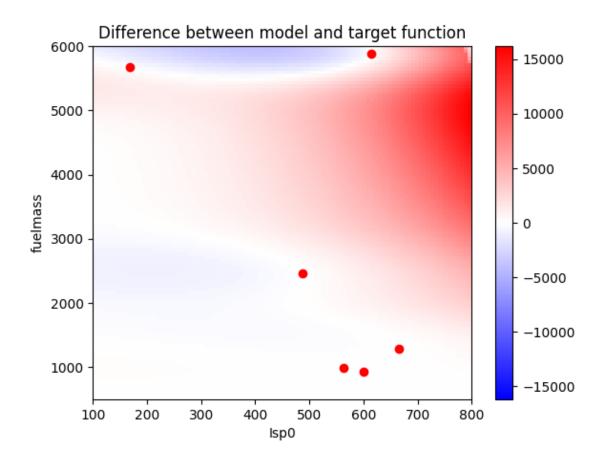
module://matplotlib\_inline.backend\_inline, which is a non-GUI backend, so cannot show the figure.

/var/folders/98/fv11ygzs4p51c21s8jln0jzc0000gn/T/ipykernel\_12821/2119566484.py: 42: UserWarning:Matplotlib is currently using module://matplotlib\_inline.backend\_inline, which is a non-GUI backend, so cannot

show the figure.







# 1.2.1 Use the model created for model-based bayes optimization

use the model to decide which are the best points to collect using some data collection criteria (that we call acquisition).

/Users/ilariasartori/opt/anaconda3/envs/mlphysical/lib/python3.10/site-packages/paramz/transformations.py:111: RuntimeWarning:overflow encountered in expm1

### New simulation

fuelmass: 6000.0

Isp0: 794.360549356994

Stage 1 burnout

Velocity (km/s): 9.178508685748767 Angle (deg h): 43.65600014577831 Range (km): 686.5357746028335 Time (sec): 519.4000000000495 Simulation exceeded time limit.

Final results:

Range (km): 13730.204805621252 Apogee (km): 24848.814173837214

Time to target (sec): 20000.099999989452

# New simulation

fuelmass: 5725.99797866685

Isp0: 800.0

Stage 1 burnout

Velocity (km/s): 9.118048401086302 Angle (deg h): 43.65626668225193 Range (km): 669.0264340484053 Time (sec): 499.200000000045

Final results:

Range (km): 18662.00297949803 Apogee (km): 22913.42429568097

Time to target (sec): 19851.69999999161

## New simulation

fuelmass: 5491.501957409965

Isp0: 800.0

Stage 1 burnout

Velocity (km/s): 8.986868397237318 Angle (deg h): 43.66205072403367 Range (km): 643.8666194042343 Time (sec): 478.70000000004035

Range (km): 18068.70181252249 Apogee (km): 19560.869158892732

Time to target (sec): 16614.000000038726

#### New simulation

fuelmass: 5638.187402073278

Isp0: 800.0

Stage 1 burnout

Velocity (km/s): 9.069021152976038 Angle (deg h): 43.66061047352842 Range (km): 659.6287739181668 Time (sec): 491.50000000004326

Final results:

Range (km): 18441.599924881288 Apogee (km): 21567.716802165975

Time to target (sec): 18534.100000010785

#### New simulation

fuelmass: 5136.2218400038255

Isp0: 800.0

Stage 1 burnout

Velocity (km/s): 8.773306219479968 Angle (deg h): 43.655173745661216 Range (km): 604.2078966755495 Time (sec): 447.800000000333

Final results:

Range (km): 17084.70004943095 Apogee (km): 15480.784296271606

Time to target (sec): 12878.20000002932

# New simulation

fuelmass: 5214.108918923757
Isp0: 598.4149918308952

Stage 1 burnout

Velocity (km/s): 6.3664507172109435 Angle (deg h): 43.66125949674566 Range (km): 337.7559182400016 Time (sec): 340.000000000088

Range (km): 7259.152101533458 Apogee (km): 2747.0445220049146

Time to target (sec): 2645.899999998689

#### New simulation

fuelmass: 4580.8528879575

Isp0: 800.0

Stage 1 burnout

Velocity (km/s): 8.366900308288027 Angle (deg h): 43.6526820549504 Range (km): 535.8848511994823 Time (sec): 399.3000000000223

