

Sine:

GP EI: exact GP dEI Jacobian vs. estimated GP EI Jacobian

```
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
8
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 cholesky, solve
16 from scipy.optimize import minimize
17 from scipy.spatial.distance import cdist
18 from scipy.stats import norm
19 from mpl_toolkits.axes_grid1.inset_locator import inset_axes, mark_inset
20
21 warnings.filterwarnings("ignore", category=RuntimeWarning)
22

1 n_start_AcqFunc = 250 #multi-start iterations to avoid local optima in AcqFunc optimiza
2

1 ### Inputs:
2
3 run_num_1 = 0
4 n_test = 500
5 eps = 1e-08
6
7 util_grad_exact = 'dEI_GP'
8 util_grad_approx = 'ExpectedImprovement'
9
10 n_init = 2 # random initialisations
11 iters = 1
12 opt = True
13

1 ### Objective Function - Sin(x) 1-D:
2
3 def objfunc(x1_training):
```

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4     return operator * np.sin(x1_training)
5
6 # Constraints:
7 lb = 0
8 ub = 2 * np.pi
9 y_global_orig = 1
10
11 # Input array dimension(s):
12 dim = 1
13 operator = 1
14
15 # 1-D inputs' parameter bounds:
16 param = {'x1_training': ('cont', [lb, ub])}
17
18 # Test data:
19 x_test = np.linspace(lb, ub, n_test).reshape((n_test, 1))
20

```

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1 ### Cumulative Regret Calculator:
2

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3 def min_max_array(x):
4     new_list = []
5     for i, num in enumerate(x):
6         new_list.append(np.min(x[0:i+1]))
7     return new_list
8

```

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1 class Acquisition_new(Acquisition):
2     def __init__(self, mode, eps=1e-08, **params):
3
4         self.params = params
5         self.eps = eps
6
7         mode_dict = {
8             'dEI_GP': self.dEI_GP
9         }
10
11         self.f = mode_dict[mode]
12
13     def dEI_GP(self, tau, mean, std, ds, dm):
14         gamma = (mean - tau - self.eps) / (std + self.eps)
15         dsdx = ds / (2 * (std + self.eps))
16         dmdx = (dm - gamma * dsdx) / (std + self.eps)
17
18         f = np.array((std + self.eps) * (gamma * norm.cdf(gamma) + norm.pdf(gamma)))
19         df1 = f / (std + self.eps) * dsdx
20         df2 = (std + self.eps) * norm.cdf(gamma) * dmdx
21         df = df1 + df2
22
23         df_arr = []
24
25         for i in range(0, dim):
26             df_arr.append([df])
27         return f, np.asarray(df_arr).transpose()

```

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29     def d_eval(self, tau, mean, std, ds, dm):
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31         return self.f(tau, mean, std, ds, dm, **self.params)
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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)
34             self.logger._printInit(self)
35         for iteration in range(max_iter):
36             self.d_optimizeAcq()
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)
42         new_std = np.sqrt(new_var + eps)
43         ds, dm = self.GP.AcqGrad(xnew)
44         f, df = self.A.d_eval(-self.tau, new_mean, new_std, ds=ds, dm=dm)
45         return -f, df
46
47     def acqfunc_h(self, xnew, n_start=n_start_AcqFunc, eps=eps):
48         f = self.acqfunc(xnew)[0]
49
50         new_mean_h, new_var_h = self.GP.predict(xnew + eps, return_std=True)
51         new_std_h = np.sqrt(new_var_h + eps)
52         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         return approx_grad
57
58
59 1 ## est_GPGO:
60 2
61 3 class est_GPGO(GPGO):
62 4     n_start = n_start_AcqFunc
63 5     eps = 1e-08
64 6
65 7     def _optimizeAcq(self, method='L-BFGS-B', n_start=n_start_AcqFunc):
66 8         start_points_dict = [self._sampleParam() for i in range(n_start)]
67 9         start_points_arr = np.array([list(s.values())
68 10                                     for s in start_points_dict])
69 11         x_best = np.empty((n_start, len(self.parameter_key)))
70 12         f_best = np.empty((n_start,))
71 13         if self.n_jobs == 1:
72 14             for index, start_point in enumerate(start_points_arr):
73 15                 res = minimize(self._acqWrapper, x0=start_point, method=method,
74 16                               bounds=self.parameter_range)
75 17                 x_best[index], f_best[index] = res.x, np.atleast_1d(res.fun)[0]
76 18         else:
77 19             opt = Parallel(n_jobs=self.n_jobs)(delayed(minimize)(self._acqWrapper,
78 20                                                                    x0=start_point,
79 21                                                                    method=method,
80 22                                                                    bounds=self.parameter_

```

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23             start_points_arr)
24         x_best = np.array([res.x for res in opt])
25         f_best = np.array([np.atleast_1d(res.fun)[0] for res in opt])
26
27         self.x_best = x_best
28         self.f_best = f_best
29         self.best = x_best[np.argmin(f_best)]
30         self.start_points_arr = start_points_arr
31
32         return x_best, f_best
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996
997
998
999

```

```

43 def plot_GP_EI_jac(gpgo, param, new):
44     plt.figure(figsize=[7,5])
45     x_test = np.linspace(lb, ub, n_test).reshape((n_test, 1))
46     jac = -dGPGO.acqfunc(gpgo, x_test)[1].flatten()
47     approx_jac = -dGPGO.acqfunc_h(gpgo, x_test).flatten()
48     plt.plot(x_test, jac, color='Red', label='GP dEI$(\mathbf{x})$: exact GP EI Jacobia
49     plt.plot(x_test, approx_jac, color='Green', label='Estimated GP EI Jacobian')
50     xbest = x_test[np.argmax(-dGPGO.acqfunc(gpgo, x_test)[0])][0]
51     plt.axvline(x=xbest, color='Black', label='GP EI$(\mathbf{x})$: arg max $\mathbf{x}$
52     plt.ylim(-0.1 + min([min(approx_jac), min(jac)]), max([max(approx_jac), max(jac)]))
53     plt.xlim(0, 2 * np.pi)
54     plt.legend(loc=0)
55     plt.xlabel("$\mathbf{x}$")
56     plt.ylabel("GP dEI$(\mathbf{x})$, GP deltaEI$(\mathbf{x})$")
57     title = 'GP dEI'
58     plt.suptitle(title, weight = 'bold')
59     plt.show()
60
61 def plot_GP_dEI_vs_approx(dgpgo, est_GPGO, param, new):
62     fig, ax = plt.subplots(figsize=[7,5])
63     x_test = np.linspace(lb, ub, n_test).reshape((n_test, 1))
64     a = -dGPGO.acqfunc(dgpgo, x_test)[0].flatten()
65     plt.plot(x_test, a, color='Purple', label='GP EI$(\mathbf{x})$')
66     ybest = np.max(-dGPGO.acqfunc(dgpgo, x_test)[0])
67     xbest = x_test[np.argmax(-dGPGO.acqfunc(dgpgo, x_test)[0])][0]
68     plt.scatter(xbest, ybest, marker='D', color='Blue', label='GP EI$(\mathbf{x})$:
69     plt.ylim(-0.1 + min(a), max(a) + 0.1)
70     plt.xlim(0, 2 * np.pi)
71     xbest_approx = est_GPGO.x_best[np.argmax(np.array(-est_GPGO.f_best))][0]
72     plt.axvline(x=xbest, color='Black', label='GP EI$(\mathbf{x})$: arg max $\mathbf{x}$
73     plt.axvline(x=xbest_approx, color='Brown', ls='--', label='Alternative GP EI$(\
74     plt.legend(loc=0)
75     plt.xlabel("$\mathbf{x}$")
76     plt.ylabel("GP dEI$(\mathbf{x})$")
77     title = 'GP dEI'
78     plt.suptitle(title, weight = 'bold')
79     plt.show()
80

```

