Rosenbrock:

GP EI: derivation of exact partial-order GP EI derivatives wrt x1, x2, x3, x4

```
1 #pip install pyGPGO
 2
 1 ### Import:
 2
 3 import numpy as np
 4 import scipy as sp
 5 import pandas as pd
 6 import matplotlib.pyplot as plt
 7 import warnings
 9 from pyGPGO.GPGO import GPGO
10 from pyGPGO.surrogates.GaussianProcess import GaussianProcess
11 from pyGPGO.acquisition import Acquisition
12 from pyGPGO.covfunc import squaredExponential
13
14 from joblib import Parallel, delayed
15 from numpy.linalg import solve
16 from scipy.optimize import minimize
17 from scipy.spatial.distance import cdist
18 from scipy.stats import norm
19 import time
20
21 warnings.filterwarnings("ignore", category=RuntimeWarning)
22
 1 n_start_AcqFunc = 100 #multi-start iterations to avoid local optima in AcqFunc optimiza
 2
 1 ### Inputs:
 3 n_{\text{test}} = 500
 4 \text{ eps} = 1e-08
 6 util_grad_exact = 'dEI_GP'
 7 util_grad_approx = 'ExpectedImprovement'
 9 n init = 5 # random initialisations
10 \text{ iters} = 40
11 opt = True
 1 ### Objective Function - Rosenbrock(x) 4-D:
 3 def objfunc(x1_training, x2_training, x3_training, x4_training):
 4
               return operator * (
                   100 * (x2_training - x1_training ** 2) ** 2 + (x1_training - 1) ** 2 +
```

```
6/14/2021
                                         3. Rosenbrock GP El.ipynb - Colaboratory
                       100 * (x3_training - x2_training ** 2) ** 2 + (x2_training - 1) ** 2 +
     6
     7
                       100 * (x4_training - x3_training ** 2) ** 2 + (x3_training - 1) ** 2
     8
     9
   10 # Constraints:
   11 lb = -2.048
   12 \text{ ub} = +2.048
   14 # Input array dimension(s):
   15 \, \text{dim} = 4
   16
   17 # 4-D inputs' parameter bounds:
   18 param = {'x1_training': ('cont', [lb, ub]),
                         'x2_training': ('cont', [lb, ub]),
   20
                         'x3_training': ('cont', [lb, ub]),
                         'x4_training': ('cont', [lb, ub])}
   21
   22
   23 # True y bounds:
   24 y_1b = 0
   25 operator = -1 # targets global minimum
   26 y_global_orig = y_lb * operator # targets global minimum
   27
   28 # Test data:
   29 x1_test = np.linspace(lb, ub, n_test)
   30 x2_test = np.linspace(lb, ub, n_test)
   31 x3_test = np.linspace(lb, ub, n_test)
   32 x4_test = np.linspace(lb, ub, n_test)
   33 Xstar = np.column_stack((x1_test, x2_test, x3_test, x4_test))
   34
   35 Xstar_d = np.column_stack((x1_test, x2_test, x3_test))
     1 ### Cumulative Regret Calculator:
     3 def min_max_array(x):
     4
           new_list = []
     5
           for i, num in enumerate(x):
                   new_list.append(np.min(x[0:i+1]))
     6
     7
           return new_list
     8
     1 ### Surrogate derivatives:
     3 cov func = squaredExponential()
     4
     5 class dGaussianProcess(GaussianProcess):
     6
           1 = GaussianProcess(cov_func, optimize=opt).getcovparams()['1']
     7
           sigmaf = GaussianProcess(cov_func, optimize=opt).getcovparams()['sigmaf']
           sigman = GaussianProcess(cov_func, optimize=opt).getcovparams()['sigman']
     8
     9
           def AcqGrad(self, Xstar):
   10
               Xstar = np.atleast_2d(Xstar)
   11
   12
               Kstar = squaredExponential.K(self, self.X, Xstar).T
               dKstar = Kstar * cdist(self.X, Xstar).T * -1
   13
```

```
15
          v = solve(self.L, Kstar.T)
          dv = solve(self.L, dKstar.T)
16
17
18
          ds = -2 * np.diag(np.dot(dv.T, v))
           dm = np.dot(dKstar, self.alpha)
19
           return ds, dm
20
21
 1 class Acquisition_new(Acquisition):
       def __init__(self, mode, eps=1e-08, **params):
 2
 3
 4
           self.params = params
 5
           self.eps = eps
 6
 7
           mode dict = {
               'dEI GP': self.dEI GP
 8
 9
           }
10
           self.f = mode_dict[mode]
11
12
      def dEI_GP(self, tau, mean, std, ds, dm):
13
14
           gamma = (mean - tau - self.eps) / (std + self.eps)
15
           gamma_h = (mean - tau) / (std + self.eps)
           dsdx = ds / (2 * (std + self.eps))
16
17
           dmdx = (dm - gamma * dsdx) / (std + self.eps)
18
19
          f = (std + self.eps) * (gamma * norm.cdf(gamma) + norm.pdf(gamma))
20
           df1 = f / (std + self.eps) * dsdx
           df2 = (std + self.eps) * norm.cdf(gamma) * dmdx
21
          df = df1 + df2
22
23
          df_arr = []
24
25
26
          for j in range(0, dim):
27
             df arr.append([df])
28
           return f, np.asarray(df_arr).transpose()
29
30
       def d eval(self, tau, mean, std, ds, dm):
31
           return self.f(tau, mean, std, ds, dm, **self.params)
32
33
 1 ## dGPGO:
 2
 3 class dGPGO(GPGO):
 4
       n_start = n_start_AcqFunc
 5
       eps = 1e-08
 6
 7
       def d_optimizeAcq(self, method='L-BFGS-B', n_start=n_start_AcqFunc):
 8
           start_points_dict = [self._sampleParam() for i in range(n_start)]
 9
           start_points_arr = np.array([list(s.values())
10
                                         for s in start_points_dict])
           x hest = nn.emntv((n start. len(self.narameter kev)))
```

```
6/14/2021
                                        3. Rosenbrock GP El.ipynb - Colaboratory
                       12
              f best = np.empty((n start,))
   13
              opt = Parallel(n jobs=self.n jobs)(delayed(minimize)(self.acqfunc,
   14
                                                                         x0=start point,
   15
                                                                         method=method,
                                                                         jac = True,
   16
   17
                                                                         bounds=self.parameter_
   18
                                                       start_points_arr)
   19
              x_best = np.array([res.x for res in opt])
              f_best = np.array([np.atleast_1d(res.fun)[0] for res in opt])
   20
   21
   22
              self.x best = x best
   23
               self.f_best = f_best
               self.best = x_best[np.argmin(f_best)]
   24
               self.start points arr = start points arr
   25
   26
   27
              return x_best, f_best
   28
   29
          def run(self, max_iter=10, init_evals=3, resume=False):
   30
   31
               if not resume:
   32
                   self.init_evals = init_evals
   33
                   self._firstRun(self.init_evals)
                   self.logger._printInit(self)
   34
              for iteration in range(max_iter):
   35
                   self.d_optimizeAcq()
   36
   37
                   self.updateGP()
   38
                   self.logger._printCurrent(self)
   39
   40
          def acqfunc(self, xnew, n_start=n_start_AcqFunc):
   41
               new_mean, new_var = self.GP.predict(xnew, return_std=True)
              new_std = np.sqrt(new_var + eps)
   42
   43
              ds, dm = self.GP.AcqGrad(xnew)
              f, df = self.A.d_eval(-self.tau, new_mean, new_std, ds=ds, dm=dm)
   44
   45
   46
              return -f, df
   47
   48
          def acqfunc h(self, xnew, n start=n start AcqFunc, eps=eps):
              f = self.acqfunc(xnew)[0]
   49
   50
   51
              new mean h, new var h = self.GP.predict(xnew + eps, return std=True)
   52
              new_std_h = np.sqrt(new_var_h + eps)
              ds_h, dm_h = self.GP.AcqGrad(xnew + eps)
   53
              f_h = self.A.d_eval(-self.tau, new_mean_h, new_std_h, ds=ds_h, dm=dm_h)[0]
   54
   55
              approx\_grad = (-f_h - f)/eps
   56
   57
               return approx_grad
   58
    1 ###Reproducible set-seeds:
    2
    3 \text{ run num } 1 = 1
    4 run_num_2 = 2
    5 run_num_3 = 3
    6 \text{ run num } 4 = 4
```

7 run num 5 = 5

```
8 \text{ run num } 6 = 6
 9 \text{ run num } 7 = 7
10 \text{ run num } 8 = 8
11 run_num_9 = 9
12 run_num_10 = 10
13 \text{ run_num_} 11 = 11
14 run_num_12 = 12
15 \text{ run num } 13 = 13
16 \text{ run num } 14 = 14
17 \text{ run}_num_15 = 15
18 \text{ run num } 16 = 16
19 run num 17 = 17
20 \text{ run num } 18 = 18
21 \text{ run num } 19 = 19
22 \text{ run num } 20 = 20
23
 1 start approx = time.time()
 2 start approx
 3
    1623407545.547943
 1 ### ESTIMATED GP EI GRADIENTS
 2
 3 np.random.seed(run num 1)
 4 surrogate_approx_1 = GaussianProcess(cov_func, optimize=opt)
 5
 6 approx_1 = GPGO(surrogate_approx_1, Acquisition(util_grad_approx), objfunc, param)
 7 approx_1.run(init_evals=n_init, max_iter=iters)
 8
                     Proposed point
                                              Current eval.
                                                                    Best eval.
    Evaluation
             [-0.33987787  0.90244913  -2.04753152  -0.80964578].
    init
                                                                    -3394.123441866637
    init
              [-1.44688787 -1.66978112 -1.28507817 -0.63258326].
                                                                      -3615.357417364757
    init
              [-0.42284043 0.15899334 -0.33097927 0.75865907].
                                                                      -59.36907919270953
    init
              [-1.21056359 1.54876902 -1.93582042 0.69823492].
                                                                      -2823.036073483468
    init
              [-0.33871953  0.24039354 -1.4729751 -1.2365763 ].
                                                                      -1404.6293821132788
                                      0.52114175 1.27606514].
    1
              [-0.0490961 0.0026703
                                                                      -130.3799970253568
              [ 2.048 -2.048 2.048 -2.048].
    2
                                                      -8265.420843724798 -59.36907919
             [-2.048 2.048 2.048 2.048].
    3
                                                                             -59.36907919
                                                     -4829.447006924799
    4
                                                      -8273.612843724799
                                                                             -59.36907919
    5
                                              -1385.2811701248 -59.369079192709535
    6
              [-2.048 -2.048 2.048 2.048].
                                                      -4837.639006924799
                                                                             -59.36907919
    7
                                       0.89949977 -2.048 ]. -2364.74423245248
              [ 2.048
                           2.048
    8
              [-2.048 2.048 2.048 2.048].
                                                     -1393.4731701248
                                                                             -59.36907919
    9
              [ 2.048 -2.048 2.048 2.048].
             [ 2.048 -2.048 -2.048 -2.048].
                                                      -4829.447006924799
                                                                             -59.36907919
    10
                                                      -11709.586680524799
                                                                             -59.36907919
    11
              [-0.04486943 0.26245645 1.33015464 0.00220004]. -479.8765479489312
              12
                                                                             -59.36907919
    13
              [-2.048 -2.048 2.048 -2.048].
                                                      -8273.612843724797
                                                                             -59.36907919
              [0.39277217 0.66508874 0.36925183 0.93955179].
                                                                      -92.02035347587906
    14
    15
              [-0.3665318 -0.09024272 -0.1746368
                                                                    -419.8520995192605
```

[0.63988049 1.57185141 0.14918416 0.78089091].

[1.59540661 -0.05364952 0.14712847 1.38299872].