Final results:

Range (km): 15183.720438505185 Apogee (km): 10540.313747532786

Time to target (sec): 8656.10000001396

#### New simulation

fuelmass: 4423.650819361284 Isp0: 496.9281684185544

Stage 1 burnout

Velocity (km/s): 4.812367615463809 Angle (deg h): 43.65142941764638 Range (km): 190.566551832335 Time (sec): 239.5999999999067

Final results:

Range (km): 3499.8928831317667 Apogee (km): 1143.739479642611

Time to target (sec): 1389.399999998318

# New simulation

fuelmass: 4804.623926231683

Isp0: 800.0

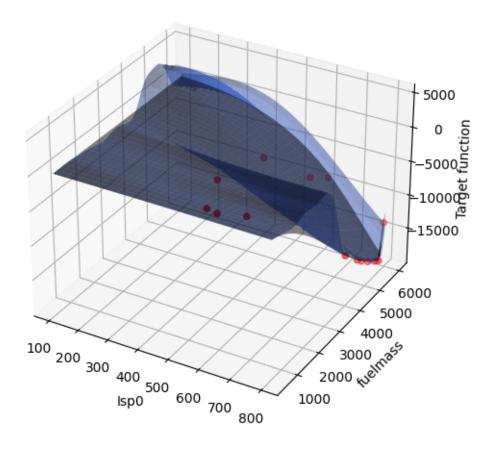
Stage 1 burnout

Velocity (km/s): 8.5433286072883 Angle (deg h): 43.6545044250496 Range (km): 564.4400146052687 Time (sec): 418.90000000002675

```
Apogee (km): 12354.506183455806
     Time to target (sec): 10168.400000019461
     New simulation
     fuelmass: 3967.1975410829014
     Isp0: 800.0
     Stage 1 burnout
     Velocity (km/s): 7.832664856369256
     Angle (deg h): 43.65434767329817
     Range (km): 455.13035058256884
     Time (sec): 345.9000000001015
     Final results:
     Range (km): 12709.242416139505
     Apogee (km): 6849.695397415779
     Time to target (sec): 5702.800000003215
[38]: results = bayesopt_loop.get_results()
      results
[38]: <emukit.bayesian_optimization.loops.bayesian_optimization_loop.BayesianOptimizat
      ionResults at 0x7fba49a43ee0>
[39]: m2_max_model_emukit.X.shape
[39]: (16, 2)
[40]: m2_max_model_emukit.__dict__
[40]: {'model': <GPy.models.gp_regression.GPRegression at 0x7fba308d0ca0>,
       'n_restarts': 1}
[41]: if run_grid_simulation:
          # Compute new prediction
          m2_mu_plot_grid_pred2, var_plot_grid_pred2 = m2_max_model_emukit.predict(m2_x_plot)
          m2_mu_plot_pred2 = m2_mu_plot_grid_pred2.reshape(m2_x_plot_mesh.shape)
          m2_var_plot_pred2 = var_plot_grid_pred2.reshape(m2_x_plot_mesh.shape)
          m2_max_rmse = evaluate_prediction(y_actual=m2_y_plot,__
       →y_predicted=m2_mu_plot_grid_pred2)
          print("RMSE m2 (post bayes opt loop): ", m2_max_rmse)
     RMSE m2 (post bayes opt loop): 1896.673493025905
[42]: if run_grid_simulation:
          # 3D Plot
          add_bands = False
```

