IDENTIFICATION OF OPTIMAL SOLUTIONS IN BAYESIAN OPTIMIZATION FOR NOISY PROBLEMS

Chenxi Li
Department of Information Systems and Management Engineering
Southern University of Science and Technology
Shenzhen, China
12333226@mail.sustech.edu.cn

ABSTRACT

We consider the identification of optimal solutions in Bayesian optimization (BO) when dealing with noisy problems. Given a limited budget, BO iteratively searches for and evaluates decision points from the decision space to optimize the objective function. When the budget is exhausted, BO identifies one point to return as its suggestion of the optimal solution. In noise-free scenarios, the typical suggestion is the best point that BO has evaluated. However, in noisy settings where points are observed with random noise, it is difficult to identify the true best evaluated point. We thus investigate alternatives to decide what to return in noisy settings. Three possible types of point to return under investigation in this work include: the evaluated point with the best observed value, the evaluated point with the best surrogate model value, and the point with the best surrogate model value among the entire decision space. The surrogate model is a statistical model in BO to predict the response values for any points. The model, to some extent, is able to 'denoise' the response with its prediction and thus may provide more stable inference compared with the raw observations. We empirically compare these three choices under different circumstances of noise levels, response smoothness and the dimensionality of the search space. We provide some informed recommendations for identification approaches.

Keywords Bayesian optimization · Gaussian process · blackbox optimization · noisy problems · BBOB

1 Introduction

Bayesian optimization (BO) is recognized as an advanced framework for black-box optimization due its efficiency under limited computing budget. This efficiency has led to its widespread adoption across various fields, including material design[Zhang Yichi, 2020], robot control[Martinez-Cantin, 2017], and machine learning [Snoek et al., 2012]. BO is a surrogate-assisted sequential optimization approach. In each iteration, it selects the next evaluation point to balance exploration and exploitation based on the observed results from the past iterations. There are two core components of BO: the surrogate model and the acquisition function. The surrogate model, typically a Gaussian process (GP) model [Rasmussen and Williams, 2005], is a statistical predictive model built with the current observations. The acquisition function then leverages this model to determine the location of the next evaluation point. As the surrogate model can summarize all the current observations to inform the response value at any unobserved point, the search under its guidance becomes more efficient. Readers can refer to [Shahriari et al., 2016],[Frazier, 2018] and [Garnett, 2023] for details of BO and GP.

BO has demonstrated its well-accepted performances in many scenarios, especially in low-dimensional, noise-free, and expensive problems. When the objective function is noisy, BO faces a critical challenge: the observations are no longer perfectly accurate. This issue impacts BO in several different aspects, such as the accuracy of the acquisition function and the quality of the final optimal point returned by BO. The most commonly used acquisition function is Expected Improvement (EI) [Jones et al., 1998]. At a candidate point, EI computes the expected improvement of the response at this point over the current best value, which typically is the best objective value at already evaluated points in noiseless case. We then select the point with the highest EI value as the next observation point. In cases of high noise

levels, the current optimal value may be significantly disturbed, affecting the point selection strategy of EI and leading to a tendency to over-exploration. As aforementioned, the noise level also impacts the final solution returned by BO. In a real-world application, the budget for decision-making stage is typically restricted, limiting the possible number of iterations for BO. When the budget is exhausted, BO should identify a solution to return to the decision maker. This solution can be treated as the 'best decision' BO suggests. An intuitive choice of this solution is the best point that has been tried by BO. However, in noisy settings, the evaluated point with best observed value may not be the true best and thus returning this point could affect the quality of the decision. A possible alternative is to return the evaluated point with the best surrogate value. As the GP model could provide a prediction of the 'denoised' response, its prediction are potentially more reliable than the raw observations. Furthermore, as the GP model can also predict the response value at all un-evaluated points, the points that has never been evaluated by BO, we could also extend the candidate set of the returned points to the entire space, i.e., return the point with the best surrogate value from the whole decision space.

This work provides an empirical study to examine the influences of noise objective functions to these two aspects. To the best of our knowledge, this topic has not been well discussed in literature. Specifically, in EI function, we test two choices of the current best value: the best observed and predictive value at evaluated points. For the point to return, we compare three choices: the evaluated point with the best observed value, the evaluated point with the best surrogate model value, and the point with the best surrogate model value among the entire decision space. The numerical studies are conducted with the BBOB [Hansen et al., 2010] test functions. BBOB is a set of challenging and representative synthetic test functions with varying characteristics and complexities for optimization, including function shapes, smoothness, and dimensionality.