16

-732.8030854206354

-865.0662183090815

```
1.32621188 -2.02981529 -1.67272649].
18
         [ 1.92664281
                                                                    -5370.451989240503
19
         [-1.38940861 -0.20044123 0.5322671
                                                0.92704531].
                                                                    -527.0965669464073
20
           1.89620782 -0.14839589 -1.53922942
                                                0.68600274].
                                                                    -1937.3981285399177
21
           0.75241121 -0.58888911
                                   0.39295842
                                                1.31362989].
                                                                    -270.9503393195663!
22
           0.08259405
                      1.94781598
                                   1.35341898 -1.16334885].
                                                                    -1871.3054961770968
23
           1.8307373
                       0.45568333 -1.22143559 -0.95524121].
                                                                    -1647.6341694210719
24
                      0.3710531
                                    1.78740995
                                                1.56979854].
                                                                    -551.8556278894023
         [-0.06298569
25
         [ 0.79734412 -0.83463689 -1.80414999 -1.60545318].
                                                                    -3215.219531243629
                      -0.68994974
                                               -1.19194178].
                                                                    -1616.8340348753732
26
         [-0.1582911
                                  1.6102458
27
         [-0.22926075
                       1.4608557
                                    1.28246287 -1.03341029].
                                                                    -989.8946435008918
28
           2.0062999
                      -1.50296352
                                   1.08688969 -0.29540852].
                                                                    -3418.8237640549432
29
         [-0.79647557
                       0.5219737
                                  -0.52585479 -1.74939235].
                                                                    -481.21093988613774
30
         [-1.67298376 -0.62270762 -1.80623959
                                                1.82093967].
                                                                    -1877.5510989093145
31
           1.55656109 -0.57199926
                                   0.1756522
                                                1.30094652].
                                                                    -1064.001858558137
32
         [-1.98935079
                      1.82470542
                                   0.7078706
                                               -0.53078398].
                                                                    -1258.384739357216
33
         [-0.06966701 0.83377973 -0.92724163
                                               1.716628381.
                                                                    -410.2453655200145
34
         [ 0.56787983 -0.70452346  0.6459641
                                              -2.00969127].
                                                                    -699.9448688633819
35
         [0.49704515 0.93111689 1.6178312 0.1594768 ].
                                                                    -707.9393288226192
36
         [ 0.87715693 -0.5909966 -1.62091187 -1.99652745].
                                                                    -2720.678153604498
37
                      1.32287606 -1.67441492
                                               1.95053983].
                                                                    -1259.1691178659573
         [-1.08501802
38
         [-1.73681667
                       0.33276035
                                  0.5322298
                                               -0.61463567].
                                                                    -826.8067343838653
39
         [ 1.69661485 -1.31722849 -1.50498054 0.6533503 ].
                                                                    -3082.082077592921
40
         [-0.38001736 -1.73073496 1.72122227 -1.51184018].
                                                                    -2525.930515971026
```

```
1 ### ESTIMATED GP EI GRADIENTS
2
3 np.random.seed(run_num_2)
4 surrogate_approx_2 = GaussianProcess(cov_func, optimize=opt)
5
6 approx_2 = GPGO(surrogate_approx_2, Acquisition(util_grad_approx), objfunc, param)
7 approx_2.run(init_evals=n_init, max_iter=iters)
8
```

```
Proposed point
Evaluation
                                            Current eval.
                                                                    Best eval.
init
         [-0.26216488 -1.94180615 0.20341751 -0.26491948].
                                                                     -1696.9764582030693
init
         [-0.32617348 -0.69494857 -1.20975919
                                                 0.48853388].
                                                                     -455.3157381798458
init
         [-0.82061446 -0.95507548 0.49616418
                                                 0.11936602].
                                                                     -291.50084682592353
init
         [-1.49676054 0.05561598 -1.29253431
                                                 1.16873277].
                                                                     -682.7190038869136
init
                      -0.02360591
                                    1.41951584 -1.72177213].
                                                                     -2051.02408589455
         [ 1.4498828
         [-1.86778037 0.18049011
                                    2.00280848
                                                                     -2718.2474715699536
1
                                                 0.51009437].
2
           2.048
                   2.048 -2.048
                                 2.048].
                                                    -4829.447006924799
                                                                             -291.5008468
3
         [-2.048
                  2.048 -2.048 -2.048].
                                                    -8273.612843724799
                                                                             -291.5008468
4
         [2.048 2.048 2.048 2.048].
                                                                    -291.50084682592353
                                            -1385.2811701248
5
         [ 2.048 -2.048 2.048 2.048].
                                                    -4829,447006924799
                                                                             -291.5008468
6
           2.048 -2.048 -2.048 -2.048].
                                                    -11709.586680524799
                                                                             -291.5008468
7
                  2.048 -2.048 -2.048].
                                                    -8265.4208437248
                                                                             -291.5008468
           2.048
8
         [ 2.048 -2.048 -2.048
                                 2.048].
                                                    -8273.612843724803
                                                                             -291.5008468
9
         [-2.048 -2.048 -2.048 -2.048].
                                                    -11717.778680524798
                                                                             -291.5008468
10
         [-2.048
                  2.048
                          2.048 -2.048].
                                                    -4829.447006924799
                                                                             -291.5008468
         [-2.048 -2.048
                         2.048 -2.048].
                                                    -8273.612843724797
                                                                             -291.5008468
11
12
         [-2.048 - 2.048 - 2.048
                                 2.048].
                                                    -8281.8048437248
                                                                             -291.5008468
13
                  2.048 -2.048
                                 2.048].
                                                    -4837.639006924799
                                                                             -291.5008468
         [-2.048
14
         [0.18190488 2.048
                                 0.3253766
                                             0.25448714].
                                                                     -1907.2778122193617
15
         [-2.048 -2.048
                         2.048
                                 2.048].
                                                    -4837.639006924799
                                                                             -291.5008468
16
         [-2.048]
                        2.048
                                    1.32278726
                                                 2.048
                                                            1.
                                                                     -1304.6100652644307
                      -0.03488486
17
           0.3123691
                                    0.27467449
                                                 2.048
                                                            1.
                                                                     -400.3992688360985
           2.048
18
                  2.048
                         2.048 -2.048].
                                                    -4821.255006924799
                                                                             -291.5008468
19
         [ 2.048 -2.048
                         2.048 -2.048].
                                                    -8265.420843724798
                                                                             -291.5008468
```

```
20
                       0.05069028 -0.01457087 0.46404581].
         [ 2.048
                                                                    -1741.525845293071
21
           0.04462302 0.26846403 -2.048
                                               -0.09134914].
                                                                    -2303.9921807495207
22
         [0.27344559 0.455541
                                 2.048
                                                                    -815.8207189943965
                                            2.048
23
         [-0.54044064 0.20470646 0.04701984 -2.048
                                                                    -425.0160411278497!
24
         [-2.048]
                      -0.02157205 -0.3367943 -0.11652646].
                                                                    -1806.1444402871912
25
         [-1.24663827 -0.00408505 -0.43085572 1.90844862].
                                                                    -566.2723726921901
26
                       1.84388246 -0.275985
                                               -2.02519151].
                                                                    -2128.652409333823
         [-0.14563468
         [ 0.51129315 -0.04674546
27
                                  1.82266245 -0.02252549].
                                                                    -1461.5725858804212
         [-0.03619105 -0.9793058
                                    0.0457563
                                                                    -604.0445860660286
28
                                                2.048
29
         [-0.38043746 -0.47436586 -0.14851725 -1.90468684].
                                                                    -428.91430783919856
         [ 1.82143212 0.73311298 -2.04727183 -1.88527067].
30
                                                                    -5038.575769519586
         [-0.47465946  0.42283806  -0.85595954  -1.68383769].
31
                                                                    -700.8748323801497
32
         [-0.68527262 -0.58563323 1.51289546
                                                0.58564071].
                                                                    -543.9353731860382
33
         [0.55223936 0.46147771 1.27238896 0.21156894].
                                                                    -313.3316330394328
34
                       2.04339184 -0.29528961 -2.00670871].
                                                                    -2448.8503389948387
         [ 1.32173857
35
         [-0.34823756 -0.05469126 0.43322284
                                                1.88093636].
                                                                    -311.56852523404655
36
         [-0.03706493 0.9732862 -0.44071488
                                                1.85148322].
                                                                    -564.9168528854626
37
           1.28905706
                       0.32105178 -1.58817841 -1.93695353].
                                                                    -2461.505686335076
38
         [-1.87234884 -1.86175433 1.40728674 -0.66191861].
                                                                    -4019.649521955219
39
                                    1.75923584
                                                                    -959.8960097161256
         [-1.75988164
                       0.58497024
                                                2.00126065].
40
                       0.37549186
                                   0.96577463
                                                1.93190576].
                                                                    -183.26676877682718
         [-0.05047861
```

```
1 ### ESTIMATED GP EI GRADIENTS
2
3 np.random.seed(run_num_3)
4 surrogate_approx_3 = GaussianProcess(cov_func, optimize=opt)
5
6 approx_3 = GPGO(surrogate_approx_3, Acquisition(util_grad_approx), objfunc, param)
7 approx_3.run(init_evals=n_init, max_iter=iters)
8
```

```
Proposed point
Evaluation
                                            Current eval.
                                                                    Best eval.
         [ 0.20806821  0.85257348 -0.85645419  0.04434987].
                                                                     -367.7787956485136
init
                       1.62321649 -1.53360257 -1.19913317].
           1.60951073
                                                                     -3099.341888277455
init
         [-1.83719034 -0.24244288 -1.92562704 -0.17681111].
                                                                     -3229.929027395333
init
         [ 0.61089402 -0.90731609 0.72194008 0.3721741 ].
                                                                     -171.0831542888061
         [-1.94977021 0.24106634 -0.98610198 -0.3477455 ].
init
                                                                     -1564.2806119712143
1
         [-2.048
                 2.048 2.048
                                2.0481.
                                                    -1393.4731701248
                                                                            -171.0831542
2
         [-2.048 -2.048
                         2.048 -2.048].
                                                    -8273.612843724797
                                                                            -171.0831542
3
         [ 2.048 -2.048 -2.048
                                                    -8273.612843724799
                                 2.048].
                                                                            -171.0831542
                                            -1385.2811701248
4
         [2.048 2.048 2.048 2.048].
                                                                    -171.0831542888061
5
         [-0.35345106 2.048
                                    2.048
                                                -2.048
                                                           ].
                                                                     -4731.147173102215
6
                       -2.048
                                    0.13981966 -2.048
                                                                     -5979.124878992427
         [ 2.048
                                                           ].
7
         [-2.048 -2.048 2.048
                                 2.0481.
                                                    -4837.639006924799
                                                                            -171.0831542
8
           2.048 -2.048
                                                    -4829.447006924799
                          2.048
                                 2.048].
                                                                            -171.0831542
9
           0.05316528 2.048
                                                 2.048
                                                           ].
                                                                     -4786.856558033743
                                   -2.048
10
         [-2.048]
                  2.048 -2.048 -2.048].
                                                    -8273.612843724799
                                                                            -171.0831542
11
         [-2.048 -2.048 -2.048
                                2.048].
                                                    -8281.8048437248
                                                                            -171.0831542
12
                        0.42594084 2.048
                                                -0.53999331].
                                                                     -4012.3493497212075
         [ 2.048
13
         [-0.04134587 0.1948249
                                    0.61106596
                                                                     -318.88672890835636
                                                2.048
         [-0.4678158 -2.048
                                                                     -8327.868564032846
14
                                 -2.048
                                             -2.048
                                                       ].
         [-2.048
15
                        0.53467127 2.048
                                                 0.01790337].
                                                                     -3404.6375654877966
                        0.71210795 -0.20409272
16
           2.048
                                                 2.048
                                                            1.
                                                                     -1668.3216340955314
17
         [-0.03729572 -2.048
                                    0.33790576
                                                                     -1926.2602326634894
                                                 0.40183461].
18
                        1.10706136 -0.28643562
                                                 2.048
                                                                     -1579.1817487520102
         [-2.048]
19
           0.25492497 -0.07302655
                                    0.71993566
                                                 1.23744619].
                                                                     -106.47150583456444
                                   1.60406172 -0.66830816].
20
           1.49239847 0.49268641
                                                                     -1537.6735410119732
21
         [0.48719489 1.84629116 0.39103139 0.64259933].
                                                                     -1194.8836625814954
```

```
22
         [ 1.2299417 -1.91096248 1.4133729
                                                1.99191587].
                                                                    -1681.9314991104627
23
           0.00550859 -0.87056605 1.11029903
                                                1.51331117].
                                                                    -100.5842275200599
24
         [-0.06327872 -0.49098943 1.10261026
                                                1.83591466].
                                                                    -140.55156137310982
25
         [-1.92125593 0.53080971 -1.93881188
                                               1.72743047].
                                                                    -1922.030053518997
26
         [1.4605204 1.90918656 1.41415443 0.55762362].
                                                                    -711.8857692267823
27
                      -0.63259091 -1.96439414 -1.85587058].
                                                                    -4106.041253375681
           1.0047818
28
           0.98492504 1.17178375 -0.22453846 -1.97200959].
                                                                    -669.856486331395
29
          1.10614155 0.98623714 1.95858435 -0.70898671].
                                                                    -2169.50428747307
                                   0.21589641 -1.32198484].
                                                                    -2592.7693977126632
30
           0.94417659 -2.0345752
           1.69980461 1.46618113 -0.57797751
31
                                                1.0150917 ].
                                                                    -996.1300770680594
32
         [-0.7850228]
                       1.3368284
                                    1.82024652
                                               0.724710131.
                                                                    -726.0825390658513
33
         [-0.90364346 -1.40881445 -0.01203534 -1.32845648].
                                                                    -1080.9212981095382
34
         [ 1.23334546 -0.45172328  0.65487468 -1.43597748].
                                                                    -759.5865546206971
35
         [0.74524341 1.03355023 1.41376536 0.64124483].
                                                                    -219.31817541039308
36
         [-1.76099243 0.62045344 -0.09891249
                                               1.63585396].
                                                                    -912.1566142299126
37
         [ 0.74426082 -0.067332
                                   -0.27796404 -1.07523988].
                                                                    -182.24072574245946
         [0.1481922 1.19051691 2.038487
38
                                            1.78777272].
                                                                    -737.5559124439973
39
         [-0.29245864 -0.98054645 -0.12680832 -0.08144759].
                                                                    -239.90148247899936
40
         [ 0.94174472 1.35912663 0.63783186 -1.03478984].
                                                                    -376.6547766751747
```

```
1 ### ESTIMATED GP EI GRADIENTS
2
3 np.random.seed(run_num_4)
4 surrogate_approx_4 = GaussianProcess(cov_func, optimize=opt)
5
6 approx_4 = GPGO(surrogate_approx_4, Acquisition(util_grad_approx), objfunc, param)
7 approx_4.run(init_evals=n_init, max_iter=iters)
```

```
Evaluation
                 Proposed point
                                           Current eval.
                                                                   Best eval.
init
         [1.91295422 0.19346329 1.93611514 0.87988631].
                                                                    -2387.047477734054
init
         [ 0.80989727 -1.16289743 1.95082017 -2.02248087].
                                                                    -3769.0203854501506
init
         [-1.01178424 -0.26709388 1.14435245 -1.23828193].
                                                                    -936.5671269056027
         -3042.500138281922
init
                                               0.39867983].
init
         [-2.01119294 -0.46460403 -1.8671204
                                                1.87045056].
                                                                    -2747.9169599921197
1
         [-2.048
                 2.048 2.048
                                2.048].
                                                   -1393.4731701248
                                                                           -936.5671269
2
         [ 2.048 -2.048 -2.048
                                 2.048].
                                                   -8273.612843724799
                                                                           -936.5671269
3
         [-2.048
                  2.048 -2.048 -2.048].
                                                    -8273.612843724799
                                                                           -936.5671269
         [-2.048 -2.048 2.048
4
                                 2.048].
                                                    -4837.639006924799
                                                                           -936.5671269
5
         [ 0.01575257 -2.048
                                               -2.048
                                   -2.048
                                                           1.
                                                                    -8232.353242429861
6
           2.048
                  2.048
                         2.048 -2.048].
                                                    -4821.255006924799
                                                                           -936.5671269
7
         [-2.048
                  2.048
                         2.048 -2.048].
                                                    -4829.447006924799
                                                                           -936.5671269
8
                       0.73200004 -2.048
                                                           1.
                                                                    -5773.465902750279
         [ 2.048
                                               -2.048
9
         [-1.09601054
                       2.048
                                   -0.67176639
                                               2.048
                                                           1.
                                                                    -2702.80551795556
10
         [-2.048 - 2.048]
                         2.048 -2.048].
                                                    -8273.612843724797
                                                                           -936.5671269
         [ 2.048 -2.048
                        2.048
                                                    -4829.447006924799
11
                                 2.048].
                                                                           -936.5671269
12
         [0.66116829 2.048
                                 2.048
                                            2.048
                                                       1.
                                                                    -1183.121451473477
13
         [-0.28151045 -2.048
                                   -0.05260156
                                                0.59319317].
                                                                    -2303.0400014507027
14
         [-2.048]
                       0.44849204 0.40482431
                                                0.17278744].
                                                                    -1417.2158768631639
15
                                   -0.04026037 -0.76597681].
                                                                    -5760.180837294365
         [ 2.048
                      -2.048
                                   -2.048
                                                                    -9621.59195594188
16
         [-2.048]
                      -2.048
                                               -0.048866041.
17
         [ 2.048
                       0.59387418 -0.27488977
                                                2.048
                                                                    -1727.6335017846045
18
         [-0.03004513
                       2.048
                                    0.91355985 -0.24276783].
                                                                    -1613.6260512468998
19
         [-0.45086815
                       0.12775493
                                    2.048
                                                                    -877.9684801032818
                                                2.048
20
         [-0.15138668
                       0.64645298 -0.09549713 -2.048
                                                           1.
                                                                    -491.0623555759303
21
           0.10188111
                       0.16515724 -2.048
                                                0.484562361.
                                                                    -1820.0852185987146
22
         [-2.048]
                       -0.33483485 -0.37828314 -2.048
                                                                    -2568.421703134025
23
         [ 0.33784187
                       2.048
                                   -0.22811678 -2.048
                                                           ].
                                                                    -2773.8237975556917
```

```
-0.01108954
24
         [-0.7049028
                                   2.048
                                                0.14702181].
                                                                    -2088.260756294008
25
          [ 2.048  2.048  -2.048  2.048].
                                                    -4829.447006924799
                                                                           -491.062355!
26
          [-0.07877363 -0.32061305 0.12502611
                                                2.048
                                                           1.
                                                                    -427.455965971639
27
          [-0.07930562 -0.31974969
                                   0.12833224
                                                2.048
                                                           1.
                                                                    -427.07642680575424
28
          [-1.83504592 0.57272321
                                   0.36396613
                                                1.78672103].
                                                                    -1063.4262741118819
29
           0.24012772 -0.73428516
                                   0.54309972
                                                1.94719065].
                                                                    -339.50087645842956
30
          [-1.22276768
                        0.7543545
                                   -0.37217706 -1.22703467].
                                                                    -336.8270745465934
31
                       1.39105073 1.36951294 -1.83395094].
                                                                    -1421.9880420840564
         [ 1.32638545
32
         [2.04198784 1.97328923 1.95800832 0.59914916].
                                                                    -1906.4297312958206
33
         [-0.87122222
                       2.04692871 0.45878489 -0.82666467].
                                                                    -1670.4616530704325
34
          [-0.33218589 0.75505643 0.15995792 -1.25506911].
                                                                    -224.93573110971306
35
         [ 0.53907861  0.80105769 -0.13294576
                                               1.03329548].
                                                                    -190.74687989954148
36
           0.60276928 1.49878963 0.26705322 -1.09257692].
                                                                    -657.1050982695266
37
         [1.17707935 1.45523333 0.8341324 0.29449966].
                                                                    -181.6101171300378
38
         [-0.08973767 1.69880134 -0.38553909 -0.15508577].
                                                                    -1368.9319491647348
39
          0.74821824 1.78306464 -1.78430824
                                               0.915498931.
                                                                    -3136.318146218995
          [ 1.01737435 -1.68893479 1.62333127 -1.74129535].
40
                                                                    -2816.089596716538
4
```

```
1 ### ESTIMATED GP EI GRADIENTS
2
3 np.random.seed(run_num_5)
4 surrogate_approx_5 = GaussianProcess(cov_func, optimize=opt)
5
6 approx_5 = GPGO(surrogate_approx_5, Acquisition(util_grad_approx), objfunc, param)
7 approx_5.run(init_evals=n_init, max_iter=iters)
8
```

```
Evaluation
                 Proposed point
                                          Current eval.
                                                                 Best eval.
init
                       1.51851953 -1.20127834
                                              1.71463028].
                                                                  -1252.0157320257063
         [-1.13871597
init
         [-0.04746777 0.45770286 1.08915858
                                               0.07544008].
                                                                  -222.91752416760144
init
         [-0.83230515 -1.27909385 -1.71728376
                                                                  -1918.291410223084
                                               0.97665145].
init
         [-0.24039742 -1.39956278 1.55622208 -0.92534185].
                                                                  -1356.5528565009568
init
         [-0.35129336 -0.8352566
                                   0.52751527
                                               0.32701567].
                                                                   -100.45329155979191
1
                  2.048 -2.048 -2.048].
         [ 2.048
                                                  -8265.4208437248
                                                                          -100.453291
2
         [ 2.048
                      -2.048
                                   1.01658064
                                               2.048
                                                         ].
                                                                  -5019.751351509129
3
         [-2.048
                 2.048 2.048 -2.048].
                                                  -4829.447006924799
                                                                          -100.4532915
4
         [2.048 2.048 2.048 2.048].
                                          -1385.2811701248
                                                                  -100.45329155979191
5
         [-2.048
                      -0.78793203 2.048
                                               2.048
                                                                   -3160.1944342868937
                                                         1.
6
         [ 2.048 -2.048 -2.048 -2.048].
                                                  -11709.586680524799
                                                                          -100.453291!
7
                     0.874058 -2.048
                                        -2.048
         [-2.048]
                                                 ].
                                                          -5808.357426017814
                                                                                  -100
8
           2.048
                  2.048
                        2.048 -2.048].
                                                  -4821.255006924799
                                                                          -100.4532915
9
           2.048
                  2.048 -2.048
                                2.048].
                                                  -4829.447006924799
                                                                          -100.4532915
10
                     -2.048
                                -0.3237166 -2.048
                                                                   -6421.671297259764
         [-2.048
                                                     1.
11
         [ 2.048 -2.048 2.048 -2.048].
                                                  -8265.420843724798
                                                                          -100.4532915
         [-1.07641781 2.048
12
                                   2.048
                                               2.048
                                                                   -1006.9221316360523
13
                     0.33814809 0.06721482 0.12593329].
                                                                   -1491.0965688074964
         [2.048
14
         -2380.899556956846
15
         [ 1.80499795  0.05340004 -1.61819437
                                               0.9156279 ].
                                                                   -1588.1307824603793
16
         [-0.18792405 -0.41670073
                                  0.6961813
                                               1.12251394].
                                                                   -91.93205825222469
17
         [-2.00979377 1.45046548 1.91636392
                                              1.91286092].
                                                                   -993.4236305943057
         [0.42690547 0.44271243 1.85937242 1.71486174].
                                                                   -588.4415514651023
18
19
           0.6927607
                       0.97949297 -1.32818922
                                              1.7809417 ].
                                                                   -553.8106806602497
20
           0.86866932 0.5076431 -1.82363683 -0.78598627].
                                                                   -2138.083968068359
21
         [ 1.94994465 -0.35355171 -1.53741326 -1.48909156].
                                                                   -3496.9851843806637
22
         0.1473329
                     -1.7247022
                                 -1.41938966
                                              0.59671559].
                                                                   -2450.7700890745095
         [-1.37505296 -1.32512161 1.12550758 -1.87113142].
23
                                                                   -2069.6453850731227
24
         [0.75502349 0.74256749 1.84303871 0.46968966].
                                                                  -1027.436879763098
25
         [ 1.32475783 -0.8915516 -0.21088425 -0.78154481].
                                                                  -874.9477914351841
```

```
26
          [ 1.15487158 -0.834299
                                     1.05481692
                                                 0.2559162 ].
                                                                      -559.694281885498
27
          [-0.3107496
                        1.66980759 -0.84551918
                                                  0.41760558].
                                                                      -1582.353544675686
28
          [-1.07255585 -0.11466322 -1.92503864
                                                                      -1264.7418425813808
                                                  1.03190207].
29
           1.28272724 -1.39964435 -0.12724209 -1.20591634].
                                                                      -1518.928737142175:
30
          [-1.20365786 0.31174043
                                   0.0297163
                                                  1.38762166].
                                                                      -328.3195031335746
31
          [-1.6109904
                        0.8590569
                                     0.45648285 -1.77930314].
                                                                      -711.5941755565317
32
          [-0.13522102 -2.00678675
                                     0.85543304
                                                  0.21808611].
                                                                      -1452.8346714359607
                        0.46429525 -0.96362403
33
          [-1.3997181
                                                 1.3682138 ].
                                                                      -391.7571103590943
34
                                     0.87587592 -2.02996793].
                                                                      -840.5237144476857
          [-0.61004237
                        1.06835669
35
          [-0.02002553 -0.03632827
                                     0.21463406
                                                  1.80302799].
                                                                      -316.10734839035746
36
          [-0.31390776]
                        0.79157762
                                     1.3836017
                                                  1.465092441.
                                                                      -127.43678379889838
37
                                                  0.83116248].
                                                                      -391.92643983382715
          [-1.38834774
                        1.34558751
                                     1.64297275
38
          [-1.00480104 -1.63478392
                                     0.45813346 -1.68836468].
                                                                      -1561.230607409748
39
          [-0.03997327
                        1.87412011
                                     1.35086415
                                                -0.98530202].
                                                                      -1609.4809120635457
40
          [-0.49490898 -0.61553645 -0.38107717
                                                  1.124754
                                                                      -234.496171179621
4
```

```
1 ### ESTIMATED GP EI GRADIENTS
2
3 np.random.seed(run_num_6)
4 surrogate_approx_6 = GaussianProcess(cov_func, optimize=opt)
5
6 approx_6 = GPGO(surrogate_approx_6, Acquisition(util_grad_approx), objfunc, param)
7 approx_6.run(init_evals=n_init, max_iter=iters)
8
```

```
Proposed point
                                            Current eval.
                                                                    Best eval.
Evaluation
init
         [ 1.60915518 -0.68821072
                                    1.31575449 -1.87721062].
                                                                     -2450.5677149947023
init
         [-1.60703824 0.38933325 0.12213192 -0.33256477].
                                                                     -501.1308148976547
init
         [-0.67416945 0.50183959 -0.25337272
                                                0.96617311].
                                                                     -111.72625934007624
init
         [0.07387714 0.32300483 0.59537447 2.00795862].
                                                                     -309.0778245045886!
init
           1.31013917 -0.35552897 1.54119232 1.32611864].
                                                                     -741.7784291682051
1
         [ 2.048
                        2.048
                                   -2.048
                                                -0.16855141].
                                                                     -6272.235654950075
2
         [-2.048 - 2.048 - 2.048]
                                2.048].
                                                    -8281.8048437248
                                                                            -111.7262593
3
                                                -2.048
         [-0.31768625 -2.048
                                   -2.048
                                                            ].
                                                                     -8275.376423859392
4
         [-2.048 -2.048 2.048 -2.048].
                                                    -8273.612843724797
                                                                            -111.7262593
5
         [ 2.048 -2.048 -2.048
                                 2.048].
                                                    -8273.612843724799
                                                                            -111.7262593
6
         [-2.048]
                  2.048 -2.048
                                 2.0481.
                                                    -4837.639006924799
                                                                            -111.7262593
7
         [-2.048
                  2.048
                          2.048
                                 2.0481.
                                                    -1393.4731701248
                                                                            -111.7262593
8
                                                    -8273.612843724799
         [-2.048]
                  2.048 -2.048 -2.048].
                                                                            -111.7262593
9
                                                    -4837.639006924799
         [-2.048 - 2.048]
                          2.048
                                 2.048].
                                                                            -111.7262593
                                    2.048
10
         [-0.89746264
                        2.048
                                                -2.048
                                                            ].
                                                                     -4517.490718018506
11
         [2.048 2.048 2.048 2.048].
                                            -1385.2811701248
                                                                    -111.72625934007624
12
                       2.048
                                             -0.8927154].
                                                                     -3512.395725008554
         [ 2.048
                                  2.048
           2.048 -2.048 2.048 2.048].
13
                                                    -4829.447006924799
                                                                            -111.7262593
         [-0.10283764 2.048
14
                                    0.25893936
                                                0.88721162].
                                                                     -2033.949610524387
15
           0.28919478 -0.27590698 -0.320587
                                                -0.29969978].
                                                                     -48.740768932182
16
           0.03514236 -0.01962668 -1.27974723
                                                0.16995172].
                                                                     -386.5293127271378
17
         [-0.1433454
                       -1.65451769
                                    0.71253363 -0.09213704].
                                                                     -735.0218045780138
18
         [-0.71508768 -1.06298624
                                    1.48028271 -0.75758851].
                                                                     -1137.112846776038
19
         [ 0.94214099 -1.57354766 -0.74644094
                                                                     -1689.576343784932
                                                 1.15478747].
20
         [1.8909089 0.28940522 0.85682419 1.06069847].
                                                                     -1151.6121108178433
21
         [ 1.89109499 -0.64451329
                                    0.19246157
                                                 1.0232119 ].
                                                                     -1887.8498992613063
22
         [-1.48289855
                        1.9603708
                                    0.88014879
                                                 1.04657615].
                                                                     -898.0695517217156
23
         [0.33873613 1.06893801 0.88105688 1.03917139].
                                                                     -105.25928491494603
24
         [-1.61922811
                        1.23481322
                                   2.02363183
                                                 1.9101849 ].
                                                                     -702.6303179178191
25
           0.15810568
                        1.97152737 -0.44674798 -1.31645352].
                                                                     -2490.5484677296968
26
         [-0.14395639
                        0.83083395
                                    0.48969449 -1.25888407].
                                                                     -295.85482689009353
27
         [-1.04837812 -1.02335261
                                    0.62386577
                                                 1.73596787].
                                                                     -658.211927766007
```

```
28
          [-0.95422001 -0.54737772 -0.44854888 -1.1889234 ].
                                                                    -470.0820820835665
29
           1.96181723 -1.56127344 0.47070345 -0.43759404].
                                                                    -3364.882590614902
30
           1.33981188 0.49177975 -1.7059087 -1.64398766].
                                                                    -2630.928106036733
31
          [-2.04650648 1.44371507 -1.98550922
                                                1.9251675 ].
                                                                    -2834.811304710729!
                       1.23904023 -1.04353373 -0.39191513].
32
          [-1.06066992
                                                                    -894.0769169135324
33
          [-0.35702929
                        1.09433763 -0.51713564 -1.56045156].
                                                                    -725.7734812165357
34
           1.85564941 -0.68981499
                                   0.2899382
                                               -1.66918129].
                                                                    -2023.3102026099407
35
                        0.30413893 1.58954197 -1.24066722].
           0.62057554
                                                                    -1645.007906836277!
                        1.36094253 -1.70864839
36
           0.78309714
                                                1.38494553].
                                                                    -1566.8381453248673
37
                        1.34467199 -0.60828857
          [-0.17324013
                                                 1.01354448].
                                                                    -802.2419906375629
38
          [-0.07967532 -0.56041942 -0.53123136 -0.08364451].
                                                                    -122.90596687337347
39
                        1.98328736 -1.20424388
                                                                    -3025.401390343327
          [ 0.18867716
                                                 1.44766517].
40
          [ 1.41638326 -0.57018461 -1.27636987 -0.21078604].
                                                                    -1266.5657344000517
4
```

```
1 ### ESTIMATED GP EI GRADIENTS
2
3 np.random.seed(run_num_7)
4 surrogate_approx_7 = GaussianProcess(cov_func, optimize=opt)
5
6 approx_7 = GPGO(surrogate_approx_7, Acquisition(util_grad_approx), objfunc, param)
7 approx_7.run(init_evals=n_init, max_iter=iters)
8
```

```
Proposed point
                                           Current eval.
                                                                   Best eval.
Evaluation
init
         [-1.73544125 \quad 1.14654737 \quad -0.25227579 \quad 0.91531337].
                                                                    -675.0078283253545
init
         [ 1.95784504  0.15767909  0.00458942  -1.75287856].
                                                                    -1660.8385633941034
init
         [-9.48473938e-01 -4.81276619e-04 7.34126064e-01 1.24411509e+00].
         [-0.48766512 -1.77792472 -0.86775563 1.67769509].
init
                                                                    -2128.346574385609
init
         [-1.17397359 -0.19610025 1.76621986 -1.94601276].
                                                                    -3119.0824429471622
1
         [2.048 2.048 2.048 2.048].
                                           -1385.2811701248
                                                                   -189.504451516756
2
         2.048].
                                                    -4829.447006924799
                                                                            -189.504451!
3
         [-2.048 - 2.048 - 2.048 - 2.048].
                                                    -11717.778680524798
                                                                            -189.5044515
4
         [ 2.048 -2.048
                         2.048
                                 2.048].
                                                    -4829.447006924799
                                                                            -189.5044515
5
         [-0.76407837
                       2.048
                                   -2.048
                                               -2.048
                                                           ].
                                                                     -8021.155976492433
6
         [-2.048 -2.048 2.048
                                 2.048].
                                                    -4837.639006924799
                                                                           -189.5044515
7
         [ 2.048
                      -2.048
                                   -2.048
                                               -0.37337285].
                                                                     -9899.31793886073
8
         [-2.048
                 2.048
                          2.048
                                 2.048].
                                                    -1393.4731701248
                                                                           -189.5044515
9
           2.048 -2.048
                          2.048 -2.048].
                                                    -8265.420843724798
                                                                            -189.504451!
10
                  2.048
                         2.048 -2.048].
                                                    -4821.255006924799
         [ 2.048
                                                                            -189.504451
11
                  2.048 -2.048
                                                    -4837.639006924799
         [-2.048]
                                2.048].
                                                                            -189.504451
12
         [0.23281682 2.048
                                 0.58845417 0.34515969].
                                                                     -1699.5940462166436
13
         [-2.048
                        2.048
                                    2.048
                                               -0.81077604].
                                                                    -3437.8937007665054
                                                    -8265.4208437248
14
         [ 2.048
                  2.048 -2.048 -2.048].
                                                                            -189.504451
15
         [-0.00297184 0.30307921 2.048
                                                2.048
                                                           1.
                                                                     -855.0867475003914
         [-0.48933097 -2.048
16
                                    0.75506552 -0.40143431].
                                                                    -1812.037447386919
17
         [-0.14976047
                      0.22071614 -2.048
                                                0.51479887].
                                                                    -1808.6487825828783
18
         [ 2.048
                       -0.24637753 -0.25108972
                                                2.048
                                                                    -2379.907852848156
                                                           1.
19
           1.57724724 -1.43419739 1.0000704
                                                1.67615355].
                                                                    -1701.786289068928
20
           1.30254556
                       0.86457258 -1.9212007
                                                                     -1193.738652806666
                                                1.68184436].
21
         [-0.09917108 -0.39295794 -0.47187016 -1.06023994].
                                                                    -225.34614242670636
22
                      -0.13259573 0.13386717
                                                0.59127733].
                                                                     -1062.9030231974123
         [-1.7492046
23
           0.92456199 -0.14870572
                                    1.83949158 -0.27586851].
                                                                     -1772.2872617658254
24
         [1.09755539 0.06000333 0.40179989 0.72821809].
                                                                     -180.2471447384382
25
         [-0.4259852
                        1.41530979 1.2169289
                                                0.21733628].
                                                                    -375.96080556137713
26
           0.36525072
                       1.67723443
                                    1.54157949 -0.61270067].
                                                                    -1294.6877030790056
27
           1.69057861
                       0.50218671
                                    0.64506916 -1.67216904].
                                                                    -1007.3907003780754
28
         [-0.38966076
                       0.92146266
                                    0.23916367
                                                1.98130549].
                                                                    -469.1687000785605
29
         [ 1.29833014 -1.73994269 -1.37322401 -2.00185139].
                                                                    -4634.594219963464
```

```
30
         [-1.37706882 -1.78891816 -1.78812293 0.9528631 ].
                                                                    -4371.451001526354
31
         [-1.34271262 0.64109026 -0.54198534 -0.83191675].
                                                                    -360.49934374026805
                       1.00488362 1.58181641 -0.42751198].
32
           1.10499416
                                                                    -896.0299290520137
33
           0.28125263 1.49538692 -1.05695459 0.37020686].
                                                                    -1345.846818341517
34
         [-1.4033467]
                       0.70593538  0.53780605  -0.57026152].
                                                                    -239.7351017763423
35
                     1.98553896 0.30785905 1.872358
                                                                    -1672.687784979123
         [1.1833041
36
         [-0.28567618 -0.1544846 -1.63190891 1.11871168].
                                                                    -528.1675091303345
                       1.13095515 0.8477285
                                               -1.307918
37
         [ 0.60536907
                                                                    -487.9394065197489
                      0.30745523 -1.78135793 -0.53039286].
                                                                    -1734.6847866522687
38
         [-0.60314838
39
         [-0.88676012 -1.24914685 -1.92922663 -0.26139304].
                                                                    -3235.9225444273907
40
         [ 0.37336764  0.79031767  1.15239768  -0.30730899].
                                                                    -338.11584891777335
```

```
1 ### ESTIMATED GP EI GRADIENTS
2
3 np.random.seed(run_num_8)
4 surrogate_approx_8 = GaussianProcess(cov_func, optimize=opt)
5
6 approx_8 = GPGO(surrogate_approx_8, Acquisition(util_grad_approx), objfunc, param)
7 approx_8.run(init_evals=n_init, max_iter=iters)
8
```

```
Evaluation
                 Proposed point
                                           Current eval.
                                                                   Best eval.
init
         [1.52956683 1.91914255 1.51222084 0.12638491].
                                                                    -957.0835831104033
init
         [-1.09474477 -2.0013105 -0.28479972 -0.39996883].
                                                                    -2902.49459403014
init
         [ 0.09287545 -0.0885072
                                    0.22674012
                                                0.17770913].
                                                                    -9.936266004845226
init
         [ 1.06862828  0.86988626  0.49021787 -0.30272811].
                                                                    -44.27508698465467
         [-0.86394869
init
                       1.94091107 -0.68086151 -1.15179085].
                                                                     -2389.276657793903
                                                                    -2875.9237346807367
1
                       -0.23418835 -2.048
                                                 2.048
         [ 2.048
2
         [ 2.048 -2.048 2.048
                                 2.048].
                                                    -4829.447006924799
                                                                            -9.936266004
3
         [-2.048]
                       0.8073882 2.048
                                             2.048
                                                                     -1813.12396018947
4
                       -0.77107626 -2.048
                                                -2.048
                                                           1.
                                                                     -7073.972948181394
           2.048
5
         [ 2.048 -2.048 2.048 -2.048].
                                                    -8265.420843724798
                                                                            -9.936266004
                                                    -4837.639006924799
6
         [-2.048]
                  2.048 -2.048 2.048].
                                                                            -9.936266004
7
                                                -2.048
         [-2.048
                       0.14199525
                                    2.048
                                                           1.
                                                                     -5961.093756570441
8
         [-1.77290669 -1.83187185
                                    1.97229377
                                                1.78585986].
                                                                     -3125.8988203363256
9
         [ 0.25243216  0.65132557 -0.14650052
                                                1.22684164].
                                                                     -214.38936491229418
                       1.90294575 -1.45125373
10
           1.61594834
                                                0.11664432].
                                                                     -3026.1678727420663
11
         [-1.37465317 -1.27719736 -1.7759979
                                                 1.52146912].
                                                                     -2448.929554584813
                                                                     -94.62044362780631
12
         [0.84504065 0.08611254 0.72124982 0.70162738].
13
         [-1.76613656 - 0.49780973 - 2.03029569 - 1.76491398].
                                                                     -5312.05401906433
14
         [0.118439
                     1.92378152 0.60865592 1.89654088].
                                                                     -1555.6104609220843
15
           0.30464581 -0.18781366 0.41570432 -0.22592534].
                                                                     -40.48245078294073
           0.91790074 0.6354423
                                    0.94951529 -1.81924204].
                                                                     -774.5000287298005
16
17
           0.27539419 -0.26838424 1.63171554 0.09632702].
                                                                     -916.1660775772639
18
           1.56847741
                       0.24316373 -0.69881531 -1.01761465].
                                                                     -779.5107598624428
19
           0.35484129 -1.86816284 -0.14451651
                                                                     -1862.7217634316391
                                                 1.179078
20
           0.79611724
                       0.59266256 -1.75214302
                                                1.71347332].
                                                                     -634.3946569537112
21
           0.33342699
                       0.85744112 -1.39013062 -0.70905999].
                                                                     -1211.338605679206
22
           1.96447046 -1.1253884
                                   -1.00393877 -0.3542284 ].
                                                                     -3195.0460205517234
23
         [-1.90505287e+00 -3.38086882e-01 -1.13311058e-03 -6.45533451e-01].
                                                                                     -16
24
           0.06932344 - 0.82987684
                                   1.31480695
                                                1.92426221].
                                                                     -117.00853922429148
25
           0.96841336
                       1.43567499 1.34995083 -0.09034321].
                                                                     -441.5271478713890
26
         [-1.94029947 -0.86847316 -1.27079134
                                                1.67313391].
                                                                     -2574.3963586969853
27
           0.3863695
                        0.15426794 0.8482894
                                               -1.47726505].
                                                                     -551.715179290625
28
           1.27554452 -1.33772913 -0.69806032 -0.96771911].
                                                                     -1717.9042203681279
29
           1.22309047
                       0.50266748 -1.68360001 -0.00168864].
                                                                     -1285.4775424217082
30
         [-1.2854068
                        1.68828179 -0.69504045
                                                1.83299086].
                                                                    -1447.8658969833066
31
         [-1.62809426 -1.9138781
                                    1.87257031 -0.31780317].
                                                                     -3882.7709730274632
```

```
32
         [ 0.01115185 -1.04402107 -0.98431878 -1.62553599].
                                                                -1221.4900994190507
33
         1.85061772].
                                                                -1344.8892697299098
34
         [-1.59478187 -1.15323929 -1.63623257
                                             1.79534308].
                                                                -2342.3884903861576
35
         [-0.69785189 -0.2136039 -0.78857984
                                             1.22944205].
                                                                -163.14461373860414
36
         [-0.12161189 0.78179848
                                0.84265519
                                             0.85241509].
                                                                -67.54368335296114
37
         [-1.99255462 -0.04453909
                                 0.05325667 -1.23906119].
                                                                -1777.308949498485
38
                      1.14762359
                                  1.95274426 -1.61966174].
                                                                -3507.4826376379906
         [-1.84338287
39
         [ 0.52225599 -0.55066016
                                 0.5964857
                                            -0.79658913].
                                                                -211.9953091401932
40
         [-0.85267003 -1.01769894 -1.92553885 -0.87200242].
                                                                -3294.7432895001366
```

```
1 ### ESTIMATED GP EI GRADIENTS
2
3 np.random.seed(run_num_9)
4 surrogate_approx_9 = GaussianProcess(cov_func, optimize=opt)
5
6 approx_9 = GPGO(surrogate_approx_9, Acquisition(util_grad_approx), objfunc, param)
7 approx_9.run(init_evals=n_init, max_iter=iters)
8
```

```
Evaluation
                 Proposed point
                                            Current eval.
                                                                    Best eval.
init
         [-2.00550747 \quad 0.00767833 \quad -0.01731259 \quad -1.49983425].
                                                                     -1847.6492499405208
init
         [-1.46591299 -1.15278366 -0.33379049 -1.03177761].
                                                                     -1509.7528388540472
         [-1.70369167 -0.63283757 -1.36488408
init
                                                1.55057801].
                                                                     -1586.883400641493
init
         [ 1.84714867 -1.88928665 0.81554388 0.2980242 ].
                                                                     -3591.2693050622433
init
         [1.63023716 0.68361819 0.19594356 0.82914273].
                                                                     -460.72675701107613
                         2.048 2.048].
                                                    -1393.4731701248
1
         [-2.048]
                  2.048
                                                                             -460.7267576
2
           2.048
                  2.048 -2.048 -2.048].
                                                    -8265.4208437248
                                                                             -460.7267576
3
                                                                                     -466
         0.745632
                     2.048
                                2.048
                                          -2.048
                                                             -4582.175544663847
4
         [-2.048 -2.048 2.048 2.048].
                                                    -4837.639006924799
                                                                             -460.7267576
5
         [ 2.048 -2.048 -2.048 -2.048].
                                                    -11709.586680524799
                                                                            -460.7267576
6
           0.62170517 2.048
                                   -2.048
                                                 2.048
                                                                     -4643.882194751861
                                                           1.
7
         [2.048 2.048 2.048 2.048].
                                            -1385.2811701248
                                                                    -460.72675701107613
8
         [ 2.048 -2.048 -2.048 2.048].
                                                    -8273.612843724799
                                                                            -460.7267570
9
                  2.048 -2.048 -2.048].
         [-2.048
                                                    -8273.612843724799
                                                                             -460.7267576
10
         [-2.048 -2.048 2.048 -2.048].
                                                    -8273.612843724797
                                                                            -460.7267576
11
         [-2.048]
                        2.048
                                    2.048
                                                -0.80668396].
                                                                     -3433.7991374968947
                       -0.95145748 2.048
12
         [ 2.048
                                                -2.048
                                                            1.
                                                                     -6681.109716094484
13
         [-2.048 -2.048 -2.048 -2.048].
                                                    -11717.778680524798
                                                                             -460.7267576
14
         [3.28483590e-01\ 1.07302868e-03\ 2.04800000e+00\ 2.04800000e+00].
15
                                                                     -3108.5581318496816
         [-2.048]
                        2.048
                                   -0.69351776 2.048
                                                            1.
16
         [ 0.17594119  0.02738846 -2.048
                                                -0.14495646].
                                                                     -2313.572463111283
17
         [2.048
                      2.048
                                 0.33949458 0.12864949].
                                                                     -1949.2684627312997
                                                 0.075972371.
18
         [-0.37661966 -0.13446282 2.048
                                                                     -2120.037805189611
19
                      0.27236274 0.13244069 2.048
                                                                     -1953.158724111358
20
         [-0.36993991 -2.048
                                   -0.19617604 2.048
                                                            ].
                                                                     -2821.4037856093846
21
         [ 2.048 -2.048 2.048 2.048].
                                                    -4829.447006924799
                                                                             -460.7267576
22
         [0.04008396 2.048
                                 1.08914878 2.048
                                                       1.
                                                                     -1459.261284448879
23
         0.34857918
                       0.19648048 -0.1790552 -2.048
                                                                     -440.4251160806338
24
         [-0.37124428
                        2.048
                                   -0.20447809 -0.27325156].
                                                                     -2314.162110380757
25
         [-2.048]
                        0.40384289 2.048
                                                                     -2263.454562520175
                                                 2.048
         [ 1.57214197  0.36938666  -0.88856352  -0.03117535].
                                                                     -618.6573179161406
26
           0.1852866 -2.048
27
                                    0.27614645 -2.048
                                                                     -2430.530897116609
         [1.49748654 0.51290318 1.64385257 0.78999404].
28
                                                                     -856.3669505790126
                       -0.18471497 0.26383397
29
                                                 0.57584231].
                                                                     -1959.7206610568678
         [-2.048]
30
         [-2.048 -2.048 -2.048 2.048].
                                                    -8281.8048437248
                                                                             -440.4251160
31
         [-1.26346914 1.78296691 -1.07923439
                                                 0.06511644].
                                                                     -1947.6919928049658
32
           2.048
                        0.15261037 -0.33715839 -0.46397146].
                                                                     -1683.4930406443598
33
         [ 2.04376527
                        1.03643392 -1.98979889
                                                 1.0844969 ].
                                                                     -2761.5855185307337
```

```
34
         [ 1.08857292
                        1.4669949
                                    0.92814686 -1.956494
                                                                     -952.068037210575
35
           0.26887127
                        0.50500011 -0.13630092 -2.048
                                                                     -463.1824494648608
         [-1.22825293
36
                        1.74001646
                                    0.68661992
                                                 1.13566625].
                                                                     -603.1303835990793
37
           0.22168689 -1.83113965
                                    0.22192424 -0.32233273].
                                                                     -1356.9898885879918
38
           0.24948113
                        1.19516488 -1.28774391 -1.39570007].
                                                                     -1804.6230797860508
39
         [-1.04158977 -0.41917658
                                    1.97191901 -1.03991655].
                                                                     -2984.8853118097572
40
         [ 1.29290756 -0.74402798
                                    1.47624219
                                                 2.00947067].
                                                                     -674.8997870657305
```

```
1 ### ESTIMATED GP EI GRADIENTS
2
3 np.random.seed(run_num_10)
4 surrogate_approx_10 = GaussianProcess(cov_func, optimize=opt)
5
6 approx_10 = GPGO(surrogate_approx_10, Acquisition(util_grad_approx), objfunc, param)
7 approx_10.run(init_evals=n_init, max_iter=iters)
8
```

```
Proposed point
                                            Current eval.
                                                                    Best eval.
Evaluation
init
         [ 1.11132935 -1.96300002 0.54742317
                                                 1.0191007
                                                                     -2176.436426889387
init
         [-0.00611528 -1.12723294 -1.23673451
                                                 1.0671338 1.
                                                                     -787.6933551437477
init
         [-1.35532201 -1.68616012 0.75923382
                                                 1.85709915].
                                                                     -1852.2892745062024
init
         [-2.0318279]
                        0.04993951
                                    1.28049546
                                                0.46090677].
                                                                     -1975.7725172569656
init
         [ 0.90830978 -0.85247562
                                    1.71120281
                                                 0.87890241].
                                                                     -802.2371849082838
1
         [ 2.048
                  2.048 -2.048 -2.048].
                                                    -8265.4208437248
                                                                            -787.6933551
2
         [-2.048 - 2.048 - 2.048 - 2.048].
                                                    -11717.778680524798
                                                                            -787.6933552
3
                  2.048 -2.048
                                                    -4837.639006924799
                                                                            -787.6933553
         [-2.048
                                 2.048].
4
           0.47780069
                       2.048
                                    2.048
                                                -2.048
                                                           1.
                                                                     -4690.900483469856
5
           2.048
                        2.048
                                   -0.02364472
                                                2.048
                                                           ].
                                                                     -2662.217114217972
6
         [ 2.048 -2.048 -2.048 -2.048].
                                                    -11709.586680524799
                                                                            -787.6933552
7
         [-2.048]
                        2.048
                                   -1.33138042 -2.048
                                                           ].
                                                                     -4989.483281183711
8
         [-0.56720242 -2.048
                                    2.048
                                                -2.048
                                                                     -4931.699360052157
9
         [-0.57377178 2.048
                                    2.048
                                                 2.048
                                                           1.
                                                                     -1221.4200510491394
10
         [-2.048 -2.048 -2.048 2.048].
                                                    -8281.8048437248
                                                                            -787.6933552
                                                                     -3293.2874943139245
11
           2.048
                       -0.56117744 -2.048
                                                 2.048
12
         [ 2.048
                       -0.57575421 1.28315288 -2.048
                                                                     -3734.491905382689
13
         [2.048
                      1.23206354 2.048
                                             0.55848702].
                                                                     -2229.7458889033796
                                                -0.06188899].
14
         [-0.1317889
                        0.56530118 -2.048
                                                                     -2412.8377317794775
15
                       0.7855277
                                  2.048
                                             -2.048
                                                       1.
                                                                     -5273.806829078712
         [-2.048
         [-0.39565453
                        2.048
                                    0.18726931
                                                 0.31931271].
                                                                     -1975.179933602968!
16
17
         [ 2.048 -2.048 2.048
                                 2.048].
                                                    -4829.447006924799
                                                                            -787.6933552
18
           2.048
                        2.048
                                   -2.048
                                                 1.02940829].
                                                                     -5370.4414049733505
19
         [-0.12950152 -0.03638543 -0.35623638 -2.048
                                                                     -490.2776334980217
                                    0.86913613
                                                 2.048
20
         [-2.048]
                        2.048
                                                                     -1743.8240457428547
21
                       -2.048
                                    2.048
                                                 0.26287683].
                                                                     -5922.58887818761
         [-2.048]
22
         [0.00922389 0.05280625 2.048
                                             2.048
                                                       1.
                                                                     -882.2061634329553
23
         -405.0282723148539!
                                                 2.048
24
         [ 2.048
                       -0.0626217
                                   -0.26329595 -0.04185903].
                                                                     -1824.341728731095
25
         [-0.70612861
                      0.04459932 -0.53963139
                                                 1.51068639].
                                                                     -204.85687590049463
26
           0.27699119 -0.52941187
                                    0.98432743
                                                 1.32497665].
                                                                     -101.84990573719982
27
         [-1.09101046 - 0.78721212 - 0.18121539 - 1.02716706].
                                                                     -576.5269503988607
                        0.85525047
                                    0.09269607
                                                                     -895.5226497615581
28
         [-1.84683074
                                                 1.39674932].
29
         [-1.10782382
                        1.08678957
                                    1.83591093
                                                 0.79947953].
                                                                     -711.0490742497022
30
           1.8866903
                      -0.12687083
                                    0.40402276
                                                 1.86449239].
                                                                     -1665.8947477686202
31
           0.08049474 -1.5649912
                                    0.34922937 -0.81227962].
                                                                     -783.0673403408462
32
         [ 1.34205403
                        2.01618533
                                    1.56150399 -1.66922673].
                                                                     -2320.0148127725156
33
         [0.86506562 1.08373241 0.70537686 0.11630819].
                                                                     -47.901348809022956
34
           1.45206965
                        1.18898007
                                    1.01897055 -1.15126377].
                                                                     -579.7917141619665
35
         [-0.52727733 -0.75829671
                                    0.98954076 -1.48721947].
                                                                     -738.3210826217644
```

```
36
         [-0.75155978 1.3610957
                                    1.14781785
                                                1.31613751].
                                                                    -116.29154433379108
37
         [2.02714091 0.73764233 1.18728261 1.92488869].
                                                                    -1205.8810803418426
         [ 0.15851054 -0.76533319 -0.06448037 -0.23312002].
38
                                                                    -115.3481941524951
39
         [-1.42267809 1.18387659 -0.61381498
                                                1.74883739].
                                                                    -673.5228586952437
40
         [-0.82339488 -1.42360596
                                   1.4478472
                                                0.39763342].
                                                                    -773.1006601987814
```

```
1 ### ESTIMATED GP EI GRADIENTS
2
3 np.random.seed(run_num_11)
4 surrogate_approx_11 = GaussianProcess(cov_func, optimize=opt)
5
6 approx_11 = GPGO(surrogate_approx_11, Acquisition(util_grad_approx), objfunc, param)
7 approx_11.run(init_evals=n_init, max_iter=iters)
```

```
Evaluation
                 Proposed point
                                           Current eval.
                                                                   Best eval.
init
         [-1.30961535 -1.96822941 -0.15065692 0.92132937].
                                                                    -3072.6361628465456
init
         [-0.32684604 -0.05969061 -1.99564978 -0.0517259 ].
                                                                    -2041.908514926983
init
         [ 1.80964005
                       1.43685669 0.94193447 -1.60261705].
                                                                    -1084.6194797620587
init
           1.61343148 1.4629038 -1.37180521
                                                0.542040121.
                                                                    -1549.0827052305292
         [-1.96409912 -1.56984415 -0.75215949 -1.40119119].
init
                                                                    -4385.783412609677
1
         [-2.048]
                  2.048 2.048
                                2.048].
                                                   -1393.4731701248
                                                                           -1084.619479
2
         [ 2.048
                       -0.91250438 2.048
                                                2.048
                                                           ].
                                                                    -3222.169648290899
3
         [-2.048
                 2.048
                         2.048 -2.048].
                                                   -4829.447006924799
                                                                           -1084.619479
4
         [ 2.048 -2.048
                        2.048 -2.048].
                                                   -8265.420843724798
                                                                           -1084.619479
5
           2.048 -2.048 -2.048
                                 2.048].
                                                   -8273.612843724799
                                                                           -1084.619479
         [-2.048
6
                  2.048 -2.048
                                 2.0481.
                                                   -4837.639006924799
                                                                           -1084.619479
7
         [ 2.048 -2.048 -2.048 -2.048].
                                                   -11709.586680524799
                                                                           -1084.619479
8
                 2.048 -2.048 -2.048].
                                                   -8273.612843724799
         [-2.048
                                                                           -1084.619479
9
         [1.08886219 2.048
                                 2.048
                                            1.24541998].
                                                                    -1406.8280653788652
10
                  2.048 -2.048 -2.048].
         [ 2.048
                                                   -8265.4208437248
                                                                           -1084.619479
         [-2.048 -2.048 2.048 -2.048].
                                                   -8273.612843724797
11
                                                                           -1084.619479
12
         [-2.048]
                      -0.82499621
                                   2.048
                                                2.048
                                                           1.
                                                                    -3180.6919127661913
                                               -0.29959423].
13
         [-0.05076564 0.12352942
                                   2.048
                                                                    -2437.1490792312607
14
         [ 0.06656225  0.7470947
                                   -0.00641287
                                                2.048
                                                                    -508.38987529902107
15
         [-2.048]
                      -1.18077181 -2.048
                                                2.048
                                                                    -4558.031738878403
                                                           ].
16
         [-0.90574639 2.048
                                    0.16575045
                                                0.19860708].
                                                                    -1781.9851379289514
17
                     2.048
                                 0.05711203 2.048
                                                      1.
                                                                    -2593.478908866238
         [2.048
                                                                    -2269.882924180482
                      -0.559388
                                                0.03599057].
18
         [ 2.048
                                    0.07527866
19
           ].
                                                                    -431.2197229866473
                                                                    -4512.882639400185
20
           0.89974518
                       2.048
                                    2.048
                                               -2.048
                                                           ].
                                                   -4829.447006924799
21
           2.048
                 2.048 -2.048
                                 2.048].
                                                                           -431.2197229
           0.01805574 -2.048
                                                           1.
                                                                    -1352.2409388680248
22
                                    2.048
                                                2.048
23
           0.24415386 -0.01483553 -0.16655859 -2.048
                                                           1.
                                                                    -437.16818284212917
24
           0.15547624 -0.09977176 -0.11715715
                                               2.048
                                                                    -420.14987269616694
25
         [-0.22887801 -0.1728996
                                 -2.048
                                               -2.048
                                                           ].
                                                                    -4345.651842457049!
26
         [ 0.15234581 -2.048
                                    2.048
                                                0.13182734].
                                                                    -2551.131648064501
27
                       0.77177479
                                   0.22070694
                                                2.048
                                                                    -1595.0929430712267
         [-2.048]
28
         [-2.04131249 -0.0225987
                                    1.47106294 -0.24288256].
                                                                    -2561.327976178364
29
         [ 0.32288174  0.5738954
                                   -0.62374632
                                                                    -343.1949329045258
                                                1.89578275].
30
           1.34553372 -0.06390034 -0.99376889 -1.73517952].
                                                                    -1197.460412286185
31
         [-0.02847015
                       0.82695272
                                    1.12184468
                                               2.01272622].
                                                                    -145.41785962811852
32
           0.2861566
                      -1.26320465
                                    0.4953292
                                               -1.70534049].
                                                                    -688.4113843347533
33
           1.48161712 0.84992301
                                   0.13479361 -0.9666187 ].
                                                                    -313.48243984588396
34
         [ 1.59888422 -0.78668892
                                   0.27709365 -0.43610009].
                                                                    -1159.7048682449756
35
         [-0.29021798 -0.77532859 -0.74730451 -1.16249637].
                                                                    -559.7522407393208
36
           0.05360964
                       1.85146916 -1.71137361
                                                1.11723377].
                                                                    -3320.132125181345
37
         [-1.57643092
                       1.74419672
                                   1.13557999
                                                0.27545106].
                                                                    -528.4755615940201
```

```
      38
      [1.20334288 0.20165943 1.35940674 0.92703019].
      -414.8765148103328

      39
      [-0.1140311 -1.40990782 -0.03519657 -0.91024241].
      -702.9354119031176

      40
      [1.91214941 -1.81467173 1.45340086 0.88242509].
      -3491.8322277538705
```

```
1 ### ESTIMATED GP EI GRADIENTS
2
3 np.random.seed(run_num_12)
4 surrogate_approx_12 = GaussianProcess(cov_func, optimize=opt)
5
6 approx_12 = GPGO(surrogate_approx_12, Acquisition(util_grad_approx), objfunc, param)
7 approx_12.run(init_evals=n_init, max_iter=iters)
```

```
Evaluation
                 Proposed point
                                            Current eval.
                                                                    Best eval.
                                                 0.13819656].
init
         [-1.416549
                        0.98324356 -0.9694617
                                                                     -553.611160809845
init
         [-1.98830095
                        1.71518775 1.64132804 -1.91110583].
                                                                     -2800.5873266661606
init
         [ 1.87166448 -1.48599062 -0.88543907
                                                 0.43451672].
                                                                     -3468.8797831248744
init
                       1.44480478 -2.03874618
                                                                     -3716.955397581154
         [ 1.81954616
                                                 0.08694181].
         [ 0.21314615 -0.05989411 1.0982775
init
                                                -1.38970418].
                                                                     -796.5750150214192
1
         [-2.048 -2.048 2.048
                                 2.0481.
                                                    -4837.639006924799
                                                                             -553.6111608
2
         [2.048 2.048 2.048 2.048].
                                            -1385.2811701248
                                                                    -553.611160809845
3
         [-2.048 - 2.048 - 2.048 - 2.048].
                                                    -11717.778680524798
                                                                             -553.6111608
4
                  2.048
                         2.048
                                 2.048].
         [-2.048
                                                    -1393.4731701248
                                                                             -553.6111608
5
         [-2.048 -2.048 -2.048
                                 2.048].
                                                    -8281.8048437248
                                                                             -553.6111608
6
         [ 2.048
                  2.048
                          2.048 -2.048].
                                                    -4821.255006924799
                                                                             -553.6111608
7
         [-2.048 -2.048
                          2.048 -2.048].
                                                    -8273.612843724797
                                                                             -553.6111608
8
           2.048 -2.048
                          2.048
                                 2.0481.
                                                    -4829.447006924799
                                                                             -553.6111608
9
                         2.048 -2.048].
         [ 2.048 -2.048
                                                    -8265.420843724798
                                                                             -553.6111608
10
         [-2.048
                  2.048 -2.048 -2.048].
                                                    -8273.612843724799
                                                                             -553.6111608
11
         [-2.048
                  2.048 -2.048
                                 2.048].
                                                    -4837.639006924799
                                                                             -553.6111608
         [0.04117651 0.47958604 0.3467295
                                                        1.
                                                                      -397.45043729468136
12
                                             2.048
         [ 2.048 -2.048 -2.048 -2.048].
                                                    -11709.586680524799
13
                                                                             -397.4504372
                                 0.71016894 0.38172922].
14
         [0.05649917 2.048
                                                                     -1635.6194622319063
                                    0.33324272 0.30310824].
15
         [-2.048
                       -0.1548642
                                                                     -1915.847757453209
16
         [ 1.0056466
                        2.048
                                    -0.80769352 -2.048
                                                                     -3343.0326671625003
                                                            ].
17
         [ 0.46500357  0.00928405 -2.048
                                                 2.048
                                                            ].
                                                                     -894.9684280766043
18
         [0.03866676 0.26551502 2.048
                                             2.048
                                                        1.
                                                                     -861.2459969869678
19
         [ 2.048
                       2.048
                                 -0.4124581 2.048
                                                                     -2939.722130793758
                                                        1.
                      0.28214534 2.048
20
                                             0.27954581].
                                                                     -3453.2011315078116
         [2.048
21
         [-0.30084609 -2.048
                                    0.45304837
                                                0.12705278].
                                                                     -1868.9143570998028
22
         [-0.53249325 -0.03014277 -2.048
                                                -0.10402547].
                                                                     -2289.906549816028
23
           2.048 -2.048 -2.048 2.048].
                                                    -8273.612843724799
                                                                             -397.4504372
24
         [-0.18882818 -0.31727506 -0.13967788 -2.048
                                                            1.
                                                                     -450.1395502899814
25
         [-0.24181274 -0.10292764 -0.04916385
                                                 2.048
                                                            1.
                                                                     -425.26237065687735
26
                                    0.36659492
         [-2.048]
                        0.77718535
                                                 2.048
                                                                     -1549.237684431107
27
           0.31497503 -0.25975828
                                    0.12303257
                                                                     -429.2729555580485
                                                 2.048
28
         [-0.05173221
                        0.07898024 -0.15437385
                                                 1.77356224].
                                                                     -312.60467986457553
29
           0.49248519 -0.36364078
                                    0.1241312
                                                -0.46128554].
                                                                     -62.36024219297695
30
         [-1.69090131
                        1.78595323
                                    1.92890053
                                                 1.11252811].
                                                                     -963.0734459791341
31
         [-1.83621103
                        1.87903779 -0.68162285 -1.26546617].
                                                                     -2308.192588094473
32
         [ 1.92156215
                        1.40944334 1.51577691 -1.70996176].
                                                                     -2150.6722660038395
33
           0.0919898
                       -0.08568237 -1.11132262 -1.62208438].
                                                                     -948.8029306342575
34
           0.89455542 -1.05435484 -1.37244859 -0.5642034 ].
                                                                     -1570.0714421606326
35
         [-1.89442692
                        1.28025951
                                    1.41878095
                                                 0.88925994].
                                                                     -672.7102189249384
36
         [-1.58683532]
                        0.93332869
                                    0.12508988 -0.19690846].
                                                                     -318.7661115293826
37
         [-1.40446844 -0.06409175 -1.4736892
                                                 1.11702579].
                                                                     -757.4511493361595
38
         [-0.22075864
                        0.21300348 -0.04241919
                                                 1.590926531.
                                                                     -259.1978979660242
```

```
39 [0.78784188 0.56687636 1.60738668 0.53712367]. -585.1246700385428
40 [-0.908832 -1.12747314 -1.62090109 -1.33948435]. -2806.611413418693
```

```
1 ### ESTIMATED GP EI GRADIENTS
2
3 np.random.seed(run_num_13)
4 surrogate_approx_13 = GaussianProcess(cov_func, optimize=opt)
5
6 approx_13 = GPGO(surrogate_approx_13, Acquisition(util_grad_approx), objfunc, param)
7 approx_13.run(init_evals=n_init, max_iter=iters)
8
```

```
Proposed point
Evaluation
                                            Current eval.
                                                                    Best eval.
init
         [ 1.13746907 -1.07503116
                                    1.32824487
                                                 1.90770872].
                                                                     -570.621446040192
init
         [ 1.93577416 -0.19067188  0.44663793
                                                 1.1285566 ].
                                                                     -1656.450565242978
init
           0.58004826
                        0.90938667 -1.9044904
                                                -0.82555097].
                                                                      -2770.1364153691793
init
         [-1.80833283
                       1.46252162 -0.5207899
                                                 0.73665721].
                                                                     -1066.23070619416
init
         [-0.99827733 -0.62430734 -2.00944529 -0.58026483].
                                                                      -2986.7442974027663
1
         [-2.048 - 2.048]
                          2.048 -2.048].
                                                     -8273.612843724797
                                                                             -570.6214466
2
           2.048
                  2.048
                          2.048 -2.0481.
                                                     -4821.255006924799
                                                                             -570.6214460
3
         [-2.048 -2.048
                          2.048
                                2.048].
                                                     -4837.639006924799
                                                                             -570.6214460
4
         [ 2.048
                       -2.048
                                     0.37059336 -2.048
                                                            ].
                                                                      -5847.067836379805
5
                  2.048 2.048 -2.048].
         [-2.048
                                                     -4829.447006924799
                                                                             -570.6214460
6
         [-0.18697538 2.048
                                     2.048
                                                 2.048
                                                            ].
                                                                      -1330.1627783340607
7
         [ 2.048 -2.048 -2.048
                                 2.048].
                                                     -8273.612843724799
                                                                             -570.6214466
8
                  2.048 -2.048
                                 2.048].
                                                     -4829.447006924799
           2.048
                                                                             -570.6214466
                                 2.048].
9
         [-2.048 -2.048 -2.048
                                                     -8281.8048437248
                                                                             -570.6214460
10
         [-2.048
                  2.048 -2.048 -2.048].
                                                     -8273.612843724799
                                                                             -570.6214460
         [-0.03981162 0.00450934
                                     2.048
                                                -0.18063442].
11
                                                                      -2336.6020548002925
12
         [-2.048
                  2.048 -2.048
                                 2.048].
                                                     -4837.639006924799
                                                                             -570.6214466
         [2.048 2.048 2.048 2.048].
13
                                            -1385.2811701248
                                                                     -570.621446040192
         [ 2.048 -2.048
                                                     -4829.447006924799
                                                                             -570.6214460
14
                        2.048 2.048].
15
         [-2.048]
                       -2.048
                                    -1.25877398 -2.048
                                                            1.
                                                                     -8213.438842569785
16
         [-0.32794879 -0.2005761
                                     0.16409003
                                                 2.048
                                                                      -423.40608061954134
17
                        1.06419756 2.048
                                                 2.048
                                                                      -1534.6224602689977
         [-2.048
18
         [ 2.048
                        2.048
                                    -1.02321284 -2.048
                                                            ].
                                                                      -4147.0808258024235
19
         [-0.02608303 -2.048
                                    0.2158432
                                                 0.4942587 ].
                                                                      -2033.5230741897465
20
         [0.30759815 2.048
                                 0.31526354 0.30328507].
                                                                      -1892.4700128372444
                                                     -11709.586680524799
21
         [ 2.048 -2.048 -2.048 -2.048].
                                                                             -423.4060806
22
                       0.271603
         [-0.23105505
                                     0.37655836 -2.048
                                                            1.
                                                                      -495.88551459455795
23
           0.00563474
                        0.20532564 -1.13214298
                                                 2.048
                                                                      -206.99354023572508
24
         [-0.36314152]
                        1.48132021 -0.81174684
                                                 1.60396981].
                                                                      -1180.4203342459014
25
         [ 1.21516934
                       0.30106952 -1.50517253
                                                                      -508.70625179966345
                                                 1.22133599].
26
         [-1.954652]
                        0.28185696 0.66734217 -0.53116287].
                                                                      -1391.5915819891713
27
         [-0.7642521]
                       -0.55159498
                                    0.98612647
                                                 0.44030284].
                                                                      -209.3084449600003
28
         [-0.57801656 -0.89346951 -0.48374123
                                                                      -324.3432054652136
                                                 0.33465638].
29
         [-1.55232093 -0.83414065 -0.91616803
                                                 1.68889364].
                                                                      -1397.811662780371
30
           1.25552684
                        0.98228179 -0.01194804
                                                 0.60380272].
                                                                      -168.2404221329065
31
           1.86866832
                        1.80735286
                                    0.88218609
                                                -1.31606209].
                                                                      -1292.3195428932797
32
         [-0.60816258 -1.48369319
                                    1.19762397 -0.3389362 ].
                                                                      -767.5440279170598
33
         [ 0.9372928
                       -0.43945546
                                     1.53552677
                                                                      -613.6859570054377
                                                 0.75343429].
34
         [-0.66508622
                        0.66638952
                                    0.87959599 -0.22493756].
                                                                      -126.61151527058537
35
         [-0.07484835
                        0.02857783 -1.34884795
                                                 0.8967764 ].
                                                                      -274.95003109985123
36
         [0.96418378 0.51201859 1.579638
                                             1.98711879].
                                                                      -217.4114104120697
37
         [-0.03576572
                        1.04072633
                                    0.05068127 -0.63198527].
                                                                      -256.8777483425788
38
         [-1.69813972
                        1.3940542
                                     0.19151705 -1.17115017].
                                                                      -682.7768916967663
39
         [-0.2194799
                        1.51724609 -1.91465659
                                                 1.68166585].
                                                                      -2397.8397335966574
40
         [-0.2367588
                        1.06158386 -0.87110555 -1.24039047].
                                                                      -905.0561957506699
```

```
1 ### ESTIMATED GP EI GRADIENTS
2
3 np.random.seed(run_num_14)
4 surrogate_approx_14 = GaussianProcess(cov_func, optimize=opt)
5
6 approx 14 = GPGO(surrogate_approx 14, Acquisition(util_grad_approx), objfunc, param)
7 approx 14.run(init evals=n init, max iter=iters)
8
   Evaluation
                     Proposed point
                                               Current eval.
                                                                       Best eval.
   init
             [ 0.05711194 1.11888405
                                        1.5172718 -2.0150397 ].
                                                                        -1996.4555487728376
   init
             [-0.77932165]
                           1.87434492
                                       0.05372605 -0.744307
                                                                        -1417.9597465038332
   init
               0.16056294 -1.14173976
                                        1.25534764 -0.64612505].
                                                                        -635.6383005184798
   init
             [ 0.15928873 -2.02394097
                                        0.70923255 -1.18774062].
                                                                        -1863.0160368222728
   init
             [ 1.7717559
                          -0.51509351
                                        1.0339079
                                                    1.07781735].
                                                                        -1397.2995170993763
   1
             [-2.048 -2.048 -2.048
                                     2.048].
                                                        -8281.8048437248
                                                                                -635.6383005
    2
               2.048
                      2.048 -2.048
                                     2.0481.
                                                        -4829.447006924799
                                                                               -635.6383005
    3
                           0.19015951 2.048
                                                               1.
             [-2.048]
                                                    2.048
                                                                        -2479.773608431594
   4
             [ 2.048
                           0.13381568 -2.048
                                                   -2.048
                                                               1.
                                                                        -5983.328365860246
    5
                          -0.89703731 -2.048
                                                   -2.048
             [-2.048
                                                               1.
                                                                        -7324.766917562415
   6
             [-2.048
                     2.048 -2.048
                                     2.048].
                                                        -4837.639006924799
                                                                                -635.638300!
   7
             [ 2.048 -2.048 -2.048
                                     2.048].
                                                        -8273.612843724799
                                                                                -635.638300!
   8
             [2.048 2.048 2.048 2.048].
                                               -1385.2811701248
                                                                       -635.6383005184798
   9
             [-2.048 -2.048 2.048 -2.048].
                                                        -8273.612843724797
                                                                               -635.6383005
             [-0.05222314 - 2.048]
                                                    2.048
   10
                                        2.048
                                                                        -1353.3681815099549
                                                               ].
   11
             [ 2.048 -2.048 2.048 -2.048].
                                                        -8265.420843724798
                                                                               -635.638300
   12
              2.048
                           2.048
                                        0.4283162
                                                   -0.52864382].
                                                                        -1932.160369297066
   13
             [-2.048]
                      2.048 -2.048 -2.048].
                                                        -8273.612843724799
                                                                                -635.638300!
                                                   -0.211789931.
   14
                           2.048
             [-2.048]
                                        2.048
                                                                        -2874.1774548197186
                           2.048
                                        0.57182985 2.048
   15
             [-0.18596147
                                                                        -2016.4931333612099
                                                               ].
   16
             [-2.03022918e-03 1.37755447e-01 -2.04800000e+00 4.45042371e-01].
                                                                                         -18
   17
             [-2.048]
                          -2.048
                                        0.8889762
                                                    0.92617433].
                                                                        -5009.594808535263
   18
             [ 0.6232987
                          -2.048
                                       -2.048
                                                   -0.91509642].
                                                                        -7119.609541343871
   19
               2.048 -2.048 2.048 2.048].
                                                        -4829.447006924799
                                                                               -635.638300!
                     2.048 2.048 -2.048].
   20
               2.048
                                                        -4821.255006924799
                                                                                -635.638300!
   21
             [0.11536007 0.06270944 2.048
                                                0.211005891.
                                                                        -2007.4910473264222
    22
             [ 0.01481728 -0.33890332 -0.23658632 2.048
                                                                        -424.9610797451489
                                                               1.
   23
                                                                        -1475.4151549972482
             [-2.048]
                           0.40820797 -0.3414399
                                                    0.33358286].
    24
               0.76148406
                           2.048
                                       -2.048
                                                   -0.604053361.
                                                                        -6425.048858017759
   25
             [-2.048]
                           -2024.500482228336
   26
             [ 2.048
                          -0.44452611 -0.02236963 -0.20696218].
                                                                        -2165,2475707317885
    27
               0.10133251 -0.37903082 -0.2183316
                                                    2.048
                                                                        -432.58568317757556
    28
             [2.048
                         0.61235701 0.19607215 2.048
                                                                        -1691.9615551863224
    29
             [0.27633111 1.37392905 0.39697562 1.34790169].
                                                                        -533.300532385822
                                                    0.48859879].
    30
               1.26069459 -1.83565215 -0.15960944
                                                                        -2449.5116865562186
    31
               0.41185065
                           0.14704051 -0.06999008 -1.30219395].
                                                                        -173.9576811616067
    32
               0.75138373 -1.42916731 1.02061145 -1.76094883].
                                                                        -1293.3492207589115
    33
               0.67610656 -1.34656751 -1.92469412
                                                    0.225962331.
                                                                        -2946.698074040383
    34
               1.7588149
                          -0.78739493 -1.93213096 -0.323968
                                                                        -3815.7850490240958
    35
             [-1.68214821
                           0.54217423 -0.6400704
                                                                        -635.9778142669621
                                                    0.01722999].
    36
               0.13865086 -2.01545562 -1.0926892
                                                   -1.01367946].
                                                                        -3572.723172473937
    37
             [ 1.82238011 -1.1194483
                                      -1.31534249 -1.06360491].
                                                                        -3422.564769724855
    38
               1.94381142
                           1.54603653 -1.04249393
                                                                        -1754.025378051432
                                                    0.23850074].
    39
               0.12795405 -1.82551184 -0.52381359
                                                    1.82879896].
                                                                        -2079.0517374677465
             [ 0.86929247 -1.73849869 -0.68259678
                                                                        -2016.3556549384557
    40
                                                    0.13072152].
```

```
1 ### ESIIMAIED GP EI GRADIENIS
2
3 np.random.seed(run_num_15)
4 surrogate_approx_15 = GaussianProcess(cov_func, optimize=opt)
5
6 approx_15 = GPGO(surrogate_approx_15, Acquisition(util_grad_approx), objfunc, param)
7 approx_15.run(init_evals=n_init, max_iter=iters)
8
```

```
Evaluation
                 Proposed point
                                           Current eval.
                                                                   Best eval.
         [ 1.42875729 -1.31524229 -1.82532827 -0.56713852].
init
                                                                    -3924.3244166004847
init
         [-0.9199578
                        0.12288092 -0.79495612 -0.80087302].
                                                                     -330.9329217994366
                                   1.71061206 -0.96605449].
init
         [-1.59030773 -1.02441364
                                                                     -2832.720279494954
init
         [ 0.89200102  1.49796878  1.25779756  -1.18558481].
                                                                     -912.8737542795088
init
         [-1.36297254 -1.85669062 -1.88652621 -1.2278546 ].
                                                                     -6538.09169222112
1
                                                    -4837.639006924799
         [-2.048]
                  2.048 -2.048
                                 2.048].
                                                                            -330.9329217
2
           2.048 -2.048
                         2.048
                                 2.048].
                                                    -4829.447006924799
                                                                            -330.9329217
3
                        2.048
         [ 2.048
                                   -0.61717139 2.048
                                                           1.
                                                                     -3058.425547776612
4
         [-2.048]
                  2.048
                         2.048
                                 2.0481.
                                                    -1393.4731701248
                                                                            -330.9329217
5
         [ 2.048 -2.048
                         2.048 -2.048].
                                                    -8265.420843724798
                                                                            -330.9329217
6
         [-2.048]
                  2.048 -2.048 -2.048].
                                                    -8273.612843724799
                                                                            -330.9329217
7
         [ 2.048
                  2.048 -2.048 -2.048].
                                                    -8265.4208437248
                                                                            -330.9329217
8
         [-2.048]
                       -2.048
                                    0.06336705 2.048
                                                           1.
                                                                     -6040.345130709454
9
         [-2.048]
                  2.048 2.048 -2.0481.
                                                    -4829.447006924799
                                                                            -330.9329217
         [0.78148219 1.171678
                                             2.048
                                                                     -538.8911694302681
10
                                 2.048
11
         [ 2.048 -2.048 -2.048 2.048].
                                                    -8273.612843724799
                                                                            -330.9329217
12
         [-0.41727943 0.7286777 -0.08004661
                                                 0.60203821].
                                                                     -106.81386008776019
13
         [-0.42371819
                        0.73697565 -0.09322079
                                                 0.57974363].
                                                                     -107.46990013897214
14
         [-0.42282605
                       0.73423031 -0.09505403
                                                 0.57912959].
                                                                     -106.86165148800532
15
         [-0.42294488]
                       0.73374591 -0.09577858
                                                 0.578285171.
                                                                     -106.6886528388227
16
         [-0.42293975
                        0.7333189
                                   -0.09602753
                                                 0.57807904].
                                                                     -106.56576860193543
17
         [-0.42299246
                       0.73312964 -0.09616131
                                                 0.577897811.
                                                                     -106.49862465015939
18
         [-0.63800826
                       1.47861284 0.78310532
                                                 0.49005971].
                                                                     -316.19497070996584
19
         [-0.16822643  0.33475194  -0.33065132
                                                 0.9251936 ].
                                                                     -99.13173520839142
20
         [ 0.26688853
                        0.20936951 -0.6210786
                                                 1.35714168].
                                                                     -144.27218723033783
21
         [-0.3085223]
                        0.5010192 -0.42658561
                                                 0.61100899].
                                                                     -84.78837818867335
22
         [0.17772393 0.1991617 0.26683836 1.71255526].
                                                                     -279.22774861285706
23
         [-0.43166503
                        2.02717788 -0.53820554
                                                 0.10309167].
                                                                     -2507.8924983256666
24
         [-0.40048572
                       0.13615201
                                   0.13819333
                                                 0.637080621.
                                                                     -43.131128264833166
25
         [-0.24109876
                       1.33577466
                                    1.78268983 -1.85506578].
                                                                     -2698.6619273246047
26
         [-0.40492792
                       0.15454405
                                    0.10815035
                                                 0.669863541.
                                                                     -47.52136236925384
27
                        0.28219844 0.86944369
                                                                     -70.73280373721906
         [-0.18451579
                                                 0.80690847].
28
         [-0.46733727
                        0.10240915 -0.61502547
                                                 0.94540471].
                                                                     -78.20493126216306
29
         [1.81050034 0.47345101 1.28230842 0.59391931].
                                                                     -1009.8154756480709
30
         [1.71257789 2.00766758 2.04074396 0.40774124].
                                                                     -1895.645937778416
31
         [-0.52169408 0.19912293 0.11130422
                                                0.71416331].
                                                                     -54.04245125354495
32
         [-0.50564748]
                       0.19940494
                                    0.10039974
                                                0.71204968].
                                                                     -53.6777056698185
33
         [-1.20652286
                       0.1849986
                                    0.06717931
                                                 0.663275821.
                                                                     -211.37610860589193
34
         [0.14477367 0.39221492 0.25811707 0.9599007 ].
                                                                     -96.31604791279474
35
         [-0.82829673 0.53154598 0.3162951
                                                                     -101.34450578089117
                                                 1.0737626 ].
36
         [-1.41747201
                        1.65781696 -1.49014706 -0.13005055].
                                                                     -2373.845117759311
37
         [ 0.06343646 -0.22959915
                                   0.21978558
                                                 0.62914234].
                                                                     -44.98413780442068
38
         [-2.04536301
                        1.59960423 -1.37306242
                                                 1.3677816
                                                                     -2255.6066494918728
39
           1.75116601 -1.15766379 -0.02397232 -1.2176205 ].
                                                                     -2125.1864546978345
         [-0.38595516 0.67898545 0.91808058
                                                                     -51.079035130825176
40
                                                0.81727359].
```

```
1 ### ESTIMATED GP EI GRADIENTS
```

