
Supplementary Materials

Physics Driven Correction for Inverse Estimation

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1 A Studied Inverse Problems

2 A.1 Problem Description

3 **Problem 1, Turbofan Design:** Turbofan is one of the most complex gas aero engine systems, and
4 it is the dominant propulsion system favoured by commercial airliners [1]. The inverse problem
5 for turbofan design is to find a group of design parameters modelled as the state to achieve the
6 desired performance modelled as observation. The observation includes two performance parameters,
7 including the thrust y_t and the thrust specific fuel consumption y_f . The state includes 11 design
8 parameters that control the performance of the engine, including the bypass ratio r_{bp} , the fan pressure
9 ratio π_{fan} , the fan efficiency η_{fan} , the low-pressure compressor pressure ratio π_{LC} , the low-pressure
10 compressor efficiency η_{LC} , the high-pressure compressor pressure ratio π_{HC} , the high-pressure
11 compressor efficiency η_{HC} , the combustor efficiency η_{LC} , the combustion temperature in the burner
12 T_B , the efficiency of high-pressure turbine η_{HT} , and the efficiency of low-pressure turbine η_{LT} .
13 Following the same setting as in [2], the goal is to estimate the design parameters that can achieve the
14 performance of a CFM-56 turbofan engine, for which the thrust should be 121 KN and the thrust
15 specific fuel consumption should be 10.63 g/(kN.s) [3]. This corresponds to the observation vector
16 $\mathbf{y} = [y_t, y_f] = [121, 10.63]$. The 100 experiment cases tested on this problem differ from the state to
17 correct, which is randomly sampled from the feasible region of the design parameter space provided
18 by [2]. Table 1 reports the allowed range of each design parameter, which all together define the
19 feasible region.

Table 1: Feasible region of the design parameter space for problem 1.

Range	r_{bp}	π_{fan}	π_{LC}	π_{HC}	T_B	η_{fan}	η_{HC}	η_{LC}	η_B	η_{HT}	η_{LT}
Min	5	1.3	1.2	8	1300 K	0.85	0.82	0.84	0.95	0.86	0.87
Max	6	2.5	2	15	1800 K	0.95	0.92	0.94	0.995	0.96	0.97

20 **Problem 2, Electro-mechanical Actuator Design:** An electro-mechanical actuator is a device
21 that converts electrical energy into mechanical energy [4], by using a combination of an electric
22 motor and mechanical components to convert an electrical signal into a mechanical movement. It
23 is commonly used in industrial automation[4], medical devices[5], and aircraft control systems [6],
24 etc. We consider the design of an electro-mechanical actuator with a three-stage spur gears. Its
25 corresponding inverse problem is to find 20 design parameters modelled as the state, according to
26 the requirements for the overall cost y_c and safety factor y_s modelled as the observation. The 100
27 experiment cases tested on this problem differ from the observation $\mathbf{y} = [y_c, y_s]$. We have randomly
28 selected 100 combinations of the safety factor and overall cost from the known Pareto front [7], which
29 is shown in Fig. 1a. For each observation, the state to correct is obtained by using an untrained ML
30 model to provide a naturally failed design.

31 **Problem 3, Pulse-width Modulation of 13-level Inverters:** Pulse-width modulation (PWM) of
32 n-level inverters is a technique for controlling the output voltage of an inverter that converts DC

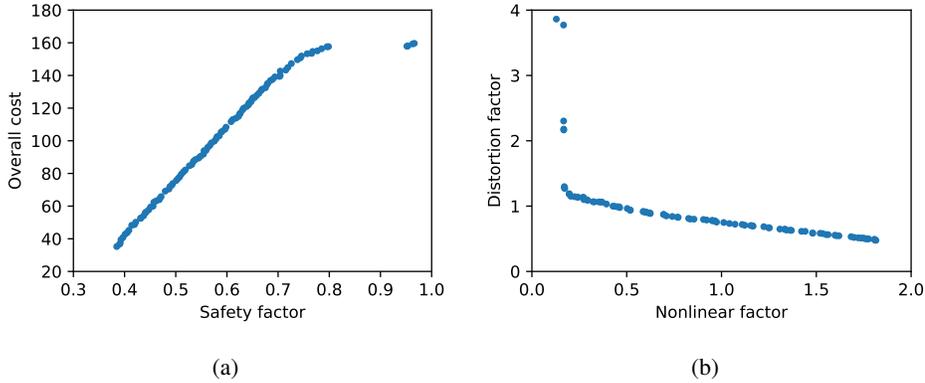


Figure 1: Illustration of the 100 used test cases in the 2-dimensional observation space for problem 2 (subfigure a) and 3 (subfigure b).