```

1 ### Random-initialisation: Bayesian optimisation
2
3 ### EXACT GP EI Jacobian
4
5 np.random.seed(run_num_1)
6 surrogate_exact_0 = dGaussianProcess(cov_func, optimize=opt)
7
8 exact_0 = dGPGO(surrogate_exact_0, Acquisition_new(util_grad_exact), objfunc, param)
9 exact_0.run(init_evals=n_init, max_iter=iters-1)
10

```

	Evaluation	Proposed point	Current eval.	Best eval.
init	[3.44829694].	-0.301918370765691	-0.301918370765691	
init	[4.49366732].	-0.9761756231500798	-0.301918370765691	

```

1 ### Random initialisation: Bayesian optimisation

```

```

1 ### Random-initialisation: Bayesian optimisation
2
3 ### versus ESTIMATED GP EI Jacobian
4
5 np.random.seed(run_num_1)
6 surrogate_approx_0 = GaussianProcess(cov_func, optimize=opt)
7
8 approx_0 = est_GPGO(surrogate_approx_0, Acquisition(util_grad_approx), objfunc, param)
9 approx_0.run(init_evals=n_init, max_iter=iters-1)
10

```

	Evaluation	Proposed point	Current eval.	Best eval.
init	[3.44829694].	-0.301918370765691	-0.301918370765691	
init	[4.49366732].	-0.9761756231500798	-0.301918370765691	

```

1 ### Random-initialisation: GP EI arg max x, max
2 np.random.seed(run_num_1)
3
4 AcqFuncMaxExact_0 = np.max(-dGPGO.acqfunc(exact_0, x_test)[0])
5 XBestExact_0 = x_test[np.argmax(-dGPGO.acqfunc(exact_0, x_test)[0])][0]
6
7 XBestExactGradExact_0 = exact_0.acqfunc(XBestExact_0)[1][0][0][0]
8 XBestApproxGradExact_0 = exact_0.acqfunc_h(XBestExact_0)[0]
9
10 print("Exact GP EI Jacobian: arg max x:", np.round(XBestExactGradExact_0, 4))
11 print("Estm. GP EI Jacobian: arg max x:", np.round(XBestApproxGradExact_0, 4))
12

```

```

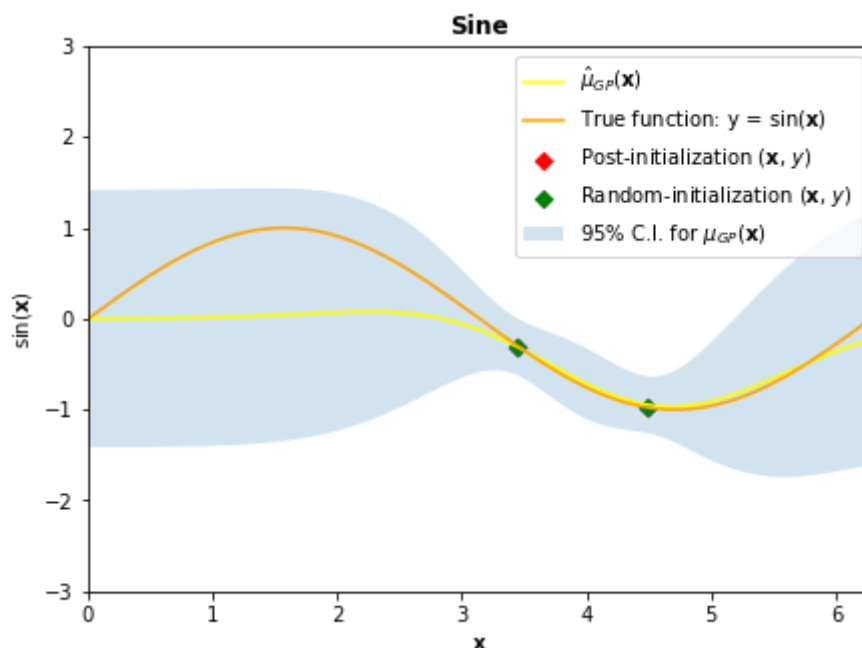
Exact GP EI Jacobian: arg max x: 0.0474
Estm. GP EI Jacobian: arg max x: -0.0001

```

```

1 ### Random-initialisation: plots
2
3 plot_sine(exact_0, param, new=True)
4

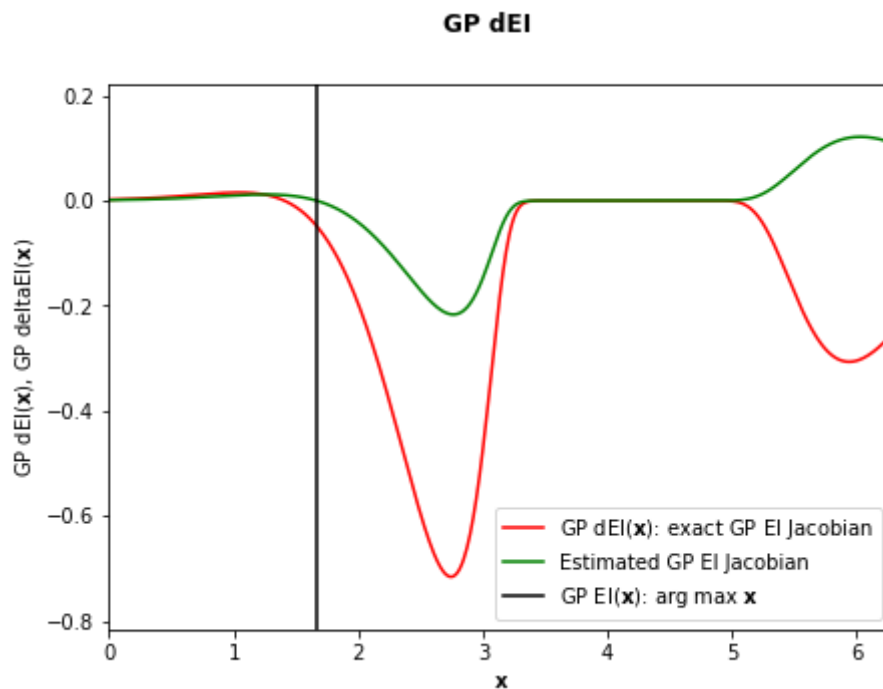
```



```

1 ### Random-initialisation: STP EI Jacobian' plots - exact versus estimated
2
3 plot_GP_EI_jac(exact_0, param, new=True)
4 print("Max. Exact GP EI Jacobian: ", np.round(max(-dGPGO.acqfunc(exact_0, x_test)[1])[0]
5 print("Min. Exact GP EI Jacobian:", np.round(min(-dGPGO.acqfunc(exact_0, x_test)[1])[0]
6 print("Max. Estm. GP EI Jacobian: ", np.round(max(-dGPGO.acqfunc_h(exact_0, x_test)), 4
7 print("Min. Estm. GP EI Jacobian:", np.round(min(-dGPGO.acqfunc_h(exact_0, x_test)), 4)
8 print("Exact Jacobian: arg max x:", np.round(XBestExactGradExact_0, 4))
9 print("Estm. Jacobian: arg max x:", np.round(XBestApproxGradExact_0, 4))
10

```