2

3 np.random.seed(run num 16)

```
4 surrogate_approx_16 = GaussianProcess(cov_func, optimize=opt)
5
6 approx_16 = GPGO(surrogate_approx_16, Acquisition(util_grad_approx), objfunc, param)
7 approx_16.run(init_evals=n_init, max_iter=iters)
8
```

```
Evaluation
                 Proposed point
                                          Current eval.
                                                                 Best eval.
         [-1.13339974 0.09487705 0.20767317 -1.86121441].
init
                                                                  -514.1403917485846
init
         [-0.57045469 -1.13426046 0.77302236 -1.37735608].
                                                                  -636.540695155299
         [-1.75994935
init
                       1.80638048 0.26083893 -1.72854338].
                                                                   -1399.5661404272828
         [ 0.91193553 -1.3989799 -1.02284777 -0.8458762 ].
init
                                                                  -1753.4526459251956
init
         [ 0.80531749 -0.1463743 -1.16710546 -0.21779963].
                                                                  -460.1166598787994!
1
         [2.048 2.048 2.048 2.048].
                                          -1385.2811701248
                                                                 -460.11665987879945
2
         [-2.048 2.048 -2.048 2.048].
                                                  -4837.639006924799
                                                                         -460.1166598
3
         [-2.048 -2.048
                        2.048 2.048].
                                                  -4837.639006924799
                                                                         -460.1166598
4
         [ 2.048 2.048
                        2.048 -2.0481.
                                                  -4821.255006924799
                                                                          -460.1166598
5
          2.048 -2.048
                        2.048
                                2.048].
                                                  -4829.447006924799
                                                                          -460.1166598
                                                  -4829.447006924799
6
         [ 2.048
                 2.048 -2.048
                                2.0481.
                                                                          -460.1166598
7
         [-2.048 -2.048 -2.048
                                2.048].
                                                  -8281.8048437248
                                                                          -460.1166598
8
         [-2.048
                 2.048
                        2.048
                               2.048].
                                                  -1393.4731701248
                                                                         -460.1166598
9
         [ 2.048
                 2.048 -2.048 -2.0481.
                                                  -8265.4208437248
                                                                          -460.1166598
10
         [ 2.048 -2.048
                       2.048 -2.048].
                                                  -8265.420843724798
                                                                         -460.1166598
11
         [-2.048 - 2.048 - 2.048 - 2.048].
                                                  -11717.778680524798
                                                                         -460.1166598
12
         [ 2.048 -2.048 -2.048 2.048].
                                                  -8273.612843724799
                                                                          -460.1166598
13
         [-2.048 -2.048 2.048 -2.048].
                                                  -8273.612843724797
                                                                          -460.1166598
14
         [-0.07853879 0.45636083 2.048
                                               0.29509575].
                                                                   -1881.6693320167167
15
                 2.048 -2.048 -2.048].
                                                  -8273.612843724799
         [-2.048
                                                                          -460.1166598
         16
                                                                   -424.49516450744443
17
         「 0.19361197
                       2.048
                                  -0.15621246 0.27605862].
                                                                   -2306.334648365382
18
                      -0.05311158 0.02817756 0.38551326].
                                                                   -1830.2628885331026
         [-2.048
19
         [-2.048 2.048 2.048 -2.048].
                                                  -4829.447006924799
                                                                          -424.495164!
20
         [ 2.048 -2.048 -2.048 -2.048].
                                                  -11709.586680524799
                                                                          -424.495164!
21
         [2.048]
                     0.04960034 0.31583126 0.39907
                                                     1.
                                                                   -1739.1059185886857
22
         [-0.11028388 0.11778902 -2.048
                                               0.28426392].
                                                                   -1966.390913702528!
                                                                   -1898.0691005385204
23
         [-0.07583815 -2.048
                                   0.3820319
                                               0.49391588].
24
         [ 0.37006987  0.21942287  0.17857812 -2.048
                                                         ].
                                                                   -436.6565406565057
25
         [0.00221686 2.048
                                2.048
                                           2.048
                                                                   -1343.9447383100664
         [ 0.23246641  0.14036431  0.22815856 -2.048
                                                         ].
                                                                   -448.0380647900797
26
27
           0.02702661 0.18776617 -0.42671713 -2.048
                                                                   -525.8111183534426
28
           0.01781265 0.14273488 2.048
                                              -2.048
                                                                   -4312.589124282656
                                                         1.
29
         [-2.048]
                       0.65997344 0.56479965
                                              2.048
                                                         1.
                                                                   -1559.3593042542104
30
         [ 0.47251379 -0.10838687 -0.02157398
                                                         ].
                                                                   -432.90076959927205
                                              2.048
31
           0.35855098 -0.0605761 -0.16931152
                                               2.048
                                                                   -417.2438331280042
                                                         1.
32
         [ 0.16100656  0.15823216 -0.50539254 -2.048
                                                                   -564.1399666632592
33
         [ 2.048
                       0.17641733 -2.048
                                               0.11636404].
                                                                   -3720.6429312222062
34
         [ 0.3616728 -0.1267279  0.1051908  2.048
                                                     1.
                                                                   -424.814902532517
35
         [-0.95071835 -0.2289704 -0.04594312 -1.93639198].
                                                                   -511.4883243438568
                     2.048
                                2.048
36
         [2.048
                                           0.39626386].
                                                                   -2367.129974975508
37
         [ 2.048
                       0.17433706 0.11280404 -2.048
                                                                   -2043.918358927217
38
         [1.23092008 1.05604526 0.35017173 1.98018267].
                                                                   -425.14324462959087
39
         [ 1.3844554
                       0.50295026 -0.30971323 2.02838352].
                                                                   -607,0844287384073
40
         [-0.44208983 1.99194991 0.15971221 0.97938317].
                                                                   -1867.703353468525
```

```
1 ### ESTIMATED GP EI GRADIENTS
2
3 np.random.seed(run_num_17)
4 surrogate_approx_17 = GaussianProcess(cov_func, optimize=opt)
5
```

```
6 approx_17 = GPGO(surrogate_approx_17, Acquisition(util_grad_approx), objfunc, param)
7 approx_17.run(init_evals=n_init, max_iter=iters)
8
```

```
Evaluation
                 Proposed point
                                          Current eval.
                                                                 Best eval.
         [-0.84105215  0.12528335  -1.26353086  -1.76988013].
                                                                  -1340.061030292479!
init
         [1.17549244 0.64034211 0.56328559 0.30966945].
                                                                  -57.67854505088549
init
         [-1.8879983 -0.58239548 1.82551833 -1.80205699].
                                                                  -4588.535377497626
init
         -1.83831075 0.62430665].
                                                                  -2599.959730636226
init
         [ 0.21197361  0.39941429 -0.06746675 -0.88888049].
                                                                  -99.66183844529772
         [ 2.048 -2.048 2.048 2.048].
                                                  -4829.447006924799
                                                                         -57.67854505
2
         [ 2.048
                       1.05649593 1.32151056 -2.048
                                                         ].
                                                                  -2429.744400124792
3
         [-0.55463032 2.048
                                   2.048
                                                                  -1228.831722957927!
                                               2.048
                                                         1.
4
         [-2.048 -2.048 -2.048
                                                  -8281.8048437248
                               2.0481.
                                                                         -57.6785450!
5
         [ 2.048 -2.048 -2.048 -2.048].
                                                  -11709.586680524799
                                                                         -57.6785450!
6
         [-2.048
                 2.048 -2.048
                                2.0481.
                                                  -4837.639006924799
                                                                         -57.6785450!
7
         [-2.048 -2.048 2.048
                                2.048].
                                                  -4837.639006924799
                                                                         -57.6785450!
8
         [ 2.048 -2.048 -2.048
                                2.048].
                                                  -8273.612843724799
                                                                         -57.6785450!
9
         [ 2.048 -2.048 2.048 -2.048].
                                                  -8265.420843724798
                                                                         -57.6785450!
10
         Γ2.048
                     2.048
                                2.048
                                           1.08031649].
                                                                  -1894.310907441302
11
         [ 0.30382411 -0.02747498  0.47507381  0.38525282].
                                                                  -28.294446786821823
12
         [ 0.49560715 -0.04984534  0.54591177
                                              0.29434606].
                                                                  -39.82580398039754!
         [-1.79497026 1.76546405
13
                                  1.28434291 -0.33941445].
                                                                  -952.0102989499331
14
         [ 0.44883056 -0.92403133  0.20514262 -0.09834762].
                                                                  -175.36017592138887
15
         [ 0.75888275 -0.05732555  0.24496585
                                                                  -49.62563349753145
                                              0.1993185 ].
16
         0.5984243
                     -0.28933658 0.28377512
                                              0.43315051].
                                                                  -60.69216986210886
17
         [0.54629375 0.25760332 0.68991895 0.80974456].
                                                                  -51.04186686389741
18
         [-0.03022147 0.23917661 0.72690777 0.58983567].
                                                                  -52.61934257570242
19
         [0.70176649 0.09840648 0.62015951 0.71873139].
                                                                  -65.00776643742648
20
         [ 0.63602298 -0.2385767
                                   0.07758818 0.1236843 ].
                                                                  -45.30261806493653
21
         [0.20652337 0.26942335 0.49977194 0.4775316 ].
                                                                  -29.99207945865354
22
         -4874.764210509927
23
                       0.19405784 -0.18651802 0.86895635].
                                                                  -80.5319508091907
         [-0.1947031
24
         [-1.84837319 -1.71996318 -1.54439013 -1.82221233].
                                                                  -6457.873681581815
25
         [-0.15921705 -0.00415956 1.37229052 0.65249987].
                                                                  -342.34884854638193
26
         [0.66745558 0.55369299 0.20408384 0.51294665].
                                                                  -25.376392217711714
27
         [ 1.30152593  0.68015254 -1.79257626 -0.43179959].
                                                                  -1948.0563208246786
28
         [0.67016107 0.07701834 0.81742873 0.9239938 ].
                                                                  -87.23597287235853
29
         [-0.03552169 -0.95576019 -0.82394689 -0.23735467].
                                                                  -485.62770529342293
30
         [-0.78940489 0.54425439 0.44427943 -1.97967394].
                                                                  -480.4916998108777
31
         [-1.55320406 -1.06992981 0.03407838 -1.14225885].
                                                                  -1478.5284734919987
32
         [0.86155625 0.68655148 0.84149486 0.31404081].
                                                                  -29.682939792261852
33
         [1.0551574 0.1735419 0.56276816 0.78510025].
                                                                  -139.51339155203266
34
         [0.25209015 0.88142615 0.22734012 0.45672361].
                                                                  -114.6713421963927
35
         [0.2098577 0.21289626 0.38236609 0.6687167 ].
                                                                  -43.1382159248404
36
         [-0.50407692 0.22632679 0.17504305 1.97008084].
                                                                  -381.29464314198236
37
         [ 0.81130009 -1.51128184 -0.00363526
                                              1.44855886].
                                                                  -1211.1614914606882
38
         [-0.43708156 -0.27418816 -0.9320137
                                              -0.23362957].
                                                                  -252.01085519104976
         [-0.88266509 -0.44579317 -1.7473574
39
                                               0.2161308 ].
                                                                  -1346.8737024339018
40
         [0.38792439 0.2615397 0.43435461 0.02195894].
                                                                  -18.644334187699467
```

```
1 ### ESTIMATED GP EI GRADIENTS
2
3 np.random.seed(run_num_18)
4 surrogate_approx_18 = GaussianProcess(cov_func, optimize=opt)
5
6 approx_18 = GPGO(surrogate_approx_18, Acquisition(util_grad_approx), objfunc, param)
7 approx_18.run(init_evals=n_init, max_iter=iters)
```

```
Evaluation
                  Proposed point
                                            Current eval.
                                                                    Best eval.
         [ 0.61593289  0.02233702  1.55075162 -1.30318244].
init
                                                                     -1629.418560245763
init
         [1.44274665 1.02455823 0.68035243 1.99841976].
                                                                      -361.44679331797425
                                                                      -2000.4660253561508
init
         [-0.99545734 -1.93205893 0.5559055
                                                 1.422591541.
init
           0.96737126 -1.96277407 -1.59087358 -0.82852355].
                                                                      -4947.239458116178
init
         [ 0.7658299
                        1.48122033 -1.23439366
                                                 0.64384627].
                                                                      -1338.1489953342577
1
         [-2.048]
                   2.048
                         2.048
                                                     -1393.4731701248
                                                                             -361.4467933
                                 2.048].
2
         [-2.048
                  2.048 -2.048 -2.048].
                                                     -8273.612843724799
                                                                             -361.4467933
3
         [-2.048 -2.048
                         2.048 -2.048].
                                                     -8273.612843724797
                                                                             -361.4467933
4
         [2.048 - 2.048]
                         2.048 2.0481.
                                                     -4829.447006924799
                                                                             -361.4467933
5
         [-2.048
                        0.39550459 -2.048
                                                 2.048
                                                            ].
                                                                      -2408.6442678719914
                  2.048 2.048 -2.0481.
6
         [-2.048]
                                                     -4829.447006924799
                                                                             -361.4467933
7
                  2.048 -2.048 -2.048].
                                                     -8265.4208437248
                                                                             -361.4467933
         [ 2.048
         [-2.048 - 2.048 - 2.048 - 2.048].
8
                                                     -11717.778680524798
                                                                             -361.446793
9
           2.048
                       -0.87618063 -2.048
                                                 2.048
                                                                      -3838.3646036629693
10
                      2.048
                                 2.048
                                             0.365806161.
                                                                      -2390.3586525055603
         Γ2.048
                         2.048 -2.048].
11
         [ 2.048 -2.048
                                                     -8265.420843724798
                                                                             -361.4467933
12
         [-2.048
                        0.5111653
                                     0.33528765
                                                 0.20084355].
                                                                      -1367.8516486916708
13
         [-0.06749412
                        0.3716805
                                     2.048
                                                 2.048
                                                                      -841.5268785235213
                                                            1.
                         2.048 -2.048].
14
           2.048
                  2.048
                                                     -4821.255006924799
                                                                             -361.4467933
15
                  2.048 -2.048
                                                     -4829.447006924799
                                                                             -361.4467933
           2.048
                                 2.048].
                                                            1.
16
         [-1.00836931 -2.048
                                    -2.048
                                                 2.048
                                                                      -5319.217376428902
17
         [-0.73923716]
                        2.048
                                    -0.12900526
                                                 2.048
                                                            1.
                                                                      -2512.598345442087
         [-2.048]
                       -0.74217147
                                                 2.048
                                                                      -3135.1201067931274
18
                                    2.048
19
         [ 2.048
                       -0.12134098
                                    0.27989241
                                                 0.35868773].
                                                                      -1880.244372998437
20
         [-0.20567022  0.28808095  -0.34036074  -2.048
                                                                      -495.94319523647704
21
         [-0.1193788
                        2.048
                                     0.21548701 -0.76652986].
                                                                      -2065.7697426972773
22
         [ 0.48981752 -0.18164856
                                    0.16862714
                                                2.048
                                                                      -429.82367542653634
                                                            1.
         [2.048 2.048 2.048 2.048].
                                            -1385.2811701248
23
                                                                     -361.44679331797425
         [-2.048]
24
                        2.048
                                    -2.048
                                                 0.80064351].
                                                                      -5528.6700698516215
25
         [-0.25529919
                        0.53518375 -1.76903814 -0.33690932].
                                                                     -1655.6380022936917
26
         [-0.72041966
                        0.43906847 1.85603283 -0.21836083].
                                                                      -1623.2039978519113
27
         [-2.048]
                        0.08735412 0.11912231 -2.048
                                                                      -2124.1087474200167
                       -2.0178505
                                  -0.29741346
                                                 1.9385005 1.
                                                                      -3142.629658146597
28
           0.9745277
29
         [1.43581515 1.70427941 0.34660858 2.02461876].
                                                                      -1030.898856822082
30
         [ 1.65420563  0.46876487 -1.15497708 -1.23229633].
                                                                      -1367.1275184848027
31
           0.48235683 -0.32152824 -0.13029186 -1.97700488].
                                                                      -437.0615453746011
         [-1.29054067 -1.01825456 -1.0846477
                                                                      -1202.9159813869048
32
                                                 0.74140891].
33
         [-0.04444255 -1.69905763 -0.81028648
                                                 0.21299648].
                                                                      -1687.5219031566799
34
         [ 1.35400996 -1.89016219 -1.89577984 -0.06905842].
                                                                      -5735.540400611233
35
         [0.80445969 0.53349022 0.88330485 1.98262236].
                                                                      -181.98014634206487
36
         [-1.30456047 -1.72741921 -1.73383645 -0.6779548 ].
                                                                      -4779.299516062846
37
         [1.50756889 1.89855338 0.12349852 2.01809109].
                                                                      -1628.7136941839224
38
         [-0.25372346
                       0.13469482 1.91152524
                                                 1.5248555 ].
                                                                      -815.4309755580788
39
         [-1.01118677
                        1.56552334 -1.07636716 -0.43010379].
                                                                      -1534.6863178834344
40
         [-0.65068038
                        1.10009825 0.05709799 -1.60403925].
                                                                      -440.72721207383967
```

```
1 ### ESTIMATED GP EI GRADIENTS
2
3 np.random.seed(run_num_19)
4 surrogate_approx_19 = GaussianProcess(cov_func, optimize=opt)
5
6 approx_19 = GPGO(surrogate_approx_19, Acquisition(util_grad_approx), objfunc, param)
7 approx_19.run(init_evals=n_init, max_iter=iters)
8
```

Evaluation Proposed point Current eval.

Best eval.

```
init
         -1412.165722504925
init
         [-0.69039488 -1.70803378 0.70441812
                                               1.2558082 ].
                                                                   -1034.97990396323
         [ 1.97731088  0.55566637 -1.16357834  0.20081636].
init
                                                                   -1480.569995327432
init
         [ 1.86613588e-01 -1.08922440e+00 -1.58217895e+00 -1.39564217e-03].
                                                                                    -1!
init
         [-1.4249639
                       0.13388219 -0.46282028 0.77138896].
                                                                   -422.6519691366176
1
         [ 2.048 -2.048 2.048 -2.048].
                                                   -8265.420843724798
                                                                          -422.6519693
2
         [0.83916702 2.048
                                2.048
                                           2.048
                                                                   -1104.1261463880821
                                                      ].
3
         -2.048
                                                                   -4640.742289311788
                                   2.048
4
         [-2.048 -2.048 2.048 -2.048].
                                                   -8273.612843724797
                                                                          -422.6519691
5
                 2.048 -2.048
         [-2.048
                                2.048].
                                                   -4837.639006924799
                                                                          -422.6519693
6
           2.048 -2.048 2.048
                                2.048].
                                                   -4829.447006924799
                                                                          -422.6519691
7
         [-2.048]
                       2.048
                                               0.70015539].
                                   2.048
                                                                   -2153.718531679629
8
         [-2.048 -2.048 -2.048 -2.048].
                                                  -11717.778680524798
                                                                         -422.6519691
9
         [-2.048 -2.048 -2.048
                                2.048].
                                                   -8281.8048437248
                                                                          -422.6519693
10
         [ 2.048 -2.048 -2.048 -2.048].
                                                  -11709.586680524799
                                                                          -422.6519691
11
         [ 2.048 -2.048 -2.048 2.048].
                                                  -8273.612843724799
                                                                          -422.6519693
12
         [ 2.048
                 2.048 -2.048 -2.048].
                                                  -8265.4208437248
                                                                          -422.6519693
13
           2.048
                  2.048 -2.048
                                2.048].
                                                   -4829.447006924799
                                                                          -422.6519691
14
         [-2.048
                      -0.60808661 2.048
                                               2.048
                                                          ].
                                                                   -3061.578011536028
15
                     0.64261857 2.048
                                           0.30303525].
                                                                   -3045.3045458801726
         [2.048
16
         [-2.048]
                       1.30097593 2.048
                                              -2.048
                                                                   -4756.8851440609
17
         [-0.05554178 2.048
                                  -0.0987187
                                               0.425149641.
                                                                   -2281.847894393856
18
         [ 0.19661126 -0.23700152  0.10816946 -2.048
                                                                   -435.0767410375057
19
         [0.43477045 0.04775423 0.09928276 2.048
                                                      ].
                                                                   -420.3769069031035
20
         [-2.048 2.048 -2.048 -2.048].
                                                   -8273.612843724799
                                                                          -420.3769069
21
                      -0.10652455 -0.01300213 -0.17740439].
                                                                   -1864.4660201487898
         [-2.048]
22
         [-0.14661242 -0.67318025 2.048
                                              -0.07349956].
                                                                   -2129.2324220954984
23
         [-0.51394201 0.18525105 -0.49302349
                                                                   -359.39259584762084
                                              2.048
24
         [ 0.04223414  0.22998796  -0.3853382
                                              -2.048
                                                                   -510.2967694207748
25
                     0.3242387 0.27704515 2.048
                                                                   -1891.3546918115003
         [2.048
                                                      ].
26
         [-1.53372405 -0.03763685 0.13687502 1.97089071].
                                                                   -962.3519514274669
27
         [-0.04871763 0.21398955 -2.048
                                               2.048
                                                                   -914.5444455566166
         [ 1.54130277 -1.40096691 0.44854182 0.28603579].
28
                                                                   -1662.6081586153343
29
         [-0.27694401 -0.87943929 1.25330768 -1.56633965].
                                                                   -1103.8287995239782
30
         [-0.63808557 \quad 0.03132333 \quad -0.59613659 \quad -0.75571869].
                                                                   -179.40284795662322
31
                      0.70642684 1.09726491 -0.37487361].
         [-0.05173137
                                                                   -335.79684363303187
32
         [ 0.71374153  2.02105291  1.40017248 -0.46276058].
                                                                   -1537.6414213532244
33
         [1.17135501 0.69985291 0.40068972 0.5299697 ].
                                                                   -60.10743371792253
34
         [ 1.47564194  0.02636049  -0.28983168  -0.78361601].
                                                                   -549.3029618091022
35
         [-2.02182177 -0.70114881 1.40662951 -0.08419685].
                                                                   -2814.800496493994
36
         [ 1.59068772    1.16671535    -0.40371861    -1.88168526].
                                                                   -917.8516733150443
37
         [ 0.35769955 -1.72257422 0.15444364 -0.55293506].
                                                                   -1175.4466417532626
38
           0.37183303 -1.45548263
                                   0.73367031 -1.47898748].
                                                                   -859.1859036805786
39
         [-1.23597818 -0.09473091 0.75009555
                                               0.3176916 ].
                                                                   -330.3961499944753
40
         [ 1.02747587 -1.86636766 -0.64418959 -1.95688314].
                                                                   -3130.985945873225
```

```
1 ### ESTIMATED GP EI GRADIENTS
2
3 np.random.seed(run num 20)
4 surrogate approx 20 = GaussianProcess(cov func, optimize=opt)
5
6 approx 20 = GPGO(surrogate approx 20, Acquisition(util grad approx), objfunc, param)
7 approx 20.run(init evals=n init, max iter=iters)
8
```