33 power into AC power [8]. It modulates the duty cycle of the output waveform of the inverter, thereby
 34 affecting the effective value of the voltage applied to a load. Particularly, a PWM of 13-level inverter
 35 adjusts its output waveform using 13 power switching devices to achieve higher precision, which
 36 is widely used in renewable power generation systems [9], electric vehicles [10], and industrial
 37 automation equipment [11]. It results in a typical inverse problem of finding the suitable control
 38 parameters including 30 switch angles modelled as the state, according to the requirements of
 39 the distortion factor y_d (which measures the harmonic distortion of the output waveform) and the
 40 nonlinear factor y_n (which avoids the malfunctioning of the inverter and the connected load) modelled
 41 as the observation. As in problem 2, the 100 experiment cases tested on this problem also differ from
 42 the observation, i.e. $\mathbf{y} = [y_d, y_n]$. They correspond to 100 randomly selected combinations of the
 43 distortion and nonlinear factors from the known Pareto front in [12], which are shown in Fig. 1b.
 44 For each observation, the state to correct is obtained by using an untrained ML model to provide a
 45 naturally failed estimation.

46 A.2 Physical Evaluation

47 We describe in this section how the physical evaluations are conducted, more specifically, how the
 48 physical errors are assessed. Overall, it includes the *observation reconstruction error*, which is based
 49 on the difference between the given observation and the reconstructed observation from the estimated
 50 state. For different problems, different physical models are used to simulate the reconstruction. It also
 51 includes the *feasible domain error*, which examines whether the estimated state is within a feasible
 52 region of the state space, and this region is often known for a given engineering problem. Apart from
 53 these, there are also other problem-specific errors.

54 A.2.1 Problem 1

55 **Observation Reconstruction Error:** The gas turbine forward model [2] is used to simulate the
 56 performance of the turbofan engine. It is constructed through the aerodynamic and thermodynamic
 57 modelling of the components in a turbofan engine, where the modelled components include the inlet,
 58 fan, low-pressure and high-pressure compressors, combustor, high-pressure and low-pressure turbines,
 59 core and fan nozzles, as well as through considering the energy losses. This model can transform the
 60 input of state into physically reasonable output of observation, which is the thrust y_t and fuel flow
 61 y_f of the engine. Let $F(\mathbf{x})$ denote a forward model. In problem 1, the performance requirement is
 62 specifically $\mathbf{y} = [y_t, y_f] = [121, 10.63]$, thus, for an estimated state $\hat{\mathbf{x}}$, the reconstruction error is

$$e_r(\hat{\mathbf{x}}) = \sum_{i=1}^2 \frac{\|F_i(\hat{\mathbf{x}}) - \mathbf{y}_i\|_1}{2\mathbf{y}_i}, \quad (1)$$

63 where, when i respectively equals to 1 or 2, $F_1(\hat{\mathbf{x}})$ and $F_2(\hat{\mathbf{x}})$ are the estimated thrust and fuel con-
 64 sumption in the engine case, respectively. Because the magnitude of the thrust and fuel consumption
 65 are different, we use the relative error to measure the reconstruction error of the two observation
 66 elements.

67 **Feasible Domain Error:** In aero engine design, the design parameters cannot exceed their feasible
68 region and such a region has already been identified by existing work [2] as in Table 1. For the i -th
69 dimension of an estimated state \hat{x}_i (an estimated design parameter), and given its maximum and
70 minimum allowed values x_{\max} and x_{\min} , we define its feasible domain error by

$$e_i^{(f)} = \max\left(\frac{\hat{x}_i - x_{\min}}{x_{\max} - x_{\min}} - 1, 0\right) + \max\left(-\frac{\hat{x}_i - x_{\min}}{x_{\max} - x_{\min}}, 0\right). \quad (2)$$

71 After normalization, all the feasible values are within the range of $[0, 1]$, while the non-feasible
72 ones outside. The above error simply examines how much the normalized state value exceeds 1
73 or below 0. We compute an accumulated feasible error for all the 11 design parameters, given by
74 $e_f(\hat{\mathbf{x}}) = \frac{1}{11} \sum_{i=1}^{11} e_i^{(f)}$.