Contributions. In this work, we (i) use the BBOB test functions to conduct noise-free optimization experiments in different dimensions, highlighting the differences between the returning the observational best evaluated point and the best predictive point from the entire space in noise-free cases. The experimental results demonstrate that the intuitive approach of using observable output in the absence of noise is indeed the best. Then, (ii) we select 9 representative functions from the 24 BBOB test functions for optimization experiments with homogeneous noise levels. We set different noise magnitudes and input dimensions. For each specific experimental setting, we provide several repetitions of experiments to ensure the validity of the results. Our findings indicate that returning the evaluated points with the largest surrogate value almost always yields relatively good optimization results. This conclusion can offer valuable guidance for selecting the identification approach in BO when dealing with noisy problems. Furthermore, (iii) we briefly discuss the influence of extreme experimental conditions and heterogeneous noise on the choice of identificaiton approach.

2 Basics of Bayesian Optimization

Denote $f(x)$ as an objective black-box function. We consider the following optimization problem:

$$x^* = \arg\max_{x \in \mathcal{X}} f(x), \tag{1}$$

where $\mathcal{X}$ is the design space, assumed to be compact. The objective function $f(x)$ has no closed form, but for any $x_0 \in \mathcal{X}$ (observation point), the objective function value $f(x_0)$ can be evaluated (observation value) by running an experiment or computer simulation at x_0. Bayesian optimization frameworks commonly employ Gaussian processes (see Section 2.1) as surrogate models to construct the posterior distribution of the objective function, providing a high degree of flexibility. With Gaussian process modeling, the model can yield the predicted mean and uncertainty for any point in the search space. Using these predicted values and uncertainties, we can design acquisition functions (see Section 2.2) to balance exploration and exploitation, thus selecting the next observation point. The specific Bayesian optimization algorithm is outlined in **Algorithm 1**.

Note that **Algorithm1** provides the standard Bayesian optimization algorithm under the assumption of a noise-free condition. In the presence of noise, outputting the point corresponding to the minimum observed value as the result may not be appropriate. Two alternative predictive output methods may be considered: outputting the point with the smallest predicted mean among the observation points or outputting the point with the smallest predicted mean throughout the entire design space. The following experimental segment will focus on comparing the output results of these output methods.

2.1 Gaussian process

Gaussian process is a nonparametric model that is fully characterized by its prior mean function $m(x) : \mathcal{X} \to \mathbb{R}$ and positive definite kernel functions(Can also be thought of as a covariance function) $k : \mathcal{X} \times \mathcal{X} \to \mathbb{R}$. For any finite set of points within the search space $x_{1:n}$, define $f_i := f(x_i)$ as the corresponding value of the objective function at x_i,

Algorithm 1: Bayesian optimization

Input: number of initial point n_0, number of max iteration n

Randomly get initial data $D_{1:n_0}$ and update GP model;

for $t = 1, 2, ..., n$ **do**

  Find x_t by optimizing the acquisition function over the GP $x_t = \arg\max_x u(x|D_{1:n_0+n})$;

  Sample the objective function: $y_t = f(x_t) + \epsilon_t$;

  Augment the data $D_{1:n_0+n} = D_{1:n_0+n-1}, (x_t, y_t)$ and update GP model;

end

Result: $(x_{t^*}, y_{t^*}) \in D_{1:n_0+n}, t^* = \arg\max y_{1:n_0+n}$

$y_i := f(x_i) + \epsilon_i$ is the corresponding noisy observation at x_i. In the Gaussian process model, we assume that $\mathbf{f} := f_{1:n}$ follows a joint Gaussian distribution, and that $\mathbf{y} := y_{1:n}$ obeys a normal distribution given $\mathbf{f}$, which is expressed as follows:

$$\mathbf{f} \mid \mathcal{X} \sim \mathcal{N}(\mathbf{m}, \mathbf{K}) \tag{2}$$

$$\mathbf{y} \mid \mathbf{f}, \sigma^2 \sim \mathcal{N}(\mathbf{f}, \sigma^2\mathbf{I}]) \tag{3}$$