Proposed point Evaluation Current eval. Best eval. init [0.36098376 1.62903543 1.60370987 1.29367031]. -499.4296468486902! init [-1.90099626 0.78543905 -0.49692286 0.07582083]. -937.6489569337288

```
[ 0.6469692 -1.25398951 -0.93259202 0.8954099 ].
init
                                                                 -916.294647636079
         init
                                                                 -1092.029190829674
         [-1.57002246 1.02924575 -1.06816219 -1.00431457].
init
                                                                 -1129.8679642787797
1
         [-2.048 -2.048 2.048 -2.048].
                                                 -8273.612843724797
                                                                       -499,4296468
2
         2.0481.
                                                 -4829.447006924799
                                                                       -499.4296468
3
         [ 2.048 -2.048 2.048
                                                 -4829.447006924799
                              2.048].
                                                                       -499.4296468
4
         [ 2.048 -2.048 -2.048 -2.048].
                                                 -11709.586680524799
                                                                        -499.4296468
5
        [-2.048
                     -1.31218948 2.048
                                              2.048
                                                                 -3519.181909230178
                                                        ].
6
         [-2.048 -2.048 -2.048 2.048].
                                                 -8281.8048437248
                                                                        -499.4296468
7
         [ 2.048 -2.048 2.048 -2.048].
                                                 -8265.420843724798
                                                                       -499.4296468
                                                 -8265.4208437248
8
                 2.048 -2.048 -2.048].
                                                                        -499.4296468
          2.048
9
         [-2.048 2.048 2.048 -2.048].
                                                 -4829.447006924799
                                                                       -499.4296468
10
         [-2.048 - 2.048 - 2.048 - 2.048].
                                                 -11717.778680524798
                                                                       -499.4296468
                 2.048 -2.048
                              2.048].
11
         [-2.048
                                                 -4837.639006924799
                                                                        -499.4296468
12
         [-2.048
                2.048 2.048 2.048].
                                                 -1393.4731701248
                                                                        -499.4296468
13
         [ 2.048 -2.048 -2.048 2.048].
                                                 -8273.612843724799
                                                                        -499.4296468
                                                                -499.42964684869025
14
         [2.048 2.048 2.048 2.048].
                                         -1385.2811701248
15
         Γ2.048
                    0.33222157 0.34513924 0.24223786].
                                                                 -1500.5685230639801
         [-0.17531963 -0.01006597 2.048
                                             -0.03965709].
16
                                                                 -2215.697948272316
17
         [-2.048 2.048 -2.048 -2.048].
                                                 -8273.612843724799
                                                                        -499.4296468
         -449.5372127249809
18
                                                       1.
19
         [ 0.06416532  0.28150094 -2.048
                                              0.028649921.
                                                                 -2206.1600814157714
         [-0.29064905 -2.048
20
                                  0.2339401
                                              0.07333681].
                                                                 -2034.7715422772617
21
         [ 2.048
                      2.048
                                  2.048
                                             -0.51091938].
                                                                 -3138.5317901644034
22
         [-1.64017903e-01 1.48217285e-03 -2.92206995e-02 -2.04800000e+00].
23
         [-0.03419113 2.048
                                  0.32453199 2.048
                                                                 -2296.489515799192
                                                        ].
24
         [-0.18129873 2.048
                                  0.0556355 -0.57412625].
                                                                 -2155.636963961828
25
         [ 0.04155987 -0.47044916  0.12063162
                                                                 -440.6541161105476
                                             2.048
                                                        1.
26
         [-2.048]
                      0.26333078
                                 0.08099687
                                              2.048
                                                        1.
                                                                 -1972.6937060511932
         [ 0.04678099 -0.35812747  0.00551397 -2.048
27
                                                                 -437.6742928880651
28
         [-0.1176829
                      0.52535607 1.25800185
                                             2.04523084].
                                                                 -145.54357766986558
29
         [0.63753141 1.39167152 0.03172582 0.39546635].
                                                                 -476.76064164378056
30
         [-1.87196263 -0.79279469 -0.91608427 -0.35078485].
                                                                 -2241.778048936678
31
         [-0.04876514  0.40945054  1.30688952  0.19211095].
                                                                 -377.6802644324403
32
         [-1.04514726 -0.18482258 0.96996067 -1.16480678].
                                                                 -699.6403016208243
33
         [ 0.24018362 -0.11406655 -0.02327053 0.19288687].
                                                                 -9.646826040884186
34
         [-1.7380717 -1.16787012 -1.20464654 0.92155594].
                                                                 -2459.4341831400907
35
         [ 0.37665898   1.49622433   -0.6456347   -0.86106668].
                                                                 -1182.006847432322!
36
         [-0.83423098  0.87355459  -1.03564615  1.6428321 ].
                                                                 -366.747503263408
37
         [ 0.99818601  0.88294004  1.42843553  -0.2987412 ].
                                                                 -590.7562504994663
38
         [ 0.13639
                     -1.98625677 -1.18880173
                                             1.99566803].
                                                                 -3086.1352358019253
39
         [-0.37295724 -0.45068957 -1.20087908 0.35091761].
                                                                 -359.81006888936713
40
         [ 1.40096206 -0.67822828 -0.22506665 -2.00215088].
                                                                 -1170.257381297159
```

```
1 end approx = time.time()
2 end approx
3
4 time approx = end approx - start approx
5 time approx
6
7 start exact = time.time()
8 start exact
    1623408371.1556969
```

```
1 ### EXACT GP EI GRADIENTS
2 nn nandom cood/nun num 1\
```

```
5 inp.ranuom.seeu(run_num_1)
4 surrogate_exact_1 = dGaussianProcess(cov_func, optimize=opt)
5
6 exact_1 = dGPGO(surrogate_exact_1, Acquisition_new(util_grad_exact), objfunc, param)
7 exact_1.run(init_evals=n_init, max_iter=iters)
8
```

```
Current eval.
                                                                  Best eval.
Evaluation
                 Proposed point
                       0.90244913 -2.04753152 -0.80964578].
init
         [-0.33987787]
                                                                   -3394.123441866637
init
         [-1.44688787 -1.66978112 -1.28507817 -0.63258326].
                                                                   -3615.357417364757
init
         [-0.42284043 0.15899334 -0.33097927
                                               0.75865907].
                                                                   -59.369079192709535
init
         [-1.21056359
                       1.54876902 -1.93582042
                                               0.69823492].
                                                                   -2823.036073483468
init
         [-0.33871953
                       0.24039354 -1.4729751
                                              -1.2365763 ].
                                                                   -1404.6293821132788
1
         [ 0.47982557 -0.71006248  0.11082999
                                               1.58081884].
                                                                   -353.9044857665011
2
         [-0.06378109
                       1.47176573
                                   1.35331664
                                               0.61093559].
                                                                   -431.9228759760618!
3
           1.37005676
                       0.81765656
                                   1.71318718 -1.88527122].
                                                                   -2545.5469796327466
4
                                   1.78238716
         [-1.81053107 -1.47940754
                                               1.59146846].
                                                                   -2545.8382380521
5
         [ 1.9232277
                      -1.98832647 -1.16650153 -1.56722413].
                                                                   -6727.49381067573
6
           1.56126543 -1.53158254
                                   0.54665558 -0.91048865].
                                                                   -2052.24859507814
7
         [-1.91249677
                       0.95620178
                                   0.92652261 -1.683623481.
                                                                   -1384.4945752368342
8
         [ 1.79630348
                      1.92819261 -0.80082844
                                               1.48474429].
                                                                   -2286.4026132497693
9
         [ 1.41062424
                      0.50059934 -1.20225809
                                               0.78433658].
                                                                   -481.8412035957267
10
                       1.97024478 -1.57773591 -1.22917739].
         [-0.47896694
                                                                   -4676.218592985641
11
         [-0.80177084
                      0.10432746 -1.2657979 -1.17103934].
                                                                   -970.2835994391748
12
         [-1.21299939 -0.61601458 0.78020353
                                               1.73140592].
                                                                   -585.3749170898446
13
         [ 1.93343763 -1.00515763 1.02813215 -0.89606058].
                                                                   -2636.316924015028
14
           0.16408403 -1.87745056 -1.08510878 -1.96427878].
                                                                   -3488.188043504941
15
          1.21927521 -1.3441189 -0.25420212 -0.95510121].
                                                                   -1337.1274101009928
         [ 0.71957744 -0.08618859 1.86832512 -0.97928598].
                                                                   -2382.8079991619197
16
17
         [-0.85563904 -0.0953072
                                   0.53507817
                                               0.88022639].
                                                                   -136.2633926140205
         [1.48287921 1.62432131 1.87436746 0.5222742 ].
                                                                   -987.3782986646119
18
         [-0.05953229 -1.85141643 -0.82367161
19
                                               0.90781219].
                                                                   -2169.3806668751913
20
         [ 1.89620782 -0.14839589 -1.53922942
                                               0.68600274].
                                                                   -1937.398128539917
21
           0.75241121 -0.58888911
                                  0.39295842
                                               1.31362989].
                                                                   -270.95033931956635
22
         [-1.91527024 1.88567789
                                   1.75165396
                                               1.9022421 ].
                                                                   -789.0627595795792
23
         [ 1.8307373
                       0.45568333 -1.22143559 -0.95524121].
                                                                   -1647.6341694210719
24
                       1.44958647 -0.0529613 -1.67199703].
                                                                   -810.1388967930725
           0.8051578
25
           0.79734412 -0.83463689 -1.80414999 -1.60545318].
                                                                   -3215.219531243629
26
         [-0.1582911
                     -0.68994974 1.6102458 -1.19194178].
                                                                   -1616.8340348753732
27
                                   1.28246287 -1.03341029].
                                                                   -989.8946435008918
         [-0.22926075
                      1.4608557
28
           2.0062999
                      -1.50296352 1.08688969 -0.29540852].
                                                                   -3418.8237640549432
29
         [-0.79647557
                       0.5219737
                                  -0.52585479 -1.74939235].
                                                                   -481.21093988613774
30
         [ 0.66119611 -0.1938156
                                   0.35461529
                                               0.57051867].
                                                                   -71.6059468847258
31
          1.55656109 -0.57199926
                                   0.1756522
                                               1.30094652].
                                                                   -1064.001858558137
32
         [-1.98935079
                       1.82470542
                                   0.7078706
                                              -0.530783981.
                                                                   -1258.384739357216
33
         [-0.06966701
                       0.83377973 -0.92724163
                                               1.71662838].
                                                                   -410.2453655200145
34
         [ 0.56787983 -0.70452346  0.6459641
                                              -2.00969127].
                                                                   -699.9448688633819
35
         [0.49704515 0.93111689 1.6178312 0.1594768 ].
                                                                   -707.9393288226192
36
         [ 0.87715693 -0.5909966
                                  -1.62091187 -1.99652745].
                                                                   -2720.678153604498
37
         1.95053983].
                                                                   -1259.1691178659573
38
         [-1.73681667 0.33276035 0.5322298
                                              -0.61463567].
                                                                   -826.8067343838653
39
           1.69661485 -1.31722849 -1.50498054
                                              0.6533503 ].
                                                                   -3082.082077592921
40
         [-0.38001736 -1.73073496 1.72122227 -1.51184018].
                                                                   -2525.930515971026
```

```
1 ### EXACT GP EI GRADIENTS
2
3 np.random.seed(run_num_2)
4 surrogate_exact_2 = dGaussianProcess(cov_func, optimize=opt)
5
```

```
6 exact_2 = dGPGO(surrogate_exact_2, Acquisition_new(util_grad_exact), objfunc, param)
7 exact_2.run(init_evals=n_init, max_iter=iters)
8
```

```
Proposed point
Evaluation
                                           Current eval.
                                                                   Best eval.
         [-0.26216488 -1.94180615 0.20341751 -0.26491948].
                                                                    -1696.9764582030693
init
init
         [-0.32617348 -0.69494857 -1.20975919
                                               0.48853388].
                                                                    -455.3157381798458
init
         [-0.82061446 -0.95507548 0.49616418
                                                0.11936602].
                                                                    -291.50084682592353
init
         [-1.49676054 0.05561598 -1.29253431
                                                1.16873277].
                                                                    -682.7190038869136
init
         [ 1.4498828
                      -0.02360591 1.41951584 -1.72177213].
                                                                    -2051.02408589455
1
         [-0.4632877]
                       1.20273901 0.32769712 -1.38322494].
                                                                    -447.6512250019873
2
         [-1.79751416 -0.52112824 -0.26988812
                                               1.94096178].
                                                                    -1797.9483083066798
3
           0.94656668 -1.40026063
                                   1.68602863 -2.04011953].
                                                                    -2925.242198220676
4
         [-0.36783662 -1.88731676 1.04396437
                                                1.21112717].
                                                                    -1054.8119304069996
5
         [ 0.49207579 -0.1936526
                                    1.21953714 -1.80202412].
                                                                    -1242.389386909326
6
                                                                    -1985.7779986308444
         [-1.91545461 -0.03437501 0.5961899
                                               -2.03028164].
7
           1.20412991 -0.51609684
                                   1.79301296
                                               1.64643946].
                                                                    -868.568370989524
8
           0.9497619 -1.00087775
                                   2.01275464 -1.90179618].
                                                                    -4013.1500050237373
9
           1.91280873 0.05792566 -1.4610237
                                               -1.744735881.
                                                                    -3023.791522215833
10
                       0.67319442 -0.29503953 -0.49728085].
           0.6711098
                                                                    -96.9852621015022
11
           1.62443908 -1.07297197
                                   0.55047237
                                                1.34488749].
                                                                    -1527.260533405431!
12
           0.70328035  0.79253662 -1.11663844
                                                0.54625177].
                                                                    -366.9920724173906
13
           0.8543915
                      -1.08588577 -0.49915066 -1.03232031].
                                                                    -782.2437551489709
14
         [-0.96817674 1.00253367
                                   0.23548821 -1.14406601].
                                                                    -207.99406890784175
15
         [-1.20514898 -0.59463617
                                   0.02209828 -1.99340305].
                                                                    -835.9401338477081
16
         [-1.79245809 0.56510131 0.01560574 -0.60648902].
                                                                    -756.0808185096352
17
         [0.88403941 0.44212308 1.24926468 0.08105246].
                                                                    -341.878459426937
18
         [-0.99411718 -0.98352436 0.78232123
                                               0.01078764].
                                                                    -436.32643069587914
19
         [-1.00984619 -2.04537038 -1.48067386
                                                                    -4433.688298840226
                                               0.56031501].
20
         [ 0.55207279 -0.01956725
                                                                    -747.8208786411448
                                   1.4668598
                                               -0.130397961.
21
         [-1.93895196
                       1.55137364
                                   0.69722405 -0.50223336].
                                                                    -886.5665471151541
22
           0.87913442
                       1.08383489 -0.5164871
                                              -0.88012047].
                                                                    -429.534789456539
23
         [ 1.68243189 -0.29617387
                                   1.20898237
                                                0.845374
                                                                    -1143.5479302987378
24
         [-1.50413177 0.89525845
                                   1.82922983
                                                0.42630423].
                                                                    -1152.0157493412569
25
           1.08619
                      -1.14804293 0.95918544
                                                1.11887641].
                                                                    -563.341210484766
26
         [1.92373852 1.90161802 1.15448994 1.02248265].
                                                                    -940.9949911919929
27
         [ 0.89051522    1.59091218    -0.85470426    -0.72790011].
                                                                    -1426.463825694853
28
           1.7952232
                       0.98917322 -0.00676112
                                               1.436821
                                                                    -804.0658058564687
                                   1.90252766 -1.75774148].
29
           0.63523663
                       1.67930549
                                                                    -3139.9508366843415
30
         [ 1.82143212  0.73311298 -2.04727183 -1.88527067].
                                                                    -5038.575769519586
31
         [-0.47465946 0.42283806 -0.85595954 -1.68383769].
                                                                    -700.8748323801497
         [-0.68527262 -0.58563323 1.51289546
32
                                                0.58564071].
                                                                    -543.9353731860382
33
         [0.55223936 0.46147771 1.27238896 0.21156894].
                                                                    -313.3316330394328
34
         [ 1.32173857  2.04339184 -0.29528961 -2.00670871].
                                                                    -2448.8503389948387
35
         [-0.34823756 -0.05469126 0.43322284
                                               1.88093636].
                                                                    -311.5685252340465
36
         [0.51395761 1.42586065 1.73124137 1.4637363 ].
                                                                    -380.1695492899531
37
         [ 1.28905706  0.32105178 -1.58817841 -1.93695353].
                                                                    -2461.505686335076
38
         [-1.87234884 -1.86175433 1.40728674 -0.66191861].
                                                                    -4019.649521955219
39
         [-1.75988164
                      0.58497024
                                    1.75923584
                                                2.00126065].
                                                                    -959.8960097161256
40
                       0.37549186
                                   0.96577463
                                                                    -183.26676877682718
         [-0.05047861
                                                1.93190576].
```

```
1 ### EXACT GP EI GRADIENTS
2
3 np.random.seed(run_num_3)
4 surrogate_exact_3 = dGaussianProcess(cov_func, optimize=opt)
5
6 exact_3 = dGPGO(surrogate_exact_3, Acquisition_new(util_grad_exact), objfunc, param)
7 exact_3.run(init_evals=n_init, max_iter=iters)
```

```
Evaluation
                 Proposed point
                                           Current eval.
                                                                  Best eval.
init
         0.20806821 0.85257348 -0.85645419
                                               0.04434987].
                                                                    -367.7787956485136
init
         1.60951073
                       1.62321649 -1.53360257 -1.19913317].
                                                                    -3099.341888277455
init
         [-1.83719034 -0.24244288 -1.92562704 -0.17681111].
                                                                    -3229.929027395333
init
           0.61089402 -0.90731609
                                   0.72194008
                                               0.3721741
                                                                    -171.0831542888061
init
         [-1.94977021
                       0.24106634 -0.98610198 -0.3477455
                                                                    -1564.280611971214
1
         [-1.67027913
                       0.62837106 0.23691576 -0.56703073].
                                                                    -516.3694433953648
2
         [-0.29100799 -0.48807482 1.00190111 -1.60624191].
                                                                    -776.2427879756497
3
           1.73122643 -0.6484088 -0.01911714
                                                1.34680056].
                                                                    -1533.9060249585593
4
         [ 0.2331452
                       0.18954322 1.52098534 -2.02444137].
                                                                    -2105.5674703812724
5
         [0.13068371 1.75340124 0.50169946 1.20414234].
                                                                    -1055.6545691701
6
         [ 1.20186817 -1.28642743 -1.13023645 -1.33955666].
                                                                    -2216.156072663885
7
         [1.75427745 1.64208478 0.672074
                                            0.7129784 ].
                                                                    -623.7616288616542
8
                      0.47902952 0.0920567
         [-1.16664765
                                                0.11458401].
                                                                    -86.60324424339615
9
         [ 2.04115885
                       1.62476609 -1.34334081 -1.03870914].
                                                                    -3047.9332791944066
10
         [-0.79508563]
                       1.14428579
                                   1.85786343
                                                1.29587167].
                                                                    -525.0293915730558
11
         [-0.49210466]
                       0.13453559 -0.0550971
                                                1.12595775].
                                                                    -131.8782605794016
12
         [ 0.15608471
                       1.42891248
                                   1.70018876 -1.78973927].
                                                                    -2400.9284253104433
13
           1.70127945
                       0.89285159
                                   1.02292007 -0.09786345].
                                                                    -537.125759480679
14
         [-0.15926852 -0.36244133 -1.73771274 -2.03864869].
                                                                    -2933.713458154941
15
                       0.9714593
                                   -0.44400853
                                                                    -368.71355924551295
           1.49026914
                                                0.61778337].
16
         [-0.46262741]
                       0.05837161
                                    1.68184685
                                                0.06103135].
                                                                    -1053.5780873033314
17
           0.16200584 -0.70881686
                                                1.16645499].
                                                                    -111.6911386063480!
                                   0.67231605
18
         [-2.03453222 -1.33622661 -1.70069197
                                                0.05220796].
                                                                    -5042.119631809486
19
          1.33696319 -1.63880317
                                   0.39971969
                                                                    -1706.1729143185794
                                                0.30947677].
20
                       0.49268641
                                                                    -1537.6735410119732
           1.49239847
                                   1.60406172 -0.668308161.
21
           1.29844154 -1.80613562
                                   0.68428634
                                                0.57604784].
                                                                    -1893.2173867997783
22
           1.2299417
                      -1.91096248
                                   1.4133729
                                                1.991915871.
                                                                    -1681.9314991104627
23
           0.00550859 -0.87056605
                                   1.11029903
                                                1.51331117].
                                                                    -100.5842275200599!
24
           1.03821088 -1.81361364 -1.15747931
                                                1.09327608].
                                                                    -2832.0132900953026
25
         [-1.92125593
                       0.53080971 -1.93881188
                                                1.72743047].
                                                                    -1922.030053518997
26
         -711.8857692267823
27
          1.0047818
                      -0.63259091 -1.96439414 -1.85587058].
                                                                    -4106.041253375681
28
           0.98492504
                      1.17178375 -0.22453846 -1.97200959].
                                                                    -669.856486331395
29
           1.10614155
                       0.98623714
                                   1.95858435 -0.70898671].
                                                                    -2169.50428747307
30
           0.94417659 -2.0345752
                                    0.21589641 -1.32198484].
                                                                    -2592.7693977126632
31
                       1.46618113 -0.57797751
                                                1.0150917 ].
                                                                    -996.1300770680594
         [ 1.69980461
32
                       1.3368284
                                    1.82024652
                                                0.72471013].
                                                                    -726.0825390658513
         [-0.7850228]
33
         [-0.90364346 -1.40881445 -0.01203534 -1.32845648].
                                                                    -1080.9212981095382
34
         [ 1.23334546 -0.45172328  0.65487468 -1.43597748].
                                                                    -759.5865546206971
35
         [0.74524341 1.03355023 1.41376536 0.64124483].
                                                                    -219.31817541039308
36
         [-1.76099243 0.62045344 -0.09891249
                                               1.63585396].
                                                                    -912.1566142299126
37
         [ 0.74426082 -0.067332
                                   -0.27796404 -1.07523988].
                                                                    -182.24072574245946
38
         [1.36215247 1.66444399 1.29525051 0.73108159].
                                                                    -311.5110661199934
39
         [-0.29245864 -0.98054645 -0.12680832 -0.08144759].
                                                                    -239.90148247899936
40
         [ 0.94174472    1.35912663    0.63783186    -1.03478984].
                                                                    -376.65477667517473
```

```
1 ### EXACT GP EI GRADIENTS
2
3 np.random.seed(run_num_4)
4 surrogate_exact_4 = dGaussianProcess(cov_func, optimize=opt)
5
6 exact_4 = dGPGO(surrogate_exact_4, Acquisition_new(util_grad_exact), objfunc, param)
7 exact_4.run(init_evals=n_init, max_iter=iters)
8
```

```
Evaluation
                 Proposed point
                                          Current eval.
                                                                 Best eval.
init
         [1.91295422 0.19346329 1.93611514 0.87988631].
                                                                  -2387.047477734054
init
         [ 0.80989727 -1.16289743 1.95082017 -2.02248087].
                                                                  -3769.0203854501506
init
         [-1.01178424 -0.26709388 1.14435245 -1.23828193].
                                                                  -936.5671269056027
init
         0.39867983].
                                                                  -3042.500138281922
init
         [-2.01119294 -0.46460403 -1.8671204
                                               1.87045056].
                                                                  -2747.9169599921197
1
          0.18515006 0.09995911
                                  0.56365156 -0.40347466].
                                                                  -84.75946556482826
2
          1.08643695 -1.32704877 0.75746856
                                              1.22708601].
                                                                  -777.5868539622428
3
          0.50108145 1.44873455 -1.9222709
                                                                  -3067.494422071646
                                               0.09215335].
4
          0.97015307 -0.14843719 -1.90712713 -0.08913273].
                                                                  -1889.173868533498
5
          0.5719512
                       0.52770101 0.01636585 -0.84311832].
                                                                  -83.39656774588515
6
          1.42806536 -1.31189144 -0.42005859 -1.21391197].
                                                                  -1782.389365571046!
7
          1.26503965 -0.57328862 0.00821153 -1.87677415].
                                                                  -838.511022269754
8
          1.32407951 -1.69087568 -1.18515526
                                              1.20351454].
                                                                  -2837.8886293809755
9
         [-1.2736561 -1.35513827 -0.00896676 -0.65844098].
                                                                  -1282.0912240841826
10
         [-1.30788384 1.6352187
                                   1.93744968 -0.47135138].
                                                                  -1846.5335472285947
11
          0.73892166 -0.30564
                                   1.8830846 -1.98827539].
                                                                  -3458.202946512108
12
          0.84366127 -0.65834373 -0.05004698 -0.57847503].
                                                                  -248.72419145669912
13
         [0.48281039 0.89101288 1.25443128 1.89276724].
                                                                  -75.02371382812068
14
         [-0.62352509 0.24447576 0.3249728
                                              -0.91682565].
                                                                  -117.3150412707675
         [ 1.63775139  0.76920136  -0.76521696  -1.80540063].
15
                                                                  -1125.32595778395
16
         [-1.86465068 -0.92999789 -1.25515852 -1.55335209].
                                                                  -3387.497726089871
         17
                                                                  -2371.8161393760843
                                              0.63114793].
18
         [-1.44955162 -0.24929692 0.99857842
                                                                  -661.1309921254697
19
         [ 0.43568332
                      1.10448031 -1.26447195
                                               1.42079957].
                                                                  -709.4880074006844
20
         [1.95857626 1.06291297 1.70378865 0.91546935].
                                                                  -1198.36545447881
21
         [-0.64020879 -0.32548536 1.10358982 0.69077064].
                                                                  -185.85029281947786
22
         [ 0.51955275 -1.53918616 -1.81726474
                                              1.82769867].
                                                                  -2311.9566892082717
23
         [-1.68797962 -1.89587099 0.53229563 -1.84784893].
                                                                  -3659.270796405538
24
         [0.19058347 0.6163165 1.52408089 0.05787768].
                                                                  -678.6412482177482
25
         [ 1.95414706 -2.00910552 0.17623568 0.51214857].
                                                                  -4920.277230184521
26
         [0.29278859 0.48443353 0.89325068 0.69622496].
                                                                  -61.07998569163262
27
         [-1.68297999 1.07256271 -1.17005342 -1.60752089].
                                                                  -1746.0517976662131
         [-1.83504592 0.57272321 0.36396613
28
                                              1.78672103].
                                                                  -1063.4262741118819
29
         [-1.82621733]
                      1.3648309
                                   1.38733792
                                              0.83316977].
                                                                  -538.2029210893229
30
                                  -0.37217706 -1.22703467].
                                                                  -336.8270745465934
         [-1.22276768
                      0.7543545
31
         [ 1.32638545
                      1.39105073 1.36951294 -1.83395094].
                                                                  -1421.9880420840564
32
         [-0.76125084 0.12963873 -0.62036409 -0.95263865].
                                                                  -246.209503333022
33
                      2.04692871 0.45878489 -0.82666467].
                                                                  -1670.4616530704325
         [-0.87122222
34
         [-0.33218589
                      0.75505643
                                  0.15995792 -1.25506911].
                                                                  -224.93573110971306
35
         [ 0.53907861
                      0.80105769 -0.13294576
                                              1.03329548].
                                                                  -190.74687989954148
36
                      1.49878963 0.26705322 -1.09257692].
                                                                  -657.1050982695266
         [ 0.60276928
37
         [1.17707935 1.45523333 0.8341324 0.29449966].
                                                                  -181.6101171300378
38
         [-0.08973767
                      1.69880134 -0.38553909 -0.15508577].
                                                                  -1368.9319491647348
39
         [ 0.74821824    1.78306464   -1.78430824    0.91549893].
                                                                  -3136.318146218995
40
         [ 1.01737435 -1.68893479 1.623333127 -1.74129535].
                                                                  -2816.089596716538
```

```
init
         [-0.04746777 0.45770286
                                    1.08915858
                                                 0.07544008].
                                                                     -222.91752416760144
init
         [-0.83230515 -1.27909385 -1.71728376
                                                 0.97665145].
                                                                     -1918.291410223084
init
                                    1.55622208 -0.92534185].
         [-0.24039742 -1.39956278
                                                                     -1356.5528565009568
init
         [-0.35129336 -0.8352566
                                    0.52751527
                                                 0.32701567].
                                                                     -100.45329155979191
1
         [ 0.31810707 -2.04127366
                                    0.06337582
                                                 0.57260104].
                                                                     -2185.7438722645497
2
           0.93417407 -0.95713874
                                    0.04788205
                                                 0.51617412].
                                                                     -441.35553809915314
3
         [-0.44059633
                        1.95260162
                                    0.98851101
                                                                     -1121.749022773105
                                                 1.32304877].
4
         [-0.69240508 -1.69821421
                                    1.05569041
                                                 0.3397459 ].
                                                                     -878.6270483712931
5
                                                                     -365.539811259935
         [-0.62007949 -0.59387599 -1.14516255
                                                 0.71394031].
6
         [-0.77079598
                        1.5938349
                                   -1.67587878 -1.06932543].
                                                                     -3392.021959788046
7
           0.08440215
                        0.09678137 -0.68591607
                                                 1.2573758 ].
                                                                     -115.56245509730319
8
         [-0.05157625 -0.67724132
                                    1.83878851
                                                 0.29903289].
                                                                     -1191.2661216102438
                                    0.54879247 -1.08623221].
9
         [ 0.5080949
                        1.05243414
                                                                     -287.2533091457605
10
         [-0.91327357
                        1.24112404
                                    1.78933104 -0.59901106].
                                                                     -1471.6531056871854
                       0.27037259
                                    0.45464854 -1.32530474].
                                                                     -370.0513563419816
11
         [ 1.16854508
12
         [-1.62959076
                        1.6064982
                                   -0.65160286
                                                 1.3152801 ].
                                                                     -1244.2646588595474
13
         [-1.18632711]
                        2.02375049
                                    0.31679644 -0.89218401].
                                                                     -1570.711430108154
14
         [-1.96247991
                        1.30933862
                                    0.78091536
                                                 1.12353327].
                                                                     -768.6132013299593
15
         [ 1.80499795
                        0.05340004 -1.61819437
                                                 0.9156279 ].
                                                                     -1588.1307824603791
16
         [-1.61562475
                        1.12448258
                                    0.36308353
                                                 1.13101629].
                                                                     -409.0966974363194
17
         [-2.00979377
                        1.45046548
                                    1.91636392
                                                 1.91286092].
                                                                     -993.4236305943057
18
         [-0.01686843 -1.65674521
                                    0.67476732
                                                 0.436646981.
                                                                     -711.3131631801381
                        0.97949297 -1.32818922
                                                 1.7809417 ].
19
           0.6927607
                                                                     -553.8106806602497
20
           0.86866932 0.5076431
                                   -1.82363683 -0.78598627].
                                                                     -2138.083968068359
           1.94994465 -0.35355171 -1.53741326 -1.48909156].
21
                                                                     -3496.9851843806637
                      -1.7247022 -1.41938966
22
                                                0.59671559].
                                                                     -2450.770089074509!
           0.1473329
23
         [-1.37505296 -1.32512161
                                   1.12550758 -1.87113142].
                                                                     -2069.6453850731227
         [0.75502349 0.74256749 1.84303871 0.46968966].
                                                                     -1027.436879763098
24
25
           1.32475783 -0.8915516
                                  -0.21088425 -0.78154481].
                                                                     -874.9477914351841
           1.15487158 -0.834299
                                    1.05481692
                                                0.2559162 ].
                                                                     -559.694281885498
26
27
         [-0.3107496
                        1.66980759 -0.84551918
                                                                     -1582.353544675686
                                                 0.41760558].
28
         [-1.07255585 -0.11466322 -1.92503864
                                                 1.03190207].
                                                                     -1264.7418425813808
29
           1.28272724 -1.39964435 -0.12724209 -1.20591634].
                                                                     -1518.9287371421751
30
         [-1.20365786
                       0.31174043
                                   0.0297163
                                                 1.38762166].
                                                                     -328.3195031335746
31
         [-1.6109904
                        0.8590569
                                    0.45648285 -1.77930314].
                                                                     -711.5941755565317
32
         [-0.13522102 -2.00678675
                                    0.85543304
                                                 0.21808611].
                                                                     -1452.8346714359607
33
         [-1.3997181
                        0.46429525 -0.96362403
                                                 1.3682138 ].
                                                                     -391.7571103590943
34
         [-0.61004237
                        1.06835669
                                    0.87587592 -2.02996793].
                                                                     -840.5237144476857
35
                                    1.24874948 -1.89400768].
                                                                     -1200.554415721937
         [-1.12910189
                        1.09708521
         [-0.31390776
                        0.79157762
                                    1.3836017
                                                 1.46509244].
                                                                     -127.43678379889838
36
37
         [-1.38834774
                        1.34558751
                                    1.64297275
                                                 0.83116248].
                                                                     -391.9264398338271
38
         [-1.00480104 -1.63478392
                                    0.45813346 -1.68836468].
                                                                     -1561.230607409748
39
         [-0.03997327
                        1.87412011
                                    1.35086415
                                               -0.98530202].
                                                                     -1609.480912063545
40
         [-0.49490898 -0.61553645 -0.38107717
                                                 1.124754
                                                                     -234.496171179621
```

```
1 ### EXACT GP EI GRADIENTS
2
3 np.random.seed(run num 6)
4 surrogate_exact_6 = dGaussianProcess(cov_func, optimize=opt)
5
6 exact 6 = dGPGO(surrogate exact 6, Acquisition new(util grad exact), objfunc, param)
7 exact 6.run(init evals=n init, max iter=iters)
8
                     Proposed point
                                               Current eval.
                                                                       Best eval.
   Evaluation
    init
              1.60915518 -0.68821072
                                        1.31575449 -1.87721062].
                                                                        -2450.5677149947023
   init
             [-1.60703824
                           0.38933325
                                       0.12213192 -0.33256477].
                                                                        -501.1308148976547
```

0.96617311].

0.50183959 -0.25337272

[-0.67416945

init

-111.72625934007624

```
[0.07387714 0.32300483 0.59537447 2.00795862].
init
                                                                    -309.0778245045886
init
         [ 1.31013917 -0.35552897 1.54119232
                                                1.32611864].
                                                                    -741.7784291682051
1
           0.89019247
                       1.79138369 -0.60698719 -1.00911474].
                                                                    -1748.991187524451
2
         [-1.14213156 0.58137556 0.92917136
                                               0.01684862].
                                                                    -163.6614524559984
3
         1.75433426
                      0.20493592 -1.15829832
                                                0.97976468].
                                                                    -988.298019147344
4
         [-0.79474745 -0.73843181
                                   0.53990645 -1.68693428].
                                                                    -585.5828092278404
5
         [-1.00900642 -1.66327098 -0.76191645 -2.04296494].
                                                                    -2666.4221910336314
6
         [ 0.04661632  0.04813664  1.80385034 -1.54175126].
                                                                    -2627.0287468897136
7
         [-1.74092098 -0.28326251 0.05425427 -0.54902337].
                                                                    -1138.8930209663592
8
         [-0.62606658 -0.58785451 0.50109625
                                               1.05568426].
                                                                    -168.57254616905388
9
         [-0.44297594 0.21604389
                                   1.09977188 -1.18858878].
                                                                    -688.7294077105599
         [-0.39873712 -1.5352345 -0.18194884 -1.01176645].
10
                                                                    -1050.5948765150392
                       0.73488137
                                   2.01182067 -0.80229802].
                                                                    -2584.45765645506
11
         [ 1.0579262
12
         [-0.86349482 -0.11862378
                                   0.83160281
                                                1.00745874].
                                                                    -156.25931898296886
         [-2.02192246
                                  -0.68755355
                                                1.22030758].
                                                                    -1390.5670773286477
13
                       1.2686919
14
         [-1.90383044 -1.71776218
                                  1.30135346
                                               2.00336669].
                                                                    -3151.598091384067
15
         [-1.33861412
                      1.23201025 -0.96307082 -0.24365355].
                                                                    -793.3806495510584
         [-1.20433764 -1.7806771 -1.09423599
                                                0.66747467].
                                                                    -2908.121430619087
16
17
         [-1.86392832 1.13826433 0.68259296
                                                1.42921976].
                                                                    -684.3704195020284
         [-0.71508768 -1.06298624
                                   1.48028271 -0.75758851].
                                                                    -1137.112846776038
18
         [ 0.94214099 -1.57354766 -0.74644094
19
                                                1.15478747].
                                                                    -1689.576343784932
20
         [1.8909089 0.28940522 0.85682419 1.06069847].
                                                                    -1151.612110817843
         [ 1.89109499 -0.64451329 0.19246157
21
                                                1.0232119 ].
                                                                    -1887.8498992613063
                                                1.04657615].
22
         [-1.48289855 1.9603708
                                    0.88014879
                                                                    -898.0695517217156
23
         [0.33873613 1.06893801 0.88105688 1.03917139].
                                                                    -105.25928491494603
24
         [-1.61922811
                       1.23481322 2.02363183
                                                1.9101849 ].
                                                                    -702.6303179178191
25
         [ 0.15810568
                       1.97152737 -0.44674798 -1.31645352].
                                                                    -2490.5484677296968
                       0.83083395
                                  0.48969449 -1.25888407].
26
         [-0.14395639
                                                                    -295.85482689009353
27
         [-1.04837812 -1.02335261
                                   0.62386577
                                                1.73596787].
                                                                    -658.211927766007
28
         [-0.95422001 -0.54737772 -0.44854888 -1.1889234 ].
                                                                    -470.0820820835665
29
         [ 1.96181723 -1.56127344 0.47070345 -0.43759404].
                                                                    -3364.8825906149023
30
           1.33981188 0.49177975 -1.7059087
                                               -1.64398766].
                                                                    -2630.928106036733
                       1.44371507 -1.98550922
                                                                    -2834.811304710729!
31
         [-2.04650648
                                               1.9251675 ].
32
         [-1.06066992
                      1.23904023 -1.04353373 -0.39191513].
                                                                    -894.0769169135324
         [-0.35702929
33
                       1.09433763 -0.51713564 -1.56045156].
                                                                    -725.7734812165357
34
           1.85564941 -0.68981499
                                   0.2899382
                                               -1.66918129].
                                                                    -2023.3102026099407
35
           0.62057554
                       0.30413893 1.58954197 -1.24066722].
                                                                    -1645.007906836277!
36
         [ 0.78309714
                       1.36094253 -1.70864839
                                               1.38494553].
                                                                    -1566.8381453248673
37
                       1.34467199 -0.60828857
         [-0.17324013
                                                1.01354448].
                                                                    -802.2419906375629
         [-0.07967532 -0.56041942 -0.53123136 -0.08364451].
                                                                    -122.90596687337347
38
39
                       1.98328736 -1.20424388
           0.18867716
                                                1.44766517].
                                                                    -3025.401390343327
40
          1.41638326 -0.57018461 -1.27636987 -0.21078604].
                                                                    -1266.5657344000517
```

[-9.48473938e-01 -4.81276619e-04 7.34126064e-01 1.24411509e+00].

1.67769509].

[1.95784504 0.15767909 0.00458942 -1.75287856].

[-1.17397359 -0.19610025 1.76621986 -1.94601276].