75 **Design Balance Error:** Another desired property by aero engine design is a low disparity among the
76 values of the design parameters after normalizing them by their feasible ranges, which indicates a
77 more balanced design, offering better cooperation between the design components and resulting in
78 lower cost [2, 1]. Standard deviation is a suitable measure to assess this balance property, resulting in
79 another physical error

$$e_\sigma(\hat{\mathbf{x}}) = \sigma\left(\left\{\frac{\hat{x}_i - x_{\min}}{x_{\max} - x_{\min}}\right\}_{i=1}^{11}\right). \quad (3)$$

80 where $\sigma(\cdot)$ denotes the standard deviation of the elements from its input set.

81 **Accumulated Physical Error:** The above three types of errors are combined to form the following
82 accumulated physical error:

$$\hat{e}(\hat{\mathbf{x}}) = e_r(\hat{\mathbf{x}}) + 0.1e_f(\hat{\mathbf{x}}) + 0.1e_\sigma(\hat{\mathbf{x}}). \quad (4)$$

83 The weights are given as 1, 0.1 and 0.1, respectively. This is because the reconstruction error
84 determines whether the estimated state is feasible, while the other two errors are used to further
85 improve the quality of the estimated state from the perspective of the design preference. Here $e_r(\hat{\mathbf{x}})$ is
86 obtained using a forward simulation process thus is an implicit error, while e_f and e_σ have analytical
87 expressions and simple gradient forms, and thus are explicit errors.

88 A.2.2 Problem 2

89 **Observation Reconstruction Error:** The used forward model for electro-mechanical actuator design
90 is a performance simulation model, considering a stepper motor, three stages of spur gears and a
91 housing to hold the components (i.e., stepper motor, and three stages of spur gears) [7]. It consists
92 of a physical model that predicts its output speed and torque and component-specific constraints, a
93 cost model and a geometric model that creates 3-D meshes for the components and the assembled
94 system. The integrated model predicts the observation $\mathbf{y} = \{y_c, y_s\}$, and is named as the "CS1"
95 model in [7]. After reconstructing by CS1 the safety factor y_s and total cost y_c from the estimated
96 design parameters $\hat{\mathbf{x}}$, the reconstruction error is computed using Eq. 1.

97 **Feasible Domain Error:** The same feasible domain error e_f as in Eq. (2) is used for each design
98 parameter of problem 2. The only difference is that the allowed parameter ranges for defining the
99 feasible region have changed. We use the region identified by [7]. There are 20 design parameters,
100 thus e_f is an average of 20 individual errors.

101 **Inequality Constraint Error:** We adopt another seven inequality constraints provided by the forward
102 model [7] to examine how reasonable the estimated design parameters are. These constraints do not
103 have analytical forms, and we express them as $c_i(\hat{\mathbf{x}}) \leq 0$ for $i = 1, 2, \dots, 7$. Based on these, we
104 define the following inequality constraint error

$$e_c(\hat{\mathbf{x}}) = \frac{1}{7} \sum_{i=1}^7 \max(c_i(\hat{\mathbf{x}}), 0). \quad (5)$$

105 **Accumulated Physical Error:** We then combine the above three types of errors, given as

$$\hat{e}(\hat{\mathbf{x}}) = e_r(\hat{\mathbf{x}}) + 0.1e_f(\hat{\mathbf{x}}) + e_c(\hat{\mathbf{x}}), \quad (6)$$

106 where both $e_r(\hat{\mathbf{x}})$ and $e_c(\hat{\mathbf{x}})$ are implicit errors computed using a black-box simulation model, while
107 e_f is an explicit error. In this case, we increase the weight for inequality constraint error to be the

108 same as the reconstruction error, this is because we regard the implicit errors irrespective of their
 109 types as the same. Of course, one can also use different weights for different types of errors according
 110 to their expertise.