Range (km): 16009.045083093062

```
# REVERSE
  fig = plt.figure()
  ax = fig.add_subplot(projection='3d')
   # True surface
   surf = ax.plot_surface(m2_y_plot_mesh, m2_x_plot_mesh, (m2_Z).transpose(),
                         alpha = .5,
                         label='target function',
                         color='black'
   # Mean predicted
   surf = ax.plot_surface(m2_y_plot_mesh, m2_x_plot_mesh, (m2_mu_plot_pred2).
→transpose(),
                         alpha = .5,
                         label='model', # Mean
                         color='royalblue'
   # True points observed
   ax.scatter(np.array(m2_max_model_emukit.X)[:,1],
             np.array(m2_max_model_emukit.X)[:,0], m2_max_model_emukit.Y,_
ax.set_xlabel(m2_param_2)
  ax.set_ylabel(m2_param_1)
  ax.set_zlabel('Target function')
  plt.tight_layout()
```



```
[43]: if run_grid_simulation:
          ## Heatmaps
          extents = [m2_space.parameters[1].min, m2_space.parameters[1].max,
                     m2_space.parameters[0].min, m2_space.parameters[0].max]
          # True values
          fig, ax = plt.subplots()
          im = ax.imshow(m2_Z, extent=extents, aspect='auto', origin='lower')
          ax.set_title('Target function')
          ax.set_xlabel(m2_param_2)
          ax.set_ylabel(m2_param_1)
          fig.colorbar(im, ax=ax)
          fig.show()
          # Model
          fig, ax = plt.subplots()
          im = ax.imshow(m2_mu_plot_pred2, extent=extents, aspect='auto', origin='lower')
          ax.set_title('Model (mean)')
          ax.set_xlabel(m2_param_2)
          ax.set_ylabel(m2_param_1)
```

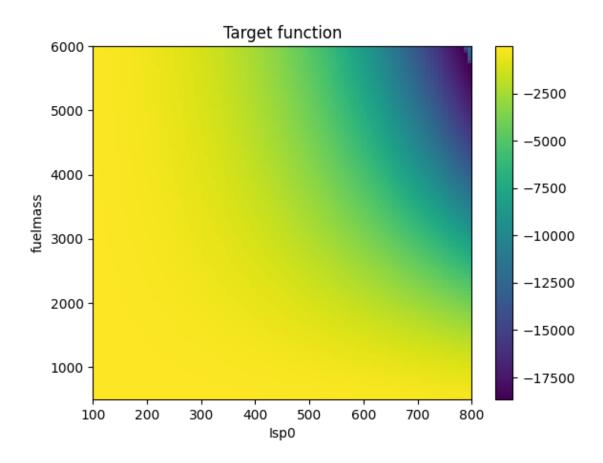
```
fig.colorbar(im, ax=ax)
   fig.show()
   # Difference
   fig, ax = plt.subplots()
   vmin = (m2_mu_plot_pred2-m2_Z).min()
   vmax = (m2_mu_plot_pred2-m2_Z).max()
   vmin_max = max(abs(vmin), abs(vmax))
   divnorm=colors.TwoSlopeNorm(vcenter=0., vmin=-vmin_max, vmax=vmin_max) # vmin=-5.,u
\rightarrow vcenter=0., vmax=10
   im = ax.imshow(m2_mu_plot_pred2-m2_Z, extent=extents, aspect='auto', cmap="bwr", u
→norm=divnorm, origin='lower')
   ax.set_title('Difference between model and target function')
   ax.set_xlabel(m2_param_2)
   ax.set_ylabel(m2_param_1)
   # Add points where simulation evaluated
     ax.plot(m2\_x[:,0], m2\_x[:,1], 'ro')
     ax.plot(m2_x[:,1], m2_x[:,0], 'ro')
   ax.plot(np.array(m2_max_model_emukit.X)[:,1], np.array(m2_max_model_emukit.X)[:
→,0], 'ro')
   fig.colorbar(im, ax=ax)
   fig.show()
```

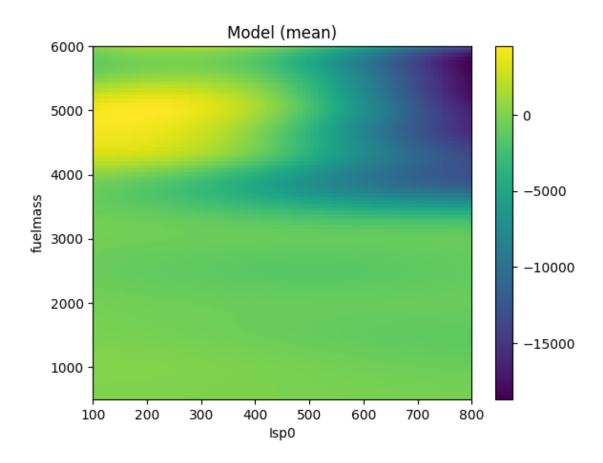
/var/folders/98/fv11ygzs4p51c21s8jln0jzc0000gn/T/ipykernel\_12821/2525306052.py: 14: UserWarning:Matplotlib is currently using module://matplotlib\_inline.backend\_inline, which is a non-GUI backend, so cannot show the figure.