[-0.48766512 -1.77792472 -0.86775563

init

init

init

init

-1660.8385633941034

-2128.346574385609

-3119.0824429471622

```
1
         [ 1.3841121
                       1.10038019 -0.7618778
                                               0.29747336].
                                                                   -466.91549800810617
2
         [-0.46462418 -1.01739574 -0.63627658 -1.21236035].
                                                                   -701.8724792881038
                       0.45704385 1.94337688 -0.92807062].
3
         [-1.46678761
                                                                   -2808.7207648117214
4
           0.88038975
                      0.42831332 -1.19910716 -0.98216741].
                                                                   -794.0017025703881
5
         T 1.1357617
                      -0.39564146 -0.88860615
                                               1.99053848].
                                                                   -543.1082177327809
6
         [-1.69941301
                      0.52314958 0.44742864 -1.63861248].
                                                                   -908.2124698408273
7
         [-0.89608508 -0.10949347 -1.06104869
                                               0.94295889].
                                                                   -210.81764308842642
8
                      1.61933938 -0.32876869 -0.63556608].
         0.22065276
                                                                   -1175.610596343472
9
           0.88589231 1.97042035 -2.00774073
                                                                   -4590.454863252045
                                               0.91601832].
10
           2.0309589
                      -0.60175451 -0.05136673 -1.39521684].
                                                                   -2451.256149086253
11
           0.99588388 1.9687159 -1.0789958
                                              -1.908739831.
                                                                   -3500.057706047198
         [-1.46915487 -0.99321291 1.31221829
12
                                               0.19699703].
                                                                   -1246.592726306397
13
         [-0.40008565 -0.92090559 -0.11573164 -1.38791558].
                                                                   -413.0030842698699
14
         [-0.8124053
                      -1.03583082
                                   1.46649275 -0.71060039].
                                                                   -1129.3673394317823
15
         [ 0.44977671 1.70397743
                                   0.71330121 -1.63729986].
                                                                   -1166.6723629796802
16
           0.29053641 0.21600328 -0.96070099
                                               1.099978241.
                                                                   -111.30510281931322
17
         [-1.50508243 -0.57055302 0.39945733 -1.0990935 ].
                                                                   -972.2626464144971
18
         [-1.24710295
                       0.95762102 -1.73052056 -1.50459248].
                                                                   -2773.546119260599
19
         [ 1.57724724 -1.43419739 1.0000704
                                               1.67615355].
                                                                   -1701.786289068928
20
         [ 1.30254556
                      0.86457258 -1.9212007
                                                                   -1193.738652806666
                                               1.68184436].
         [-0.09917108 -0.39295794 -0.47187016 -1.06023994].
21
                                                                   -225.34614242670636
                       1.74048623 0.48743567 -0.60968492].
22
         [ 0.1774199
                                                                   -1011.4502620486527
         [-0.31346838 -0.90223615 -1.67879094
                                              1.18131619].
23
                                                                   -1002.0194042116342
24
         [1.09755539 0.06000333 0.40179989 0.72821809].
                                                                   -180.2471447384382
25
         [-0.4259852
                       1.41530979 1.2169289
                                               0.21733628].
                                                                   -375.96080556137713
26
         1.54157949 -0.61270067].
                                                                   -1294.6877030790056
27
         [ 1.69057861  0.50218671
                                   0.64506916 -1.67216904].
                                                                   -1007.3907003780754
         [-1.74730148 -1.48302988 -1.77713273
                                                                   -4159.123649942196
28
                                               0.9247701 ].
29
           1.29833014 -1.73994269 -1.37322401 -2.00185139].
                                                                   -4634.594219963464
30
         [-1.37706882 -1.78891816 -1.78812293
                                               0.9528631 ].
                                                                   -4371.451001526354
31
         [-1.34271262 \quad 0.64109026 \quad -0.54198534 \quad -0.83191675].
                                                                   -360.49934374026805
32
           1.10499416 1.00488362 1.58181641 -0.42751198].
                                                                   -896.0299290520137
                      1.49538692 -1.05695459
                                               0.37020686].
                                                                   -1345.846818341517
33
         [ 0.28125263
34
         [-1.4033467
                       0.70593538  0.53780605  -0.57026152].
                                                                   -239.7351017763423
35
         -1672.687784979123
                                  -1.63190891
36
         [-0.28567618 -0.1544846
                                               1.11871168].
                                                                   -528.1675091303345
37
         [ 0.60536907
                       1.13095515 0.8477285
                                              -1.307918
                                                                   -487.9394065197489
38
         [-0.60314838  0.30745523 -1.78135793 -0.53039286].
                                                                   -1734.6847866522687
39
         [-0.88676012 -1.24914685 -1.92922663 -0.26139304].
                                                                   -3235.9225444273907
40
         [ 0.37336764  0.79031767  1.15239768  -0.30730899].
                                                                   -338.1158489177733!
4
```

```
1 ### EXACT GP EI GRADIENTS
2
3 np.random.seed(run_num_8)
4 surrogate_exact_8 = dGaussianProcess(cov_func, optimize=opt)
5
6 exact_8 = dGPGO(surrogate_exact_8, Acquisition_new(util_grad_exact), objfunc, param)
7 exact_8.run(init_evals=n_init, max_iter=iters)
8
```

```
Evaluation
                 Proposed point
                                           Current eval.
                                                                  Best eval.
init
         [1.52956683 1.91914255 1.51222084 0.12638491].
                                                                    -957.0835831104033
init
         [-1.09474477 -2.0013105
                                 -0.28479972 -0.39996883].
                                                                    -2902.49459403014
         [ 0.09287545 -0.0885072
                                    0.22674012
init
                                                0.17770913].
                                                                    -9.936266004845226
init
         1.06862828
                      0.86988626 0.49021787 -0.30272811].
                                                                    -44.27508698465467
init
         [-0.86394869
                       1.94091107 -0.68086151 -1.15179085].
                                                                    -2389.276657793903
1
         [-1.63681569
                       0.94682494
                                   1.80081066
                                                1.81583128].
                                                                    -593.1371362732267
2
         [ 2.0241536
                      -0.6796886
                                  -1.83302627
                                                0.24753545].
                                                                    -3789.198897659005
```

```
3
                                              1.94051986].
         [-1.25453515 0.6570893
                                 -1.93700116
                                                                  -987.1154357131456
4
         [ 1.61665153 -1.94173538 1.76024883
                                              0.7901011 ].
                                                                  -3021.590236385825
5
          1.61690965 0.28689875 0.72519754 -1.78512954].
                                                                  -1118.110716909711
6
         [0.38306717 0.28451289 0.20902794 1.06419821].
                                                                  -109.19990161751558
7
         [-0.70002706 1.15319997 2.04529378 -2.01252415].
                                                                  -3937.9004813257
8
         [-1.77290669 -1.83187185
                                  1.97229377
                                               1.78585986].
                                                                  -3125.8988203363256
9
                      1.89824598 -1.54249073
                                              0.81909326].
                                                                  -2927.810244765299
          1.16552122
         [ 0.10812383 -0.51758335 -2.03090377 -1.90582035].
10
                                                                  -4205.305325106837
         [ 1.35410927 -1.84798102 0.27464388
                                                                  -2485.474846971902
11
                                              1.23773193].
         [-0.64051136  0.65756381 -1.43646501
12
                                               1.19262726].
                                                                  -439.9530863865007
13
         [-0.14971546 0.50775422 0.63444506
                                              0.460895061.
                                                                  -39.77905313856528
14
         [-0.06069706 1.17252573 -1.39191537
                                              0.21232906].
                                                                  -1206.5725167417554
15
         [ 1.94676455  0.73444973  0.5608725
                                              -0.22515299].
                                                                  -963.9095824792869
16
         [-1.77262273 -2.03776117 -0.16499829 -1.11504552].
                                                                  -4695.995287267862
17
         [0.20993332 0.5569241 0.8493887 0.54120142].
                                                                  -59.4705694381346
18
         [ 1.56847741  0.24316373  -0.69881531  -1.01761465].
                                                                  -779.5107598624428
19
          0.35484129 -1.86816284 -0.14451651
                                               1.179078 ].
                                                                  -1862.721763431639:
20
          1.71347332].
                                                                  -634.3946569537112
21
         [0.06425197 1.96587622 0.90111521 1.97688995].
                                                                  -1400.6239448847728
22
         [ 1.96447046 -1.1253884 -1.00393877 -0.3542284 ].
                                                                  -3195.0460205517234
         [-1.90505287e+00 -3.38086882e-01 -1.13311058e-03 -6.45533451e-01].
23
                                                                                  -16
          0.06932344 -0.82987684 1.31480695
24
                                              1.924262211.
                                                                  -117.00853922429148
25
          1.94956957 1.98306302 -1.11386725 -2.04089036].
                                                                  -3960.2663481731424
26
         [-1.94029947 -0.86847316 -1.27079134
                                              1.67313391].
                                                                  -2574.3963586969853
                       0.15426794 0.8482894
27
          0.3863695
                                             -1.47726505].
                                                                  -551.715179290625
28
          1.27554452 -1.33772913 -0.69806032 -0.96771911].
                                                                  -1717.9042203681279
29
         [ 1.22309047  0.50266748 -1.68360001 -0.00168864].
                                                                  -1285.4775424217082
30
                       1.68828179 -0.69504045
                                              1.83299086].
                                                                  -1447.8658969833066
         [-1.2854068
31
         [-1.62809426 -1.9138781
                                   1.87257031 -0.31780317].
                                                                  -3882.7709730274632
32
         [ 0.01115185 -1.04402107 -0.98431878 -1.62553599].
                                                                  -1221.4900994190507
33
         1.85061772].
                                                                  -1344.8892697299098
34
         [-1.59478187 -1.15323929 -1.63623257
                                               1.79534308].
                                                                  -2342.3884903861576
35
         [-0.69785189 -0.2136039 -0.78857984
                                                                  -163.14461373860414
                                              1.22944205].
36
         [-0.12161189 0.78179848 0.84265519
                                              0.85241509].
                                                                  -67.54368335296114
37
         [-1.99255462 -0.04453909
                                  0.05325667 -1.23906119].
                                                                  -1777.308949498485
                                   1.95274426 -1.61966174].
38
         [-1.84338287
                       1.14762359
                                                                  -3507.4826376379906
39
         [ 0.52225599 -0.55066016
                                  0.5964857
                                              -0.79658913].
                                                                  -211.9953091401932
40
         [0.0662418 0.0768072 1.03349554 0.33770486].
                                                                  -161.19477034947843
```

```
1 ### EXACT GP EI GRADIENTS
2
3 np.random.seed(run_num_9)
4 surrogate_exact_9 = dGaussianProcess(cov_func, optimize=opt)
5
6 exact_9 = dGPGO(surrogate_exact_9, Acquisition_new(util_grad_exact), objfunc, param)
7 exact_9.run(init_evals=n_init, max_iter=iters)
8
```

```
Evaluation
                 Proposed point
                                          Current eval.
                                                                  Best eval.
init
         [-2.00550747 0.00767833 -0.01731259 -1.49983425].
                                                                   -1847.6492499405208
init
         [-1.46591299 -1.15278366 -0.33379049 -1.03177761].
                                                                   -1509.7528388540472
         [-1.70369167 -0.63283757 -1.36488408
init
                                               1.55057801].
                                                                   -1586.883400641493
init
         [ 1.84714867 -1.88928665 0.81554388
                                                0.2980242 ].
                                                                   -3591.269305062243
init
         [1.63023716 0.68361819 0.19594356 0.82914273].
                                                                   -460.72675701107613
1
         1.52944985
                       1.66411173 1.05790663 -0.6270896 ].
                                                                   -644.1181418882177
2
           0.36691068
                       1.35867799 -0.37546878 -1.8128426 ].
                                                                   -1027.4883118151865
3
           1.91082423 -1.54166834 -1.15314338 -0.10428515].
                                                                   -4160.216262988813!
         [ 1.8941372 -1.08190004 1.39260512
                                               1.90549007].
                                                                   -2190.903816870602
```

```
5
         [-0.77748103 -1.36916658 1.33978041
                                                 1.79642139].
                                                                     -427.01987106211254
6
         [ 0.43540538
                       1.01380899 -1.90982985 -1.97512192].
                                                                     -4101.0253414933
7
         [-0.53922054   0.42288161   -1.65103556
                                                 1.59059735].
                                                                     -475.2116658321254
8
         [-1.50294447 -1.23674694 0.70406135
                                                1.57347334].
                                                                     -1417.570625638267
9
         [ 0.93681476 -0.46414781  0.86557214 -1.01655719].
                                                                     -536.263637801552
                                                0.34947216].
10
           1.2087894
                      -0.20026847 -1.51486286
                                                                     -904.0741546959051
                      1.14973778 -1.5407734
                                                                     -1602.8351337940483
11
           0.77052113
                                               -0.35713227].
         [-0.57410591 -1.15922655 -1.47822393 -1.45918156].
12
                                                                     -2359.4391147680835
         [ 0.94016196 -1.35872001 0.53165354 -0.50916564].
13
                                                                     -744.2032650905579
         [-1.37454807 -0.82899214
14
                                    1.16351592
                                                0.83737527].
                                                                     -797.3177408401876
15
           1.79796123
                       1.63136227
                                    1.09539079 -0.195229351.
                                                                     -697.3152311893124
         [-1.22972822
                       1.34093876 -0.72463508
16
                                                1.99718201].
                                                                     -864.1278242321243
         [ 0.9448242
17
                      -1.63675234 -0.80095414
                                                0.52073276].
                                                                     -1862.4463434291495
18
         [-0.45272639
                      0.24594195 -1.37697682 -1.70214641].
                                                                     -1509.8399823581478
19
         [-0.82137149 -0.0716439
                                    1.76308515
                                                0.19802656].
                                                                    -1216.8510398242117
20
         [ 0.15589795  0.83672932
                                    0.91785406 -0.67661491].
                                                                     -302.24803204814896
21
         [-0.39164466 -0.83932236 0.5986962
                                               -1.42650476].
                                                                     -423.7481242317493
22
         [-0.30577308
                       1.59623401 -0.09521891 -0.07634192].
                                                                     -928.4523825651771
                                                                     -1554.5173837772443
23
           1.02842179 -1.06051989 -1.41518039 -0.12016884].
24
                        1.54077152 -0.65082177 -1.69000317].
                                                                     -1377.213943907618
         [ 1.089408
25
         [-1.10293183 -1.23710514 -1.70721259 -0.99154435].
                                                                     -3192.762557425501
26
           1.76694719 -0.66753681
                                    1.5391013
                                                 0.678210621.
                                                                     -1845.1897093751204
27
         [ 1.55595475 -0.04915379
                                    1.86520262
                                                1.8685069 ].
                                                                     -1218.6819553360144
28
         [-0.16132052
                       1.87369501
                                    0.42650489
                                                1.87382795].
                                                                     -1581.3357400333223
29
         [-1.97729446 -0.30654351
                                    0.20585548
                                                 0.68478427].
                                                                     -1831.3879932990244
30
         [ 0.53323654 -0.34523495 -0.90883618
                                                1.48485433].
                                                                     -194.4021115076707!
31
         [-1.26346914
                       1.78296691 -1.07923439
                                                 0.06511644].
                                                                     -1947.6919928049658
32
         [-0.24277585]
                       0.08353605 -1.35071151
                                                                    -198.34783344424238
                                                 1.57855697].
33
           0.79555608 -1.11052001 -1.44027944 -1.73988948].
                                                                     -2484.0683153676932
34
           1.08857292
                       1.4669949
                                    0.92814686 -1.956494
                                                                    -952.068037210575
35
           0.62710801 -1.37936141
                                    1.87632722
                                                0.78688539].
                                                                     -1068.1794944818805
36
         [-1.22825293
                       1.74001646
                                    0.68661992
                                                1.13566625].
                                                                     -603.1303835990793
37
                                    0.22192424 -0.32233273].
                                                                     -1356.9898885879918
           0.22168689 -1.83113965
38
           0.24948113
                       1.19516488 -1.28774391 -1.39570007].
                                                                    -1804.6230797860508
39
         [-1.04158977 -0.41917658
                                    1.97191901 -1.03991655].
                                                                     -2984.8853118097572
40
           1.29290756 -0.74402798
                                    1.47624219
                                                 2.00947067].
                                                                     -674.8997870657305
```

```
1 ### EXACT GP EI GRADIENTS
2
3 np.random.seed(run_num_10)
4 surrogate_exact_10 = dGaussianProcess(cov_func, optimize=opt)
5
6 exact_10 = dGPGO(surrogate_exact_10, Acquisition_new(util_grad_exact), objfunc, param)
7 exact_10.run(init_evals=n_init, max_iter=iters)
8
```

```
Evaluation
                 Proposed point
                                            Current eval.
                                                                    Best eval.
         [ 1.11132935 -1.96300002 0.54742317
init
                                                 1.0191007 ].
                                                                     -2176.436426889387
init
         [-0.00611528 -1.12723294 -1.23673451
                                                                     -787.6933551437477
                                                 1.0671338 ].
                                   0.75923382
                                                1.85709915].
init
         [-1.35532201 -1.68616012
                                                                     -1852.2892745062024
                        0.04993951
                                    1.28049546
                                                                     -1975.7725172569656
init
         [-2.0318279]
                                                 0.46090677].
init
           0.90830978 -0.85247562
                                    1.71120281
                                                 0.87890241].
                                                                     -802.2371849082838
1
         [-0.81633257 -1.58112005
                                    1.34627871 -1.85591268].
                                                                     -1994.0093456433356
2
                       1.39217912 -1.61809444
         [ 1.07342562
                                                 0.04354584].
                                                                     -1940.366717616157
3
         [-1.43008917 -1.54327785 -0.09024326 -0.99359866].
                                                                     -2012.6496423727694
4
         [-0.36623728
                        0.66682619 -0.29800586
                                                 0.3236784 1.
                                                                     -92.71025043943006
5
           0.94867509 -2.00602812 -1.86802941
                                                 0.10104421].
                                                                     -5481.717992918238
         [-1.60488548 -0.26364021 -1.58688116 -0.53910029].
                                                                     -2030.3006701793129
```

```
7
         [-1.79898003 -0.90849921 0.74067811
                                             1.84460761].
                                                                 -1898.1839215181774
8
         -1834.248967261895
9
         [0.09221679 1.75138084 0.80469637 1.1725351 ].
                                                                 -844.7044503699319
10
         [ 0.25385502 -0.56137304 -1.02847848 -0.94794006].
                                                                 -629.0912858575092
11
         [-1.08914015 -0.86926364 0.27263031 -0.44518991].
                                                                 -481.2092416961812
12
         [-1.47012591 -0.73192944
                                  0.84283469 -0.53623689].
                                                                 -1011.0210744828247
13
                      1.76383678
                                  1.45961371 -1.58350427].
                                                                 -1730.8910014293738
         [-0.95001787
         [0.90499836 1.10141346 1.28603698 0.54893986].
14
                                                                 -130.69915689422186
         15
                                                                 -5121.14606532571
         [-0.35390856 -0.84421579 -0.44549616
16
                                             1.32577765].
                                                                 -362.535168310281
17
          0.82928393 -0.24396943 1.8187735
                                              0.205781261.
                                                                 -1360.8839400930592
         [-0.64646938 1.72808184 -1.32611196 -1.14608907].
18
                                                                 -2883.670679994826
19
         [ 1.77563892 -0.90998601 -0.54683595
                                              1.45418423].
                                                                 -1979.8175305753468
20
          1.48857256
                      0.88094911 -0.84988613 -0.64237975].
                                                                 -632.4811382199022
         [-0.38511662
                     2.04739557
                                 0.37558093 -1.28295932].
                                                                 -2023.214311202851
21
22
         [-0.70082677 -1.96912104 -0.68708509
                                             1.5540179 1.
                                                                 -2820.396617607148
23
         [ 0.01423615 -0.75885146 -2.00485552 -1.56799862].
                                                                 -3858.671075563624!
24
         [-1.295827]
                      1.12800061 -0.65775574
                                              2.02362631].
                                                                 -664.0812506500738
25
         [-1.74537717 -0.72709154 -2.02712967 -0.4807217 ].
                                                                 -4203.558594573616
         [ 0.27699119 -0.52941187
                                  0.98432743
                                                                 -101.84990573719982
26
                                              1.32497665].
27
         [-1.09101046 - 0.78721212 - 0.18121539 - 1.02716706].
                                                                 -576.5269503988607
28
         [-1.84683074 0.85525047
                                  0.09269607
                                              1.396749321.
                                                                 -895.5226497615581
29
         [-1.10782382 1.08678957
                                  1.83591093
                                              0.79947953].
                                                                 -711.0490742497022
30
         [ 1.8866903 -0.12687083 0.40402276
                                              1.86449239].
                                                                 -1665.8947477686202
31
          0.08049474 -1.5649912
                                  0.34922937 -0.81227962].
                                                                 -783.0673403408462
32
         [ 1.34205403  2.01618533  1.56150399 -1.66922673].
                                                                 -2320.0148127725156
33
         [0.86506562 1.08373241 0.70537686 0.11630819].
                                                                 -47.901348809022956
                                                                 -579.7917141619665
34
         1.45206965
                      1.18898007
                                  1.01897055 -1.15126377].
35
         [-0.52727733 -0.75829671
                                  0.98954076 -1.48721947].
                                                                 -738.3210826217644
36
         [-0.75155978 1.3610957
                                  1.14781785
                                              1.31613751].
                                                                 -116.29154433379108
37
         [2.02714091 0.73764233 1.18728261 1.92488869].
                                                                 -1205.8810803418426
38
         [ 0.15851054 -0.76533319 -0.06448037 -0.23312002].
                                                                 -115.3481941524951
39
                      1.18387659 -0.61381498
         [-1.42267809
                                              1.74883739].
                                                                 -673.5228586952437
40
         [-0.82339488 -1.42360596 1.4478472
                                              0.39763342].
                                                                 -773.1006601987814
```

```
1 ### EXACT GP EI GRADIENTS
2
3 np.random.seed(run_num_11)
4 surrogate_exact_11 = dGaussianProcess(cov_func, optimize=opt)
5
6 exact_11 = dGPGO(surrogate_exact_11, Acquisition_new(util_grad_exact), objfunc, param)
7 exact_11.run(init_evals=n_init, max_iter=iters)
8
```

```
Evaluation
                 Proposed point
                                           Current eval.
                                                                   Best eval.
init
         [-1.30961535 -1.96822941 -0.15065692
                                               0.92132937].
                                                                    -3072.6361628465456
init
         [-0.32684604 -0.05969061 -1.99564978 -0.0517259 ].
                                                                    -2041.908514926983
init
         [ 1.80964005
                       1.43685669 0.94193447 -1.60261705].
                                                                    -1084.6194797620587
init
           1.61343148
                       1.4629038
                                   -1.37180521
                                                0.54204012].
                                                                    -1549.0827052305292
         [-1.96409912 -1.56984415 -0.75215949 -1.40119119].
                                                                    -4385.783412609677
init
1
                      1.99341396 -0.66333061 -1.06547331].
         [ 1.83952342
                                                                    -2574.640397190391
2
         [-0.50547507 -1.49511739 -0.59683872 0.57939828].
                                                                    -1124.6348986589117
3
           1.75448183
                       0.59941317
                                    1.722094
                                               -1.87233294].
                                                                    -3141.9815488207764
4
           1.79525537 -0.77193875
                                   0.07904719 -0.83005758].
                                                                    -1697.18081013564
5
           0.08235597
                       1.20351735 -1.38078313 -1.82955343].
                                                                    -2346.083214352141
6
         [-1.96031946
                       0.99863466 -1.22105629
                                                0.799686691.
                                                                    -1362.5401457795633
7
           1.32122758 -1.57765635 1.52175549 -0.96298413].
                                                                    -2280.010270656378
         [ 1.35923303 -1.24567748 -0.76853718 -1.15385311].
                                                                    -1807.7681589140548
```

```
9
         [ 0.28340268 -1.24036592 -1.99635595 -1.88565185].
                                                                    -4885.425833430284
10
           0.00333095 -1.11448453 0.85634639 -0.32611189].
                                                                    -256.8153273481155
           1.45797774 -1.45580172 -0.7585601
                                               -0.09951625].
11
                                                                    -2165.8426680648963
12
           0.69901164 1.51409958 -0.05184924 -0.14638403].
                                                                    -658.4411064717772
13
           0.861473
                      -0.43280607 0.46623865
                                                0.24889164].
                                                                    -148.2846556243542
14
         [-1.70615562 -0.5940618
                                    0.52920458
                                                0.51918329].
                                                                    -1247.4347520846834
15
                       1.4817917
                                   -1.66154637 -1.03228681].
                                                                    -3114.9645271636496
         [-0.37830153
16
         [-1.78058023 -0.56425788
                                  1.90591314
                                                0.77617674].
                                                                    -2473.700423571399
                       1.91236701 -0.65876847
17
         [-0.45001579
                                                1.49172643].
                                                                    -2272.6428997106177
18
           0.12524724 -1.95276106
                                   1.81441315
                                                1.78963802].
                                                                    -1022.9088869615543
19
           1.09908957 -0.43405758
                                   0.61859251
                                                0.407667641.
                                                                    -290.41502747795874
           0.36103998 0.36582851
                                   0.27979328 -0.22574481].
20
                                                                    -18.248042387909766
21
         [-1.97672755
                       1.41145903
                                   0.92901769 -1.88026378].
                                                                    -1497.6625627387957
22
         [1.75283337 1.24073503 1.75641149 1.78801317].
                                                                    -509.6266415521887
23
         [0.51683445 0.5694324 1.20893699 0.63536788].
                                                                    -156.12259244782246
24
         [ 1.72074709  0.38575114 -0.43076513
                                                0.281164661.
                                                                    -700.6234481962055
25
         [-1.52142811 -1.53003023 0.99039518
                                                0.91216498].
                                                                    -1673.8707621117673
26
         [-1.42079613 -1.38032598 -1.31102534
                                                1.61117467].
                                                                    -2207.8115269992472
27
         [-0.88544558 0.3188642
                                    0.27497829 -0.10211445].
                                                                    -32.34306084978883
         [-0.70003402 -2.0232322
                                   -1.40257619
                                                                    -3748.4851170194092
28
                                                1.08192701].
29
         [-1.77840172 -1.11020889 -1.99052581 -0.45637993].
                                                                    -4838.110916540896
           1.34553372 -0.06390034 -0.99376889 -1.73517952].
30
                                                                    -1197.460412286185
         [-0.28513591 1.70128455 -0.35440022 0.21816641].
                                                                    -1322.7190569437453
31
32
           0.2861566 -1.26320465 0.4953292
                                               -1.70534049].
                                                                    -688.4113843347533
                                   0.13479361 -0.9666187 ].
33
           1.48161712 0.84992301
                                                                    -313.48243984588396
34
           1.59888422 -0.78668892 0.27709365 -0.43610009].
                                                                    -1159.7048682449756
35
         [-0.29021798 - 0.77532859 - 0.74730451 - 1.16249637].
                                                                    -559.7522407393208
36
                      1.85146916 -1.71137361
                                                                    -3320.132125181345
           0.05360964
                                                1.11723377].
37
         [-1.57643092
                       1.74419672 1.13557999
                                                0.27545106].
                                                                    -528.4755615940201
38
         [1.20334288 0.20165943 1.35940674 0.92703019].
                                                                    -414.8765148103328
39
         [-0.1140311 -1.40990782 -0.03519657 -0.91024241].
                                                                    -702.9354119031176
40
         [ 1.91214941 -1.81467173 1.45340086
                                                0.88242509].
                                                                    -3491.832227753870
```

```
1 ### EXACT GP EI GRADIENTS
2
3 np.random.seed(run_num_12)
4 surrogate_exact_12 = dGaussianProcess(cov_func, optimize=opt)
5
6 exact_12 = dGPGO(surrogate_exact_12, Acquisition_new(util_grad_exact), objfunc, param)
7 exact_12.run(init_evals=n_init, max_iter=iters)
8
```

```
Evaluation
                 Proposed point
                                           Current eval.
                                                                   Best eval.
init
                        0.98324356 -0.9694617
                                                 0.13819656].
                                                                     -553.611160809845
         [-1.416549
                       1.71518775 1.64132804 -1.91110583].
init
         [-1.98830095
                                                                     -2800.5873266661606
           1.87166448 -1.48599062 -0.88543907
init
                                                 0.43451672].
                                                                     -3468.8797831248744
init
         [ 1.81954616
                       1.44480478 -2.03874618
                                                0.08694181].
                                                                     -3716.955397581154
init
           0.21314615 -0.05989411
                                    1.0982775
                                               -1.38970418].
                                                                     -796.5750150214192
1
                        1.09558026
                                    1.3312379
                                                                     -998.7882904772749
           1.8444842
                                               -0.38240132].
2
         [1.66129593 0.87073672 0.5816198 0.10572224].
                                                                     -366.0502544279664
3
         [1.44989773 0.86205149 1.70214109 1.20890877].
                                                                     -531.5430041745518
4
           0.74784519 -0.87913124 0.68208437
                                                 1.38327915].
                                                                     -295.7002912929996
5
           0.62898362 -0.72891718 -1.22436402 -0.53895578].
                                                                     -858.129586262932
6
                       0.68633941 -0.37528478 -0.0720933 ].
                                                                     -585.8498109295922
         [-1.70973589
7
         [-1.38708707]
                       1.21965328
                                   0.90740933
                                                 0.51329934].
                                                                     -98.63944356233895
8
           1.86689185 -1.93569271
                                    2.04039957
                                                 1.10854027].
                                                                     -4173.482040007393
9
         [-0.11129628
                       1.41579596 -0.63186892
                                                 0.16351787].
                                                                     -901.6165373650053
         [ 2.02281781 -1.96033515 -1.49693588 -0.58386694].
                                                                     -7328.152102380102
```

```
11
         [-1.64158863
                       0.88855344 -1.86185311 -1.04514634].
                                                                     -3079.912385424591
12
         [-1.57870863
                        1.8513935
                                   -0.303098
                                                 1.40030235].
                                                                     -1613.2053794572441
13
           1.6802252
                       -1.8192295
                                   -0.01445017
                                                 1.38147967].
                                                                     -3460.3340637458464
14
         [-1.16680679
                        1.27539561
                                   1.70702369
                                                1.91886518].
                                                                     -105.67273264192974
15
         [-1.18355784 -1.03286419 -1.59607503 -0.21520693].
                                                                     -2080.241860998364
                        0.9654606
           0.96578729
                                   -0.43353335
                                                 1.07326823].
                                                                     -267.042357821699
16
         [-1.59936356
                        0.05202077 -1.68099862 -1.36931641].
                                                                     -2686.1678997041663
17
18
         [-1.93196624
                       1.1203768
                                   -0.36986941
                                                0.15225688].
                                                                     -956.9261517599865
                                                                     -309.2552412962974
19
         [ 0.7072878
                        0.6559028
                                   -1.10801994
                                                0.4179542 ].
20
         [-1.78114909 -0.69041045 -1.87445089 -0.16824127].
                                                                     -3419.402257969233
21
           2.03701021
                        0.84977593
                                    1.88576638 -0.40654752].
                                                                     -2796.318245152882
22
         [-1.93415834
                       1.60900614 -1.1198731
                                                -0.56720358].
                                                                     -2175.221159522027
23
         [-1.2991774
                       -0.66905575
                                    1.72276999 -0.06727684].
                                                                     -1647.9491977105322
24
           0.86179156
                        1.80144989 -1.16981236
                                                 1.63366197].
                                                                     -2073.7536293335856
25
           0.47150925 -0.19129195
                                    1.71696357 -0.56016155].
                                                                     -1532.3791517552193
26
         [-0.92510619]
                        0.21502146
                                    1.34712889
                                                1.00119717].
                                                                     -280.9257146505063
27
           0.73593244 -0.93145875
                                    1.79902655 -1.02205019].
                                                                     -2121.7026042201296
28
           0.58013731 -1.25518042
                                    1.01801776
                                                 0.76034697].
                                                                     -297.3204888518643!
                                    0.1241312
29
           0.49248519 -0.36364078
                                               -0.46128554].
                                                                     -62.36024219297695!
                                                                     -963.0734459791341
30
         [-1.69090131
                        1.78595323
                                    1.92890053
                                                1.11252811].
31
         [-1.83621103
                        1.87903779 -0.68162285 -1.26546617].
                                                                     -2308.192588094473
32
           1.92156215
                       1.40944334
                                    1.51577691 -1.709961761.
                                                                     -2150.6722660038395
                      -0.08568237 -1.11132262 -1.62208438].
33
           0.0919898
                                                                     -948.8029306342575
34
         [-0.1542413
                       -0.44101939
                                    0.49396321
                                                 1.62342477].
                                                                     -224.5189959433865
35
         [-1.89442692
                        1.28025951
                                    1.41878095
                                                 0.88925994].
                                                                     -672.7102189249384
36
         [-1.58683532
                       0.93332869
                                    0.12508988 -0.19690846].
                                                                     -318.7661115293826
37
         [-1.40446844 -0.06409175 -1.4736892
                                                 1.11702579].
                                                                     -757.4511493361595
         [-0.22075864 0.21300348 -0.04241919
                                                                     -259.1978979660242
38
                                                 1.59092653].
39
         [0.78784188 0.56687636 1.60738668 0.53712367].
                                                                     -585.1246700385428
40
                       -1.12747314 -1.62090109 -1.33948435].
                                                                     -2806.611413418693
         [-0.908832
```

```
1 ### EXACT GP EI GRADIENTS
2
3 np.random.seed(run_num_13)
4 surrogate_exact_13 = dGaussianProcess(cov_func, optimize=opt)
5
6 exact_13 = dGPGO(surrogate_exact_13, Acquisition_new(util_grad_exact), objfunc, param)
7 exact_13.run(init_evals=n_init, max_iter=iters)
8
```

```
Evaluation
                 Proposed point
                                           Current eval.
                                                                   Best eval.
init
         [ 1.13746907 -1.07503116
                                    1.32824487
                                                1.90770872].
                                                                    -570.621446040192
init
           1.93577416 -0.19067188 0.44663793
                                                1.1285566 ].
                                                                    -1656.450565242978
init
           0.58004826 0.90938667 -1.9044904
                                                -0.82555097].
                                                                    -2770.1364153691793
init
         [-1.80833283
                       1.46252162 -0.5207899
                                                0.73665721].
                                                                     -1066.23070619416
         [-0.99827733 -0.62430734 -2.00944529 -0.58026483].
                                                                     -2986.7442974027663
init
1
         [ 1.8660317
                      -2.04795071 -1.03637524
                                                0.86930505].
                                                                     -5812.2868484529
2
         [-1.99093343 -1.57541334 -1.27558555
                                                1.5579621 ].
                                                                     -4501.431269415862
3
                       0.04375793 -1.84819292 -1.21433545].
                                                                     -3329.025935220234
         [-1.7084272]
4
         [ 1.20977231  0.68296146 -1.42178533 -0.28413332].
                                                                     -955.0616727742835
5
         [0.73870568 0.44692721 0.01696619 0.92994009].
                                                                     -92.08194989676083
6
         [-1.66395119 -0.80730287 -1.84496721
                                                0.13029281].
                                                                     -2992.267160837443
7
         [-1.81799706 -1.22894338 -1.59166549
                                                1.27851928].
                                                                     -3195.085476637445
8
         [ 0.13435789 -1.36913607 1.48107155 -1.66219771].
                                                                    -1701.200626347697
9
         [ 1.49280048 -1.10459031
                                   1.9369463
                                                0.58144526].
                                                                    -2172.9421677440087
10
         [-1.76484225]
                       1.52616774 -1.96596454 -0.41212094].
                                                                     -3943.275554929836
11
         [-1.02843701 -0.74279767 -1.33933376 -0.48197864].
                                                                    -1212.340125948955
12
         [ 1.90955169 -1.50253651 1.13409201
                                                1.80691212].
                                                                    -2811.5983744767746
```

```
13
         [-0.15542593 0.77543219 -0.32110269 -0.50675733].
                                                                     -181.84736821629252
14
           0.50991521
                        0.22600793 -1.46246783
                                                 1.59299728].
                                                                     -265.89259682563846
15
           0.98814807 -1.58991753 0.55997626
                                                 1.08080517].
                                                                     -1111.631134123834
         [-0.23675551 0.13543324 -0.00873668
                                                 0.81396943].
                                                                     -70.24023282169031
16
17
         [0.15455253 1.64946528 1.57544879 0.02949059].
                                                                     -998.3859062868203
           1.24746474
                        1.90552036 0.8662623
                                                -0.00290784].
                                                                     -834.2343974023479
18
19
         [-0.13364844
                        0.3340454
                                   -0.34606933
                                                 1.03498846].
                                                                     -118.24621245130742
20
         [-1.29091789 -0.9704555
                                    1.94901953
                                                 1.88212017].
                                                                     -1174.1401451615682
                        1.97398803 -0.19739056 -1.64338008].
21
         [ 1.53455042
                                                                     -1976.3005900039768
                        1.50796225 -0.51658438
22
         [-0.54607875
                                                 1.23602916].
                                                                     -1023.9376977250108
23
         [-1.69647431 -0.13849044 -0.85437537 -1.77819124].
                                                                     -1627.3331486126021
         [-0.36314152
                        1.48132021 -0.81174684
24
                                                 1.60396981].
                                                                     -1180.4203342459014
25
         [ 1.21516934
                       0.30106952 -1.50517253
                                                 1.22133599].
                                                                     -508.70625179966345
26
         [-1.74787857
                        0.92605445
                                    0.44786136
                                                 1.67306986].
                                                                     -694.7452976294811
27
         [-0.7642521
                      -0.55159498
                                    0.98612647
                                                 0.44030284].
                                                                     -209.3084449600003
28
         [-0.57801656 -0.89346951 -0.48374123
                                                 0.33465638].
                                                                     -324.3432054652136
29
         [-1.55232093 -0.83414065 -0.91616803
                                                 1.68889364].
                                                                     -1397.811662780371
30
           1.25552684
                        0.98228179 -0.01194804
                                                 0.60380272].
                                                                     -168.2404221329065
31
         [ 1.86866832
                       1.80735286
                                    0.88218609 -1.31606209].
                                                                     -1292.3195428932797
32
         [-0.60816258 -1.48369319
                                    1.19762397 -0.3389362 ].
                                                                     -767.5440279170598
33
           0.9372928
                       -0.43945546
                                    1.53552677
                                                 0.75343429].
                                                                     -613.6859570054377
34
         [-0.66508622
                       0.66638952
                                    0.87959599 -0.224937561.
                                                                     -126.61151527058537
         [-0.07484835
                       0.02857783 -1.34884795
                                                 0.8967764 ].
                                                                     -274.95003109985123
35
36
         [0.96418378 0.51201859 1.579638
                                             1.98711879].
                                                                     -217.4114104120697
37
         [-0.03576572
                        1.04072633
                                   0.05068127 -0.63198527].
                                                                     -256.8777483425788
38
         [-1.69813972
                       1.3940542
                                    0.19151705 -1.17115017].
                                                                     -682.7768916967663
39
         [-0.2194799]
                        1.51724609 -1.91465659
                                                 1.68166585].
                                                                     -2397.8397335966574
                                                                     -905.0561957506699
40
         [-0.2367588
                        1.06158386 -0.87110555 -1.24039047].
```

```
1 ### EXACT GP EI GRADIENTS
2
3 np.random.seed(run_num_14)
4 surrogate_exact_14 = dGaussianProcess(cov_func, optimize=opt)
5
6 exact_14 = dGPGO(surrogate_exact_14, Acquisition_new(util_grad_exact), objfunc, param)
7 exact_14.run(init_evals=n_init, max_iter=iters)
8
```

```
Evaluation
                 Proposed point
                                           Current eval.
                                                                  Best eval.
                                   1.5172718
                                                                   -1996.4555487728376
init
         [ 0.05711194
                       1.11888405
                                              -2.0150397
init
         [-0.77932165]
                       1.87434492
                                   0.05372605 -0.744307
                                                                   -1417.9597465038332
init
           0.16056294 -1.14173976
                                   1.25534764 -0.64612505].
                                                                   -635.6383005184798
           0.15928873 -2.02394097
                                   0.70923255 -1.18774062].
init
                                                                   -1863.0160368222728
init
           1.7717559
                      -0.51509351
                                   1.0339079
                                                1.07781735].
                                                                   -1397.2995170993763
1
           0.99332651 -0.37717683
                                   2.01270476 -0.19604562].
                                                                   -2342.516103819445
2
         [-0.97786591 -1.99526909
                                   0.19679333 -1.95785246].
                                                                   -2715.3884769596207
3
         [-2.03313668 -0.93462245 -0.00775355 -1.32427274].
                                                                   -2835.7413982504854
4
         [0.0398087
                     0.42157067 0.33954241 1.06185617].
                                                                   -111.54909229033513
5
         [-0.26998621 -0.47520129 -0.51714112 -1.39745282].
                                                                   -368.51517593058196
6
          0.04971751 -0.84388258
                                  0.45380972
                                                                   -284.52532843827254
                                               1.62586983].
7
           -495.6539924024287
                                               1.56748659].
8
         [-1.76432072]
                       1.75373419
                                   1.76096656 -0.17849612].
                                                                   -1441.8355353693546
9
         [-0.25013786]
                       0.58131844
                                   0.74150156
                                                1.21362059].
                                                                   -89.06448998253701
10
         [ 0.52069338 -0.46443599
                                   1.37184847 -0.8653678 ].
                                                                   -945.0703467819066
11
           1.03203137 -0.02147058 -1.41823377
                                                0.92455831].
                                                                   -444.3425429441072
12
           1.39730886 -0.01876222 -0.41538171
                                                1.80457934].
                                                                   -675.413538554842
13
         [-1.83683859 -2.00726755 -1.26585638 -0.1341597 ].
                                                                   -6023.245600609232
         [-1.39208894
                      1.36606172 -0.85438521 -0.2751843 ].
                                                                   -883.147772405993
```

```
15
         [-1.2605655
                       0.59505477 1.88176971 -1.84227427].
                                                                    -3236.2557170776927
16
         [-0.70663261 -0.788236
                                    1.25868644 -0.82944904].
                                                                    -795.1983064011594
17
           1.2943011
                      -1.65891147
                                    1.28764649
                                                0.76212883].
                                                                    -1413.5732294508307
18
         [-0.85939116]
                      1.79062222
                                   0.63035876 -0.70415994].
                                                                    -899.798599656544
19
         [ 1.54956234
                       0.2443581
                                    1.59720447 -0.44513779].
                                                                    -1600.51201005209
20
         [-1.59175313
                       0.59075894 -1.18001661
                                                0.91206296].
                                                                    -645.9947182472462
21
         [-0.02537064
                                   0.18305542 -1.16579367].
                                                                    -1223.984452437756!
                       1.72531768
22
         [-1.26484967
                       1.1756304
                                    0.57576666 -0.62946688].
                                                                    -180.70171640777548
23
         [ 1.07007622
                       1.97358001
                                   0.14598518 -1.34343711].
                                                                    -1662.1048140846456
24
           0.64750203 -1.51918159
                                    1.91248765 -1.53072617].
                                                                    -3090.576598668522
25
         [-1.10900046 -1.28899246
                                   1.80112137 -1.10237781].
                                                                    -2535.8846171355544
         [-0.44884526 - 0.20569578 - 1.34067759 - 1.77079305].
26
                                                                    -1490.086931665832
27
         [-1.64083647 -0.08188128 0.53807534
                                                1.50857328].
                                                                    -954.8339772285511
28
         [-0.32302589 0.4282859
                                   -0.1091979
                                                1.49674112].
                                                                    -242.83247253126913
29
         [0.27633111 1.37392905 0.39697562 1.34790169].
                                                                    -533.300532385822
30
         [ 1.26069459 -1.83565215 -0.15960944
                                                0.488598791.
                                                                    -2449.5116865562186
31
           0.41185065 0.14704051 -0.06999008 -1.30219395].
                                                                    -173.9576811616067
32
           0.75138373 -1.42916731 1.02061145 -1.76094883].
                                                                    -1293.349220758911!
33
           0.67610656 -1.34656751 -1.92469412
                                                0.22596233].
                                                                    -2946.698074040383
34
                      -0.78739493 -1.93213096 -0.323968
                                                                    -3815.7850490240958
         [ 1.7588149
35
         [-1.68214821 0.54217423 -0.6400704
                                                0.01722999].
                                                                    -635.9778142669621
36
           0.13865086 -2.01545562 -1.0926892
                                               -1.013679461.
                                                                    -3572.723172473937
           1.82238011 -1.1194483 -1.31534249 -1.06360491].
                                                                    -3422.564769724855
37
38
           1.94381142 1.54603653 -1.04249393
                                                0.23850074].
                                                                    -1754.0253780514327
39
           0.12795405 -1.82551184 -0.52381359
                                                1.82879896].
                                                                    -2079.0517374677465
40
         [ 0.86929247 -1.73849869 -0.68259678
                                                0.13072152].
                                                                    -2016.3556549384557
```

```
1 ### EXACT GP EI GRADIENTS
2
3 np.random.seed(run_num_15)
4 surrogate_exact_15 = dGaussianProcess(cov_func, optimize=opt)
5
6 exact_15 = dGPGO(surrogate_exact_15, Acquisition_new(util_grad_exact), objfunc, param)
7 exact_15.run(init_evals=n_init, max_iter=iters)
```

```
Evaluation
                 Proposed point
                                          Current eval.
                                                                 Best eval.
init
         [ 1.42875729 -1.31524229 -1.82532827 -0.56713852].
                                                                  -3924.3244166004847
                       0.12288092 -0.79495612 -0.80087302].
init
         [-0.9199578
                                                                  -330.9329217994366
init
         [-1.59030773 -1.02441364
                                  1.71061206 -0.96605449].
                                                                  -2832.720279494954
init
         [ 0.89200102
                       1.49796878
                                  1.25779756 -1.18558481].
                                                                  -912.8737542795088
init
         [-1.36297254 -1.85669062 -1.88652621 -1.2278546 ].
                                                                  -6538.09169222112
1
         [ 0.58460113 -0.32775446 -0.39631899 -0.44883834].
                                                                  -110.79789128159267
2
         -61.63957624806721!
3
         [1.17524651 0.81266714 0.06578144 1.87055775].
                                                                  -416.9041118681516
                                                                  -1945.0028201943212
4
         [-1.37601528 2.01548466 0.00408975
                                               1.70012238].
5
         [ 1.38289251
                      2.04145711 -1.69811698 -0.4971158 ].
                                                                  -4593.703203221396
6
          1.58556031 -1.16178674
                                   1.82715306
                                               0.55767211].
                                                                  -2152.927698875604
7
         [-1.9457908
                     -1.62753648
                                  0.90927685
                                               2.04416103].
                                                                  -3397.158605260719
8
         [-1.47661357 0.9182499
                                  -1.01377724 -1.54885025].
                                                                  -1178.208793385813
9
         [-0.02651074 -0.92941848
                                  1.00534467
                                              0.957772831.
                                                                  -93.57224973285331
10
         [-0.18573446
                       0.83886291
                                   1.4122079
                                              -1.25290689].
                                                                  -1170.9573549500035
11
         [ 0.57370594 -1.10128151 -1.02032557
                                               0.01089391].
                                                                  -818.1084051893896
12
                       0.02289176 -1.63283341
         [-1.0655448
                                               0.71785545].
                                                                  -782.2861555773686
13
         [-0.4994855]
                       1.64957649
                                  0.57379538 -1.81250558].
                                                                  -1118.6781915959964
14
         [-1.08497521
                       0.84636257
                                   0.49280125 -1.81616963].
                                                                  -444.52535472196007
15
          1.03136549 -0.3112375
                                   0.45622147 -1.36849795].
                                                                  -452.5569342228273!
         [-1.25906869 -0.08959343
                                  0.7303103
                                              -0.45009119].
                                                                  -435.7603115490442
```

```
17
          0.26669857 -1.68266996 1.01018804
                                                2.03422787].
                                                                    -749.7571901059255
18
          [1.51360165 1.98828678 1.70815557 1.18950089].
                                                                    -813.6654166220812
19
          [ 0.23371844  0.85794796 -1.13695059 -1.46894332].
                                                                    -1183.1726294017064
20
          [-2.01176549 0.83883047 -0.0157342 -0.16909236].
                                                                    -1094.109201736202
21
          [ 0.48578938  2.0011167  -0.76894845  -0.91579566].
                                                                    -2821.641308934085
22
          [-2.04286803
                       1.33193982 -1.84903679
                                                1.30743019].
                                                                    -2583.356388762627
23
          [-1.44755121 -2.02169385
                                   1.96860149 -0.83865247].
                                                                    -4382.196027042846
                       1.62661238 -1.56239402 1.62635524].
24
          [-1.70112205
                                                                    -2012.1587440723067
25
          [-0.24109876 1.33577466 1.78268983 -1.85506578].
                                                                    -2698.6619273246047
           0.38949032 -1.37982152 -0.45361363 -0.78642501].
26
                                                                    -896.9406318394908
27
           1.14701612 -0.79378236 -1.07987956 -1.48697064].
                                                                    -1448.833233472687
28
          [-1.43303668 -1.93865232 -1.95336332 -1.12318036].
                                                                    -7318.656924336549
29
          [ 1.03832863 -1.16145392 1.70120691
                                                0.87975459].
                                                                    -924.9044843772957
30
          [1.71257789 2.00766758 2.04074396 0.40774124].
                                                                    -1895.645937778416
31
          [ 1.28582099 -1.49887299 0.06383655
                                                1.77795686].
                                                                    -1791.964482589178
32
          0.81334184 -0.16141846 -1.32866259
                                                0.48226796].
                                                                    -422.68469495337126
33
          [-0.74818958 0.94692366 -0.04901244 -1.17932449].
                                                                    -248.2251143656931
34
          [-1.92520942 -1.82842073 -0.73296963
                                                0.94338598].
                                                                    -4760.966359727565
35
          [1.06801719 0.30765051 1.6121512 0.52897123].
                                                                    -729.0455971122695
36
          [-1.41747201 1.65781696 -1.49014706 -0.13005055].
                                                                    -2373.8451177593115
37
                        1.37206471 -2.0436346
          [-0.4844244
                                                0.79540728].
                                                                    -2825.6144824265625
38
          [-2.04536301 1.59960423 -1.37306242
                                                1.3677816 ].
                                                                    -2255.6066494918728
39
          [ 1.75116601 -1.15766379 -0.02397232 -1.2176205 ].
                                                                    -2125.1864546978345
40
          [-1.25806394 -1.84417246 -1.25807903 -0.61869265].
                                                                    -3847.965947792774
4
```

```
1 ### EXACT GP EI GRADIENTS
2
3 np.random.seed(run_num_16)
4 surrogate_exact_16 = dGaussianProcess(cov_func, optimize=opt)
5
6 exact_16 = dGPGO(surrogate_exact_16, Acquisition_new(util_grad_exact), objfunc, param)
7 exact_16.run(init_evals=n_init, max_iter=iters)
8
```

```
Evaluation
                 Proposed point
                                          Current eval.
                                                                  Best eval.
init
         [-1.13339974 0.09487705 0.20767317 -1.86121441].
                                                                   -514.1403917485846
init
         [-0.57045469 -1.13426046 0.77302236 -1.37735608].
                                                                   -636.540695155299
init
         [-1.75994935]
                       1.80638048
                                   0.26083893 -1.72854338].
                                                                   -1399.5661404272828
         [ 0.91193553 -1.3989799 -1.02284777 -0.8458762 ].
init
                                                                   -1753.4526459251950
init
                                  -1.16710546 -0.21779963].
         [ 0.80531749 -0.1463743
                                                                   -460.1166598787994!
1
         [-0.13108778 0.65969904
                                  0.77810332 -0.96940243].
                                                                   -302.4994095893768
2
           1.22573358 -1.62776275 -0.59572774
                                               1.86643276].
                                                                   -2271.007002774895
3
           0.09704324 -1.45330609 -1.31939395 0.64367914].
                                                                   -1524.0512445841719
4
           1.13175832 0.95270927 0.6939976 -1.85842868].
                                                                   -563.0362907121892
5
           0.87766015 -0.56988658 1.86040774 0.55181588].
                                                                   -1265.0478080730422
6
         [0.38324944 1.15320791 0.7361225 0.87331715].
                                                                   -147.9841514380348
7
         [1.52761822 1.05335325 1.86698362 1.69312043].
                                                                   -543.6189085901927
8
         0.25466755
                       1.95777246 -1.96183909
                                                1.6941066 ].
                                                                   -4190.703432069714
9
         [-0.63259733]
                       1.23580709 1.66993686
                                               0.07586134].
                                                                   -810.9774526850983
10
         [-0.25142728 0.6963049 -0.15196989 -1.98024137].
                                                                   -484.95388046833204
         [ 1.82271043 -1.73186874 0.86059175
                                               0.559603441.
                                                                   -3023.308191163494!
11
12
         [-0.62557716
                       1.77178749 -1.72549473 -0.03016737].
                                                                   -3472.288969003308
13
         [ 1.35578327 -0.8312143 -0.91182455 -0.38361047].
                                                                   -1124.1936478797918
         [0.53777153 0.09512887 0.09037536 0.48936688].
                                                                   -29.44280902753841
14
15
         [-1.62152026 -1.77709901 1.61597695
                                               2.032436691.
                                                                   -2227.950104164753
16
         [-1.87707151 -1.6480133 -1.77751135 -1.61557787].
                                                                   -6996.651917829854
17
         [1.97250323 1.79523848 0.12675634 0.0337621 ].
                                                                   -1400.095758841347
18
         [-0.84563711 -1.32015721 -1.96163582
                                               1.97171453].
                                                                   -2156.13484709627
```

4

```
19
         [ 0.89972157 -1.87913879 -1.5988437
                                                1.66792078].
                                                                    -3448.5491609045444
20
         [-1.7958477]
                       1.44665275 0.41079517
                                                1.92766293].
                                                                    -916.9318079383902
21
           1.41428035 -1.8667259
                                                                    -4036.7975536056283
                                   -1.45290667
                                                1.16687183].
22
           1.53805572
                       0.16820999 -1.68697563 -1.72537074].
                                                                    -2874.914984625272
23
         [-1.60757224
                       0.37443735 -1.22386642
                                                1.96901563].
                                                                    -708.7489798501717
24
           1.94242514
                       1.39930119
                                   1.09479611 -0.08147982].
                                                                    -802.8831214032763
25
         [-0.37698257 -1.1846033
                                   -0.67927416
                                                1.96327194].
                                                                    -844.7700735312142
26
         [ 0.76097357 -0.7554043
                                   -1.68858591
                                                1.96761798].
                                                                    -776.9536659413799
27
                       0.76600669 -0.77466918 -1.968011
           0.56605901
                                                                    -868.1233995856558
28
         [-0.33820064
                       1.50267429 1.45033202
                                                1.42829275].
                                                                    -305.80554799968826
29
           1.12705548 -1.87015347 -0.18151034 -0.32981433].
                                                                    -2362.517922860184
30
           0.75743389
                       1.00544326
                                   0.75450434 -1.43491909].
                                                                    -427.0136528381095
31
         [-1.49994631 0.11419392
                                   1.97504145
                                                0.95615802].
                                                                    -1716.1129143999592
32
         [-1.58705473 -0.11125429 -0.30949866 -1.51669008].
                                                                    -971.7003995977981
33
           1.16945483 -1.66995561 1.14717628 -1.43539411].
                                                                    -1956.3697290903986
34
           1.66267478 -1.91018957 -0.49616571
                                               0.87781687].
                                                                    -3954.3979714222473
35
           1.12235304 -0.08782422 -0.83101542 -1.32571468].
                                                                    -663.0203749314862
36
           0.61165069
                       1.29386844 -2.0006338
                                               -1.22259168].
                                                                    -4174.394427951614!
37
         [-0.88630481 -1.6866546 -1.46697368 -1.76056431].
                                                                    -4018.002599228690!
         [-1.95200933 -2.03845899 1.73236918 -2.03702153].
38
                                                                    -6564.664954368759
39
         [-0.79495387]
                       0.97135031 -1.58578895 -1.44407326].
                                                                    -2228.378864665281
40
         [-0.44208983]
                       1.99194991 0.15971221
                                                0.97938317].
                                                                    -1867.703353468525
```

```
1 ### EXACT GP EI GRADIENTS
2
3 np.random.seed(run_num_17)
4 surrogate_exact_17 = dGaussianProcess(cov_func, optimize=opt)
5
6 exact_17 = dGPGO(surrogate_exact_17, Acquisition_new(util_grad_exact), objfunc, param)
7 exact_17.run(init_evals=n_init, max_iter=iters)
8
```

```
Evaluation
                 Proposed point
                                           Current eval.
                                                                   Best eval.
         [-0.84105215  0.12528335  -1.26353086  -1.76988013].
init
                                                                    -1340.0610302924795
init
         [1.17549244 0.64034211 0.56328559 0.30966945].
                                                                     -57.67854505088549
init
         [-1.8879983 -0.58239548 1.82551833 -1.80205699].
                                                                     -4588.535377497626
init
           1.49111646 1.545382
                                   -1.83831075
                                                0.624306651.
                                                                     -2599.959730636226
init
           0.21197361
                       0.39941429 -0.06746675 -0.88888049].
                                                                     -99.66183844529772
         [ 0.42203482 -2.00904097
                                   1.09846332
                                                 1.90827245].
1
                                                                     -1400.0503426825965
2
         [0.09299641 1.76547411 2.00100021 1.86818336].
                                                                     -891.7493177411302
3
           1.03524528
                       2.01791497
                                    0.66692259 -1.76993414].
                                                                     -1740.6149776893044
4
           1.79060021 -1.63794888
                                    0.78010485 -1.24596241].
                                                                     -3060.238268647078
5
         [-1.98982343 -1.90350839 -1.70179203
                                                1.51123826].
                                                                     -6489.526096787567
6
         [-1.31799397
                       2.01514826 -0.77630285
                                                1.85071305].
                                                                     -2512.8348079919515
7
         [-1.70500609
                       0.22690576 -1.80045119
                                                 1.65595213].
                                                                     -1328.4751987733005
           1.86062044 -1.55616452
8
                                                                     -3197.3762049513903
                                   0.75643756 -1.41436721].
9
         [-0.23805299 -1.5834918
                                    0.80621095
                                                 0.72568851].
                                                                     -567.2509761868196
10
           1.61865995 -1.8818946
                                   -2.00305014
                                                 1.10989172].
                                                                     -5961.044846880138
11
         [-0.72789992 -0.26871933
                                    1.28346906
                                                 0.91848902].
                                                                     -268.275398760704
12
         [ 0.52172695 -1.90390253
                                    1.43290056 -1.37482193].
                                                                     -2137.9887660512804
13
           0.69165667 0.09427389 -1.05529447
                                                                     -133.60784178022286
                                                 1.04542536].
14
         [-1.98093256 -1.81212483
                                    0.95420026
                                                0.17949747].
                                                                     -3903.3545575055746
15
           0.88962951
                        1.27603683
                                    1.37351323 -1.12492908].
                                                                     -937.0950833794803
         [-0.67968804 -1.44603439
                                    1.68593438
16
                                                 1.83708789].
                                                                     -490.7944754048813
17
         [-0.82342883 -1.84286467
                                    0.32791642
                                                 1.7467644 ].
                                                                     -1857.4670492161945
18
           1.81352625
                       0.97294554
                                    0.21198954 -0.34099275].
                                                                     -606.5005846326469
19
         [1.26977767 1.58392248 1.26092496 0.00980864].
                                                                     -405.9632770929851
20
         [-1.00359125 -1.85000404
                                   1.26277177
                                                0.24557093].
                                                                     -1476.9998000770709
```