111 A.2.3 Problem 3

112 We use the forward model from [12] to reconstruct the observation for the 13-level inverter. It takes
 113 the control parameters as the input and returns the distortion factor y_d and the nonlinear factor y_n .
 114 Based the reconstructed y_d and y_n , the observation reconstruction error e_r is computed by Eq. (1) in
 115 the same way as in problems 1 and 2. Similarly, the same feasible boundary error e_f as in Eq. (2) is
 116 computed, but the feasible region is different where the range of $[0, \frac{\pi}{2}]$ is applied for all the 30 control
 117 parameters, which is defined in [12]. A similar inequality constraint error as in Eq. (5) is used, which
 118 contains 29 inequality constraints in the form of

$$c_i(\hat{\mathbf{x}}) = \hat{\mathbf{x}}_i - \hat{\mathbf{x}}_{i+1} < 0, \text{ for } i = 1, 2, \dots 29. \quad (7)$$

119 Finally, the accumulated physical error is given by

$$\hat{e}(\hat{\mathbf{x}}) = e_r(\hat{\mathbf{x}}) + 0.1e_f(\hat{\mathbf{x}}) + 10e_c(\hat{\mathbf{x}}), \quad (8)$$

120 where a large weight is used for $e_c(\hat{\mathbf{x}})$ because the inequality constraints that it involves are very
 121 critical for the design. Among the three types of errors, $e_r(\hat{\mathbf{x}})$ is an implicit error, while $e_f(\hat{\mathbf{x}})$ and
 122 $e_c(\hat{\mathbf{x}})$ are explicit errors.

123 B Extra Implementation Information

124 In this section, we introduce extra implementation information for GEESE and the compared methods,
 125 in addition to what has been mentioned in the main text. In GEESE implementation, the latent vector
 126 \mathbf{z} has the same dimension as the state \mathbf{x} in problems 1 and 2, because the optimization is done
 127 directly on the latent vectors. In problem 3, the dimension of \mathbf{z} is set be 1, and transformed into a
 128 30-dimensional vector \mathbf{x} by the state generator. The number of the latent vector \mathbf{z} used for sampling
 129 distribution of generators is set increasingly as $d = 64, 128, 256$ for problems 1, 2, and 3, due to the
 130 increasing dimension of the state space of the three problems. Although, the budget query number
 131 equals to 1000, because GEESE may query two times per iteration, thus, the maximum iteration
 132 number is smaller than 1000, which is determined when the budget is used up.

133 For BOGP, its Bayesian optimization is implemented using the package [13]. The prior is set to be a
 134 Gaussian process, and its kernel is set as Matern 5/2. The acquisition function is set to be the upper
 135 confidence bound (UCB). The parameter kappa, which indicates how closed the next parameters are
 136 sampled, is set to be 2.5. The other hyperparameters are kept as default. Since Bayesian optimization
 137 only queries one state-error pair in each iteration, its maximum iteration number is equal to the
 138 maximum number of queries, i.e., 1000.

139 The other methods of GA, PSO, CMAES, ISRES, NSGA2, and UNSGA3 are implemented using
 140 the package pymoo [14]. For ISRES, we apply a 1/7 success rule to generate seven times more
 141 candidates than that in the current population in order to perform a sufficient search. The other
 142 parameters are kept as default. Since these algorithms need to query the whole population in each
 143 iteration, their maximum iteration number is thus much smaller than the query budget 1000. In the
 144 experiments, these algorithms are terminated when the maximum query number 1000 is reached.

145 To implement SVPEN [2], we use the default setting for problem 1. As for problems 2 and 3, to
 146 construct the state estimator and the error estimator for SVPEN, the same structures of the base neural
 147 networks and the exploitation generator as used by GEESE are adopted, respectively. Also the same
 148 learning rate as used by GEESE is used for SVPEN, while the other settings are kept as default for
 149 problems 2 and 3. In each iteration, SVPEN queries three times the physical errors for simulating the
 150 exploitation, as well as the regional and global exploration. Thus, the maximum iteration number of
 151 SVPEN is set as 333 to match the query budget 1000.