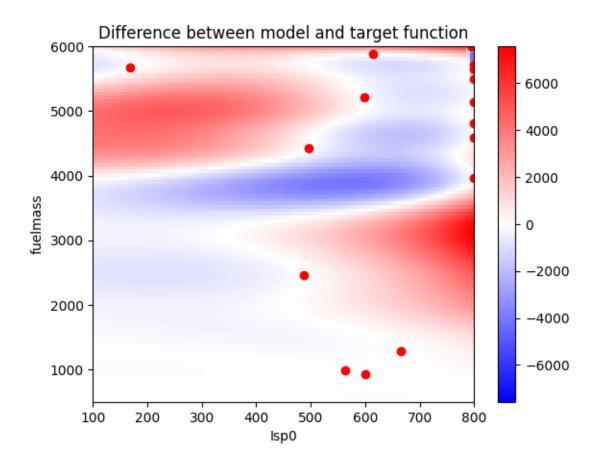
/var/folders/98/fv11ygzs4p51c21s8jln0jzc0000gn/T/ipykernel\_12821/2525306052.py: 23: UserWarning:Matplotlib is currently using

module://matplotlib\_inline.backend\_inline, which is a non-GUI backend, so cannot show the figure.

/var/folders/98/fv11ygzs4p51c21s8jln0jzc0000gn/T/ipykernel\_12821/2525306052.py: 41: UserWarning:Matplotlib is currently using module://matplotlib\_inline.backend\_inline, which is a non-GUI backend, so cannot show the figure.







```
[44]: ## Greedy maximization using the simulator
      # # opt 1
      from collections import namedtuple
      Min_val = namedtuple('Min_val', 'fun x')
      min_idx = np.argmin(m2_y_plot)
      true_minim = Min_val( m2_y_plot[min_idx], m2_x_plot[min_idx])
      print("True min value: ", m2_y_plot[min_idx])
      print("True min location: ", m2_x_plot[min_idx])
      # # # opt2
      \# nr\_custom\_params = 2
      # wirte_output_txt = False
      # from scipy.optimize import minimize
      # # func_{to_{minimize}} = lambda x: (x[0] - 1)**2 + (x[1] - 2.5)**2
      # def func_to_minimize(x):
            print(x)
            return neg_run_missile_sim(np.array(x).reshape(1,nr_custom_params))
      # bnds = [(m2_domain_param_1),
                (m2_domain_param_2),
```

```
# #
             (m3_domain_param_3),
 # #
             (m3_domain_param_4),
# #
             (m3_domain_param_5),
             (m3_domain_param_6)
# initial_guess = [np.mean(m2_domain_param_1),
                    np.mean(m2_domain_param_2),
                      np.mean(m3_domain_param_3),
 # #
                      np.mean(m3_domain_param_4),
# #
                      np.mean(m3_domain_param_5),
 # #
                      np.mean(m3_domain_param_6)
 # true_minim = minimize(func_to_minimize, initial_guess, bounds=bnds) # ,u
 \rightarrow method='SLSQP'constraints=cons
True min value: [-18655.87990491]
True min location: [5725. 800.]
```

```
[]:
```

```
[45]: min_val_from_sim = true_minim.fun
      min_loc_from_sim = true_minim.x
      min_val_from_emu = results.minimum_value
      min_loc_from_emu = results.minimum_location
      min_val_diff = min_val_from_sim - min_val_from_emu
      min_loc_diff = min_loc_from_sim - min_loc_from_emu
      print("Min val from sim - min val from em: \n", min_val_diff)
      print('\n')
      print("Min location from sim - min location from em: \n", min_loc_diff)
      print('\n')
      print('\n')
      print("Min location from sim: \n", min_loc_from_sim)
      print("Min location from emu: \n", min_loc_from_emu)
      print('\n')
      print('\n')
      print("Min value from sim: \n", min_val_from_sim)
      print("Min value from emu: \n", min_val_from_emu)
```

Min val from sim - min val from em: [5.35667777]

Min location from sim - min location from em: [-0.99797867 0. ]

Min location from sim: [5725. 800.]

	Min location from emu: [5725.99797867 800.	]
	Min value from sim: [-18655.87990491] Min value from emu: -18661.23658268512	
[]:		
r 1		
[]:		