•

```
21
         0.86881634].
                                                                   -118.18502924934323
22
         [-1.26489958 -1.73404299
                                   1.8423527
                                              -0.61024919].
                                                                   -2864.10960753177
23
                       -1.24370359 -0.30735697 -1.17185651].
                                                                   -723.3642477988516
           0.461464
24
           0.91600734 -0.49890457
                                   0.24883577 -0.18646842].
                                                                   -188.00510674115222
25
         [-0.75299319
                       0.66639061
                                  0.10740529
                                               1.37821958].
                                                                   -203.08605659574272
26
                       1.30454928 -1.64569473
                                               1.21466059].
                                                                   -1520.9682958377457
         [-0.06645649
27
         [ 1.30152593  0.68015254 -1.79257626 -0.43179959].
                                                                   -1948.0563208246786
         [0.67016107 0.07701834 0.81742873 0.9239938 ].
28
                                                                   -87.23597287235853
29
         [-0.03552169 -0.95576019 -0.82394689 -0.23735467].
                                                                   -485.62770529342293
         [-0.78940489 0.54425439 0.44427943 -1.97967394].
30
                                                                   -480.4916998108777
31
         [-1.55320406 -1.06992981 0.03407838 -1.14225885].
                                                                   -1478.5284734919987
32
         [-0.72040874 -1.13875366 0.00904431 -0.9410444 ].
                                                                   -537.7200524503019
33
         [-0.99120872 0.74885557 0.52254111 -1.08124627].
                                                                   -193.2725609651687
34
         [0.7461642 0.1028982 0.17156515 0.68392102].
                                                                   -67.58128471883002
35
                     0.21289626 0.38236609 0.6687167 ].
                                                                   -43.1382159248404
         [0.2098577
36
                       1.25092555 -0.04996177
                                               0.01012974].
                                                                   -357.2324422499452
37
           0.81130009 -1.51128184 -0.00363526
                                               1.44855886].
                                                                   -1211.1614914606882
38
         [-0.43708156 -0.27418816 -0.9320137
                                              -0.23362957].
                                                                   -252.01085519104976
39
         [-0.88266509 -0.44579317 -1.7473574
                                               0.2161308 ].
                                                                   -1346.8737024339018
40
         [ 1.78607808
                       0.95245947 -1.33129278
                                               0.76786254].
                                                                   -1108.720591515662
4
                                                                                    •
```

```
1 ### EXACT GP EI GRADIENTS
2
3 np.random.seed(run_num_18)
4 surrogate_exact_18 = dGaussianProcess(cov_func, optimize=opt)
5
6 exact_18 = dGPGO(surrogate_exact_18, Acquisition_new(util_grad_exact), objfunc, param)
7 exact_18.run(init_evals=n_init, max_iter=iters)
8
```

```
Proposed point
                                           Current eval.
                                                                   Best eval.
Evaluation
init
         [ 0.61593289  0.02233702  1.55075162 -1.30318244].
                                                                    -1629.4185602457633
init
         [1.44274665 1.02455823 0.68035243 1.99841976].
                                                                    -361.44679331797425
init
         [-0.99545734 -1.93205893 0.5559055
                                                1.42259154].
                                                                    -2000.4660253561508
init
         [ 0.96737126 -1.96277407 -1.59087358 -0.82852355].
                                                                    -4947.239458116178
init
         [ 0.7658299
                        1.48122033 -1.23439366
                                                0.64384627].
                                                                    -1338.1489953342577
1
         [-1.26288935
                       0.87759561 0.57290898
                                                0.13600289].
                                                                    -64.35538477553783
2
         [-1.74446096
                        1.39314865 -1.6298479
                                               -1.01881068].
                                                                    -2912.5693898788636
3
         [-2.03346864
                       1.78025771
                                    1.7144816
                                                1.78378342].
                                                                    -910.0104665352812
4
         [ 1.64588817 -1.61712998
                                    1.57846447
                                                0.25331343].
                                                                    -2487.5297271973463
5
           1.95846595 -1.61619238
                                   0.37536288
                                                1.15289237].
                                                                    -3583.047935120242
6
         [-1.08847274 -0.9436667
                                   -0.60971513 -1.62513327].
                                                                    -1087.57814364623
7
         [ 0.93115609
                       1.78128986
                                   0.00350732 -1.34043722].
                                                                    -1269.4360904655873
8
           0.47395153 -0.51406193
                                    1.77573504
                                                1.99418243].
                                                                    -420.5335147655135
9
           1.72008428 -0.94304356 -1.59657826
                                                2.04264977].
                                                                    -2177.0084861325863
10
                                    1.44182572 -0.94212871].
                                                                    -2153.557278841074
           1.73561417 -0.21946425
11
         [-0.9051035
                        0.56081845
                                    0.04174753
                                                1.09781341].
                                                                    -138.99469085785802
12
         [-0.10366618
                       0.58328748
                                   0.52458188 -1.52649207].
                                                                    -362.40126070791297
13
         [-1.80142378 -1.30992486
                                    1.37594861 -1.5878291 ].
                                                                    -3311.51273381473
                                    0.07765978 -1.53921094].
14
         [-1.10045743
                      1.6279866
                                                                    -923.690049821954
15
         [-1.36911015 -1.26106733 -1.10497762 -0.42321055].
                                                                    -1995.092818765097
16
           1.34874724 -0.66725668 -0.11233362 -0.10276976].
                                                                    -654.7644544144575
17
         [-2.03840758 -1.02306318 -0.43795472 -1.41361415].
                                                                    -3174.879884791438
18
         [ 0.92417415 -1.2766809
                                    1.53075985 0.38222458].
                                                                    -845.0282471213242
19
         [-0.90884815 -1.07971857 1.82699941 -0.71338556].
                                                                    -2056.863779476655
20
         [1.92104964 0.85427448 1.75285377 1.75741926].
                                                                    -1083.4249072866344
21
         [-0.80950738 1.53213968 -1.19707279 -1.54218491].
                                                                    -2226.797190219007!
22
         [-0.77674369 -0.9601174 -1.23380575 -0.73873945].
                                                                    -1232.3197232684288
```

```
23
         [-0.30424501 -1.41566203 1.07316125 -1.41254683].
                                                                    -979.2046094688227
24
         [-1.37188790e+00 -1.91343383e+00 1.89013899e+00 -3.61196141e-05].
                                                                                     -36
25
         [ 1.03643217  0.37351182 -1.27503057 -0.76182749].
                                                                    -824.7877668149931
26
         [0.48476226 1.63508301 0.47961728 0.28471247].
                                                                    -678.5739686000503
27
         [-1.11289949 -0.01153869 0.60452205
                                                0.40918519].
                                                                    -198.63485011926758
28
         [-0.78606796 -1.73543614 0.22726162
                                                0.37670767].
                                                                    -1350.987793773297
29
                      -1.06418723 -0.73216872
                                                1.03400931].
                                                                    -512.1013127048446
         [-0.2812224
         [ 1.65420563  0.46876487 -1.15497708 -1.23229633].
30
                                                                    -1367.1275184848027
31
         [ 0.45561251 -1.2856581
                                    0.69185979
                                                0.74844961].
                                                                    -328.23351842940116
         [-1.29054067 -1.01825456 -1.0846477
32
                                                0.74140891].
                                                                    -1202.9159813869048
33
         [-0.04444255 -1.69905763 -0.81028648
                                                0.212996481.
                                                                    -1687.5219031566799
         [ 1.35400996 -1.89016219 -1.89577984 -0.06905842].
                                                                    -5735.540400611233
34
35
         [-1.95646766 1.00206324 1.19245359
                                                0.86058453].
                                                                    -842.2963684080944
36
         [-1.30456047 -1.72741921 -1.73383645 -0.6779548
                                                                    -4779.299516062846
37
         [1.50756889 1.89855338 0.12349852 2.01809109].
                                                                    -1628.7136941839224
38
         [-0.25372346 0.13469482 1.91152524
                                                1.5248555 ].
                                                                    -815.4309755580788
39
         [-1.01118677
                        1.56552334 -1.07636716 -0.43010379].
                                                                    -1534.6863178834344
40
                       1.10009825 0.05709799 -1.60403925].
                                                                    -440.72721207383967
         [-0.65068038
```

```
1 ### EXACT GP EI GRADIENTS
2
3 np.random.seed(run_num_19)
4 surrogate_exact_19 = dGaussianProcess(cov_func, optimize=opt)
5
6 exact_19 = dGPGO(surrogate_exact_19, Acquisition_new(util_grad_exact), objfunc, param)
7 exact_19.run(init_evals=n_init, max_iter=iters)
8
```

```
Proposed point
                                           Current eval.
                                                                  Best eval.
Evaluation
init
         [-1.64850237 1.07007884 -1.03654206 -1.48221261].
                                                                   -1412.165722504925
init
         [-0.69039488 -1.70803378 0.70441812
                                                1.2558082 ].
                                                                    -1034.97990396323
init
         [ 1.97731088  0.55566637 -1.16357834
                                               0.20081636].
                                                                   -1480.569995327432
init
         [ 1.86613588e-01 -1.08922440e+00 -1.58217895e+00 -1.39564217e-03].
init
         [-1.4249639
                       0.13388219 -0.46282028
                                               0.77138896].
                                                                    -422.6519691366176
1
         [-1.34097732 0.17175608 -1.835954
                                                1.33348398].
                                                                   -1041.7752034870423
2
         [-0.47183857 -1.08051498 -1.98692162 -0.26910445].
                                                                   -2958.5580127023322
3
         [ 0.95635377 -0.09333769 -1.3606779 -1.10736771].
                                                                   -1171.346180444734
4
         [-1.87182651 -1.16011981
                                   1.01228468
                                               1.7311966 ].
                                                                    -2249.1066694975525
5
                      1.95053524
                                   0.9782044
                                                                    -1770.3793486483364
         [-0.82657301
                                              -1.88333914].
6
         [-0.98994087 -0.49943038
                                   0.93011811
                                                1.25314217].
                                                                    -286.469091399597
7
         [-0.35663689 -0.46273206 -0.95591287 -1.52972143].
                                                                    -776.5691012170619
8
           0.69425194 -0.71523599 -1.65736387
                                                2.044584231.
                                                                    -673.1736856574765
9
           0.09943037 -1.35763835
                                  1.3172727
                                               -1.33848286].
                                                                   -1165.8977469871683
10
         [-0.20349371
                      1.59029297 -0.67841032 -1.64335141].
                                                                   -1715.7962272986503
11
           0.34129079 -1.7134077
                                  -1.60651937
                                                1.63754837].
                                                                    -2501.6667856875133
                       0.76206533 -0.52972482
                                                                    -215.25607256241028
12
         [-1.04533355
                                                1.14332856].
13
         [ 0.58688618 -0.06914282
                                  0.19680719
                                              -0.94155176].
                                                                    -118.8467931993781
14
         [-1.95802936
                      0.22155234 -0.41099883
                                                0.89883213].
                                                                    -1390.6821336092044
15
           0.48118595 -0.64255789
                                   0.64678184
                                                                    -543.1455287201588
                                               -1.72218236].
         0.38281773
                                                                    -74.08684814103536
16
                                                0.88220296].
17
         [1.00553932 1.91351647 1.76932332 1.640034
                                                                    -663.0610478743334
18
           1.86717929 -0.93208909 0.38747913
                                                1.57727232].
                                                                    -2183.9647223240972
19
         [-0.47227969 -1.06617946 -0.03278646
                                                0.888563941.
                                                                    -389.25668712151105
20
         [ 1.9488119
                      -1.80752078 -0.48920473 -0.57007702].
                                                                    -4629.556928154609
21
           0.28847414 -0.14003924 -0.42148983
                                                0.935595371.
                                                                    -85.71549541447347
22
           1.94014221 -0.57875769 -2.04442496
                                              -1.87321588].
                                                                    -6128.625545737622
23
           0.51513501 -0.94655805
                                   2.04317749
                                                0.992688641.
                                                                   -1296.0355377370665
24
         [-1.42772146 0.04964094
                                   1.11089206
                                                1.30022216].
                                                                    -525.6197156403487
```

```
25
         [-0.83544783  0.36907882  -0.68553566  -1.27956431].
                                                                    -391.03643711296587
26
         [-1.93097095
                       1.84046418 0.77938391 -1.19947924].
                                                                    -1372.4922405179746
27
           0.93135423 -0.04191946 -0.28813248 -0.77884995].
                                                                    -168.12518908427677
28
           1.64128941
                       0.48224145 -1.28233846
                                                1.33374014].
                                                                    -734.142421431925
29
         [-0.27694401 -0.87943929 1.25330768 -1.56633965].
                                                                    -1103.8287995239782
30
         [-0.63808557
                       0.03132333 -0.59613659 -0.75571869].
                                                                    -179.40284795662322
31
                       0.70642684
                                    1.09726491 -0.37487361].
                                                                    -335.79684363303187
         [-0.05173137
                       2.02105291
32
         [ 0.71374153
                                  1.40017248 -0.46276058].
                                                                    -1537.6414213532244
         [1.17135501 0.69985291 0.40068972 0.5299697 ].
                                                                    -60.10743371792253
33
         [ 1.47564194  0.02636049  -0.28983168  -0.78361601].
34
                                                                    -549.3029618091022
35
         [-2.02182177 -0.70114881
                                   1.40662951 -0.08419685].
                                                                    -2814.800496493994
           1.59068772 1.16671535 -0.40371861 -1.88168526].
36
                                                                    -917.8516733150443
37
           0.35769955 -1.72257422 0.15444364 -0.55293506].
                                                                    -1175.4466417532626
38
           0.37183303 -1.45548263
                                    0.73367031 -1.47898748].
                                                                    -859.1859036805786
39
         [-1.23597818 -0.09473091 0.75009555
                                                0.3176916 ].
                                                                    -330.3961499944753
40
         [ 1.02747587 -1.86636766 -0.64418959 -1.95688314].
                                                                    -3130.985945873225
```

```
1 ### EXACT GP EI GRADIENTS
2
3 np.random.seed(run_num_20)
4 surrogate_exact_20 = dGaussianProcess(cov_func, optimize=opt)
5
6 exact_20 = dGPGO(surrogate_exact_20, Acquisition_new(util_grad_exact), objfunc, param)
7 exact_20.run(init_evals=n_init, max_iter=iters)
```

```
Evaluation
                 Proposed point
                                           Current eval.
                                                                   Best eval.
init
         [0.36098376 1.62903543 1.60370987 1.29367031].
                                                                    -499.4296468486902!
init
         [-1.90099626 0.78543905 -0.49692286
                                                                    -937.6489569337288
                                                0.07582083].
init
         [ 0.6469692 -1.25398951 -0.93259202
                                                0.8954099
                                                                    -916.294647636079
           1.15918278 1.43494201
                                   1.12740309 -1.897823
                                                                    -1092.029190829674
init
init
         [-1.57002246
                      1.02924575 -1.06816219 -1.00431457].
                                                                    -1129.8679642787797
1
         [-0.07788899 -0.69957055
                                   0.04358577 -0.96817632].
                                                                    -168.73719780046255
2
           0.46111926 -1.76732302
                                    1.4924756
                                                1.87484522].
                                                                    -678.6495892411331
3
         [-0.41017193 -1.04370263
                                   0.10465761
                                                1.36986945].
                                                                    -435.46806705922864
4
         [-0.68337633
                      1.04340582 -0.02893697 -1.71758559].
                                                                    -457.32636617313904
5
         [-0.76890696
                       1.43771268 0.93871157 -1.25103137].
                                                                    -656.9194881080607
6
           0.87400662
                       0.25583496 -0.98932062 -1.26131996].
                                                                    -643.3869394235138
7
                       0.05885878 -1.79915953 -1.23751637].
                                                                    -2341.220945994441!
           0.53628406
8
                       0.63274154 -0.16463738
         1.48676537
                                                2.033608421.
                                                                    -685.1791327179618
9
         [-0.03479318 -1.72142218
                                   0.08490681 -1.4905188 ].
                                                                    -1358.8910688226583
10
         [-0.71679575]
                       0.1183272
                                    0.44250923 -0.43806832].
                                                                    -78.21773357648438
           0.93174174 -1.80043821 -1.11231057
                                                0.9157171 ].
11
                                                                    -2630.413075041978
12
         [-0.14497107 -1.88923506 -1.24191093
                                                2.04331784].
                                                                    -2719.37616469843
13
           1.77606792
                       1.00107966
                                   0.41432244 -0.82536097].
                                                                    -598.5926340581475
14
           1.95153786
                                    1.34480077 -1.0042522 ].
                       1.39205014
                                                                    -1411.417628244256
15
           0.35184308
                       0.38504659
                                    0.24691546 -1.49409436].
                                                                    -250.98565692044613
           1.9572054
                       1.55274861
                                    0.42376897 -1.22554584].
                                                                    -1112.7964838243277
16
17
         [-1.94567723 -2.03159091
                                    0.59649137
                                                1.63019238].
                                                                    -4811.182622250396
                       1.35057717 -0.27348387
                                                                    -573.4146307103362
18
         [-0.46124676
                                                0.043036351.
19
         [-0.29968836 -0.36181771 -0.56648986
                                                                    -348.08624989049326
                                                1.97334726].
20
         [-0.33426003 -0.39091638 1.4649311
                                               -0.6427726 ].
                                                                    -979.0992443779695
21
         [0.93135994 0.60897708 0.52812793 0.52804205].
                                                                    -15.73989562308487
22
         [ 1.91938095 -1.53492843 1.86274858 -1.29906807].
                                                                    -5030.332344932889
23
         [-0.97155197
                       1.66050876 -1.54658613
                                                2.027757621.
                                                                    -1927.7557869919847
24
         [-1.14859456
                       1.41782234 -0.00329371
                                                1.37715507].
                                                                    -601.8453472714374
25
         [1.41562305 0.87537359 1.77578706 0.95501074].
                                                                    -713.378163906437
26
         [ 0.37538949  0.83543473 -2.04526569 -1.58776789].
                                                                    -4140.755353505755
```

-1487.3603438687906

-2447.058902331077

[-0.45927725 -1.89064134 0.5847654 -0.84621611].

[1.14127524 -1.81378399 -0.41349412 1.14333225].

27

28

```
29
              [-1.565668
                          -1.65420093 -1.89373656 -1.70995388].
                                                                       -6656.291951536386!
     30
              [-1.87196263 -0.79279469 -0.91608427 -0.35078485].
                                                                       -2241.778048936678
    31
              [-0.04876514 0.40945054 1.30688952 0.19211095].
                                                                      -377.6802644324403
    32
              [-1.04514726 -0.18482258 0.96996067 -1.16480678].
                                                                      -699.6403016208243
    33
              [ 0.24018362 -0.11406655 -0.02327053 0.19288687].
                                                                       -9.646826040884186
    34
              [-1.7380717 -1.16787012 -1.20464654 0.92155594].
                                                                      -2459.4341831400907
    35
              -1182.006847432322!
              [-0.83423098  0.87355459  -1.03564615  1.6428321 ].
    36
                                                                      -366.747503263408
    37
              [ 0.99818601  0.88294004  1.42843553  -0.2987412 ].
                                                                      -590.7562504994663
    38
                          -1.98625677 -1.18880173
                                                   1.99566803].
              [ 0.13639
                                                                      -3086.135235801925
    39
              [-0.37295724 -0.45068957 -1.20087908 0.35091761].
                                                                      -359.81006888936713
    40
              [ 1.40096206 -0.67822828 -0.22506665 -2.00215088].
                                                                       -1170.257381297159
 1 end_exact = time.time()
 2 end exact
 3
 4 time_exact = end_exact - start_exact
 5 time_exact
    210.44350624084473
 1 ### Simple regret minimization: run number = 1
 2
 3 approx_output_1 = np.append(np.min(approx_1.GP.y[0:n_init]),approx_1.GP.y[n_init:(n_ini
 4 exact_output_1 = np.append(np.min(exact_1.GP.y[0:n_init]),exact_1.GP.y[n_init:(n_init+i
 5
 6 regret_approx_1 = np.log(-approx_output_1 + y_global_orig)
 7 regret_exact_1 = np.log(-exact_output_1 + y_global_orig)
 8
 9 simple_regret_approx_1 = min_max_array(regret_approx_1)
10 simple_regret_exact_1 = min_max_array(regret_exact_1)
11
12 min_simple_regret_approx_1 = min(simple_regret_approx_1)
13 min simple regret exact 1 = min(simple regret exact 1)
15 min_simple_regret_approx_1, min_simple_regret_exact_1
     (4.522009786014001, 4.271178127566797)
 1 ### Simple regret minimization: run number = 2
 2
 3 approx_output_2 = np.append(np.min(approx_2.GP.y[0:n_init]),approx_2.GP.y[n_init:(n_ini
 4 exact_output_2 = np.append(np.min(exact_2.GP.y[0:n_init]),exact_2.GP.y[n_init:(n_init+i
 5
 6 regret_approx_2 = np.log(-approx_output_2 + y_global_orig)
 7 regret_exact_2 = np.log(-exact_output_2 + y_global_orig)
 9 simple regret approx 2 = min max array(regret approx 2)
10 simple regret exact 2 = min max array(regret exact 2)
11
12 min simple regret approx 2 = min(simple regret approx 2)
13 min_simple_regret_exact_2 = min(simple_regret_exact_2)
```

```
14
15 min simple regret approx 2, min simple regret exact 2
     (5.210942844229998, 4.574559029861857)
 1 ### Simple regret minimization: run number = 3
 3 approx_output_3 = np.append(np.min(approx_3.GP.y[0:n_init]),approx_3.GP.y[n_init:(n_ini
 4 exact_output_3 = np.append(np.min(exact_3.GP.y[0:n_init]),exact_3.GP.y[n_init:(n_init+i
 6 regret_approx_3 = np.log(-approx_output_3 + y_global_orig)
 7 regret_exact_3 = np.log(-exact_output_3 + y_global_orig)
 9 simple_regret_approx_3 = min_max_array(regret_approx_3)
10 simple_regret_exact_3 = min_max_array(regret_exact_3)
11
12 min_simple_regret_approx_3 = min(simple_regret_approx_3)
13 min_simple_regret_exact_3 = min(simple_regret_exact_3)
14
15 min_simple_regret_approx_3, min_simple_regret_exact_3
     (4.610995461278897, 4.461337277261566)
 1 ### Simple regret minimization: run number = 4
 2
 3 approx_output_4 = np.append(np.min(approx_4.GP.y[0:n_init]),approx_4.GP.y[n_init:(n_ini
 4 exact_output_4 = np.append(np.min(exact_4.GP.y[0:n_init]),exact_4.GP.y[n_init:(n_init+i
 6 regret_approx_4 = np.log(-approx_output_4 + y_global_orig)
 7 regret_exact_4 = np.log(-exact_output_4 + y_global_orig)
 9 simple_regret_approx_4 = min_max_array(regret_approx_4)
10 simple_regret_exact_4 = min_max_array(regret_exact_4)
11
12 min_simple_regret_approx_4 = min(simple_regret_approx_4)
13 min_simple_regret_exact_4 = min(simple_regret_exact_4)
14
15 min_simple_regret_approx_4, min_simple_regret_exact_4
     (5.201862175683879, 4.112184246094226)
 1 ### Simple regret minimization: run number = 5
 2
 3 approx output 5 = np.append(np.min(approx 5.GP.y[0:n init]),approx 5.GP.y[n init:(n ini
 4 exact_output_5 = np.append(np.min(exact_5.GP.y[0:n_init]),exact_5.GP.y[n_init:(n_init+i
 6 regret_approx_5 = np.log(-approx_output_5 + y_global_orig)
 7 regret_exact_5 = np.log(-exact_output_5 + y_global_orig)
 8
 9 simple_regret_approx_5 = min_max_array(regret_approx_5)
10 simple regret exact 5 = min max array(regret exact 5)
11
12 min_simple_regret_approx_5 = min(simple_regret_approx_5)
```

```
6/14/2021
                                        3. Rosenbrock GP El.ipynb - Colaboratory
   13 min_simple_regret_exact_5 = min(simple_regret_exact_5)
   14
   15 min_simple_regret_approx_5, min_simple_regret_exact_5
         (4.521049806967185, 4.749811120589589)
    1 ### Simple regret minimization: run number = 6
    2
    3 approx_output_6 = np.append(np.min(approx_6.GP.y[0:n_init]),approx_6.GP.y[n_init:(n_ini
    4 exact_output_6 = np.append(np.min(exact_6.GP.y[0:n_init]),exact_6.GP.y[n_init:(n_init+i
    5
    6 regret_approx_6 = np.log(-approx_output_6 + y_global_orig)
    7 regret_exact_6 = np.log(-exact_output_6 + y_global_orig)
    9 simple_regret_approx_6 = min_max_array(regret_approx_6)
   10 simple_regret_exact_6 = min_max_array(regret_exact_6)
   12 min_simple_regret_approx_6 = min(simple_regret_approx_6)
   13 min_simple_regret_exact_6 = min(simple_regret_exact_6)
   14
   15 min_simple_regret_approx_6, min_simple_regret_exact_6
         (3.8865158242765974, 4.656426686390739)
    1 ### Simple regret minimization: run number = 7
    3 approx_output_7 = np.append(np.min(approx_7.GP.y[0:n_init]),approx_7.GP.y[n_init:(n_ini
    4 exact_output_7 = np.append(np.min(exact_7.GP.y[0:n_init]),exact_7.GP.y[n_init:(n_init+i
    6 regret_approx_7 = np.log(-approx_output_7 + y_global_orig)
    7 regret_exact_7 = np.log(-exact_output_7 + y_global_orig)
    9 simple_regret_approx_7 = min_max_array(regret_approx_7)
   10 simple_regret_exact_7 = min_max_array(regret_exact_7)
   12 min_simple_regret_approx_7 = min(simple_regret_approx_7)
   13 min_simple_regret_exact_7 = min(simple_regret_exact_7)
   14
   15 min_simple_regret_approx_7, min_simple_regret_exact_7
         (5.194328935476146, 4.71227510466372)
    1 ### Simple regret minimization: run number = 8
     3 approx_output_8 = np.append(np.min(approx_8.GP.y[0:n_init]),approx_8.GP.y[n_init:(n_ini
    4 exact_output_8 = np.append(np.min(exact_8.GP.y[0:n_init]),exact_8.GP.y[n_init:(n_init+i
    6 regret_approx_8 = np.log(-approx_output_8 + y_global_orig)
    7 regret_exact_8 = np.log(-exact_output_8 + y_global_orig)
    9 simple_regret_approx_8 = min_max_array(regret_approx_8)
   10 simple_regret_exact_8 = min_max_array(regret_exact_8)
   11
   12 min_simple_regret_approx_8 = min(simple_regret_approx_8)
```

```
13 min_simple_regret_exact_8 = min(simple_regret_exact_8)
14
15 min_simple_regret_approx_8, min_simple_regret_exact_8
     (3.7008685662033893, 3.683340470693204)
 1 ### Simple regret minimization: run number = 9
 3 approx_output_9 = np.append(np.min(approx_9.GP.y[0:n_init]),approx_9.GP.y[n_init:(n_ini
 4 exact_output_9 = np.append(np.min(exact_9.GP.y[0:n_init]),exact_9.GP.y[n_init:(n_init+i
 5
 6 regret_approx_9 = np.log(-approx_output_9 + y_global_orig)
 7 regret_exact_9 = np.log(-exact_output_9 + y_global_orig)
 8
 9 simple_regret_approx_9 = min_max_array(regret_approx_9)
10 simple_regret_exact_9 = min_max_array(regret_exact_9)
11
12 min_simple_regret_approx_9 = min(simple_regret_approx_9)
13 min_simple_regret_exact_9 = min(simple_regret_exact_9)
14
15 min_simple_regret_approx_9, min_simple_regret_exact_9
     (6.087740433378212, 5.269928753632324)
 1 ### Simple regret minimization: run number = 10
 2
 3 approx_output_10 = np.append(np.min(approx_10.GP.y[0:n_init]),approx_10.GP.y[n_init:(n_
 4 exact_output_10 = np.append(np.min(exact_10.GP.y[0:n_init]),exact_10.GP.y[n_init:(n_ini
 5
 6 regret_approx_10 = np.log(-approx_output_10 + y_global_orig)
 7 regret_exact_10 = np.log(-exact_output_10 + y_global_orig)
 8
 9 simple_regret_approx_10 = min_max_array(regret_approx_10)
10 simple regret exact 10 = min max array(regret exact 10)
11
12 min simple regret approx 10 = min(simple regret approx 10)
13 min simple regret exact 10 = min(simple regret exact 10)
14
15 min_simple_regret_approx_10, min_simple_regret_exact_10
     (3.8691436628726703, 3.8691436628726703)
 1 ### Simple regret minimization: run number = 11
 2
 3 approx_output_11 = np.append(np.min(approx_11.GP.y[0:n_init]),approx_11.GP.y[n_init:(n_
 4 exact_output_11 = np.append(np.min(exact_11.GP.y[0:n_init]),exact_11.GP.y[n_init:(n_ini
 5
 6 regret_approx_11 = np.log(-approx_output_11 + y_global_orig)
 7 regret_exact_11 = np.log(-exact_output_11 + y_global_orig)
 9 simple regret approx 11 = min max array(regret approx 11)
10 simple_regret_exact_11 = min_max_array(regret_exact_11)
11
```