```

Max. Exact GP EI Jacobian:  0.0153
Min. Exact GP EI Jacobian: -0.7158
Max. Estm. GP EI Jacobian:  0.1214
Min. Estm. GP EI Jacobian: -0.2168
Exact Jacobian: arg max x: 0.0474
Estm. Jacobian: arg max x: -0.0001

```

```
1 min(-dGPGO.acqfunc(exact_0, x_test)[1])[0][0]
```

```
-0.7158356355687903
```

```

1 ### Post-initialisation: iteration 1 Bayesian optimisation
2
3 ### EXACT GP EI Jacobian
4
5 np.random.seed(run_num_1)
6 surrogate_exact_1 = dGaussianProcess(cov_func, optimize=opt)
7
8 exact_1 = dGPGO(surrogate_exact_1, Acquisition_new(util_grad_exact), objfunc, param)
9 exact_1.run(init_evals=n_init, max_iter=iters)
10
11 a_exact_1 = np.array(-exact_1.f_best)
12 xbest_exact_1 = exact_1.x_best[np.argmax(a_exact_1)][0]
13 regret_exact_1 = y_global_orig - objfunc(xbest_exact_1)
14

```



```

14

```

```

15 print("Exact GP EI Jacobian: Max. GP EI", np.round(np.max(a_exact_1), 4))
16 print("Exact GP EI Jacobian: regret", np.round(regret_exact_1, 4))
17

```

Evaluation	Proposed point	Current eval.	Best eval.
init	[3.44829694].	-0.301918370765691	-0.301918370765691
init	[4.49366732].	-0.9761756231500798	-0.301918370765691
1	[1.66399209].	0.9956604172034629	0.9956604172034629

Exact GP EI Jacobian: Max. GP EI 0.173
Exact GP EI Jacobian: regret 0.0043

```

1 ### Post-initialisation: iteration 1 Bayesian optimisation
2
3 ### versus ESTIMATED GP EI Jacobian
4
5 np.random.seed(run_num_1)
6 surrogate_approx_1 = GaussianProcess(cov_func, optimize=opt)
7
8 approx_1 = est_GPGO(surrogate_approx_1, Acquisition(util_grad_approx), objfunc, param)
9 approx_1.run(init_evals=n_init, max_iter=iters)
10
11 a_approx_1 = np.array(-approx_1.f_best)
12 xbest_approx_1 = approx_1.x_best[np.argmax(a_approx_1)][0]
13 regret_approx_1 = y_global_orig - objfunc(xbest_approx_1)
14
15 print("Estimated GP EI Jacobian: Max. GP EI", np.round(np.max(a_approx_1), 4))
16 print("Estimated GP EI Jacobian: regret", np.round(regret_approx_1, 4))
17

```

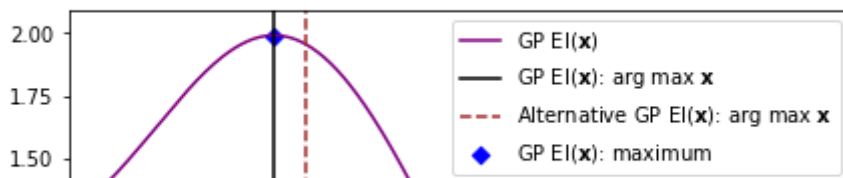
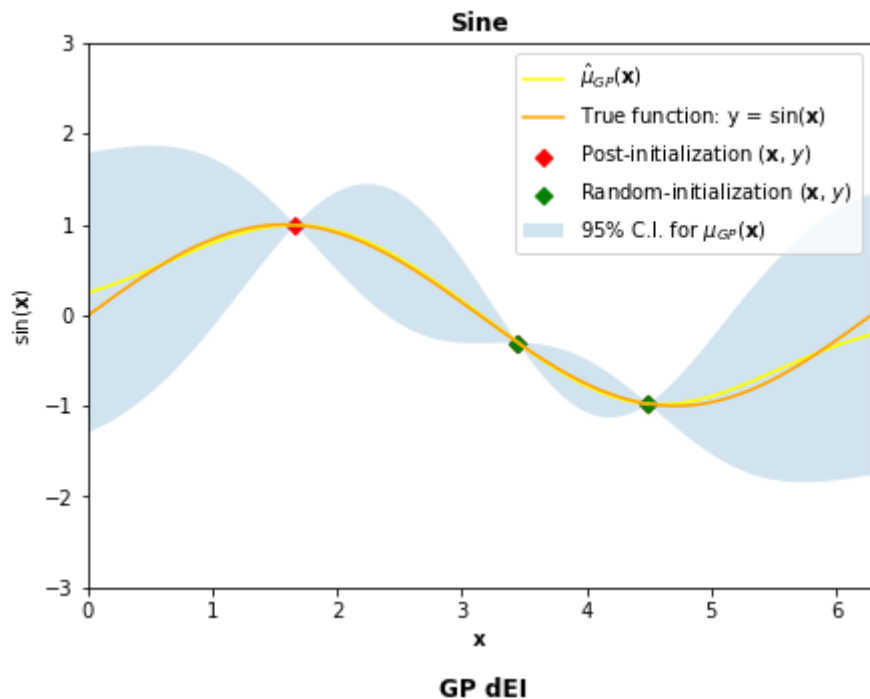
Evaluation	Proposed point	Current eval.	Best eval.
init	[3.44829694].	-0.301918370765691	-0.301918370765691
init	[4.49366732].	-0.9761756231500798	-0.301918370765691
1	[1.90357748].	0.9451374717390602	0.9451374717390602

Estimated GP EI Jacobian: Max. GP EI 0.4955
Estimated GP EI Jacobian: regret 0.0549

```

1 ### Post-initialisation: iteration 1 plots
2
3 plot_sine(exact_1, param, new=True)
4 plot_GP_dEI_vs_approx(exact_1, approx_1, param, new=True)
5

```



```

1 ### Post-initialisation: iteration 1 GP EI arg max x, max
2
3 np.random.seed(run_num_1)
4
5 AcqFuncMaxExact_1 = np.max(-dGPGO.acqfunc(exact_1, x_test)[0])
6 XBestExact_1 = x_test[np.argmax(-dGPGO.acqfunc(exact_1, x_test)[0])][0]
7
8 XBestExactGradExact_1 = exact_1.acqfunc(XBestExact_1)[1][0][0][0]
9 XBestApproxGradExact_1 = exact_1.acqfunc_h(XBestExact_1)[0]
10
11 print("Exact GP EI Jacobian: arg max x:", np.round(XBestExactGradExact_1, 4))
12 print("Estm. GP EI Jacobian: arg max x:", np.round(XBestApproxGradExact_1, 4))
13

```