Note here we treat the objective function $f(x)$ as a random variable, and equation(2) represents the prior distribution of the variable $f(x)$. where $\mathbf{m}$ represents the prior mean function, and $K_{i,j} := k(x_i, x_j)$ is the covariance matrix. After obtaining the observation data $\mathcal{D}_n = (x_i, y_i)_{i=1}^n$, $f(x)$ given the observed data $\mathcal{D}_n$, for the new value to be predicted $f(x^*)$, we have the following joint distribution:

$$\begin{bmatrix} \mathbf{y} \\ f(x^*) \end{bmatrix} \sim \mathcal{N}\left(\mathbf{m}, \begin{bmatrix} \mathbf{K} + \sigma^2\mathbf{I} & \mathbf{k}(x^*) \\ \mathbf{k}(x^*)^T & k(x^*, x^*) \end{bmatrix} \right)$$

Using the conditional probability distribution formula of normal distribution, it is easy to deduce the mean and variance functions of $f(x^*)$ as follows:

$$\mathbf{m}_n(x^*) = \mathbf{m}(x^*) + \mathbf{k}(x^*)^T(\mathbf{K} + \sigma^2\mathbf{I})^{-1}(\mathbf{y} - \mathbf{m}(\mathbf{x})) \tag{4}$$

$$\sigma_n^2(x^*) = k(\mathbf{x}, \mathbf{x}) - \mathbf{k}(\mathbf{x})^T(\mathbf{K} + \sigma^2\mathbf{I})^{-1}\mathbf{k}(\mathbf{x}) \tag{5}$$

The $\mathbf{k}(x^*)$ in the formula is the vector of covariance between x^* and $\mathbf{x}_{1:n}$. By employing the Gaussian process model, we can obtain the predicted mean and predicted variance for each point in the search space, which provides an important basis for the design of the acquisition function.

2.2 Expected improvement

BO has a variety of acquisition fuction options, including Expected improvement[Jones et al., 1998], GP upper confiddences bound[Srinivas et al., 2009], Thompson sampling[Thompson, 1933], and Entropy search methods[Hennig and Schuler, 2012]. This paper concentrates on the most commonly used method EI. The main idea of EI is to select the point with the greatest improvement expectation compared to the current optimal value as the next observation point. Specifically, we first define the improvement function **I**(improvement function):

$$I(\mathbf{x}, v, \theta) := (v - f_n^*)\mathbb{I}(v > f_n^*) \tag{6}$$

where $v \sim \mathcal{N}(m_n(\mathbf{x}), \sigma^2(\mathbf{x}))$, $\mathbb{I}$ is the indicator function, θ is the hyperparameter set. f_n^* is the current optimal value, $m_n(\mathbf{x}), \sigma_n(\mathbf{x})$ are respectively the values returned by the Gaussian process model for the input value **x** Predicted mean and predicted variance. Take expectation for v to get the acquisition function EI:

$$u(\mathbf{x}; D_{1:n}) := \mathbb{E}[I(\mathbf{x}, v, \theta)] = (m_n(\mathbf{x}) - f_n^*)\Phi\Big(\frac{m_n(\mathbf{x}) - f_n^*}{\sigma(\mathbf{x})}\Big) + \sigma_n(\mathbf{x})\phi\Big(\frac{m_n(\mathbf{x}) - f_n^*}{\sigma_n(\mathbf{x})}\Big) \tag{7}$$

Where Φ and ϕ are the cumulative distribution (CDF) and probability density distribution (PDF) of the standard normal distribution, respectively.

When there is noise in the objective function, the current optimal value f_n^* is inaccurate. In situations of high noise level, the value of f_n^* may be more extreme, causing EI to mistakenly believe that most points have minimal improvement expectations, making EI overly biased towards exploration rather than exploitation. One of the most intuitive solutions is to use the minimum predicted mean m_n^* of the surrogate model among the observed points to replace f_n^*. This actually improves EI from optimizing the optimal observation value with noise to optimizing the optimal predicted value of the surrogate model, thereby improving the algorithm's robustness to noise. We record the improved EI as EIM, and its expression is as follows:

$$u'(\mathbf{x}; D_{1:n}) := (m_n(\mathbf{x}) - m_n^*)\Phi\Big(\frac{m_n(\mathbf{x}) - m_n^*}{\sigma(\mathbf{x})}\Big) + \sigma_n(\mathbf{x})\phi\Big(\frac{m_n(\mathbf{x}) - m_n^*}{\sigma_n(\mathbf{x})}\Big) \tag{8}$$

In fact, there are many other variants of EI designed to deal with noisy problems, such as Augmented expected improvement(AEI)[Huang et al., 2006], the reinterpolation procedure(RI)[Forrester et al., 2006], Expected quantile improvement(EQI)[Picheny et al., 2012] and so on. The behavior of these methods has been detailed discussed in [Picheny et al., 2013]. The experiments in this article will not involve too many variations of EI, since there is no direct relationship between the output method of the final result and the point selection method of the acquisition function.