11

```
12 min simple regret approx 14 = min(simple regret approx 14)
13 min_simple_regret_exact_14 = min(simple_regret_exact_14)
15 min_simple_regret_approx_14, min_simple_regret_exact_14
     (5.158812057918859, 4.489360713876927)
 1 ### Simple regret minimization: run number = 15
 2
 3 approx_output_15 = np.append(np.min(approx_15.GP.y[0:n_init]),approx_15.GP.y[n_init:(n_
 4 exact_output_15 = np.append(np.min(exact_15.GP.y[0:n_init]),exact_15.GP.y[n_init:(n_ini
 5
 6 regret_approx_15 = np.log(-approx_output_15 + y_global_orig)
 7 regret_exact_15 = np.log(-exact_output_15 + y_global_orig)
 9 simple regret approx 15 = min max array(regret approx 15)
10 simple_regret_exact_15 = min_max_array(regret_exact_15)
12 min_simple_regret_approx_15 = min(simple_regret_approx_15)
13 min_simple_regret_exact_15 = min(simple_regret_exact_15)
14
15 min_simple_regret_approx_15, min_simple_regret_exact_15
     (3.764244969947392, 4.121304135802509)
 1 ### Simple regret minimization: run number = 16
 3 approx_output_16 = np.append(np.min(approx_16.GP.y[0:n_init]),approx_16.GP.y[n_init:(n_
 4 exact_output_16 = np.append(np.min(exact_16.GP.y[0:n_init]),exact_16.GP.y[n_init:(n_ini
 6 regret_approx_16 = np.log(-approx_output_16 + y_global_orig)
 7 regret_exact_16 = np.log(-exact_output_16 + y_global_orig)
 9 simple_regret_approx_16 = min_max_array(regret_approx_16)
10 simple_regret_exact_16 = min_max_array(regret_exact_16)
12 min_simple_regret_approx_16 = min(simple_regret_approx_16)
13 min_simple_regret_exact_16 = min(simple_regret_exact_16)
14
15 min_simple_regret_approx_16, min_simple_regret_exact_16
     (6.033670782631654, 3.3824497046465036)
 1 ### Simple regret minimization: run number = 17
 3 approx_output_17 = np.append(np.min(approx_17.GP.y[0:n_init]),approx_17.GP.y[n_init:(n_
 4 exact output 17 = np.append(np.min(exact 17.GP.y[0:n init]),exact 17.GP.y[n init:(n ini
 6 regret_approx_17 = np.log(-approx_output_17 + y_global_orig)
 7 regret_exact_17 = np.log(-exact_output_17 + y_global_orig)
 9 simple_regret_approx_17 = min_max_array(regret_approx_17)
10 simple_regret_exact_17 = min_max_array(regret_exact_17)
```

```
6/14/2021
                                        3. Rosenbrock GP El.ipynb - Colaboratory
   11
   12 min_simple_regret_approx_17 = min(simple_regret_approx_17)
   13 min simple regret exact 17 = min(simple regret exact 17)
   14
   15 min_simple_regret_approx_17, min_simple_regret_exact_17
         (2.9255423030280014, 3.7644092846315886)
    1 ### Simple regret minimization: run number = 18
    3 approx_output_18 = np.append(np.min(approx_18.GP.y[0:n_init]),approx_18.GP.y[n_init:(n_
    4 exact_output_18 = np.append(np.min(exact_18.GP.y[0:n_init]),exact_18.GP.y[n_init:(n_ini
    5
    6 regret_approx_18 = np.log(-approx_output_18 + y_global_orig)
    7 regret_exact_18 = np.log(-exact_output_18 + y_global_orig)
    8
    9 simple_regret_approx_18 = min_max_array(regret_approx_18)
   10 simple_regret_exact_18 = min_max_array(regret_exact_18)
   11
   12 min_simple_regret_approx_18 = min(simple_regret_approx_18)
   13 min simple regret exact 18 = min(simple regret exact 18)
   14
   15 min_simple_regret_approx_18, min_simple_regret_exact_18
         (5.203897595093871, 4.164420610036739)
    1 ### Simple regret minimization: run number = 19
    2
    3 approx_output_19 = np.append(np.min(approx_19.GP.y[0:n_init]),approx_19.GP.y[n_init:(n_
    4 exact_output_19 = np.append(np.min(exact_19.GP.y[0:n_init]),exact_19.GP.y[n_init:(n_ini
    5
    6 regret_approx_19 = np.log(-approx_output_19 + y_global_orig)
    7 regret_exact_19 = np.log(-exact_output_19 + y_global_orig)
    8
    9 simple regret approx 19 = min max array(regret approx 19)
   10 simple regret exact 19 = min max array(regret exact 19)
   11
   12 min simple regret approx 19 = min(simple regret approx 19)
   13 min simple regret exact 19 = min(simple regret exact 19)
   14
   15 min_simple_regret_approx_19, min_simple_regret_exact_19
         (4.096133523042415, 4.096133523042415)
    1 ### Simple regret minimization: run number = 20
    2
    3 approx_output_20 = np.append(np.min(approx_20.GP.y[0:n_init]),approx_20.GP.y[n_init:(n_
    4 exact_output_20 = np.append(np.min(exact_20.GP.y[0:n_init]),exact_20.GP.y[n_init:(n_ini
    5
    6 regret_approx_20 = np.log(-approx_output_20 + y_global_orig)
    7 regret_exact_20 = np.log(-exact_output_20 + y_global_orig)
    8
    9 simple regret approx 20 = min max array(regret approx 20)
   10 simple regret exact 20 = min max arrav(regret exact 20)
```

```
11
12 min_simple_regret_approx_20 = min(simple_regret_approx_20)
13 min_simple_regret_exact_20 = min(simple_regret_exact_20)
14
15 min_simple_regret_approx_20, min_simple_regret_exact_20
     (2.266628953568505, 2.266628953568505)
 1 # Iteration1 :
 2
 3 \text{ slice1} = 0
 4
 5 approx1 = [simple_regret_approx_1[slice1],
 6
          simple_regret_approx_2[slice1],
 7
          simple regret approx 3[slice1],
 8
          simple_regret_approx_4[slice1],
 9
          simple_regret_approx_5[slice1],
10
          simple_regret_approx_6[slice1],
11
          simple_regret_approx_7[slice1],
12
          simple_regret_approx_8[slice1],
13
          simple_regret_approx_9[slice1],
14
          simple_regret_approx_10[slice1],
15
          simple_regret_approx_11[slice1],
16
          simple_regret_approx_12[slice1],
17
          simple regret approx 13[slice1],
18
          simple_regret_approx_14[slice1],
19
          simple_regret_approx_15[slice1],
20
          simple_regret_approx_16[slice1],
21
          simple_regret_approx_17[slice1],
22
          simple_regret_approx_18[slice1],
23
          simple_regret_approx_19[slice1],
24
          simple_regret_approx_20[slice1]]
25
26 exact1 = [simple_regret_exact_1[slice1],
27
          simple regret exact 2[slice1],
28
          simple regret exact 3[slice1],
29
          simple_regret_exact_4[slice1],
30
          simple regret exact 5[slice1],
31
          simple regret exact 6[slice1],
32
          simple_regret_exact_7[slice1],
33
          simple_regret_exact_8[slice1],
34
          simple_regret_exact_9[slice1],
35
          simple_regret_exact_10[slice1],
36
          simple_regret_exact_11[slice1],
37
          simple regret exact 12[slice1],
38
          simple_regret_exact_13[slice1],
39
          simple_regret_exact_14[slice1],
40
          simple regret exact 15[slice1],
41
          simple regret exact 16[slice1],
42
          simple regret exact 17[slice1],
43
          simple regret exact 18[slice1],
44
          simple_regret_exact_19[slice1],
45
          simple_regret_exact_20[slice1]]
46
```

```
47 approx1 results = pd.DataFrame(approx1).sort values(by=|0|, ascending=False)
48 exact1_results = pd.DataFrame(exact1).sort_values(by=[0], ascending=False)
49
50 ### Best simple regret minimization IQR - approx:
51 lower approx1 = np.asarray(approx1 results[4:5][0])[0]
52 median_approx1 = np.asarray(approx1_results[9:10][0])[0]
53 upper approx1 = np.asarray(approx1 results[14:15][0])[0]
55 lower_exact1 = np.asarray(exact1_results[4:5][0])[0]
56 median_exact1 = np.asarray(exact1_results[9:10][0])[0]
57 upper_exact1 = np.asarray(exact1_results[14:15][0])[0]
 1 # Iteration11:
 2
 3 \text{ slice} 11 = 10
 4
 5 approx11 = [simple_regret_approx_1[slice11],
 6
          simple_regret_approx_2[slice11],
 7
          simple_regret_approx_3[slice11],
 8
          simple regret approx 4[slice11],
 9
          simple_regret_approx_5[slice11],
10
          simple_regret_approx_6[slice11],
11
          simple_regret_approx_7[slice11],
12
          simple regret approx 8[slice11],
13
          simple regret approx 9[slice11],
14
          simple_regret_approx_10[slice11],
15
          simple regret approx 11[slice11],
16
          simple_regret_approx_12[slice11],
17
          simple_regret_approx_13[slice11],
18
          simple_regret_approx_14[slice11],
19
          simple_regret_approx_15[slice11],
20
          simple_regret_approx_16[slice11],
21
          simple regret approx 17[slice11],
22
          simple_regret_approx_18[slice11],
23
          simple regret approx 19[slice11],
24
          simple regret approx 20[slice11]]
25
26 exact11 = [simple regret exact 1[slice11],
27
          simple_regret_exact_2[slice11],
28
          simple regret exact 3[slice11],
29
          simple_regret_exact_4[slice11],
30
          simple_regret_exact_5[slice11],
31
          simple regret exact 6[slice11],
32
          simple regret exact 7[slice11],
33
          simple_regret_exact_8[slice11],
34
          simple regret exact 9[slice11],
35
          simple regret exact 10[slice11],
36
          simple regret exact 11[slice11],
37
          simple regret exact 12[slice11],
38
          simple regret exact 13[slice11],
39
          simple regret exact 14[slice11],
40
          simple_regret_exact_15[slice11],
41
          simple regret exact 16[slice11],
42
          simple_regret_exact_17[slice11],
          simple regret exact 18[slice11].
```

```
6/14/2021
                                         3. Rosenbrock GP El.ipynb - Colaboratory
                     . Chi ce chace
   44
              simple regret exact 19[slice11],
   45
              simple regret exact 20[slice11]]
   46
   47 approx11 results = pd.DataFrame(approx11).sort values(by=[0], ascending=False)
   48 exact11_results = pd.DataFrame(exact11).sort_values(by=[0], ascending=False)
   49
   50 ### Best simple regret minimization IQR - approx:
   51 lower_approx11 = np.asarray(approx11_results[4:5][0])[0]
   52 median_approx11 = np.asarray(approx11_results[9:10][0])[0]
   53 upper_approx11 = np.asarray(approx11_results[14:15][0])[0]
   54
   55 lower_exact11 = np.asarray(exact11_results[4:5][0])[0]
   56 median_exact11 = np.asarray(exact11_results[9:10][0])[0]
   57 upper exact11 = np.asarray(exact11 results[14:15][0])[0]
     1 # Iteration21 :
     2
     3 \text{ slice21} = 20
     4
     5 approx21 = [simple_regret_approx_1[slice21],
     6
              simple regret approx 2[slice21],
     7
              simple_regret_approx_3[slice21],
     8
              simple_regret_approx_4[slice21],
     9
              simple_regret_approx_5[slice21],
   10
              simple_regret_approx_6[slice21],
   11
              simple_regret_approx_7[slice21],
   12
              simple_regret_approx_8[slice21],
   13
              simple_regret_approx_9[slice21],
   14
              simple_regret_approx_10[slice21],
   15
              simple_regret_approx_11[slice21],
   16
              simple_regret_approx_12[slice21],
   17
              simple_regret_approx_13[slice21],
   18
              simple_regret_approx_14[slice21],
   19
              simple_regret_approx_15[slice21],
   20
              simple regret approx 16[slice21],
   21
              simple_regret_approx_17[slice21],
   22
              simple regret approx 18[slice21],
   23
              simple_regret_approx_19[slice21],
   24
              simple_regret_approx_20[slice21]]
   25
   26 exact21 = [simple regret exact 1[slice21],
   27
              simple_regret_exact_2[slice21],
   28
              simple_regret_exact_3[slice21],
   29
              simple regret exact 4[slice21],
   30
              simple regret exact 5[slice21],
   31
              simple_regret_exact_6[slice21],
   32
              simple regret exact 7[slice21],
   33
              simple regret exact 8[slice21],
   34
              simple_regret_exact_9[slice21],
   35
              simple regret exact 10[slice21],
   36
              simple_regret_exact_11[slice21],
   37
              simple_regret_exact_12[slice21],
   38
              simple_regret_exact_13[slice21],
   39
              simple_regret_exact_14[slice21],
```

```
6/14/2021
                                         3. Rosenbrock GP El.ipynb - Colaboratory
              simple regret exact II|SIIce3I|,
   36
   37
              simple_regret_exact_12[slice31],
   38
              simple_regret_exact_13[slice31],
   39
              simple regret exact 14[slice31],
   40
              simple_regret_exact_15[slice31],
   41
              simple_regret_exact_16[slice31],
   42
              simple regret exact 17[slice31],
   43
              simple_regret_exact_18[slice31],
   44
              simple_regret_exact_19[slice31],
   45
              simple regret exact 20[slice31]]
   46
   47 approx31 results = pd.DataFrame(approx31).sort values(by=[0], ascending=False)
   48 exact31_results = pd.DataFrame(exact31).sort_values(by=[0], ascending=False)
   49
   50 ### Best simple regret minimization IQR - approx:
   51 lower_approx31 = np.asarray(approx31_results[4:5][0])[0]
   52 median_approx31 = np.asarray(approx31_results[9:10][0])[0]
   53 upper_approx31 = np.asarray(approx31_results[14:15][0])[0]
   54
   55 lower exact31 = np.asarray(exact31 results[4:5][0])[0]
   56 median_exact31 = np.asarray(exact31_results[9:10][0])[0]
   57 upper_exact31 = np.asarray(exact31_results[14:15][0])[0]
   58
     1 # Iteration41 :
     2
     3 \text{ slice} 41 = 40
     4
     5 approx41 = [simple_regret_approx_1[slice41],
              simple_regret_approx_2[slice41],
     6
     7
              simple regret approx 3[slice41],
     8
              simple_regret_approx_4[slice41],
     9
              simple_regret_approx_5[slice41],
   10
              simple_regret_approx_6[slice41],
   11
              simple_regret_approx_7[slice41],
   12
              simple_regret_approx_8[slice41],
   13
              simple regret approx 9[slice41],
   14
              simple regret approx 10[slice41],
              simple_regret_approx_11[slice41],
   15
   16
              simple regret approx 12[slice41],
   17
              simple regret approx 13[slice41],
   18
              simple regret approx 14[slice41],
   19
              simple_regret_approx_15[slice41],
   20
              simple regret approx 16[slice41],
   21
              simple_regret_approx_17[slice41],
   22
              simple_regret_approx_18[slice41],
   23
              simple regret approx 19[slice41],
   24
              simple_regret_approx_20[slice41]]
   25
   26 exact41 = [simple regret exact 1[slice41],
   27
              simple regret exact 2[slice41],
   28
              simple_regret_exact_3[slice41],
   29
              simple_regret_exact_4[slice41],
   30
              simple regret exact 5[slice41],
    31
              simple regret exact 6[slice41].
```

```
32
          simple regret exact 7[slice41],
33
          simple_regret_exact_8[slice41],
34
          simple_regret_exact_9[slice41],
35
          simple regret exact 10[slice41],
36
          simple regret exact 11[slice41],
37
          simple_regret_exact_12[slice41],
38
          simple_regret_exact_13[slice41],
39
          simple regret exact 14[slice41],
40
          simple regret exact 15[slice41],
41
          simple_regret_exact_16[slice41],
42
          simple regret exact 17[slice41],
43
          simple_regret_exact_18[slice41],
44
          simple_regret_exact_19[slice41],
45
          simple regret exact 20[slice41]]
46
47 approx41_results = pd.DataFrame(approx41).sort_values(by=[0], ascending=False)
48 exact41_results = pd.DataFrame(exact41).sort_values(by=[0], ascending=False)
49
50 ### Best simple regret minimization IQR - approx:
51 lower_approx41 = np.asarray(approx41_results[4:5][0])[0]
52 median approx41 = np.asarray(approx41 results[9:10][0])[0]
53 upper_approx41 = np.asarray(approx41_results[14:15][0])[0]
54
55 lower exact41 = np.asarray(exact41 results[4:5][0])[0]
56 median_exact41 = np.asarray(exact41_results[9:10][0])[0]
57 upper_exact41 = np.asarray(exact41_results[14:15][0])[0]
58
 1 # Iteration2 :
 2
 3 \text{ slice2} = 1
 5 approx2 = [simple_regret_approx_1[slice2],
 6
          simple_regret_approx_2[slice2],
 7
          simple regret approx 3[slice2],
 8
          simple_regret_approx_4[slice2],
 9
          simple_regret_approx_5[slice2],
10
          simple regret approx 6[slice2],
11
          simple regret approx 7[slice2],
12
          simple_regret_approx_8[slice2],
13
          simple regret approx 9[slice2],
14
          simple regret approx 10[slice2],
15
          simple_regret_approx_11[slice2],
16
          simple regret approx 12[slice2],
17
          simple_regret_approx_13[slice2],
18
          simple_regret_approx_14[slice2],
19
          simple regret approx 15[slice2],
20
          simple regret approx 16[slice2],
21
          simple_regret_approx_17[slice2],
22
          simple_regret_approx_18[slice2],
23
          simple regret approx 19[slice2],
24
          simple regret approx 20[slice2]]
25
26 exact2 = [simple regret exact 1[slice2],
```

```
6/14/2021
                                         3. Rosenbrock GP El.ipynb - Colaboratory
              >TIIIhTeTi.eRi.erTabhi.nxTaf2TTCeT7]
    ۷٥
   24
              simple_regret_approx_20[slice12]]
   25
   26 exact12 = [simple regret exact 1[slice12],
   27
              simple regret exact 2[slice12],
   28
              simple_regret_exact_3[slice12],
   29
              simple_regret_exact_4[slice12],
   30
              simple_regret_exact_5[slice12],
   31
              simple_regret_exact_6[slice12],
   32
              simple_regret_exact_7[slice12],
   33
              simple_regret_exact_8[slice12],
   34
              simple_regret_exact_9[slice12],
              simple_regret_exact_10[slice12],
   35
   36
              simple regret exact 11[slice12],
   37
              simple_regret_exact_12[slice12],
   38
              simple_regret_exact_13[slice12],
   39
              simple_regret_exact_14[slice12],
   40
              simple regret exact 15[slice12],
   41
              simple_regret_exact_16[slice12],
   42
              simple_regret_exact_17[slice12],
   43
              simple_regret_exact_18[slice12],
   44
              simple_regret_exact_19[slice12],
   45
              simple_regret_exact_20[slice12]]
   46
   47 approx12_results = pd.DataFrame(approx12).sort_values(by=[0], ascending=False)
   48 exact12_results = pd.DataFrame(exact12).sort_values(by=[0], ascending=False)
   49
   50 ### Best simple regret minimization IQR - approx:
   51 lower_approx12 = np.asarray(approx12_results[4:5][0])[0]
   52 median_approx12 = np.asarray(approx12_results[9:10][0])[0]
   53 upper_approx12 = np.asarray(approx12_results[14:15][0])[0]
   54
   55 lower_exact12 = np.asarray(exact12_results[4:5][0])[0]
   56 median exact12 = np.asarray(exact12 results[9:10][0])[0]
   57 upper_exact12 = np.asarray(exact12_results[14:15][0])[0]
     1 # Iteration22 :
     2
     3 \text{ slice22} = 21
     4
     5 approx22 = [simple regret approx 1[slice22],
     6
              simple_regret_approx_2[slice22],
     7
              simple_regret_approx_3[slice22],
     8
              simple regret approx 4[slice22],
     9
              simple regret approx 5[slice22],
              simple_regret_approx_6[slice22],
   10
   11
              simple regret approx 7[slice22],
   12
              simple regret approx 8[slice22],
              simple regret approx 9[slice22],
   13
   14
              simple_regret_approx_10[slice22],
   15
              simple regret approx 11[slice22],
   16
              simple regret approx 12[slice22],
   17
              simple_regret_approx_13[slice22],
   18
              simple regret approx 14[slice22],
   19
              simple regret approx 15[slice22],
```

```
simple_regret_approx_16[slice22],
20
21
          simple regret approx 17[slice22],
22
          simple regret approx 18[slice22],
23
          simple_regret_approx_19[slice22],
24
          simple regret approx 20[slice22]]
25
26 exact22 = [simple_regret_exact_1[slice22],
27
          simple_regret_exact_2[slice22],
28
          simple_regret_exact_3[slice22],
29
          simple_regret_exact_4[slice22],
30
          simple regret exact 5[slice22],
31
          simple_regret_exact_6[slice22],
32
          simple_regret_exact_7[slice22],
33
          simple_regret_exact_8[slice22],
34
          simple regret exact 9[slice22],
          simple_regret_exact_10[slice22],
35
36
          simple_regret_exact_11[slice22],
37
          simple_regret_exact_12[slice22],
38
          simple_regret_exact_13[slice22],
39
          simple_regret_exact_14[slice22],
40
          simple_regret_exact_15[slice22],
41
          simple_regret_exact_16[slice22],
42
          simple_regret_exact_17[slice22],
43
          simple_regret_exact_18[slice22],
44
          simple_regret_exact_19[slice22],
45
          simple_regret_exact_20[slice22]]
46
47 approx22 results = pd.DataFrame(approx22).sort values(by=[0], ascending=False)
48 exact22_results = pd.DataFrame(exact22).sort_values(by=[0], ascending=False)
49
50 ### Best simple regret minimization IQR - approx:
51 lower_approx22 = np.asarray(approx22_results[4:5][0])[0]
52 median_approx22 = np.asarray(approx22_results[9:10][0])[0]
53 upper_approx22 = np.asarray(approx22_results[14:15][0])[0]
54
55 lower_exact22 = np.asarray(exact22_results[4:5][0])[0]
56 median_exact22 = np.asarray(exact22_results[9:10][0])[0]
57 upper exact22 = np.asarray(exact22 results[14:15][0])[0]
 1 # Iteration32 :
 2
 3 \text{ slice} 32 = 31
 4
 5 approx32 = [simple_regret_approx_1[slice32],
          simple regret approx 2[slice32],
 6
 7
          simple regret approx 3[slice32],
 8
          simple_regret_approx_4[slice32],
 9
          simple regret approx 5[slice32],
10
          simple_regret_approx_6[slice32],
          simple_regret_approx_7[slice32],
11
12
          simple regret approx 8[slice32],
13
          simple_regret_approx_9[slice32],
14
          simple_regret_approx_10[slice32],
15
          simple_regret_approx_11[slice32],
```

```
6/14/2021
                                         3. Rosenbrock GP El.ipynb - Colaboratory
   16
              simple regret approx 12[slice32],
   17
              simple regret approx 13[slice32],
   18
              simple regret approx 14[slice32],
   19
              simple regret approx 15[slice32],
   20
              simple_regret_approx_16[slice32],
   21
              simple_regret_approx_17[slice32],
   22
              simple_regret_approx_18[slice32],
   23
              simple_regret_approx_19[slice32],
   24
              simple_regret_approx_20[slice32]]
   25
   26 exact32 = [simple_regret_exact_1[slice32],
   27
              simple_regret_exact_2[slice32],
   28
              simple regret exact 3[slice32],
   29
              simple regret exact 4[slice32],
   30
              simple_regret_exact_5[slice32],
   31
              simple regret exact 6[slice32],
              simple_regret_exact_7[slice32],
   32
   33
              simple_regret_exact_8[slice32],
   34
              simple_regret_exact_9[slice32],
   35
              simple_regret_exact_10[slice32],
   36
              simple_regret_exact_11[slice32],
   37
              simple_regret_exact_12[slice32],
   38
              simple_regret_exact_13[slice32],
   39
              simple_regret_exact_14[slice32],
              simple_regret_exact_15[slice32],
   40
   41
              simple regret exact 16[slice32],
   42
              simple_regret_exact_17[slice32],
   43
              simple_regret_exact_18[slice32],
   44
              simple_regret_exact_19[slice32],
   45
              simple_regret_exact_20[slice32]]
   46
   47 approx32_results = pd.DataFrame(approx32).sort_values(by=[0], ascending=False)
   48 exact32_results = pd.DataFrame(exact32).sort_values(by=[0], ascending=False)
   49
   50 ### Best simple regret minimization IQR - approx:
   51 lower approx32 = np.asarray(approx32 results[4:5][0])[0]
   52 median approx32 = np.asarray(approx32 results[9:10][0])[0]
   53 upper approx32 = np.asarray(approx32_results[14:15][0])[0]
   54
   55 lower exact32 = np.asarray(exact32 results[4:5][0])[0]
   56 median_exact32 = np.asarray(exact32_results[9:10][0])[0]
   57 upper_exact32 = np.asarray(exact32_results[14:15][0])[0]
     1 # Iteration3 :
     2
     3 \text{ slice} 3 = 2
     4
     5 approx3 = [simple_regret_approx_1[slice3],
     6
              simple_regret_approx_2[slice3],
     7
              simple_regret_approx_3[slice3],
     8
              simple_regret_approx_4[slice3],
     9
              simple_regret_approx_5[slice3],
   10
              simple regret approx 6[slice3],
   11
              simple_regret_approx_7[slice3],
   12
              simple regret approx &[slice3]
```

```
6/14/2021
                                                                                   3. Rosenbrock GP El.ipynb - Colaboratory
                             و را عند ما مناسب من مناسب عند مناسب عدد مناسب عند مناسب عدد مناسب
        __
       13
                            simple regret approx 9[slice3],
       14
                            simple_regret_approx_10[slice3],
       15
                            simple_regret_approx_11[slice3],
       16
                            simple_regret_approx_12[slice3],
       17
                            simple_regret_approx_13[slice3],
       18
                            simple_regret_approx_14[slice3],
       19
                            simple_regret_approx_15[slice3],
       20
                            simple_regret_approx_16[slice3],
       21
                            simple_regret_approx_17[slice3],
       22
                            simple regret approx 18[slice3],
       23
                            simple regret approx 19[slice3],
       24
                            simple_regret_approx_20[slice3]]
       25
       26 exact3 = [simple regret exact 1[slice3],
       27
                            simple_regret_exact_2[slice3],
       28
                            simple_regret_exact_3[slice3],
       29
                            simple_regret_exact_4[slice3],
       30
                            simple_regret_exact_5[slice3],
       31
                            simple_regret_exact_6[slice3],
       32
                            simple_regret_exact_7[slice3],
       33
                            simple_regret_exact_8[slice3],
       34
                            simple_regret_exact_9[slice3],
       35
                            simple_regret_exact_10[slice3],
                            simple_regret_exact_11[slice3],
       36
       37
                            simple_regret_exact_12[slice3],
       38
                            simple_regret_exact_13[slice3],
       39
                            simple_regret_exact_14[slice3],
       40
                            simple_regret_exact_15[slice3],
       41
                            simple_regret_exact_16[slice3],
       42
                            simple_regret_exact_17[slice3],
       43
                            simple_regret_exact_18[slice3],
       44
                            simple_regret_exact_19[slice3],
       45
                            simple_regret_exact_20[slice3]]
       46
       47 approx3_results = pd.DataFrame(approx3).sort_values(by=[0], ascending=False)
       48 exact3_results = pd.DataFrame(exact3).sort_values(by=[0], ascending=False)
       49
       50 ### Best simple regret minimization IQR - approx:
       51 lower_approx3 = np.asarray(approx3_results[4:5][0])[0]
       52 median_approx3 = np.asarray(approx3_results[9:10][0])[0]
       53 upper_approx3 = np.asarray(approx3_results[14:15][0])[0]
       54
       55 lower exact3 = np.asarray(exact3 results[4:5][0])[0]
       56 median exact3 = np.asarray(exact3 results[9:10][0])[0]
       57 upper_exact3 = np.asarray(exact3_results[14:15][0])[0]
          1 # Iteration13 :
          2
          3 \text{ slice} 13 = 12
          4
          5 approx13 = [simple_regret_approx_1[slice13],
          6
                             simple_regret_approx_2[slice13],
          7
                             simple regret approx 3[slice13],
          8
                             simple regret approx 4[slice13],
```

```
simple_regret_approx_5[slice13],
 9
10
          simple regret approx 6[slice13],
11
          simple_regret_approx_7[slice13],
12
          simple_regret_approx_8[slice13],
13
          simple regret approx 9[slice13],
14
          simple_regret_approx_10[slice13],
15
          simple_regret_approx_11[slice13],
          simple_regret_approx_12[slice13],
16
17
          simple regret approx 13[slice13],
18
          simple_regret_approx_14[slice13],
19
          simple_regret_approx_15[slice13],
20
          simple regret approx 16[slice13],
21
          simple_regret_approx_17[slice13],
22
          simple_regret_approx_18[slice13],
23
          simple_regret_approx_19[slice13],
24
          simple_regret_approx_20[slice13]]
25
26 exact13 = [simple_regret_exact_1[slice13],
27
          simple_regret_exact_2[slice13],
          simple_regret_exact_3[slice13],
28
29
          simple_regret_exact_4[slice13],
30
          simple regret exact 5[slice13],
31
          simple_regret_exact_6[slice13],
32
          simple_regret_exact_7[slice13],
33
          simple regret exact 8[slice13],
34
          simple_regret_exact_9[slice13],
35
          simple_regret_exact_10[slice13],
36
          simple regret exact 11[slice13],
37
          simple_regret_exact_12[slice13],
38
          simple_regret_exact_13[slice13],
39
          simple_regret_exact_14[slice13],
40
          simple_regret_exact_15[slice13],
41
          simple_regret_exact_16[slice13],
42
          simple_regret_exact_17[slice13],
43
          simple regret exact 18[slice13],
44
          simple regret exact 19[slice13],
45
          simple_regret_exact_20[slice13]]
46
47 approx13 results = pd.DataFrame(approx13).sort values(by=[0], ascending=False)
48 exact13_results = pd.DataFrame(exact13).sort_values(by=[0], ascending=False)
49
50 ### Best simple regret minimization IQR - approx:
51 lower approx13 = np.asarray(approx13 results[4:5][0])[0]
52 median_approx13 = np.asarray(approx13_results[9:10][0])[0]
53 upper approx13 = np.asarray(approx13 results[14:15][0])[0]
54
55 lower exact13 = np.asarray(exact13 results[4:5][0])[0]
56 median exact13 = np.asarray(exact13_results[9:10][0])[0]
57 upper_exact13 = np.asarray(exact13_results[14:15][0])[0]
 1 # Iteration23 :
 2
 3 \text{ slice23} = 22
 4
```

```
2
 3 \text{ slice} 33 = 32
 4
 5 approx33 = [simple regret approx 1[slice33],
 6
          simple regret approx 2[slice33],
 7
          simple_regret_approx_3[slice33],
 8
          simple_regret_approx_4[slice33],
          simple_regret_approx_5[slice33],
 9
10
          simple_regret_approx_6[slice33],
11
          simple_regret_approx_7[slice33],
12
          simple_regret_approx_8[slice33],
13
          simple_regret_approx_9[slice33],
          simple_regret_approx_10[slice33],
14
15
          simple regret approx 11[slice33],
16
          simple_regret_approx_12[slice33],
17
          simple_regret_approx_13[slice33],
18
          simple regret approx 14[slice33],
19
          simple regret approx 15[slice33],
20
          simple_regret_approx_16[slice33],
21
          simple_regret_approx_17[slice33],
22
          simple_regret_approx_18[slice33],
23
          simple_regret_approx_19[slice33],
24
          simple_regret_approx_20[slice33]]
25
26 exact33 = [simple_regret_exact_1[slice33],
27
          simple_regret_exact_2[slice33],
28
          simple regret exact 3[slice33],
29
          simple_regret_exact_4[slice33],
30
          simple_regret_exact_5[slice33],
31
          simple_regret_exact_6[slice33],
32
          simple regret exact 7[slice33],
33
          simple_regret_exact_8[slice33],
34
          simple_regret_exact_9[slice33],
35
          simple_regret_exact_10[slice33],
36
          simple_regret_exact_11[slice33],
37
          simple_regret_exact_12[slice33],
38
          simple regret exact 13[slice33],
39
          simple regret exact 14[slice33],
40
          simple_regret_exact_15[slice33],
41
          simple regret exact 16[slice33],
42
          simple regret exact 17[slice33],
43
          simple regret exact 18[slice33],
44
          simple_regret_exact_19[slice33],
45
          simple regret exact 20[slice33]]
46
47 approx33_results = pd.DataFrame(approx33).sort_values(by=[0], ascending=False)
48 exact33 results = pd.DataFrame(exact33).sort values(by=[0], ascending=False)
49
50 ### Best simple regret minimization IQR - approx:
51 lower approx33 = np.asarray(approx33 results[4:5][0])[0]
52 median approx33 = np.asarray(approx33 results[9:10][0])[0]
53 upper_approx33 = np.asarray(approx33_results[14:15][0])[0]
54
55 lower_exact33 = np.asarray(exact33_results[4:5][0])[0]
56 median exact33 = np.asarrav(exact33 results[9:10][0])[0]
```

```
36-376-3
57 upper exact33 = np.asarray(exact33 results[14:15][0])[0]
 1 # Iteration4:
 2
 3 \text{ slice4} = 3
 4
 5 approx4 = [simple_regret_approx_1[slice4],
 6
          simple_regret_approx_2[slice4],
 7
          simple_regret_approx_3[slice4],
 8
          simple_regret_approx_4[slice4],
 9
          simple regret approx 5[slice4],
10
          simple_regret_approx_6[slice4],
11
          simple_regret_approx_7[slice4],
12
          simple_regret_approx_8[slice4],
13
          simple regret approx 9[slice4],
14
          simple_regret_approx_10[slice4],
15
          simple_regret_approx_11[slice4],
16
          simple regret approx 12[slice4],
17
          simple_regret_approx_13[slice4],
18
          simple_regret_approx_14[slice4],
19
          simple_regret_approx_15[slice4],
20
          simple_regret_approx_16[slice4],
21
          simple_regret_approx_17[slice4],
22
          simple_regret_approx_18[slice4],
23
          simple_regret_approx_19[slice4],
24
          simple_regret_approx_20[slice4]]
25
26 exact4 = [simple regret exact 1[slice4],
27
          simple regret exact 2[slice4],
28
          simple_regret_exact_3[slice4],
29
          simple regret exact 4[slice4],
30
          simple_regret_exact_5[slice4],
31
          simple_regret_exact_6[slice4],
32
          simple_regret_exact_7[slice4],
33
          simple regret exact 8[slice4],
          simple_regret_exact_9[slice4],
34
35
          simple_regret_exact_10[slice4],
36
          simple regret exact 11[slice4],
37
          simple regret exact 12[slice4],
38
          simple_regret_exact_13[slice4],
39
          simple regret exact 14[slice4],
40
          simple_regret_exact_15[slice4],
41
          simple_regret_exact_16[slice4],
42
          simple regret exact 17[slice4],
43
          simple_regret_exact_18[slice4],
44
          simple_regret_exact_19[slice4],
45
          simple regret exact 20[slice4]]
46
47 approx4 results = pd.DataFrame(approx4).sort values(by=[0], ascending=False)
48 exact4_results = pd.DataFrame(exact4).sort_values(by=[0], ascending=False)
49
50 ### Best simple regret minimization IQR - approx:
51 lower approx4 = np.asarray(approx4 results[4:5][0])[0]
52 median approx4 = np.asarray(approx4 results[9:10][0])[0]
```

```
53 upper_approx4 = np.asarray(approx4_results[14:15][0])[0]
54
55 lower exact4 = np.asarray(exact4 results[4:5][0])[0]
56 median_exact4 = np.asarray(exact4_results[9:10][0])[0]
57 upper_exact4 = np.asarray(exact4_results[14:15][0])[0]
 1 # Iteration14:
 2
 3 \text{ slice} 14 = 13
 4
 5 approx14 = [simple_regret_approx_1[slice14],
 6
          simple_regret_approx_2[slice14],
 7
          simple regret approx 3[slice14],
 8
          simple regret approx 4[slice14],
 9
          simple_regret_approx_5[slice14],
10
          simple regret approx 6[slice14],
11
          simple_regret_approx_7[slice14],
12
          simple_regret_approx_8[slice14],
13
          simple_regret_approx_9[slice14],
14
          simple_regret_approx_10[slice14],
15
          simple_regret_approx_11[slice14],
16
          simple_regret_approx_12[slice14],
17
          simple_regret_approx_13[slice14],
18
          simple_regret_approx_14[slice14],
19
          simple_regret_approx_15[slice14],
20
          simple regret approx 16[slice14],
21
          simple_regret_approx_17[slice14],
22
          simple_regret_approx_18[slice14],
23
          simple regret approx 19[slice14],
24
          simple_regret_approx_20[slice14]]
25
26 exact14 = [simple_regret_exact_1[slice14],
27
          simple_regret_exact_2[slice14],
28
          simple_regret_exact_3[slice14],
29
          simple_regret_exact_4[slice14],
30
          simple regret exact 5[slice14],
31
          simple regret exact 6[slice14],
32
          simple_regret_exact_7[slice14],
33
          simple regret exact 8[slice14],
34
          simple regret exact 9[slice14],
35
          simple_regret_exact_10[slice14],
36
          simple regret exact 11[slice14],
37
          simple_regret_exact_12[slice14],
38
          simple_regret_exact_13[slice14],
39
          simple_regret_exact_14[slice14],
40
          simple regret exact 15[slice14],
41
          simple_regret_exact_16[slice14],
42
          simple_regret_exact_17[slice14],
43
          simple regret exact 18[slice14],
44
          simple regret exact 19[slice14],
45
          simple_regret_exact_20[slice14]]
46
47 approx14 results = pd.DataFrame(approx14).sort values(by=[0], ascending=False)
48 exact14_results = pd.DataFrame(exact14).sort_values(by=[0], ascending=False)
4Ω
```

```
45
50 ### Best simple regret minimization IQR - approx:
51 lower approx14 = np.asarray(approx14 results[4:5][0])[0]
52 median approx14 = np.asarray(approx14 results[9:10][0])[0]
53 upper approx14 = np.asarray(approx14 results[14:15][0])[0]
54
55 lower_exact14 = np.asarray(exact14_results[4:5][0])[0]
56 median exact14 = np.asarray(exact14 results[9:10][0])[0]
57 upper_exact14 = np.asarray(exact14_results[14:15][0])[0]
 1 # Iteration24 :
 3 \text{ slice} 24 = 23
 4
 5 approx24 = [simple_regret_approx_1[slice24],
 6
          simple_regret_approx_2[slice24],
 7
          simple_regret_approx_3[slice24],
 8
          simple_regret_approx_4[slice24],
 9
          simple_regret_approx_5[slice24],
10
          simple_regret_approx_6[slice24],
11
          simple_regret_approx_7[slice24],
12
          simple_regret_approx_8[slice24],
13
          simple_regret_approx_9[slice24],
14
          simple regret approx 10[slice24],
15
          simple regret approx 11[slice24],
16
          simple_regret_approx_12[slice24],
17
          simple_regret_approx_13[slice24],
18
          simple_regret_approx_14[slice24],
19
          simple_regret_approx_15[slice24],
20
          simple_regret_approx_16[slice24],
21
          simple_regret_approx_17[slice24],
22
          simple_regret_approx_18[slice24],
23
          simple_regret_approx_19[slice24],
24
          simple regret approx 20[slice24]]
25
26 exact24 = [simple regret exact 1[slice24],
27
          simple regret exact 2[slice24],
28
          simple regret exact 3[slice24],
          simple_regret_exact_4[slice24],
29
30
          simple_regret_exact_5[slice24],
31
          simple regret exact 6[slice24],
32
          simple_regret_exact_7[slice24],
33
          simple_regret_exact_8[slice24],
34
          simple regret exact 9[slice24],
35
          simple regret exact 10[slice24],
36
          simple_regret_exact_11[slice24],
37
          simple regret exact 12[slice24],
38
          simple regret exact 13[slice24],
39
          simple regret exact 14[slice24],
40
          simple regret exact 15[slice24],
41
          simple regret exact 16[slice24],
42
          simple regret exact 17[slice24],
43
          simple_regret_exact_18[slice24],
44
          simple regret exact 19[slice24],
45
          simple regret exact 20[slice24]]
```

```
46
47 approx24 results = pd.DataFrame(approx24).sort values(by=[0], ascending=False)
48 exact24 results = pd.DataFrame(exact24).sort values(by=[0], ascending=False)
49
50 ### Best simple regret minimization IQR - approx:
51 lower_approx24 = np.asarray(approx24_results[4:5][0])[0]
52 median_approx24 = np.asarray(approx24_results[9:10][0])[0]
53 upper_approx24 = np.asarray(approx24_results[14:15][0])[0]
54
55 lower_exact24 = np.asarray(exact24_results[4:5][0])[0]
56 median exact24 = np.asarray(exact24 results[9:10][0])[0]
57 upper_exact24 = np.asarray(exact24_results[14:15][0])[0]
 1 # Iteration34:
 2
 3 \text{ slice} 34 = 33
 4
 5 approx34 = [simple_regret_approx_1[slice34],
 6
          simple_regret_approx_2[slice34],
 7
          simple_regret_approx_3[slice34],
 8
          simple_regret_approx_4[slice34],
 9
          simple_regret_approx_5[slice34],
10
          simple_regret_approx_6[slice34],
11
          simple_regret_approx_7[slice34],
12
          simple_regret_approx_8[slice34],
13
          simple_regret_approx_9[slice34],
14
          simple_regret_approx_10[slice34],
15
          simple_regret_approx_11[slice34],
16
          simple_regret_approx_12[slice34],
17
          simple_regret_approx_13[slice34],
18
          simple_regret_approx_14[slice34],
19
          simple_regret_approx_15[slice34],
20
          simple_regret_approx_16[slice34],
21
          simple_regret_approx_17[slice34],
22
          simple regret approx 18[slice34],
23
          simple_regret_approx_19[slice34],
24
          simple_regret_approx_20[slice34]]
25
26 exact34 = [simple regret exact 1[slice34],
27
          simple_regret_exact_2[slice34],
28
          simple regret exact 3[slice34],
29
          simple regret exact 4[slice34],
30
          simple_regret_exact_5[slice34],
31
          simple_regret_exact_6[slice34],
32
          simple regret exact 7[slice34],
33
          simple regret exact 8[slice34],
34
          simple_regret_exact_9[slice34],
35
          simple regret exact 10[slice34],
36
          simple regret exact 11[slice34],
37
          simple_regret_exact_12[slice34],
38
          simple regret exact 13[slice34],
39
          simple_regret_exact_14[slice34],
40
          simple_regret_exact_15[slice34],
41
          simple_regret_exact_16[slice34],
```

```
6/14/2021
                                         3. Rosenbrock GP El.ipynb - Colaboratory
   42
              simple regret exact 17[slice34],
   43
              simple regret exact 18[slice34],
              simple regret exact 19[slice34],
   44
   45
              simple regret exact 20[slice34]]
   46
   47 approx34 results = pd.DataFrame(approx34).sort values(by=[0], ascending=False)
   48 exact34_results = pd.DataFrame(exact34).sort_values(by=[0], ascending=False)
   49
   50 ### Best simple regret minimization IQR - approx:
   51 lower approx34 = np.asarray(approx34 results[4:5][0])[0]
   52 median_approx34 = np.asarray(approx34_results[9:10][0])[0]
   53 upper_approx34 = np.asarray(approx34_results[14:15][0])[0]
   54
   55 lower exact34 = np.asarray(exact34 results[4:5][0])[0]
   56 median_exact34 = np.asarray(exact34_results[9:10][0])[0]
   57 upper_exact34 = np.asarray(exact34_results[14:15][0])[0]
     1 # Iteration5 :
     2
     3 \text{ slice5} = 4
     4
     5 approx5 = [simple_regret_approx_1[slice5],
     6
              simple regret approx 2[slice5],
     7
              simple_regret_approx_3[slice5],
     8
              simple_regret_approx_4[slice5],
     9
              simple_regret_approx_5[slice5],
   10
              simple_regret_approx_6[slice5],
              simple_regret_approx_7[slice5],
   11
   12
              simple_regret_approx_8[slice5],
   13
              simple_regret_approx_9[slice5],
   14
              simple_regret_approx_10[slice5],
   15
              simple_regret_approx_11[slice5],
   16
              simple regret approx 12[slice5],
   17
              simple_regret_approx_13[slice5],
   18
              simple regret approx 14[slice5],
   19
              simple regret approx 15[slice5],
   20
              simple regret approx 16[slice5],
   21
              simple_regret_approx_17[slice5],
   22
              simple_regret_approx_18[slice5],
   23
              simple regret approx 19[slice5],
   24
              simple_regret_approx_20[slice5]]
   25
   26 exact5 = [simple regret exact 1[slice5],
   27
              simple regret exact 2[slice5],
   28
              simple regret exact 3[slice5],
   29
              simple regret exact 4[slice5],
   30
              simple regret exact 5[slice5],
   31
              simple regret exact 6[slice5],
   32
              simple_regret_exact_7[slice5],
   33
              simple regret exact 8[slice5],
   34
              simple_regret_exact_9[slice5],
   35
              simple_regret_exact_10[slice5],
   36
              simple regret exact 11[slice5],
   37
              simple_regret_exact_12[slice5],
    38
              simple regret exact 13[slice5]
```

```
6/14/2021
                                         3. Rosenbrock GP El.ipynb - Colaboratory
              JIMPIC_1 C81 CC_CNGCC_IJ[JIICCJ],
    ںر
   39
              simple regret exact 14[slice5],
   40
              simple_regret_exact_15[slice5],
   41
              simple_regret_exact_16[slice5],
   42
              simple regret exact 17[slice5],
   43
              simple_regret_exact_18[slice5],
   44
              simple_regret_exact_19[slice5],
   45
              simple_regret_exact_20[slice5]]
   46
   47 approx5_results = pd.DataFrame(approx5).sort_values(by=[0], ascending=False)
   48 exact5 results = pd.DataFrame(exact5).sort values(by=[0], ascending=False)
   49
   50 ### Best simple regret minimization IQR - approx:
   51 lower_approx5 = np.asarray(approx5_results[4:5][0])[0]
   52 median_approx5 = np.asarray(approx5_results[9:10][0])[0]
   53 upper_approx5 = np.asarray(approx5_results[14:15][0])[0]
   54
   55 lower exact5 = np.asarray(exact5 results[4:5][0])[0]
   56 median_exact5 = np.asarray(exact5_results[9:10][0])[0]
   57 upper_exact5 = np.asarray(exact5_results[14:15][0])[0]
     1 # Iteration15 :
     2
     3 \text{ slice} 15 = 14
     4
     5 approx15 = [simple_regret_approx_1[slice15],
     6
              simple_regret_approx_2[slice15],
     7
              simple_regret_approx_3[slice15],
     8
              simple_regret_approx_4[slice15],
     9
              simple_regret_approx_5[slice15],
   10
              simple_regret_approx_6[slice15],
   11
              simple regret approx 7[slice15],
   12
              simple_regret_approx_8[slice15],
   13
              simple_regret_approx_9[slice15],
   14
              simple_regret_approx_10[slice15],
   15
              simple_regret_approx_11[slice15],
   16
              simple_regret_approx_12[slice15],
   17
              simple regret approx 13[slice15],
   18
              simple_regret_approx_14[slice15],
   19
              simple_regret_approx_15[slice15],
   20
              simple regret approx 16[slice15],
   21
              simple regret approx 17[slice15],
   22
              simple regret approx 18[slice15],
   23
              simple_regret_approx_19[slice15],
   24
              simple regret approx 20[slice15]]
   25
   26 exact15 = [simple_regret_exact_1[slice15],
   27
              simple regret exact 2[slice15],
   28
              simple_regret_exact_3[slice15],
   29
              simple_regret_exact_4[slice15],
   30
              simple regret exact 5[slice15],
   31
              simple regret exact 6[slice15],
   32
              simple_regret_exact_7[slice15],
   33
              simple regret exact 8[slice15],
              simple regret exact 9[slice15],
   34
```

```
35
          simple_regret_exact_10[slice15],
36
          simple regret exact 11[slice15],
37
          simple_regret_exact_12[slice15],
38
          simple_regret_exact_13[slice15],
39
          simple regret exact 14[slice15],
40
          simple_regret_exact_15[slice15],
          simple_regret_exact_16[slice15],
41
42
          simple_regret_exact_17[slice15],
43
          simple regret exact 18[slice15],
44
          simple_regret_exact_19[slice15],
45
          simple_regret_exact_20[slice15]]
46
47 approx15_results = pd.DataFrame(approx15).sort_values(by=[0], ascending=False)
48 exact15_results = pd.DataFrame(exact15).sort_values(by=[0], ascending=False)
49
50 ### Best simple regret minimization IQR - approx:
51 lower_approx15 = np.asarray(approx15_results[4:5][0])[0]
52 median_approx15 = np.asarray(approx15_results[9:10][0])[0]
53 upper_approx15 = np.asarray(approx15_results[14:15][0])[0]
54
55 lower_exact15 = np.asarray(exact15_results[4:5][0])[0]
56 median exact15 = np.asarray(exact15 results[9:10][0])[0]
57 upper_exact15 = np.asarray(exact15_results[14:15][0])[0]
 1 # Iteration25 :
 2
 3 \text{ slice25} = 24
 4
 5 approx25 = [simple regret approx 1[slice25],
 6
          simple_regret_approx_2[slice25],
 7
          simple_regret_approx_3[slice25],
 8
          simple regret approx 4[slice25],
 9
          simple_regret_approx_5[slice25],
10
          simple_regret_approx_6[slice25],
          simple regret approx 7[slice25],
11
12
          simple regret approx 8[slice25],
13
          simple_regret_approx_9[slice25],
14
          simple regret approx 10[slice25],
15
          simple regret approx 11[slice25],
16
          simple regret approx 12[slice25],
17
          simple_regret_approx_13[slice25],
18
          simple regret approx 14[slice25],
19
          simple regret approx 15[slice25],
20
          simple_regret_approx_16[slice25],
21
          simple regret approx 17[slice25],
22
          simple_regret_approx_18[slice25],
23
          simple_regret_approx_19[slice25],
24
          simple regret approx 20[slice25]]
25
26 exact25 = [simple regret exact 1[slice25],
27
          simple_regret_exact_2[slice25],
28
          simple regret exact 3[slice25],
29
          simple_regret_exact_4[slice25],
30
          simple_regret_exact_5[slice25],
```

```
6/14/2021
                                         3. Rosenbrock GP El.ipynb - Colaboratory
              simple_regret_exact_6[slice25],
   31
   32
              simple_regret_exact_7[slice25],
   33
              simple_regret_exact_8[slice25],
   34
              simple regret exact 9[slice25],
   35
              simple_regret_exact_10[slice25],
   36
              simple_regret_exact_11[slice25],
              simple regret exact 12[slice25],
   37
   38
              simple regret exact 13[slice25],
   39
              simple_regret_exact_14[slice25],
   40
              simple regret exact 15[slice25],
   41
              simple_regret_exact_16[slice25],
   42
              simple_regret_exact_17[slice25],
   43
              simple_regret_exact_18[slice25],
   44
              simple_regret_exact_19[slice25],
   45
              simple_regret_exact_20[slice25]]
   46
   47 approx25 results = pd.DataFrame(approx25).sort values(by=[0], ascending=False)
   48 exact25_results = pd.DataFrame(exact25).sort_values(by=[0], ascending=False)
   49
   50 ### Best simple regret minimization IQR - approx:
   51 lower approx25 = np.asarray(approx25 results[4:5][0])[0]
   52 median_approx25 = np.asarray(approx25_results[9:10][0])[0]
   53 upper approx25 = np.asarray(approx25 results[14:15][0])[0]
   54
   55 lower_exact25 = np.asarray(exact25_results[4:5][0])[0]
   56 median_exact25 = np.asarray(exact25_results[9:10][0])[0]
   57 upper_exact25 = np.asarray(exact25_results[14:15][0])[0]
     1 # Iteration35 :
     2
     3 \text{ slice} 35 = 34
     4
     5 approx35 = [simple_regret_approx_1[slice35],
     6
              simple_regret_approx_2[slice35],
     7
              simple regret approx 3[slice35],
     8
              simple_regret_approx_4[slice35],
     9
              simple regret approx 5[slice35],
   10
              simple regret approx 6[slice35],
   11
              simple_regret_approx_7[slice35],
   12
              simple regret approx 8[slice35],
   13
              simple regret approx 9[slice35],
   14
              simple_regret_approx_10[slice35],
   15
              simple regret approx 11[slice35],
   16
              simple_regret_approx_12[slice35],
   17
              simple_regret_approx_13[slice35],
   18
              simple_regret_approx_14[slice35],
   19
              simple regret approx 15[slice35],
   20
              simple_regret_approx_16[slice35],
              simple_regret_approx_17[slice35],
   21
   22
              simple regret approx 18[slice35],
   23
              simple regret approx 19[slice35],
   24
              simple regret approx 20[slice35]]
   25
   26 exact35 = [simple_regret_exact_1[slice35],
   27
              simple regret exact 2[slice35].
```

```
simple_regret_approx_20[slice6]]
24
25
26 exact6 = [simple regret exact 1[slice6],
27
          simple regret exact 2[slice6],
28
          simple_regret_exact_3[slice6],
29
          simple regret exact 4[slice6],
30
          simple_regret_exact_5[slice6],
31
          simple_regret_exact_6[slice6],
32
          simple_regret_exact_7[slice6],
33
          simple_regret_exact_8[slice6],
34
          simple_regret_exact_9[slice6],
35
          simple regret exact 10[slice6],
36
          simple_regret_exact_11[slice6],
37
          simple_regret_exact_12[slice6],
38
          simple_regret_exact_13[slice6],
39
          simple regret exact 14[slice6],
40
          simple_regret_exact_15[slice6],
41
          simple_regret_exact_16[slice6],
42
          simple_regret_exact_17[slice6],
43
          simple_regret_exact_18[slice6],
44
          simple_regret_exact_19[slice6],
45
          simple_regret_exact_20[slice6]]
46
47 approx6_results = pd.DataFrame(approx6).sort_values(by=[0], ascending=False)
48 exact6_results = pd.DataFrame(exact6).sort_values(by=[0], ascending=False)
49
50 ### Best simple regret minimization IQR - approx:
51 lower_approx6 = np.asarray(approx6_results[4:5][0])[0]
52 median approx6 = np.asarray(approx6 results[9:10][0])[0]
53 upper_approx6 = np.asarray(approx6_results[14:15][0])[0]
54
55 lower exact6 = np.asarray(exact6 results[4:5][0])[0]
56 median_exact6 = np.asarray(exact6_results[9:10][0])[0]
57 upper_exact6 = np.asarray(exact6_results[14:15][0])[0]
 1 # Iteration16:
 2
 3 \text{ slice} 16 = 15
 4
 5 approx16 = [simple_regret_approx_1[slice16],
 6
          simple_regret_approx_2[slice16],
 7
          simple regret approx 3[slice16],
 8
          simple regret approx 4[slice16],
 9
          simple_regret_approx_5[slice16],
10
          simple_regret_approx_6[slice16],
11
          simple regret approx 7[slice16],
12
          simple regret approx 8[slice16],
13
          simple regret approx 9[slice16],
14
          simple regret approx 10[slice16],
15
          simple regret approx 11[slice16],
16
          simple_regret_approx_12[slice16],
17
          simple regret approx 13[slice16],
18
          simple_regret_approx_14[slice16],
19
          simple_regret_approx_15[slice16],
20
```

```
6/14/2021
                                         3. Rosenbrock GP El.ipynb - Colaboratory
              simple regret approx idjsilceid,
    20
   21
              simple_regret_approx_17[slice16],
   22
              simple regret approx 18[slice16],
   23
              simple regret approx 19[slice16],
              simple_regret_approx_20[slice16]]
   24
   25
   26 exact16 = [simple regret exact 1[slice16],
   27
              simple_regret_exact_2[slice16],
   28
              simple_regret_exact_3[slice16],
   29
              simple_regret_exact_4[slice16],
   30
              simple_regret_exact_5[slice16],
   31
              simple_regret_exact_6[slice16],
   32
              simple_regret_exact_7[slice16],
   33
              simple regret exact 8[slice16],
   34
              simple regret exact 9[slice16],
   35
              simple_regret_exact_10[slice16],
   36
              simple regret exact 11[slice16],
   37
              simple_regret_exact_12[slice16],
   38
              simple_regret_exact_13[slice16],
   39
              simple_regret_exact_14[slice16],
   40
              simple_regret_exact_15[slice16],
   41
              simple_regret_exact_16[slice16],
   42
              simple_regret_exact_17[slice16],
   43
              simple_regret_exact_18[slice16],
   44
              simple_regret_exact_19[slice16],
   45
              simple_regret_exact_20[slice16]]
   46
   47 approx16 results = pd.DataFrame(approx16).sort values(by=[0], ascending=False)
   48 exact16_results = pd.DataFrame(exact16).sort_values(by=[0], ascending=False)
   49
   50 ### Best simple regret minimization IQR - approx:
   51 lower_approx16 = np.asarray(approx16_results[4:5][0])[0]
   52 median_approx16 = np.asarray(approx16_results[9:10][0])[0]
   53 upper_approx16 = np.asarray(approx16_results[14:15][0])[0]
   54
   55 lower exact16 = np.asarray(exact16 results[4:5][0])[0]
   56 median exact16 = np.asarray(exact16 results[9:10][0])[0]
   57 upper exact16 = np.asarray(exact16 results[14:15][0])[0]
     1 # Iteration26 :
     2
     3 \text{ slice} 26 = 25
     4
     5 approx26 = [simple regret approx 1[slice26],
              simple regret approx 2[slice26],
     6
     7
              simple regret approx 3[slice26],
     8
              simple regret approx 4[slice26],
     9
              simple regret approx 5[slice26],
   10
              simple_regret_approx_6[slice26],
   11
              simple regret approx 7[slice26],
   12
              simple_regret_approx_8[slice26],
   13
              simple_regret_approx_9[slice26],
   14
              simple_regret_approx_10[slice26],
   15
              simple_regret_approx_11[slice26],
              simple regret approx 12[slice26],
   16
```

```
simple regret approx 13[slice26],
17
18
          simple regret approx 14[slice26],
19
          simple_regret_approx_15[slice26],
20
          simple_regret_approx_16[slice26],
21
          simple_regret_approx_17[slice26],
22
          simple_regret_approx_18[slice26],
23
          simple_regret_approx_19[slice26],
24
          simple_regret_approx_20[slice26]]
25
26 exact26 = [simple_regret_exact_1[slice26],
          simple regret exact 2[slice26],
27
          simple_regret_exact_3[slice26],
28
29
          simple_regret_exact_4[slice26],
30
          simple_regret_exact_5[slice26],
31
          simple_regret_exact_6[slice26],
32
          simple_regret_exact_7[slice26],
33
          simple_regret_exact_8[slice26],
34
          simple_regret_exact_9[slice26],
35
          simple_regret_exact_10[slice26],
          simple_regret_exact_11[slice26],
36
37
          simple_regret_exact_12[slice26],
          simple_regret_exact_13[slice26],
38
          simple_regret_exact_14[slice26],
39
40
          simple regret exact 15[slice26],
41
          simple_regret_exact_16[slice26],
42
          simple_regret_exact_17[slice26],
43
          simple_regret_exact_18[slice26],
44
          simple_regret_exact_19[slice26],
45
          simple_regret_exact_20[slice26]]
46
47 approx26_results = pd.DataFrame(approx26).sort_values(by=[0], ascending=False)
48 exact26_results = pd.DataFrame(exact26).sort_values(by=[0], ascending=False)
49
50 ### Best simple regret minimization IQR - approx:
51 lower_approx26 = np.asarray(approx26_results[4:5][0])[0]
52 median approx26 = np.asarray(approx26 results[9:10][0])[0]
53 upper approx26 = np.asarray(approx26 results[14:15][0])[0]
54
55 lower_exact26 = np.asarray(exact26_results[4:5][0])[0]
56 median_exact26 = np.asarray(exact26_results[9:10][0])[0]
57 upper_exact26 = np.asarray(exact26_results[14:15][0])[0]
 1 # Iteration36 :
 2
 3 \text{ slice} 36 = 35
 4
 5 approx36 = [simple_regret_approx_1[slice36],
 6
          simple regret approx 2[slice36],
 7
          simple_regret_approx_3[slice36],
 8
          simple_regret_approx_4[slice36],
 9
          simple regret approx 5[slice36],
10
          simple regret approx 6[slice36],
11
          simple_regret_approx_7[slice36],
12
          simple regret approx 8[slice36],
```

```
6/14/2021
                                         3. Rosenbrock GP El.ipynb - Colaboratory
   13
              simple regret approx 9[slice36],
   14
              simple_regret_approx_10[slice36],
   15
              simple regret approx 11[slice36],
   16
              simple_regret_approx_12[slice36],
   17
              simple_regret_approx_13[slice36],
   18
              simple regret approx 14[slice36],
   19
              simple_regret_approx_15[slice36],
   20
              simple_regret_approx_16[slice36],
   21
              simple_regret_approx_17[slice36],
   22
              simple regret approx 18[slice36],
   23
              simple_regret_approx_19[slice36],
   24
              simple_regret_approx_20[slice36]]
   25
   26 exact36 = [simple_regret_exact_1[slice36],
   27
              simple_regret_exact_2[slice36],
   28
              simple_regret_exact_3[slice36],
   29
              simple_regret_exact_4[slice36],
   30
              simple_regret_exact_5[slice36],
   31
              simple regret exact 6[slice36],
   32
              simple_regret_exact_7[slice36],
   33
              simple_regret_exact_8[slice36],
   34
              simple_regret_exact_9[slice36],
   35
              simple regret exact 10[slice36],
   36
              simple regret exact 11[slice36],
   37
              simple_regret_exact_12[slice36],
   38
              simple regret exact 13[slice36],
   39
              simple_regret_exact_14[slice36],
   40
              simple_regret_exact_15[slice36],
   41
              simple regret exact 16[slice36],
   42
              simple_regret_exact_17[slice36],
   43
              simple_regret_exact_18[slice36],
   44
              simple_regret_exact_19[slice36],
   45
              simple_regret_exact_20[slice36]]
   46
   47 approx36_results = pd.DataFrame(approx36).sort_values(by=[0], ascending=False)
   48 exact36 results = pd.DataFrame(exact36).sort values(by=[0], ascending=False)
   49
   50 ### Best simple regret minimization IQR - approx:
   51 lower approx36 = np.asarray(approx36 results[4:5][0])[0]
   52 median approx36 = np.asarray(approx36 results[9:10][0])[0]
   53 upper_approx36 = np.asarray(approx36_results[14:15][0])[0]
   54
   55 lower exact36 = np.asarray(exact36 results[4:5][0])[0]
   56 median exact36 = np.asarray(exact36 results[9:10][0])[0]
   57 upper_exact36 = np.asarray(exact36_results[14:15][0])[0]
     1 # Iteration7 :
     2
     3 \text{ slice7} = 6
     4
     5 approx7 = [simple_regret_approx_1[slice7],
     6
              simple_regret_approx_2[slice7],
     7
              simple regret approx 3[slice7],
     8
              simple regret approx 4[slice7],
              cimple regret annov 5[clice7]
```

```
6/14/2021
                                         3. Rosenbrock GP El.ipynb - Colaboratory
              otilibie i eki er ahhi ny o otice, 1
   10
              simple_regret_approx_6[slice7],
   11
              simple_regret_approx_7[slice7],
   12
              simple_regret_approx_8[slice7],
   13
              simple_regret_approx_9[slice7],
   14
              simple_regret_approx_10[slice7],
   15
              simple_regret_approx_11[slice7],
              simple regret approx 12[slice7],
   16
   17
              simple_regret_approx_13[slice7],
   18
              simple_regret_approx_14[slice7],
   19
              simple regret approx 15[slice7],
   20
              simple_regret_approx_16[slice7],
   21
              simple_regret_approx_17[slice7],
   22
              simple regret approx 18[slice7],
   23
              simple_regret_approx_19[slice7],
   24
              simple_regret_approx_20[slice7]]
   25
   26 exact7 = [simple regret exact 1[slice7],
   27
              simple_regret_exact_2[slice7],
   28
              simple_regret_exact_3[slice7],
   29
              simple regret exact 4[slice7],
   30
              simple_regret_exact_5[slice7],
   31
              simple_regret_exact_6[slice7],
   32
              simple regret exact 7[slice7],
   33
              simple_regret_exact_8[slice7],
   34
              simple_regret_exact_9[slice7],
   35
              simple_regret_exact_10[slice7],
   36
              simple_regret_exact_11[slice7],
   37
              simple_regret_exact_12[slice7],
   38
              simple_regret_exact_13[slice7],
   39
              simple regret exact 14[slice7],
   40
              simple_regret_exact_15[slice7],
   41
              simple_regret_exact_16[slice7],
   42
              simple regret exact 17[slice7],
   43
              simple_regret_exact_18[slice7],
   44
              simple_regret_exact_19[slice7],
   45
              simple regret exact 20[slice7]]
   46
   47 approx7_results = pd.DataFrame(approx7).sort_values(by=[0], ascending=False)
   48 exact7_results = pd.DataFrame(exact7).sort_values(by=[0], ascending=False)
   49
   50 ### Best simple regret minimization IQR - approx:
   51 lower_approx7 = np.asarray(approx7_results[4:5][0])[0]
   52 median approx7 = np.asarray(approx7 results[9:10][0])[0]
   53 upper approx7 = np.asarray(approx7 results[14:15][0])[0]
   54
   55 lower exact7 = np.asarray(exact7 results[4:5][0])[0]
   56 median exact7 = np.asarray(exact7 results[9:10][0])[0]
   57 upper_exact7 = np.asarray(exact7_results[14:15][0])[0]
     1 # Iteration17 :
     2
     3 \text{ slice} 17 = 16
     4
     5 approx17 = [simple regret approx 1[slice17],
```

```
6
          simple_regret_approx_2[slice17],
 7
          simple regret approx 3[slice17],
 8
          simple_regret_approx_4[slice17],
 9
          simple_regret_approx_5[slice17],
10
          simple regret approx 6[slice17],
11
          simple regret approx 7[slice17],
12
          simple_regret_approx_8[slice17],
13
          simple regret approx 9[slice17],
14
          simple_regret_approx_10[slice17],
15
          simple_regret_approx_11[slice17],
16
          simple_regret_approx_12[slice17],
17
          simple_regret_approx_13[slice17],
18
          simple_regret_approx_14[slice17],
19
          simple_regret_approx_15[slice17],
20
          simple_regret_approx_16[slice17],
21
          simple_regret_approx_17[slice17],
22
          simple_regret_approx_18[slice17],
23
          simple regret approx 19[slice17],
24
          simple regret approx 20[slice17]]
25
26 exact17 = [simple_regret_exact_1[slice17],
27
          simple regret exact 2[slice17],
28
          simple_regret_exact_3[slice17],
29
          simple_regret_exact_4[slice17],
30
          simple_regret_exact_5[slice17],
31
          simple_regret_exact_6[slice17],
32
          simple_regret_exact_7[slice17],
33
          simple regret exact 8[slice17],
34
          simple_regret_exact_9[slice17],
35
          simple_regret_exact_10[slice17],
36
          simple_regret_exact_11[slice17],
37
          simple regret exact 12[slice17],
38
          simple_regret_exact_13[slice17],
39
          simple_regret_exact_14[slice17],
40
          simple regret exact 15[slice17],
41
          simple_regret_exact_16[slice17],
42
          simple_regret_exact_17[slice17],
43
          simple regret exact 18[slice17],
44
          simple regret exact 19[slice17],
45
          simple_regret_exact_20[slice17]]
46
47 approx17 results = pd.DataFrame(approx17).sort values(by=[0], ascending=False)
48 exact17_results = pd.DataFrame(exact17).sort_values(by=[0], ascending=False)
49
50 ### Best simple regret minimization IQR - approx:
51 lower_approx17 = np.asarray(approx17_results[4:5][0])[0]
52 median_approx17 = np.asarray(approx17_results[9:10][0])[0]
53 upper approx17 = np.asarray(approx17 results[14:15][0])[0]
54
55 lower_exact17 = np.asarray(exact17_results[4:5][0])[0]
56 median exact17 = np.asarray(exact17 results[9:10][0])[0]
57 upper_exact17 = np.asarray(exact17_results[14:15][0])[0]
```