```

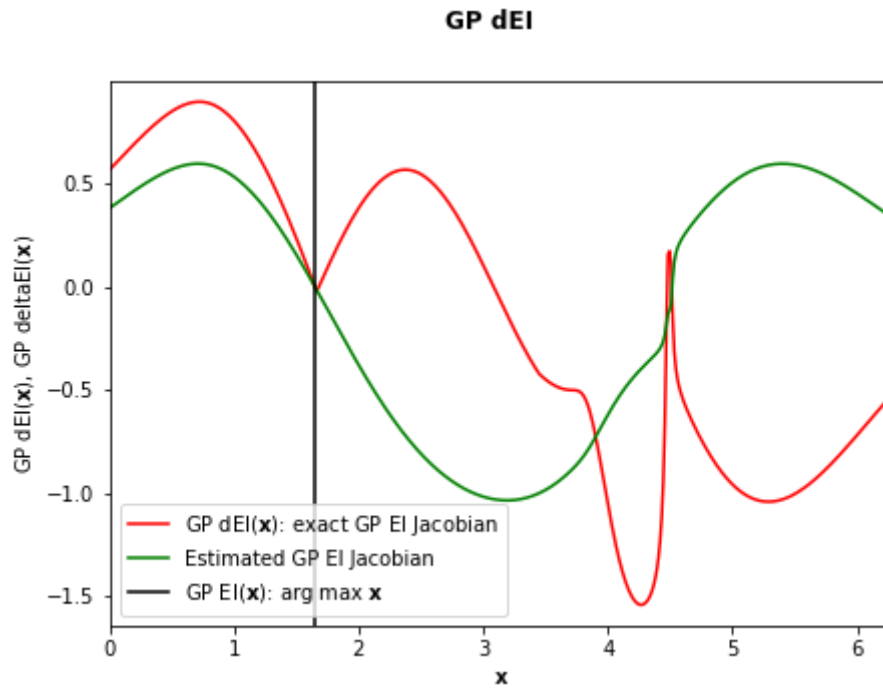
Exact GP EI Jacobian: arg max x: -0.0003
Estm. GP EI Jacobian: arg max x: -0.0002

```

```

1 ### Post-initialisation: iteration 1 GP EI Jacobian' plots - exact versus estimated
2
3 plot_GP_EI_jac(exact_1, param, new=True)
4 print("Max. Exact GP EI Jacobian: ", np.round(max(-dGPGO.acqfunc(exact_1, x_test)[1])[0], 4))
5 print("Min. Exact GP EI Jacobian:", np.round(min(-dGPGO.acqfunc(exact_1, x_test)[1])[0], 4))
6 print("Max. Estm. GP EI Jacobian: ", np.round(max(-dGPGO.acqfunc_h(exact_1, x_test)), 4))
7 print("Min. Estm. GP EI Jacobian:", np.round(min(-dGPGO.acqfunc_h(exact_1, x_test)), 4))
8 print("Exact GP EI Jacobian: arg max x:", np.round(XBestExactGradExact_1, 4))
9 print("Estm. GP EI Jacobian: arg max x:", np.round(XBestApproxGradExact_1, 4))
10

```



Max. Exact GP EI Jacobian: 0.8967
 Min. Exact GP EI Jacobian: -1.5411
 Max. Estm. GP EI Jacobian: 0.5968
 Min. Estm. GP EI Jacobian: -1.035
 Exact GP EI Jacobian: arg max x: -0.0003

```
1 ### Post-initialisation: iteration 2 Bayesian optimisation
2
3 ### EXACT GP EI Jacobian
4
5 np.random.seed(run_num_1)
6 surrogate_exact_2 = dGaussianProcess(cov_func, optimize=opt)
7
8 exact_2 = dGPGO(surrogate_exact_2, Acquisition_new(util_grad_exact), objfunc, param)
9 exact_2.run(init_evals=n_init, max_iter=iters+1)
10
11 a_exact_2 = np.array(-exact_2.f_best)
12 xbest_exact_2 = exact_2.x_best[np.argmax(a_exact_2)][0]
13 regret_exact_2 = y_global_orig - objfunc(xbest_exact_2)
14
15 print("Exact GP EI Jacobian: Max. GP EI", np.round(np.max(a_exact_2), 4))
16 print("Exact GP EI Jacobian: regret", np.round(regret_exact_2, 4))
17
```

	Evaluation	Proposed point	Current eval.	Best eval.
init	[3.44829694].	-0.301918370765691	-0.301918370765691	-0.301918370765691
init	[4.49366732].	-0.9761756231500798	-0.301918370765691	-0.301918370765691
1	[1.66399209].	0.9956604172034629	0.9956604172034629	0.9956604172034629
2	[1.64970468].	0.9968883509017231	0.9968883509017231	0.9968883509017231
Exact GP EI Jacobian: Max. GP EI 1.9914				
Exact GP EI Jacobian: regret 0.0031				

```
1 ### Post-initialisation: iteration 2 Bayesian optimisation
2
3 ### versus ESTIMATED GP EI Jacobian
4
5 np.random.seed(run_num_1)
```

```

6 surrogate_approx_2 = GaussianProcess(cov_func, optimize=opt)
7
8 approx_2 = est_GPGO(surrogate_approx_2, Acquisition(util_grad_approx), objfunc, param)
9 approx_2.run(init_evals=n_init, max_iter=iters+1)
10
11 a_approx_2 = np.array(-approx_2.f_best)
12 xbest_approx_2 = approx_2.x_best[np.argmax(a_approx_2)][0]
13 regret_approx_2 = y_global_orig - objfunc(xbest_approx_1) ### Iteration 1's y-value is
14
15 print("Estimated GP EI Jacobian: Max. GP EI", np.round(np.max(a_approx_2), 4))
16 print("Estimated GP EI Jacobian: regret", np.round(regret_approx_2, 4))
17

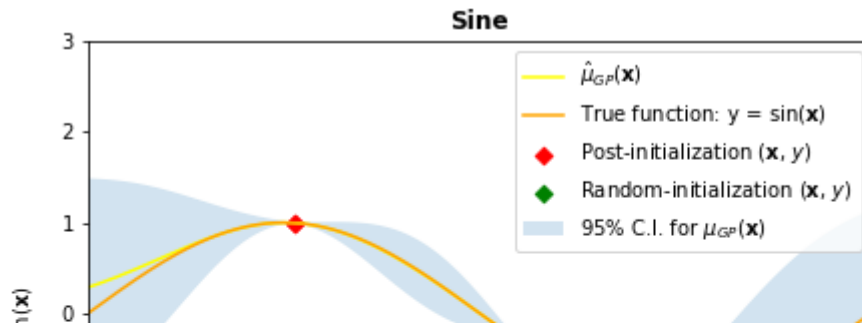
```

Evaluation	Proposed point	Current eval.	Best eval.
init	[3.44829694].	-0.301918370765691	-0.301918370765691
init	[4.49366732].	-0.9761756231500798	-0.301918370765691
1	[1.90357748].	0.9451374717390602	0.9451374717390602
2	[1.09255415].	0.8878052780090047	0.9451374717390602
Estimated GP EI Jacobian: Max. GP EI 0.1143			
Estimated GP EI Jacobian: regret 0.0549			

```

1 ### Post-initialisation: iteration 2 plots
2
3 plot_sine(exact_2, param, new=True)
4 plot_GP_dEI_vs_approx(exact_2, approx_2, param, new=True)
5

```



```

1 ### Post-initialisation: iteration 2 GP EI arg max x, max
2 np.random.seed(run_num_1)
3
4 AcqFuncMaxExact_2 = np.max(-dGPGO.acqfunc(exact_2, x_test)[0])
5 XBestExact_2 = x_test[np.argmax(-dGPGO.acqfunc(exact_2, x_test)[0])][0]
6
7 XBestExactGradExact_2 = exact_2.acqfunc(XBestExact_2)[1][0][0][0]
8 XBestApproxGradExact_2 = exact_2.acqfunc_h(XBestExact_2)[0]
9
10 print("Exact GP EI Jacobian: arg max x:", np.round(XBestExactGradExact_2, 4))
11 print("Estm. GP EI Jacobian: arg max x:", np.round(XBestApproxGradExact_2, 4))
12

```