152 All the methods are activated or initialized using the same set of N state-error pairs randomly sampled
 153 from a predefined feasible region in the state space. For GEESE and SVPEN, these samples are
 154 used to train their surrogate error models, i.e., the base neural networks in GEESE and the error
 155 estimator in SVPEN, thus their batch size for training is also set as N . For Bayesian optimization,

Table 2: Performance comparison for two different values of feasibility threshold ϵ , where the best is shown in **bold** while the second best is underlined for query times.

Threshold	Algorithm	Problem 1		Problem 2		Problem 3	
		State Dimension:11		State Dimension:20		State Dimension:30	
		Failure times	Query times	Failure times	Query times	Failure times	Query times
$\epsilon = 0.1$	BOGP	0	<u>3.04 ±0.83</u>	78	849.26 ±295.35	3	<u>86 ±200.49</u>
	GA	0	64 ±0	0	65.92 ±10.92	8	183.04 ±287.80
	PSO	0	64 ±0	0	<u>64.00 ±0</u>	8	199.92 ±284.94
	CMAES	0	12 ±0	0	73.84 ±25.81	3	127.29 ±233.71
	ISRES	0	65 ±0	0	108.52 ±41.36	10	203.30 ±297.13
	NSGA2	0	64 ±0	0	70.40 ±19.20	8	189.04 ±293.60
	UNSGA3	0	64 ±0	0	68.48 ±16.33	7	177.52 ±275.84
	SVPEN	82	932.51 ±176.38	100	1000 ±0	100	1000 ±0
	GEESE (ours)	0	2.34 ±17.99	0	23.13 ±17.99	0	35.58 ±63.82
$\epsilon = 0.05$	BOGP	0	9.24 ±3.97	100	1000 ±0	16	<u>227.63 ±364.08</u>
	GA	0	64.00 ±0	0	353.28 ±105.74	20	297.92 ±363.45
	PSO	0	64.00 ±0	1	157.84 ±137.40	18	290.96 ±373.65
	CMAES	0	77.56 ±4.38	1	302.59 ±156.24	22	344.54 ±363.18
	ISRES	0	193.00 ±0	3	391.54 ±241.22	19	313.69 ±368.78
	NSGA2	0	64.00 ±0	0	352.00 ±114.31	20	299.84 364.63
	UNSGA3	0	64.00 ±0	0	368.64 ±102.85	20	310.72 ±370.24
	SVPEN	100	1000 ±0	100	1000 ±0	100	1000 ±0
	GEESE (Ours)	0	<u>20.20 ±16.37</u>	0	<u>189.90 ±164.96</u>	2	81.26 ±155.30

156 these samples are used to construct the Gaussian process prior. For GA, PSO, ISRES, NSGA2, and
 157 UNSGA3, these samples are used as the initial population to start the search. The only special case is
 158 CMAES, as it does not need a set of samples to start the algorithm, but one sample. So we randomly
 159 select one state-error pair from the N pairs to activate its search.

160 For problem 3, we post-process the output of all the compared methods, in order to accommodate the
 161 element-wise inequality constraints in Eq. (7), by

$$\hat{\mathbf{x}}_i^{(p)} = \hat{\mathbf{x}}_1^{(p)} + \frac{1}{1 + e^{-\sum_{j=1}^i \hat{\mathbf{x}}_j^{(p)}}} \left(1 - \hat{\mathbf{x}}_1^{(p)}\right). \quad (9)$$

162 As a result, the magnitude of the element in $\hat{\mathbf{x}}^{(p)}$ is monotonically increasing, and the inequality
 163 constraints are naturally satisfied. But this can complicate the state search, as the elements are no
 164 longer independent. A balance between correlating the state elements and minimizing the accumulated
 165 physical error is needed. But in general, we have observed empirically that the above post-processing
 166 can accelerate the convergence for all the compared methods. One way to explain the effectiveness
 167 of this post-processing is that it forces the inequality constraints to hold, and this is hard for the
 168 optimization algorithms to achieve on their own.