3 Test functions and experimental settings

3.1 BBOB benchmark functions

The test functions in this article are selected from the 24 test functions of the BBOB noiseless test function group, with added noise to serve as our test benchmark problems. These functions are designated as F1-F24. In the original BBOB text's configurations, these functions are categorized into five types: separable functions (F1-F5), functions with low or moderate conditioning (F6-F9), functions with high conditioning and unimodal (F10-F14), multimodal functions with adequate global structure (F15-F19), and multi-modal functions with weak global structure (F20-F24). Every function within the BBOB test function group is capable of acquiring novel test functions through alterations like shifting or rotating. In subsequent experiments of this article, we fixed these 24 noise-free functions in advance. The optimal values, standard deviations, and simple descriptions of these functions are shown in Table 1. More detailed information on them can be found in [Hansen et al., 2010].

2Dfunctions	optimal value	std	comment
F1	79.48	12.57	sphere function,unimodal,presumably the most easy continuous domain ssearch problem
F2	66.95	10044455.67	Globally quadratic and ill-conditioned(about 10^6) function with smooth local irregularities.Conditioning is about 10^6
F3	77.66	418.57	Highly multimodal function with a comparatively regular structure for the placement of the optima.
F4	77.66	171.86	Highly multimodal function with a structured but highly asymmetric placement of the optima.
F5	66.71	29.02	Purely linear function,solution is on the domain boundary
F6	65.87	237396.11	Unimodal,highly asymmetric function,
F7	92.94	431.55	unimodal, non-separable, conditioning is about 100.The function consists of many plateaus of different sizes.
F8	98.62	46480.79	(Rosenbrock function) in larger dimensions the function has a local optimum with an attraction volume of about 25%
F9	65.61	21715.05	rotated version of the previously defined f8.
F10	59.13	9634378.45	rotated version of the previously defined f2.
F11	76.27	21241083.28	A single direction in search space is a 1000 times more sensitive than all others.Conditioning is about 10^6
F12	56.61	9607260659	conditioning is about 10^6, rotated, unimodal
F13	68.42	449.99	Resembles f12 with a non-differentiable bottom of valley
F14	77.31	41.04	The sensitivies of the z_i-variables become more and more different when approaching the optimum
F15	70.03	521.74	Prototypical highly multimodal function which has originally a very regular and symmetric structure for the placement of the optima.
F16	71.35	79.07	Highly rugged and moderately repetitive landscape, where the global optimum is not unique.
F17	69.83	19.00	A highly multimodal function where frequency and amplitude of the modulation vary.Conditioning is low
F18	119.54	308.17	Moderately ill-conditioned counterpart to f17
F19	71.69	74.72	Resembling the Rosenbrock function in a highly multimodal way.
F20	71.29	45818.02	The most prominent 2D minima are located comparatively close to the corners of the unpenalized search area.
F21	124.08	12.21	The function consists of 101 optima with position and height being unrelated and randomly chosen.
F22	51.57	24.05	The function consists of 21 optima with position and height being unrelated and randomly chosen.Conditioning is about 1000
F23	85.39	20.12	Highly rugged and highly repetitive function with more than 10D global optima.
F24	93.30	18.18	Highly multimodal function with two funnels.

Table 1: BBOB functions

3.2 Experimeental settings

- **Dimension and budget:** In the experiment, the dimensions of the function are segmented into 2 and 4 dimensions. For 2-dimensional problems, the total budget for a single experiment is 100 observation points under noise-free conditions, and escalates to 300 points in noisy conditions. For four-dimensional problems, the total budget is 200 under no-noise conditions and increases to 400 under noisy conditions.