```

Exact GP EI Jacobian: arg max x: -0.0052
Estm. GP EI Jacobian: arg max x: -0.0026

```

✓ | | \ |

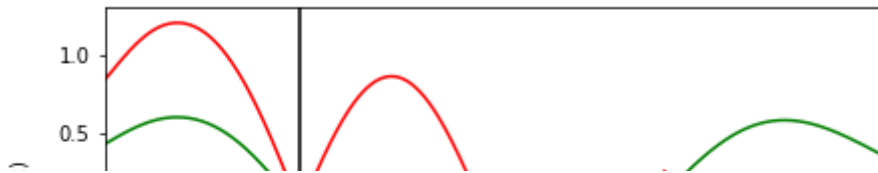
```

1 ### Post-initialisation: iteration 2 GP EI Jacobian' plots - exact versus estimated
2
3 plot_GP_EI_jac(exact_2, param, new=True)
4 print("Max. Exact GP EI Jacobian: ", np.round(max(-dGPGO.acqfunc(exact_2, x_test)[1])[0], 4))
5 print("Min. Exact GP EI Jacobian:", np.round(min(-dGPGO.acqfunc(exact_2, x_test)[1])[0], 4))
6 print("Max. Estm. GP EI Jacobian: ", np.round(max(-dGPGO.acqfunc_h(exact_2, x_test)), 4))
7 print("Min. Estm. GP EI Jacobian:", np.round(min(-dGPGO.acqfunc_h(exact_2, x_test)), 4))
8 print("Exact GP EI Jacobian: arg max x:", np.round(XBestExactGradExact_2, 4))
9 print("Estm. GP EI Jacobian: arg max x:", np.round(XBestApproxGradExact_2, 4))
10

```

☞

GP dEI



```

1 ### Post-initialisation: iteration 3 Bayesian optimisation
2
3 ### EXACT GP EI Jacobian
4
5 np.random.seed(run_num_1)
6 surrogate_exact_3 = dGaussianProcess(cov_func, optimize=opt)
7
8 exact_3 = dGPGO(surrogate_exact_3, Acquisition_new(util_grad_exact), objfunc, param)
9 exact_3.run(init_evals=n_init, max_iter=iters+2)
10
11 a_exact_3 = np.array(-exact_3.f_best)
12 xbest_exact_3 = exact_3.x_best[np.argmax(a_exact_3)][0]
13 regret_exact_3 = y_global_orig - objfunc(xbest_exact_3)
14
15 print("Exact GP EI Jacobian: Max. GP EI", np.round(np.max(a_exact_3), 4))
16 print("Exact GP EI Jacobian: regret", np.round(regret_exact_3, 4))
17

```

	Evaluation	Proposed point	Current eval.	Best eval.
init	[3.44829694].	-0.301918370765691	-0.301918370765691	-0.301918370765691
init	[4.49366732].	-0.9761756231500798	-0.301918370765691	-0.301918370765691
1	[1.66399209].	0.9956604172034629	0.9956604172034629	0.9956604172034629
2	[1.64970468].	0.9968883509017231	0.9968883509017231	0.9968883509017231
3	[1.57642514].	0.9999841582756325	0.9999841582756325	0.9999841582756325
Exact GP EI Jacobian: Max. GP EI 1.9966				
Exact GP EI Jacobian: regret 0.0				

```

1 ### Post-initialisation: iteration 3 Bayesian optimisation
2
3 ### versus ESTIMATED GP EI Jacobian
4
5 np.random.seed(run_num_1)
6 surrogate_approx_3 = GaussianProcess(cov_func, optimize=opt)
7
8 approx_3 = est_GPGO(surrogate_approx_3, Acquisition(util_grad_approx), objfunc, param)
9 approx_3.run(init_evals=n_init, max_iter=iters+2)
10
11 a_approx_3 = np.array(-approx_3.f_best)
12 xbest_approx_3 = approx_3.x_best[np.argmax(a_approx_3)][0]
13 regret_approx_3 = y_global_orig - objfunc(xbest_approx_3)
14
15 print("Estimated GP EI Jacobian: Max. GP EI", np.round(np.max(a_approx_3), 4))
16 print("Estimated GP EI Jacobian: regret", np.round(regret_approx_3, 4))
17

```

	Evaluation	Proposed point	Current eval.	Best eval.
init	[3.44829694].	-0.301918370765691	-0.301918370765691	-0.301918370765691
init	[4.49366732].	-0.9761756231500798	-0.301918370765691	-0.301918370765691

```

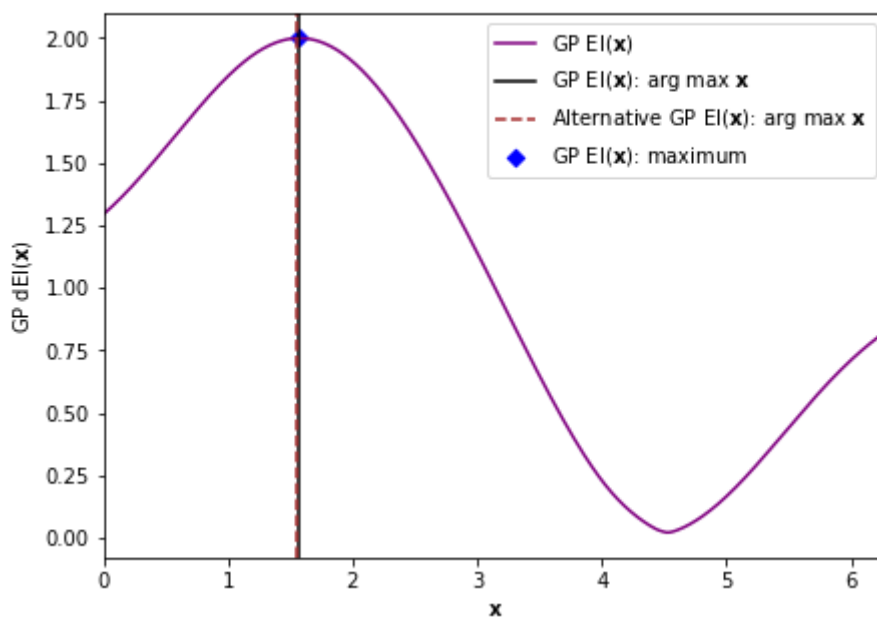
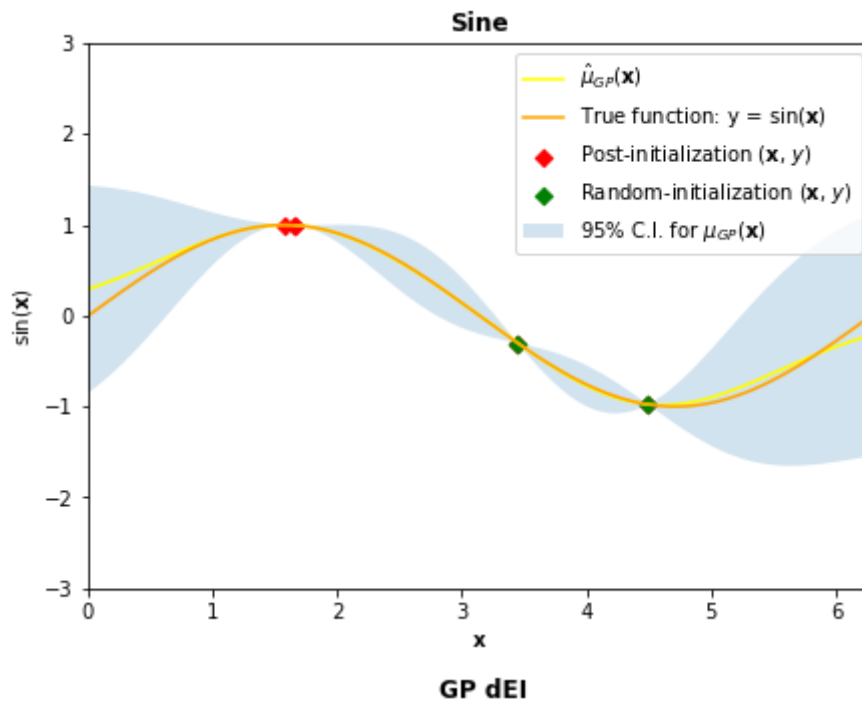
1      [1.90357748].    0.9451374717390602    0.9451374717390602
2      [1.09255415].    0.8878052780090047    0.9451374717390602
3      [1.55822889].    0.9999210308501604    0.9999210308501604
Estimated GP EI Jacobian: Max. GP EI 0.0562
Estimated GP EI Jacobian: regret 0.0001

```