169 C Extra Results

170 **Varying Feasibility Threshold:** In addition to the feasibility threshold of $\epsilon = 0.075$ as studied in the
 171 main text, we test two other threshold values, including $\epsilon = 0.05$ representing a more challenging
 172 case with lower error tolerance, and $\epsilon = 0.1$ representing a comparatively easier case with higher
 173 error tolerance. Results are reported in Table 2. In both cases, GEESE has failed the least times
 174 among all the compared methods and for all three problems studied. It is worth to mention that, in
 175 most cases, GEESE has achieved zero failure, and a very small $N_{\text{failure}} = 2$ out of 100 in only one
 176 experiment when all the other methods have failed more than fifteen times. Also, this one experiment
 177 is the most challenging, solving the most complex problem 3 with the highest state dimension $d = 30$
 178 and having the lowest error tolerance $\epsilon = 0.05$. In terms of query times, GEESE has always ranked
 179 among the top 2 most efficient methods for all the tested cases and problems, while the ranking of
 180 the other methods vary quite a lot. For instance, when $\epsilon = 0.05$, BOGP performs the best for the
 181 easiest problem 1, but it performs the worst for the more difficult problem 2 where it has failed to
 182 find a feasible solution within the allowed query budget. In the most difficult experiment that studies
 183 problem 3 under $\epsilon = 0.05$, GEESE requires much less query times and is significantly more efficient
 184 than the second most efficient method.

185 **Varying Initial Sample Size:** In addition to the studied initial sample size $N = 64$ in the main
 186 text, we further compare to more cases of $N = 16$ and $N = 32$ under $\epsilon = 0.05$. The results are
 187 shown in Table 3. Still, GEESE has the least failure times in all experiments, which is important

Table 3: Performance comparison under for two different sizes of initial samples, where the best is shown in **bold** while the second best is underlined for query times.

Initial Size	Algorithm	Problem 1		Problem 2		Problem 3	
		State Dimension:11		State Dimension:20		State Dimension:30	
		Failure times	Query times	Failure times	Query times	Failure times	Query times
$N = 32$	BOGP	0	9.60 ±3.89	100	1000 ±0	15	239.12 ±367.12
	GA	0	<u>32.00 ±0</u>	0	241.60 ±71.75	21	270.80 ±382.51
	PSO	0	<u>32.00 ±0</u>	18	311.20 ±333.45	14	283.28 ±324.54
	CMAES	0	77.56 ±4.38	1	321.01 ±188.6	22	280.54 ±363.18
	ISRES	0	64.00 ±0	3	416.24 ±209.23	21	276.24 ±386.75
	NSGA2	0	<u>32.00 ±0</u>	1	239.44 ±150.26	22	262.88 ±394.99
	UNSGA3	0	<u>32.00 ±0</u>	2	218.72 ±136.53	22	260.64 ±396.51
	SVPEN	100	1000 ±0	100	1000 ±0	100	1000 ±0
	GEESE (Ours)	0	33.63 ±19.35	0	<u>233.96 ±180.01</u>	10	167.77 ±284.31
$N = 16$	BOGP	0	10.62 ±5.53	100	1000 ±0	17	249.88 ±372.99
	GA	0	<u>16.00 ±0</u>	43	657.04 ±352.42	23	364.40 ±373.30
	PSO	0	<u>32.00 ±0</u>	10	293.76 ±271.02	21	247.76 ±392.87
	CMAES	0	77.56 ±4.38	1	333.49 ±156.24	17	320.07 ±350.84
	ISRES	0	17.00 ±0	2	<u>260.50 ±189.71</u>	20	<u>243.20 ±392.70</u>
	NSGA2	0	32.00 ±0	33	590.96 ±355.93	25	377.20 ±385.78
	UNSGA3	0	32.00 ±0	28	487.04 ±360.22	28	408.80 ±397.77
	SVPEN	100	1000 ±0	100	1000 ±0	100	1000 ±0
	GEESE(Ours)	0	36.72 ±22.52	0	248.26 ±176.64	9	163.26 ±279.34

188 in remediating failed ML estimations. In terms of query times, GESE still ranks among the top 2
189 most efficient methods for the two more complex problems 2 and 3, being the top 1 with significantly
190 less query times for the most complex problem 3. However, GESE does not show advantage in the
191 simplest problem 1 with the lowest state dimension. It performs similarly to those top 2 methods
192 under $N = 32$, e.g. 34 vs. 32 query times, while performs averagely when the initial sample size
193 drops to $N = 16$. This is in a way not surprising, because BOGP, GA, PSO, NSGA2 and UNSGA3
194 can easily explore the error distribution of low state dimensions. BOGP uses Gaussian process to
195 construct accurate distribution of errors, while GA, PSO, NSGA2, and UNSGA3 sample sufficient
196 samples in each iteration to sense the distribution of error in each iteration, and there is a high chance
197 for them to find a good candidate in early iterations when the search space has a low dimension.
198 However, the valuable samples are sparsely distributed into the higher dimensional space, and it is
199 challenging for them to explore the error distribution and find the feasible states in the early iterations.