1 # Iteration27 :

56 median_exact27 = np.asarray(exact27_results[9:10][0])[0]

```
57 upper_exact27 = np.asarray(exact27_results[14:15][0])[0]
```

```
1 # Iteration37 :
 3 \text{ slice} 37 = 36
 4
 5 approx37 = [simple_regret_approx_1[slice37],
 6
          simple_regret_approx_2[slice37],
 7
          simple_regret_approx_3[slice37],
 8
          simple_regret_approx_4[slice37],
 9
          simple_regret_approx_5[slice37],
10
          simple_regret_approx_6[slice37],
11
          simple_regret_approx_7[slice37],
12
          simple regret approx 8[slice37],
13
          simple regret approx 9[slice37],
14
          simple_regret_approx_10[slice37],
15
          simple regret approx 11[slice37],
16
          simple_regret_approx_12[slice37],
17
          simple_regret_approx_13[slice37],
18
          simple_regret_approx_14[slice37],
19
          simple_regret_approx_15[slice37],
20
          simple_regret_approx_16[slice37],
21
          simple_regret_approx_17[slice37],
22
          simple_regret_approx_18[slice37],
23
          simple_regret_approx_19[slice37],
24
          simple_regret_approx_20[slice37]]
25
26 exact37 = [simple regret exact 1[slice37],
27
          simple_regret_exact_2[slice37],
28
          simple regret exact 3[slice37],
29
          simple_regret_exact_4[slice37],
30
          simple_regret_exact_5[slice37],
31
          simple_regret_exact_6[slice37],
32
          simple_regret_exact_7[slice37],
33
          simple regret exact 8[slice37],
34
          simple_regret_exact_9[slice37],
35
          simple regret exact 10[slice37],
36
          simple regret exact 11[slice37],
37
          simple_regret_exact_12[slice37],
38
          simple regret exact 13[slice37],
39
          simple_regret_exact_14[slice37],
40
          simple_regret_exact_15[slice37],
41
          simple regret exact 16[slice37],
42
          simple_regret_exact_17[slice37],
43
          simple_regret_exact_18[slice37],
44
          simple_regret_exact_19[slice37],
45
          simple regret exact 20[slice37]]
46
47 approx37_results = pd.DataFrame(approx37).sort_values(by=[0], ascending=False)
48 exact37 results = pd.DataFrame(exact37).sort values(by=[0], ascending=False)
49
50 ### Best simple regret minimization IQR - approx:
51 lower approx37 = np.asarray(approx37 results[4:5][0])[0]
52 median_approx37 = np.asarray(approx37_results[9:10][0])[0]
53 upper approx37 = np.asarrav(approx37 results[14:15][0])[0]
```

```
54
55 lower_exact37 = np.asarray(exact37_results[4:5][0])[0]
56 median_exact37 = np.asarray(exact37_results[9:10][0])[0]
57 upper exact37 = np.asarray(exact37 results[14:15][0])[0]
 1 # Iteration8 :
 2
 3 \text{ slice8} = 7
 4
 5 approx8 = [simple_regret_approx_1[slice8],
 6
          simple regret approx 2[slice8],
 7
          simple_regret_approx_3[slice8],
 8
          simple_regret_approx_4[slice8],
 9
          simple regret approx 5[slice8],
10
          simple_regret_approx_6[slice8],
11
          simple_regret_approx_7[slice8],
12
          simple_regret_approx_8[slice8],
13
          simple_regret_approx_9[slice8],
14
          simple_regret_approx_10[slice8],
15
          simple_regret_approx_11[slice8],
          simple_regret_approx_12[slice8],
16
17
          simple_regret_approx_13[slice8],
          simple_regret_approx_14[slice8],
18
19
          simple regret approx 15[slice8],
20
          simple_regret_approx_16[slice8],
21
          simple_regret_approx_17[slice8],
22
          simple_regret_approx_18[slice8],
23
          simple_regret_approx_19[slice8],
24
          simple_regret_approx_20[slice8]]
25
26 exact8 = [simple_regret_exact_1[slice8],
27
          simple_regret_exact_2[slice8],
28
          simple_regret_exact_3[slice8],
29
          simple_regret_exact_4[slice8],
30
          simple regret exact 5[slice8],
31
          simple_regret_exact_6[slice8],
32
          simple regret exact 7[slice8],
33
          simple regret exact 8[slice8],
34
          simple_regret_exact_9[slice8],
35
          simple_regret_exact_10[slice8],
36
          simple_regret_exact_11[slice8],
37
          simple_regret_exact_12[slice8],
38
          simple_regret_exact_13[slice8],
39
          simple regret exact 14[slice8],
40
          simple_regret_exact_15[slice8],
41
          simple_regret_exact_16[slice8],
42
          simple regret exact 17[slice8],
43
          simple regret exact 18[slice8],
44
          simple_regret_exact_19[slice8],
45
          simple_regret_exact_20[slice8]]
46
47 approx8_results = pd.DataFrame(approx8).sort_values(by=[0], ascending=False)
48 exact8_results = pd.DataFrame(exact8).sort_values(by=[0], ascending=False)
49
```

```
50 ### Best simple regret minimization IQR - approx:
51 lower approx8 = np.asarray(approx8 results[4:5][0])[0]
52 median approx8 = np.asarray(approx8 results[9:10][0])[0]
53 upper_approx8 = np.asarray(approx8_results[14:15][0])[0]
54
55 lower exact8 = np.asarray(exact8 results[4:5][0])[0]
56 median_exact8 = np.asarray(exact8_results[9:10][0])[0]
57 upper_exact8 = np.asarray(exact8_results[14:15][0])[0]
 1 # Iteration18:
 2
 3 \text{ slice} 18 = 17
 4
 5 approx18 = [simple_regret_approx_1[slice18],
 6
          simple_regret_approx_2[slice18],
 7
          simple_regret_approx_3[slice18],
 8
          simple_regret_approx_4[slice18],
 9
          simple_regret_approx_5[slice18],
10
          simple_regret_approx_6[slice18],
11
          simple_regret_approx_7[slice18],
12
          simple_regret_approx_8[slice18],
13
          simple_regret_approx_9[slice18],
14
          simple_regret_approx_10[slice18],
15
          simple_regret_approx_11[slice18],
16
          simple_regret_approx_12[slice18],
17
          simple_regret_approx_13[slice18],
18
          simple_regret_approx_14[slice18],
19
          simple_regret_approx_15[slice18],
20
          simple_regret_approx_16[slice18],
21
          simple_regret_approx_17[slice18],
22
          simple_regret_approx_18[slice18],
23
          simple_regret_approx_19[slice18],
24
          simple_regret_approx_20[slice18]]
25
26 exact18 = [simple regret exact 1[slice18],
27
          simple regret exact 2[slice18],
28
          simple regret exact 3[slice18],
29
          simple_regret_exact_4[slice18],
30
          simple regret exact 5[slice18],
31
          simple_regret_exact_6[slice18],
32
          simple_regret_exact_7[slice18],
33
          simple regret exact 8[slice18],
34
          simple regret exact 9[slice18],
35
          simple_regret_exact_10[slice18],
          simple_regret_exact_11[slice18],
36
37
          simple regret exact 12[slice18],
38
          simple regret exact 13[slice18],
39
          simple regret exact 14[slice18],
40
          simple regret exact 15[slice18],
41
          simple regret exact 16[slice18],
42
          simple_regret_exact_17[slice18],
43
          simple regret exact 18[slice18],
44
          simple_regret_exact_19[slice18],
45
          simple_regret_exact_20[slice18]]
```

simple_regret_exact_12[slice38],

37

38

```
6/14/2021
                                         3. Rosenbrock GP El.ipynb - Colaboratory
    39
              simple_regret_exact_14[slice38],
   40
              simple_regret_exact_15[slice38],
              simple regret exact 16[slice38],
   41
   42
              simple_regret_exact_17[slice38],
   43
              simple_regret_exact_18[slice38],
   44
              simple regret exact 19[slice38],
   45
              simple_regret_exact_20[slice38]]
   46
   47 approx38_results = pd.DataFrame(approx38).sort_values(by=[0], ascending=False)
   48 exact38 results = pd.DataFrame(exact38).sort values(by=[0], ascending=False)
   49
   50 ### Best simple regret minimization IQR - approx:
   51 lower approx38 = np.asarray(approx38 results[4:5][0])[0]
   52 median approx38 = np.asarray(approx38 results[9:10][0])[0]
   53 upper_approx38 = np.asarray(approx38_results[14:15][0])[0]
   54
   55 lower_exact38 = np.asarray(exact38_results[4:5][0])[0]
   56 median_exact38 = np.asarray(exact38_results[9:10][0])[0]
   57 upper_exact38 = np.asarray(exact38_results[14:15][0])[0]
     1 # Iteration9 :
     2
     3 \text{ slice} 9 = 8
     4
     5 approx9 = [simple_regret_approx_1[slice9],
     6
              simple regret approx 2[slice9],
     7
              simple_regret_approx_3[slice9],
     8
              simple_regret_approx_4[slice9],
     9
              simple_regret_approx_5[slice9],
   10
              simple regret approx 6[slice9],
   11
              simple_regret_approx_7[slice9],
   12
              simple_regret_approx_8[slice9],
   13
              simple regret approx 9[slice9],
   14
              simple_regret_approx_10[slice9],
   15
              simple_regret_approx_11[slice9],
   16
              simple regret approx 12[slice9],
   17
              simple regret approx 13[slice9],
   18
              simple_regret_approx_14[slice9],
   19
              simple regret approx 15[slice9],
   20
              simple regret approx 16[slice9],
   21
              simple regret approx 17[slice9],
   22
              simple_regret_approx_18[slice9],
   23
              simple regret approx 19[slice9],
   24
              simple_regret_approx_20[slice9]]
   25
   26 exact9 = [simple regret exact 1[slice9],
   27
              simple_regret_exact_2[slice9],
   28
              simple_regret_exact_3[slice9],
   29
              simple regret exact 4[slice9],
   30
              simple regret exact 5[slice9],
   31
              simple regret exact 6[slice9],
              simple_regret_exact_7[slice9],
   32
   33
              simple regret exact 8[slice9],
   34
              simple regret exact 9[slice9],
              cimple regret evect 10[clice0]
    25
```

```
6/14/2021
                                         3. Rosenbrock GP El.ipynb - Colaboratory
              יווואדב ו בצו בר בצמר ר דמן אדורב או
   رر
   36
              simple_regret_exact_11[slice9],
   37
              simple_regret_exact_12[slice9],
   38
              simple_regret_exact_13[slice9],
   39
              simple regret exact 14[slice9],
              simple_regret_exact_15[slice9],
   40
   41
              simple_regret_exact_16[slice9],
   42
              simple regret exact 17[slice9],
   43
              simple_regret_exact_18[slice9],
   44
              simple_regret_exact_19[slice9],
   45
              simple regret exact 20[slice9]]
   46
   47 approx9_results = pd.DataFrame(approx9).sort_values(by=[0], ascending=False)
   48 exact9 results = pd.DataFrame(exact9).sort values(by=[0], ascending=False)
   49
   50 ### Best simple regret minimization IQR - approx:
   51 lower_approx9 = np.asarray(approx9_results[4:5][0])[0]
   52 median_approx9 = np.asarray(approx9_results[9:10][0])[0]
   53 upper_approx9 = np.asarray(approx9_results[14:15][0])[0]
   54
   55 lower exact9 = np.asarray(exact9 results[4:5][0])[0]
   56 median exact9 = np.asarray(exact9_results[9:10][0])[0]
   57 upper_exact9 = np.asarray(exact9_results[14:15][0])[0]
     1 # Iteration19 :
     2
     3 \text{ slice} 19 = 18
     4
     5 approx19 = [simple_regret_approx_1[slice19],
     6
              simple_regret_approx_2[slice19],
     7
              simple regret approx 3[slice19],
     8
              simple_regret_approx_4[slice19],
     9
              simple_regret_approx_5[slice19],
   10
              simple_regret_approx_6[slice19],
   11
              simple regret approx 7[slice19],
   12
              simple_regret_approx_8[slice19],
   13
              simple_regret_approx_9[slice19],
   14
              simple regret approx 10[slice19],
   15
              simple regret approx 11[slice19],
   16
              simple_regret_approx_12[slice19],
   17
              simple regret approx 13[slice19],
   18
              simple regret approx 14[slice19],
   19
              simple_regret_approx_15[slice19],
   20
              simple regret approx 16[slice19],
   21
              simple_regret_approx_17[slice19],
   22
              simple_regret_approx_18[slice19],
   23
              simple_regret_approx_19[slice19],
   24
              simple regret approx 20[slice19]]
   25
   26 exact19 = [simple_regret_exact_1[slice19],
   27
              simple regret exact 2[slice19],
   28
              simple regret exact 3[slice19],
   29
              simple regret exact 4[slice19],
   30
              simple regret exact 5[slice19],
   31
              simple regret exact 6[slice19],
```

```
32
          simple_regret_exact_7[slice19],
33
          simple regret exact 8[slice19],
34
          simple_regret_exact_9[slice19],
35
          simple_regret_exact_10[slice19],
          simple regret exact 11[slice19],
36
37
          simple regret exact 12[slice19],
38
          simple_regret_exact_13[slice19],
39
          simple regret exact 14[slice19],
40
          simple regret exact 15[slice19],
41
          simple_regret_exact_16[slice19],
42
          simple_regret_exact_17[slice19],
43
          simple_regret_exact_18[slice19],
44
          simple_regret_exact_19[slice19],
45
          simple_regret_exact_20[slice19]]
46
47 approx19_results = pd.DataFrame(approx19).sort_values(by=[0], ascending=False)
48 exact19_results = pd.DataFrame(exact19).sort_values(by=[0], ascending=False)
49
50 ### Best simple regret minimization IQR - approx:
51 lower_approx19 = np.asarray(approx19_results[4:5][0])[0]
52 median_approx19 = np.asarray(approx19_results[9:10][0])[0]
53 upper_approx19 = np.asarray(approx19_results[14:15][0])[0]
54
55 lower_exact19 = np.asarray(exact19_results[4:5][0])[0]
56 median_exact19 = np.asarray(exact19_results[9:10][0])[0]
57 upper_exact19 = np.asarray(exact19_results[14:15][0])[0]
 1 # Iteration29 :
 2
 3 \text{ slice29} = 28
 4
 5 approx29 = [simple_regret_approx_1[slice29],
          simple_regret_approx_2[slice29],
 6
 7
          simple_regret_approx_3[slice29],
 8
          simple regret approx 4[slice29],
 9
          simple regret approx 5[slice29],
10
          simple_regret_approx_6[slice29],
11
          simple regret approx 7[slice29],
12
          simple regret approx 8[slice29],
13
          simple_regret_approx_9[slice29],
14
          simple_regret_approx_10[slice29],
15
          simple regret approx 11[slice29],
16
          simple_regret_approx_12[slice29],
17
          simple_regret_approx_13[slice29],
18
          simple regret approx 14[slice29],
19
          simple regret approx 15[slice29],
20
          simple_regret_approx_16[slice29],
21
          simple regret approx 17[slice29],
22
          simple regret approx 18[slice29],
23
          simple regret approx 19[slice29],
24
          simple regret approx 20[slice29]]
25
26 exact29 = [simple_regret_exact_1[slice29],
27
          simple_regret_exact_2[slice29],
```

```
6/14/2021
                                         3. Rosenbrock GP El.ipynb - Colaboratory
   28
              simple regret exact 3[slice29],
   29
              simple_regret_exact_4[slice29],
              simple regret exact 5[slice29],
   30
   31
              simple regret exact 6[slice29],
   32
              simple_regret_exact_7[slice29],
   33
              simple_regret_exact_8[slice29],
   34
              simple_regret_exact_9[slice29],
   35
              simple_regret_exact_10[slice29],
   36
              simple_regret_exact_11[slice29],
   37
              simple_regret_exact_12[slice29],
   38
              simple_regret_exact_13[slice29],
   39
              simple_regret_exact_14[slice29],
   40
              simple regret exact 15[slice29],
   41
              simple_regret_exact_16[slice29],
   42
              simple_regret_exact_17[slice29],
              simple_regret_exact_18[slice29],
   43
   44
              simple regret exact 19[slice29],
   45
              simple_regret_exact_20[slice29]]
   46
   47 approx29 results = pd.DataFrame(approx29).sort values(by=[0], ascending=False)
   48 exact29_results = pd.DataFrame(exact29).sort_values(by=[0], ascending=False)
   49
   50 ### Best simple regret minimization IQR - approx:
   51 lower_approx29 = np.asarray(approx29_results[4:5][0])[0]
   52 median_approx29 = np.asarray(approx29_results[9:10][0])[0]
   53 upper_approx29 = np.asarray(approx29_results[14:15][0])[0]
   54
   55 lower_exact29 = np.asarray(exact29_results[4:5][0])[0]
   56 median_exact29 = np.asarray(exact29_results[9:10][0])[0]
   57 upper exact29 = np.asarray(exact29 results[14:15][0])[0]
     1 # Iteration39 :
     2
     3 \text{ slice} 39 = 38
     4
     5 approx39 = [simple regret approx 1[slice39],
     6
              simple regret approx 2[slice39],
     7
              simple regret approx 3[slice39],
     8
              simple_regret_approx_4[slice39],
     9
              simple regret approx 5[slice39],
   10
              simple_regret_approx_6[slice39],
   11
              simple_regret_approx_7[slice39],
   12
              simple regret approx 8[slice39],
              simple regret approx 9[slice39],
   13
   14
              simple_regret_approx_10[slice39],
   15
              simple regret approx 11[slice39],
   16
              simple regret approx 12[slice39],
   17
              simple regret approx 13[slice39],
   18
              simple_regret_approx_14[slice39],
   19
              simple regret approx 15[slice39],
   20
              simple regret approx 16[slice39],
   21
              simple_regret_approx_17[slice39],
   22
              simple regret approx 18[slice39],
   23
              simple_regret_approx_19[slice39],
              simple regret approx 20[slice39]]
```

```
21
          simple regret approx 17[slice10],
22
          simple regret approx 18[slice10],
23
          simple regret approx 19[slice10],
24
          simple_regret_approx_20[slice10]]
25
26 exact10 = [simple_regret_exact_1[slice10],
27
          simple_regret_exact_2[slice10],
28
          simple_regret_exact_3[slice10],
29
          simple regret exact 4[slice10],
          simple_regret_exact_5[slice10],
30
          simple_regret_exact_6[slice10],
31
32
          simple regret exact 7[slice10],
33
          simple regret exact 8[slice10],
34
          simple_regret_exact_9[slice10],
35
          simple regret exact 10[slice10],
36
          simple_regret_exact_11[slice10],
37
          simple_regret_exact_12[slice10],
38
          simple_regret_exact_13[slice10],
39
          simple_regret_exact_14[slice10],
40
          simple_regret_exact_15[slice10],
41
          simple_regret_exact_16[slice10],
42
          simple_regret_exact_17[slice10],
43
          simple_regret_exact_18[slice10],
          simple_regret_exact_19[slice10],
44
45
          simple regret exact 20[slice10]]
46
47 approx10 results = pd.DataFrame(approx10).sort values(by=[0], ascending=False)
48 exact10_results = pd.DataFrame(exact10).sort_values(by=[0], ascending=False)
49
50 ### Best simple regret minimization IQR - approx:
51 lower_approx10 = np.asarray(approx10_results[4:5][0])[0]
52 median_approx10 = np.asarray(approx10_results[9:10][0])[0]
53 upper_approx10 = np.asarray(approx10_results[14:15][0])[0]
54
55 lower exact10 = np.asarray(exact10 results[4:5][0])[0]
56 median exact10 = np.asarray(exact10 results[9:10][0])[0]
57 upper_exact10 = np.asarray(exact10_results[14:15][0])[0]
 1 # Iteration20 :
 2
 3 \text{ slice20} = 19
 4
 5 approx20 = [simple regret approx 1[slice20],
 6
          simple regret approx 2[slice20],
 7
          simple regret approx 3[slice20],
 8
          simple regret approx 4[slice20],
 9
          simple_regret_approx_5[slice20],
10
          simple_regret_approx_6[slice20],
11
          simple regret approx 7[slice20],
12
          simple_regret_approx_8[slice20],
13
          simple_regret_approx_9[slice20],
14
          simple regret approx 10[slice20],
15
          simple_regret_approx_11[slice20],
16
          simple_regret_approx_12[slice20],
```

```
6/14/2021
                                         3. Rosenbrock GP El.ipynb - Colaboratory
              simple regret approx 13|slice20|,
   1/
   18
              simple_regret_approx_14[slice20],
   19
              simple_regret_approx_15[slice20],
   20
              simple regret approx 16[slice20],
   21
              simple_regret_approx_17[slice20],
   22
              simple_regret_approx_18[slice20],
   23
              simple regret approx 19[slice20],
   24
              simple_regret_approx_20[slice20]]
   25
   26 exact20 = [simple regret exact 1[slice20],
   27
              simple regret exact 2[slice20],
   28
              simple_regret_exact_3[slice20],
   29
              simple_regret_exact_4[slice20],
   30
              simple regret exact 5[slice20],
   31
              simple_regret_exact_6[slice20],
   32
              simple_regret_exact_7[slice20],
   33
              simple_regret_exact_8[slice20],
   34
              simple_regret_exact_9[slice20],
   35
              simple_regret_exact_10[slice20],
   36
              simple regret exact 11[slice20],
   37
              simple_regret_exact_12[slice20],
              simple_regret_exact_13[slice20],
   38
   39
              simple_regret_exact_14[slice20],
              simple regret exact 15[slice20],
   40
   41
              simple_regret_exact_16[slice20],
   42
              simple_regret_exact_17[slice20],
   43
              simple regret exact 18[slice20],
   44
              simple_regret_exact_19[slice20],
   45
              simple_regret_exact_20[slice20]]
   46
   47 approx20_results = pd.DataFrame(approx20).sort_values(by=[0], ascending=False)
   48 exact20_results = pd.DataFrame(exact20).sort_values(by=[0], ascending=False)
   49
   50 ### Best simple regret minimization IQR - approx:
   51 lower_approx20 = np.asarray(approx20_results[4:5][0])[0]
   52 median approx20 = np.asarray(approx20 results[9:10][0])[0]
   53 upper approx20 = np.asarray(approx20 results[14:15][0])[0]
   54
   55 lower_exact20 = np.asarray(exact20_results[4:5][0])[0]
   56 median exact20 = np.asarray(exact20 results[9:10][0])[0]
   57 upper_exact20 = np.asarray(exact20_results[14:15][0])[0]
     1 # Iteration30:
     2
     3 \text{ slice} 30 = 29
     4
     5 approx30 = [simple regret approx 1[slice30],
     6
              simple_regret_approx_2[slice30],
     7
              simple_regret_approx_3[slice30],
     8
              simple regret approx 4[slice30],
     9
              simple regret approx 5[slice30],
   10
              simple_regret_approx_6[slice30],
   11
              simple_regret_approx_7[slice30],
   12
              simple regret approx 8[slice30],
   13
              simple regret approx 9[slice30].
```

```
simple_regret_approx_10[slice30],
14
15
          simple_regret_approx_11[slice30],
16
          simple_regret_approx_12[slice30],
17
          simple regret approx 13[slice30],
18
          simple_regret_approx_14[slice30],
19
          simple_regret_approx_15[slice30],
          simple_regret_approx_16[slice30],
20
          simple regret approx 17[slice30],
21
22
          simple_regret_approx_18[slice30],
23
          simple_regret_approx_19[slice30],
24
          simple_regret_approx_20[slice30]]
25
26 exact30 = [simple_regret_exact_1[slice30],
27
          simple_regret_exact_2[slice30],
28
          simple_regret_exact_3[slice30],
29
          simple_regret_exact_4[slice30],
30
          simple_regret_exact_5[slice30],
          simple_regret_exact_6[slice30],
31
          simple_regret_exact_7[slice30],
32
33
          simple_regret_exact_8[slice30],
          simple regret exact 9[slice30],
34
35
          simple_regret_exact_10[slice30],
36
          simple_regret_exact_11[slice30],
37
          simple_regret_exact_12[slice30],
38
          simple_regret_exact_13[slice30],
39
          simple_regret_exact_14[slice30],
40
          simple_regret_exact_15[slice30],
41
          simple_regret_exact_16[slice30],
42
          simple_regret_exact_17[slice30],
43
          simple_regret_exact_18[slice30],
44
          simple_regret_exact_19[slice30],
          simple_regret_exact_20[slice30]]
45
46
47 approx30 results = pd.DataFrame(approx30).sort values(by=[0], ascending=False)
48 exact30 results = pd.DataFrame(exact30).sort values(by=[0], ascending=False)
49
50 ### Best simple regret minimization IQR - approx:
51 lower approx30 = np.asarray(approx30 results[4:5][0])[0]
52 median_approx30 = np.asarray(approx30_results[9:10][0])[0]
53 upper_approx30 = np.asarray(approx30_results[14:15][0])[0]
54
55 lower exact30 = np.asarray(exact30 results[4:5][0])[0]
56 median_exact30 = np.asarray(exact30_results[9:10][0])[0]
57 upper exact30 = np.asarray(exact30 results[14:15][0])[0]
 1 # Iteration40:
 2
 3 \text{ slice} 40 = 39
 4
 5 approx40 = [simple_regret_approx_1[slice40],
          simple regret approx 2[slice40],
 6
 7
          simple regret approx 3[slice40],
 8
          simple_regret_approx_4[slice40],
 9
          simple regret approx 5[slice40],
```

```
6/14/2021
                    Tomei. ahhi. ox4
     7
                    lower_approx5,
     8
                    lower_approx6,
     9
                    lower approx7,
    10
                    lower approx8,
    11
                    lower_approx9,
    12
                    lower_approx10,
    13
                    lower_approx11,
    14
                    lower_approx12,
    15
                    lower_approx13,
    16
                    lower_approx14,
    17
                    lower_approx15,
    18
                    lower_approx16,
    19
                    lower_approx17,
    20
                    lower_approx18,
                    lower_approx19,
    21
    22
                    lower_approx20,
    23
                    lower approx21,
    24
                    lower_approx22,
    25
                    lower_approx23,
    26
                    lower_approx24,
    27
                    lower_approx25,
    28
                    lower_approx26,
    29
                    lower_approx27,
    30
                    lower_approx28,
    31
                    lower_approx29,
    32
                    lower_approx30,
    33
                    lower_approx31,
    34
                    lower_approx32,
    35
                    lower_approx33,
    36
                    lower approx34,
    37
                    lower_approx35,
    38
                    lower_approx36,
    39
                    lower_approx37,
    40
                    lower_approx38,
    41
                    lower_approx39,
    42
                    lower approx40,
    43
                    lower_approx41]
    44
    45 median approx = [median approx1,
    46
                    median approx2,
    47
                    median approx3,
    48
                    median approx4,
    49
                    median approx5,
    50
                    median_approx6,
    51
                    median_approx7,
    52
                    median approx8,
    53
                    median_approx9,
    54
                    median_approx10,
    55
                    median approx11,
    56
                    median approx12,
    57
                    median_approx13,
    58
                    median_approx14,
    59
                    median approx15,
    60
                    median approx16,
    ۲1
                    median annrov17
```

upper_approx29,

unner annroy30

115

116

```
מערט במאףו מאסט,
__
117
                 upper_approx31,
118
                 upper_approx32,
119
                 upper_approx33,
120
                 upper_approx34,
121
                 upper_approx35,
122
                 upper_approx36,
123
                 upper_approx37,
124
                 upper_approx38,
125
                 upper_approx39,
126
                 upper approx40,
127
                 upper_approx41]
  1 ### Summarize arrays: 'exact'
  2
  3 lower_exact = [lower_exact1,
  4
                 lower_exact2,
  5
                 lower exact3,
  6
                 lower exact4,
  7
                 lower_exact5,
  8
                 lower_exact6,
  9
                 lower_exact7,
 10
                 lower_exact8,
 11
                 lower_exact9,
 12
                 lower_exact10,
 13
                 lower_exact11,
 14
                 lower_exact12,
                 lower_exact13,
 15
                 lower_exact14,
 16
                 lower_exact15,
 17
                 lower_exact16,
 18
 19
                 lower_exact17,
 20
                 lower_exact18,
 21
                 lower_exact19,
 22
                 lower_exact20,
 23
                 lower_exact21,
 24
                 lower_exact22,
 25
                 lower exact23,
 26
                 lower_exact24,
                 lower_exact25,
 27
 28
                 lower exact26,
 29
                 lower exact27,
 30
                 lower exact28,
 31
                 lower_exact29,
 32
                 lower exact30,
 33
                 lower_exact31,
 34
                 lower_exact32,
 35
                 lower_exact33,
 36
                 lower_exact34,
 37
                 lower_exact35,
                 lower exact36,
 38
 39
                 lower_exact37,
 40
                 lower_exact38,
 41
                 lower exact39,
 42
                 lower exact40,
```

6/14/2021

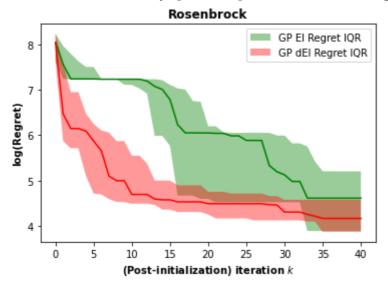
```
43
                lower_exact41]
44
45 median_exact = [median_exact1,
46
                median_exact2,
47
                median exact3,
48
                median_exact4,
                median_exact5,
49
                median_exact6,
50
                median exact7,
51
52
                median_exact8,
53
                median_exact9,
54
                median exact10,
                median_exact11,
55
56
                median_exact12,
57
                median_exact13,
58
                median_exact14,
59
                median_exact15,
                median_exact16,
60
                median_exact17,
61
                median_exact18,
62
63
                median_exact19,
                median exact20,
64
65
                median exact21,
66
                median_exact22,
67
                median_exact23,
68
                median_exact24,
69
                median_exact25,
70
                median_exact26,
71
                median_exact27,
72
                median_exact28,
                median_exact29,
73
74
                median_exact30,
75
                median_exact31,
                median_exact32,
76
77
                median exact33,
78
                median exact34,
79
                median_exact35,
80
                median exact36,
81
                median_exact37,
82
                median_exact38,
83
                median exact39,
84
                median exact40,
85
                median_exact41]
86
87 upper_exact = [upper_exact1,
88
                upper_exact2,
89
                upper_exact3,
90
                upper_exact4,
91
                upper_exact5,
92
                upper_exact6,
93
                upper_exact7,
94
                upper_exact8,
95
                upper_exact9,
96
                upper_exact10,
97
                upper_exact11,
```

20 count = len(xstar)

22 plt.show() #visualize!

21 plt.xticks(np.arange(0, count, 5))

findfont: Font family ['Arial'] not found. Falling back to DejaVu Sans. findfont: Font family ['Arial'] not found. Falling back to DejaVu Sans.



1 time_approx, time_exact

(825.6076500415802, 210.44350624084473)

1

X