```

1 ### Post-initialisation: iteration 3 plots
2
3 plot_sine(exact_3, param, new=True)
4 plot_GP_dEI_vs_approx(exact_3, approx_3, param, new=True)
5

```



```

1 ### Post-initialisation: iteration 3 STP EI arg max x, max
2 np.random.seed(run_num_1)
3
4 AcqFuncMaxExact_3 = np.max(-dGPG0.acqfunc(exact_3, x_test)[0])
5 XBestExact_3 = x_test[np.argmax(-dGPG0.acqfunc(exact_3, x_test)[0])][0]

```

```

6
7 XBestExactGradExact_3 = exact_3.acqfunc(XBestExact_3)[1][0][0][0]
8 XBestApproxGradExact_3 = exact_3.acqfunc_h(XBestExact_3)[0]
9
10 print("Exact GP EI Jacobian: arg max x:", np.round(XBestExactGradExact_3, 4))
11 print("Estm. GP EI Jacobian: arg max x:", np.round(XBestApproxGradExact_3, 4))
12

```

```

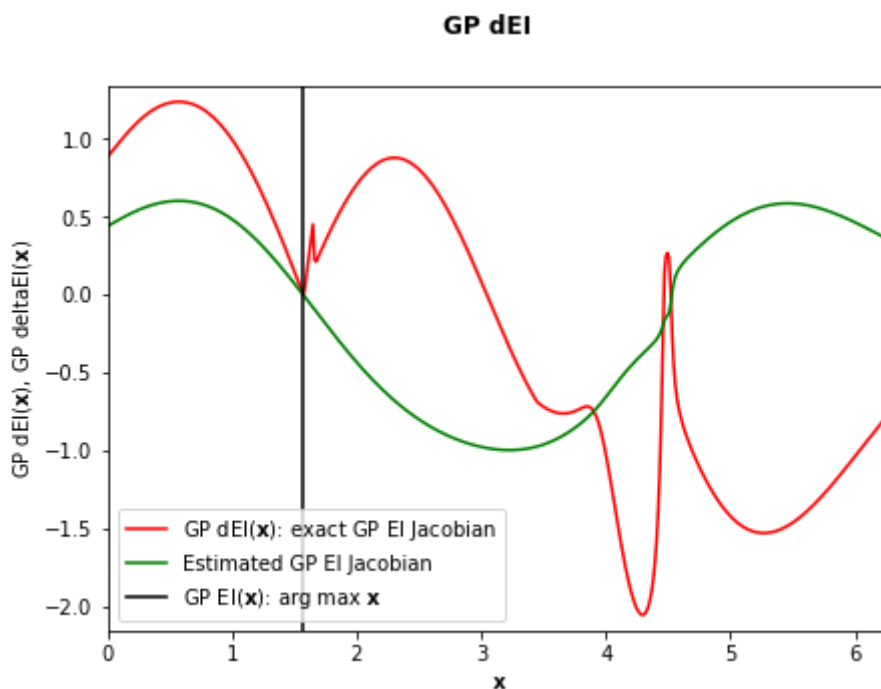
Exact GP EI Jacobian: arg max x: 0.0031
Estm. GP EI Jacobian: arg max x: 0.0015

```

```

1 ### Post-initialisation: iteration 3 GP EI Jacobian' plots - exact versus estimated
2
3 plot_GP_EI_jac(exact_3, param, new=True)
4 print("Max. Exact GP EI Jacobian: ", np.round(max(-dGPG0.acqfunc(exact_3, x_test)[1])[0]
5 print("Min. Exact GP EI Jacobian:", np.round(min(-dGPG0.acqfunc(exact_3, x_test)[1])[0]
6 print("Max. Estm. GP EI Jacobian: ", np.round(max(-dGPG0.acqfunc_h(exact_3, x_test)), 4)
7 print("Min. Estm. GP EI Jacobian:", np.round(min(-dGPG0.acqfunc_h(exact_3, x_test)), 4)
8 print("Exact GP EI Jacobian: arg max x:", np.round(XBestExactGradExact_3, 4))
9 print("Estm. GP EI Jacobian: arg max x:", np.round(XBestApproxGradExact_3, 4))
10

```



```

Max. Exact GP EI Jacobian: 1.2387
Min. Exact GP EI Jacobian: -2.0505
Max. Estm. GP EI Jacobian: 0.6034
Min. Estm. GP EI Jacobian: -0.9945
Exact GP EI Jacobian: arg max x: 0.0031
Estm. GP EI Jacobian: arg max x: 0.0015

```

```

1 ### Post-initialisation: iteration 4 Bayesian optimisation
2
3 ### EXACT GP EI Jacobian
4
5 np.random.seed(run_num_1)
6 surrogate_exact_4 = dGaussianProcess(cov_func, optimize=opt)
7

```



```

8 exact_4 = dGPG0(surrogate_exact_4, Acquisition_new(util_grad_exact), objfunc, param)
9 exact_4.run(init_evals=n_init, max_iter=iters+3)
10
11 a_exact_4 = np.array(-exact_4.f_best)
12 xbest_exact_4 = exact_4.x_best[np.argmax(a_exact_4)][0]
13 regret_exact_4 = y_global_orig - objfunc(xbest_exact_4)
14
15 print("Exact GP EI Jacobian: Max. GP EI", np.round(np.max(a_exact_4), 4))
16 print("Exact GP EI Jacobian: regret", np.round(regret_exact_4, 4))
17

```

Evaluation	Proposed point	Current eval.	Best eval.
init	[3.44829694].	-0.301918370765691	-0.301918370765691
init	[4.49366732].	-0.9761756231500798	-0.301918370765691
1	[1.66399209].	0.9956604172034629	0.9956604172034629
2	[1.64970468].	0.9968883509017231	0.9968883509017231
3	[1.57642514].	0.9999841582756325	0.9999841582756325
4	[1.57249288].	0.9999985608512583	0.9999985608512583
Exact GP EI Jacobian: Max. GP EI 2.0			
Exact GP EI Jacobian: regret 0.0			

```

1 ### Post-initialisation: iteration 4 Bayesian optimisation
2
3 ### versus ESTIMATED GP EI Jacobian
4
5 np.random.seed(run_num_1)
6 surrogate_approx_4 = GaussianProcess(cov_func, optimize=opt)
7
8 approx_4 = est_GPG0(surrogate_exact_4, Acquisition(util_grad_approx), objfunc, param)
9 approx_4.run(init_evals=n_init, max_iter=iters+3)
10
11 a_approx_4 = np.array(-approx_4.f_best)
12 xbest_approx_4 = approx_4.x_best[np.argmax(a_approx_4)][0]
13 regret_approx_4 = y_global_orig - objfunc(xbest_approx_3) ### Iteration 3's y-value is
14
15 print("Estimated GP EI Jacobian: Max. GP EI", np.round(np.max(a_approx_4), 4))
16 print("Estimated GP EI Jacobian: regret", np.round(regret_approx_4, 4))
17