200 D GESE Sensitivity Analysis

201 We conduct extra experiments to assess the hyperparameter sensitivity of GESE using problem 1
202 under $\epsilon = 0.05$. The studied hyperparameters include the number L of the base neural networks,
203 the number N_{IT} of the candidate states generated for exploitation, the learning rate for training the
204 exploitation generator η_{IT} , and the early stopping threshold ϵ_e for training the base neural networks.
205 The results are reported in Table 4. It can be seen from the table that, although the performance varies
206 versus different settings, the change is mild within an acceptable range. This makes it convenient to
207 tune the hyperparameters for GESE.

208 Below we further discuss separately the effects of different hyperparameters and analyze the reasons
209 behind: (1) We experiment with three base network numbers $L = 2, 4, 8$. It can be seen from Table
210 4 that there is a performance improvement as L increases in terms of the required query times,
211 but this is on the expense of consuming higher training cost. Thus, we choose the more balanced
212 setting $L = 4$ as the default in our main experiments. (2) We test different candidate state numbers
213 $N_{IT} = 1, 32, 64, 128$ used for exploitation. Results show a performance increase followed by a
214 decrease as N_{IT} increases. Using a candidate set containing one single state is insufficient, while
215 allowing a set with too many candidate states can also harm the efficiency. This can be caused by
216 the approximation gap between the surrogate error model and the true physical evaluation. In our
217 main experiments, we go with the setting of 64 for problem 1 as we mentioned in Appendix B,
218 because it provides a proper balance between the exploitation performance and the overfitting risk.
219 (3) We also examine different settings of the learning rate for training the exploitation generator, i.e.,
220 $\eta_{IT} = 1e^{-1}, 1e^{-2}, 1e^{-3}$. Similarly, there is a performance increase first but followed by a decrease,
221 as in changing N_{IT} . A larger learning rate can accelerate the learning of the exploitation generator
222 and subsequently enable a potentially faster search of the feasible state. But an overly high learning

223 rate can also cause fluctuation around the local optimum, and this then consumes more query times.
 224 Although a smaller learning rate can enable a more guaranteed convergence to the local optimum,
 225 it requires more iterations, thus more query times. (4) We experiment with three values of early
 226 stopping threshold, i.e., $\epsilon_e = 1e^{-3}, 1e^{-4}, 1e^{-5}$. It can be seen from Table 4 that a decreasing ϵ_e can
 227 first improve the efficiency but then reduce it, however without changing much the standard deviation.
 228 An inappropriate setting of the early stopping threshold can lead to base neural networks overfitting
 229 (or underfitting) to the actual data distribution, thus harm the performance.

Table 4: Results of sensitivity Analysis, where a better performance is highlighted in **bold**.

(1): Effect of Base Network Number		(2): Effect of Latent Vector Number	
Base Network Number	Query times	Latent vector number	Query times
$L = 2$	20.20 \pm 16.37	$N_{IT} = 1$	72.56 \pm 36.13
$L = 4$	15.44 \pm 13.86	$N_{IT} = 32$	28.21 \pm 17.05
$L = 8$	15.09 \pm13.01	$N_{IT} = 64$	20.20 \pm16.37
		$N_{IT} = 128$	26.95 \pm 14.12

(3): Effect of Learning rate for Exploration Generator		(4): Effect of Early Stopping Threshold	
Learning Rate	Query times	Early stopping threshold	Query times
$\eta_{IT} = 1e^{-1}$	27.56 \pm 9.28	$\epsilon_e = 1e^{-3}$	37.55 \pm 17.28
$\eta_{IT} = 1e^{-2}$	20.20 \pm16.37	$\epsilon_e = 1e^{-4}$	20.20 \pm16.37
$\eta_{IT} = 1e^{-3}$	64.36 \pm 44.50	$\epsilon_e = 1e^{-5}$	26.20 \pm 15.45

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