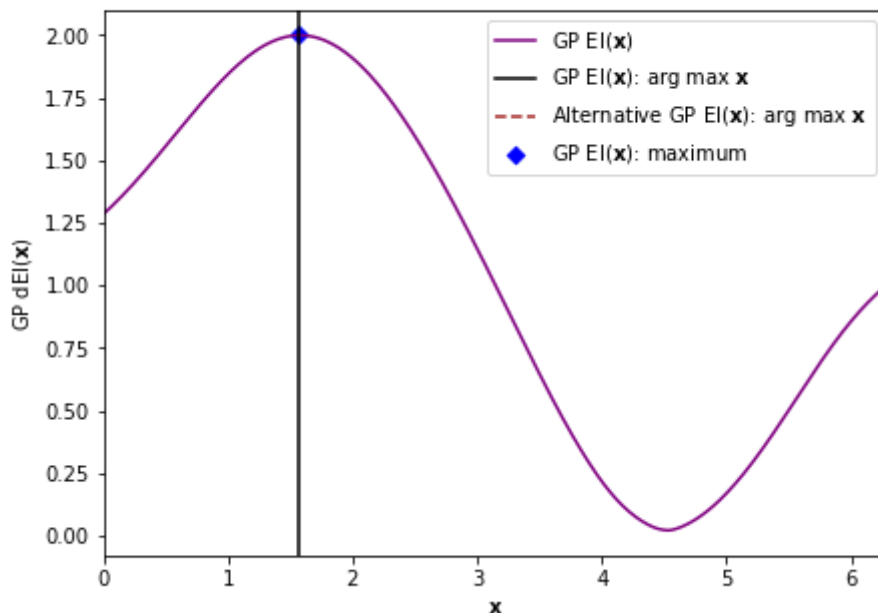
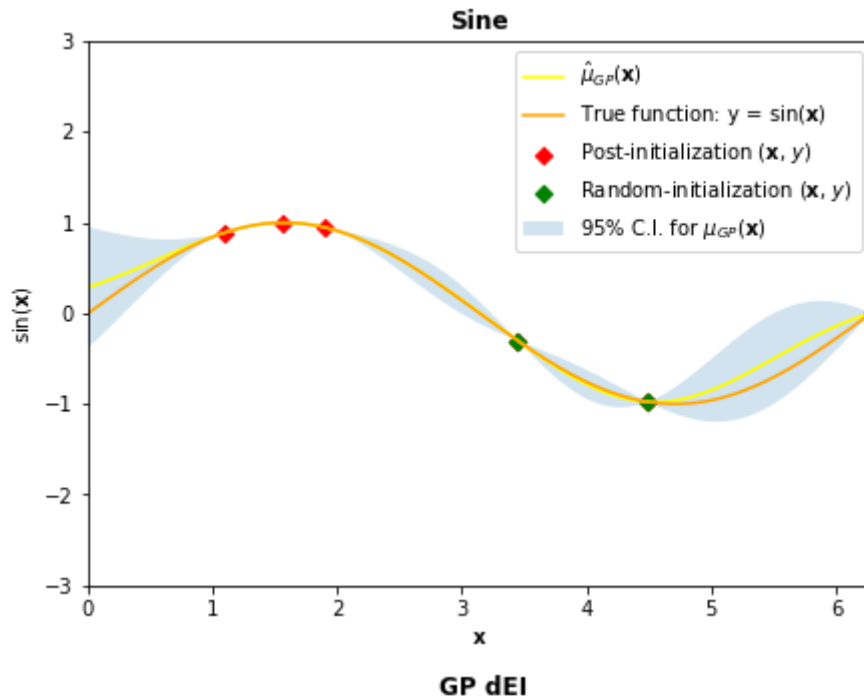
```

Evaluation	Proposed point	Current eval.	Best eval.
init	[3.44829694].	-0.301918370765691	-0.301918370765691
init	[4.49366732].	-0.9761756231500798	-0.301918370765691
1	[1.90357748].	0.9451374717390602	0.9451374717390602
2	[1.09255415].	0.8878052780090047	0.9451374717390602
3	[1.55822889].	0.9999210308501604	0.9999210308501604
4	[6.28318531].	-2.4492935982947064e-16	0.9999210308501604
Estimated GP EI Jacobian: Max. GP EI 0.0054			
Estimated GP EI Jacobian: regret 0.0001			

```

1 ### Post-initialisation: iteration 4 plots
2
3 plot_sine(exact_4, param, new=True)
4 plot_GP_dEI_vs_approx(exact_4, approx_4, param, new=True)
5

```



```

1 ### Post-initialisation: iteration 4 STP EI arg max x, max
2 np.random.seed(run_num_1)
3
4 AcqFuncMaxExact_4 = np.max(-dGPGO.acqfunc(exact_4, x_test)[0])
5 XBestExact_4 = x_test[np.argmax(-dGPGO.acqfunc(exact_4, x_test)[0])][0]
6
7 XBestExactGradExact_4 = exact_4.acqfunc(XBestExact_4)[1][0][0][0]
8 XBestApproxGradExact_4 = exact_4.acqfunc_h(XBestExact_4)[0]
9
10 print("Exact GP EI Jacobian: arg max x:", np.round(XBestExactGradExact_4, 4))
11 print("Estm. GP EI Jacobian: arg max x:", np.round(XBestApproxGradExact_4, 4))
12

```

```

Exact GP EI Jacobian: arg max x: 0.0044
Estm. GP EI Jacobian: arg max x: -0.0032

```

```

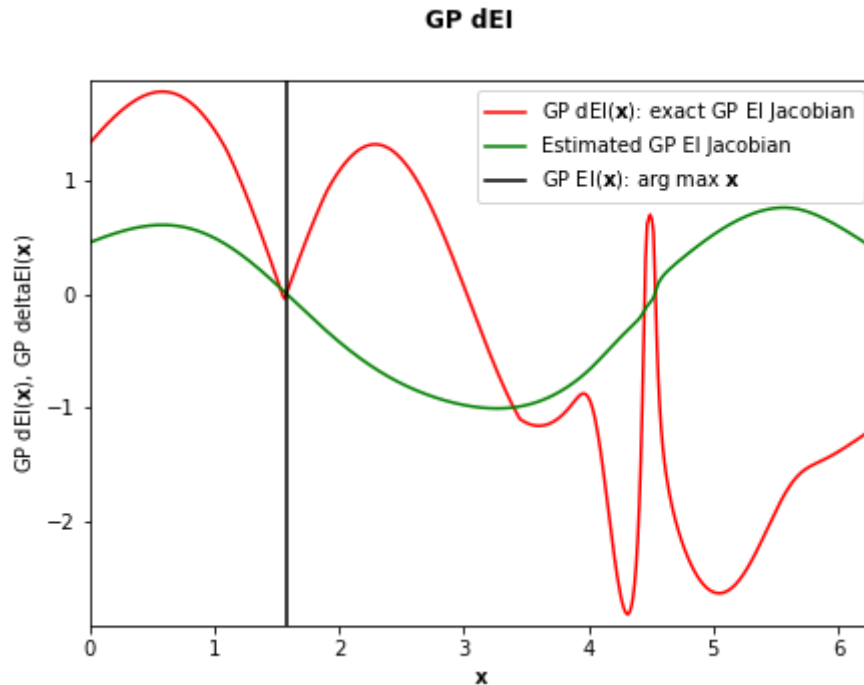
1 ### Post-initialisation: iteration 4 GP EI Jacobian' plots - exact versus estimated
2

```

```

3 plot_GP_EI_jac(exact_4, param, new=True)
4 print("Max. Exact GP EI Jacobian: ", np.round(max(-dGPG0.acqfunc(exact_4, x_test)[1])[0]
5 print("Min. Exact GP EI Jacobian:", np.round(min(-dGPG0.acqfunc(exact_4, x_test)[1])[0]
6 print("Max. Estm. GP EI Jacobian: ", np.round(max(-dGPG0.acqfunc_h(exact_4, x_test)), 4
7 print("Min. Estm. GP EI Jacobian:", np.round(min(-dGPG0.acqfunc_h(exact_4, x_test)), 4)
8 print("Exact GP EI Jacobian: arg max x:", np.round(XBestExactGradExact_4, 4))
9 print("Estm. GP EI Jacobian: arg max x:", np.round(XBestApproxGradExact_4, 4))
10

```



```

Max. Exact GP EI Jacobian: 1.7836
Min. Exact GP EI Jacobian: -2.8227
Max. Estm. GP EI Jacobian: 0.7607
Min. Estm. GP EI Jacobian: -1.0099
Exact GP EI Jacobian: arg max x: 0.0044
Estm. GP EI Jacobian: arg max x: -0.0032

```

CHECKS: exact_0 BayesOpt surrogate, exact GP EI Jacobian

```

1 ### Exact GP EI Jacobian checks: exact_0 BayesOpt surrogate
2
3 f0, df0 = exact_0.acqfunc(x_test)
4 print("Max. Exact GP EI AcqFunc: ", np.round(max(-dGPG0.acqfunc(exact_0, x_test)[0]),
5 print("Min. Exact GP EI AcqFunc: ", np.round(min(-dGPG0.acqfunc(exact_0, x_test)[0]),
6 print("Max. Exact GP EI Jacobian: ", np.round(max(-dGPG0.acqfunc(exact_0, x_test)[1][0]
7 print("Min. Exact GP EI Jacobian:", np.round(min(-dGPG0.acqfunc(exact_0, x_test)[1][0]
8

```

```

Max. Exact GP EI AcqFunc: 0.173
Min. Exact GP EI AcqFunc: 0.0
Max. Exact GP EI Jacobian: 0.002
Min. Exact GP EI Jacobian: 0.002

```

```

1 ### Exact GP EI Jacobian checks: exact_0 BayesOpt surrogate
2
3 mean0, var0 = exact_0.GP.predict(x_test, return_std=True)

```

```

4 std0 = np.sqrt(var0 + eps)
5 print("Max. GP Posterior Mean: ", np.round(max(mean0), 4))
6 print("Min. GP Posterior Mean:", np.round(min(mean0), 4))
7 print("Max. GP Posterior Std. Dev:", np.round(max(std0), 4))
8 print("Min. GP Posterior Std. Dev:", np.round(min(std0), 4))
9

```

```

Max. GP Posterior Mean:  0.081
Min. GP Posterior Mean: -0.9665
Max. GP Posterior Std. Dev: 0.7225
Min. GP Posterior Std. Dev: 0.1588

```

```

1 ### Exact GP EI Jacobian checks: exact_0 BayesOpt surrogate
2
3 ds0, dm0 = exact_0.GP.AcqGrad(x_test)
4 print("Max. GP Posterior Mean 1st Derivative:", np.round(max(dm0), 4))
5 print("Min. GP Posterior Mean 1st Derivative:", np.round(min(dm0), 4))
6 print("Max. GP Posterior Variance 1st Derivative: ", np.round(max(ds0), 4))
7 print("Min. GP Posterior Variance 1st Derivative:", np.round(min(ds0), 4))
8

```

```

Max. GP Posterior Mean 1st Derivative: 1.3703
Min. GP Posterior Mean 1st Derivative: -0.4206
Max. GP Posterior Variance 1st Derivative:  1.9477
Min. GP Posterior Variance 1st Derivative: 0.0001

```

```

1 ### Exact GP EI Jacobian checks: exact_0 BayesOpt surrogate
2
3 tau0 = -exact_0.tau
4 gamma0 = (mean0 - tau0)/(std0 + eps)
5 print("tau:", np.round(tau0, 4))
6 print("Max. gamma:", np.round(max(gamma0), 4))
7 print("Min. gamma:", np.round(min(gamma0), 4))
8

```

```

tau: 0.3019
Max. gamma: -0.3427
Min. gamma: -7.8397

```

```

1 ### Exact GP EI Jacobian checks: exact_0 BayesOpt surrogate
2
3 dsdx0 = ds0 / (2 * (std0 + eps))
4 dmdx0 = (dm0 - gamma0 * dsdx0) / (std0 + eps)
5 print("Max. GP Posterior Std. Dev. 1st Derivative: ", np.round(max(dsdx0), 4))
6 print("Min. GP Posterior Std. Dev. 1st Derivative:", np.round(min(dsdx0), 4))
7 print("Max. gamma 1st Derivative:", np.round(max(dmdx0), 4))
8 print("Min. gamma 1st Derivative:", np.round(min(dmdx0), 4))
9

```

```

Max. GP Posterior Std. Dev. 1st Derivative:  4.9228
Min. GP Posterior Std. Dev. 1st Derivative: 0.0001
Max. gamma 1st Derivative: 142.5155
Min. gamma 1st Derivative: -0.1074

```

```

1 ### Exact GP EI Jacobian checks: exact_0 BayesOpt surrogate
2
3 df0_check = -f0/(std0 + eps) * dsdx0 + (std0 + eps) * norm.cdf(gamma0) * dmdx0
4
5 print("Max. GP EI 1st Derivative - check:", np.round(max(-df0_check), 4))
6 print("Min. GP EI 1st Derivative - check:", np.round(min(-df0_check), 4))
7

```

```

Max. GP EI 1st Derivative - check: 0.0153
Min. GP EI 1st Derivative - check: -0.7158

```

```

1 ### Exact GP EI Jacobian checks: exact_0 BayesOpt surrogate
2
3 print("Max. GP EI 1st Derivative:", np.round(max(-df0)[0][0], 4))
4 print("Min. GP EI 1st Derivative:", np.round(min(-df0)[0][0], 4))
5

```

```

Max. GP EI 1st Derivative: 0.0153
Min. GP EI 1st Derivative: -0.7158

```

```

1 np.random.seed(run_num_1)
2
3 new_mean, new_var = exact_0.GP.predict(x_test, return_std=True)
4 new_std = np.sqrt(new_var + eps)
5 new_ds, new_dm = exact_0.GP.AcqGrad(x_test)
6
7 exact_0.A.dEI_GP(-exact_0.tau, new_mean, new_std, new_ds, new_dm)
8

```

```

--
[[ 1.91929115e-03]],
[[ 3.41122906e-03]],
[[ 4.98786751e-03]],
[[ 6.65191066e-03]],
[[ 8.40608782e-03]],
[[ 1.02531508e-02]],
[[ 1.21958712e-02]],
[[ 1.42370374e-02]],
[[ 1.63794516e-02]],
[[ 1.86259266e-02]],
[[ 2.09792820e-02]],
[[ 2.34423415e-02]],
[[ 2.60179282e-02]],
[[ 2.87088616e-02]],

```

```
[[ 3.15179529e-02]],  
[[ 3.44480011e-02]],  
[[ 3.75017887e-02]],  
[[ 4.06820772e-02]],  
[[ 4.39916019e-02]],  
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[[ 8.00250277e-02]],  
[[ 8.47680141e-02]],
```

1