- **Initialization:** Following the result of [Bossek et al., 2020], we set the initial number of points to 10% of the total budget, and use Latin hypercube sampling to randomly select points in the search area.
- **loss rate** Denote y_a as the true value of the result obtained by the optimization algorithm, y_{opt} as the true optimal value. We define the loss rate:

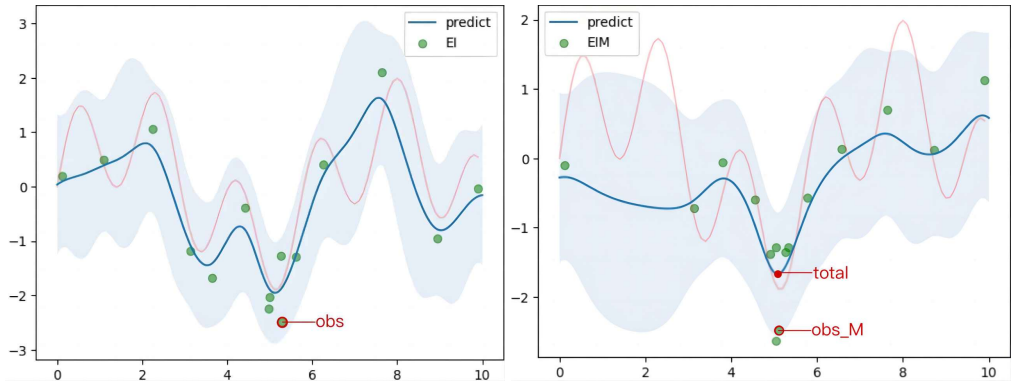
$$loss = \frac{y_a - y_{opt}}{y_{opt}} \times 100\% \tag{9}$$

as the optimization performance evaluation index of the algorithm. Note that the minimum values of the 24 functions we tested are all positive and do not approach 0, so the loss rate is well defined. Similarly, we can also define the relative loss rate between the two algorithms:

$$relloss = \frac{y_1 - y_2}{y_2} \times 100\% \tag{10}$$

where y_1 is the real value of the result obtained by optimization algorithm 1 and y_2 is the real value of the result obtained by optimization algorithm 2. If the relative loss rate is negative, it means that the optimal result of Algorithm 1 is better than Algorithm 2.

- **Randomness processing:** To ensure the generality of the results, we will use different random seeds to repeat each set of experiments 30 times(20 times for 4D problems) and then average the results. The randomness in the bayesian optimization process is mainly reflected in the initial point position and the internal optimization of the acquisition function.
- **Noise settings:** The noise added to the test functions in the experiments is Gaussian white noise, with a mean value of 0. The noise level is expressed as a proportion of the function's standard deviation(5% for small noise, 20% for medium, 50% for large noise).
- **Acquisition function and output results:** As mentioned earlier, We will discuss three output methods:
1.Directly output the minimum observation value(Abbreviated as **obs**).
2.Output observation point with the minimum predicted mean.(Abbreviated as **obs_M**).
3.Output the point with the minimum predicted mean over the total design space.(Abbreviated as **total_M**).
The choice of output method will align with the selection of the acquisition function. If the output method based on observed values (**obs**) is employed, then the Expected Improvement (EI) acquisition function will be used. Conversely, if the output method based on predicted values (**obs_M** and **total_M**) is employed, then we use EIM. The main reason for this is to ensure logical consistency. If we use **obs** as the output method, it indicates that we are more inclined to trust the observed values over the predicted values. Therefore, when selecting the acquisition function, we should correspondingly choose EI, which is optimized based on the observed values, and vice versa.



(a) Using EI for output method based on observation (b) Using EIM for output method based on prediction

Figure 1: The above two figures illustrate the results of bayesian optimization for a one-dimensional noisy function. The pale red curve represents the true function, while the blue curve depicts the predicted mean function of the Gaussian Process (GP). The green dots indicate the observation points selected by the acquisition function EI and EIM. The acquisition function used in the left figure is Expected Improvement (EI), which corresponds to the output method '**obs**', where the point with the smallest observation value is directly outputted. The acquisition function for the right figure is Expected Improvement of the Mean (EIM), showing two outputs based on the predicted values. The method '**total_M**' corresponds to the minimum value of the predicted mean function (blue curve), and '**obs_M**' is the point with the smallest predicted mean (blue curve) among all observed points (green dots).

4 Experimental results and analysis.

4.1 Noise-free experimental results

We first focus on the experimental results for the noise-free problem. In a noise-free scenario, the methods **obs** and **obs_M** are exactly the same since the observed value and predicted mean of any point are exactly equal. Therefore, we only need to compare the **obs** and **total_M** methods to analyze whether the predictive output method can yield better points as the final result. Intuitively, it is reasonable to consider **obs** as the most appropriate output method under noise-free conditions. The main purpose of our noise-free experiments is to investigate the specific gap in optimization efficiency between these two output methods. Table 2 details the specific differences between these two output methods:

2D	obs	total_M	total_M vs obs	4D	obs	total_M	total_M vs obs
F1	0.00%	0.00%	0.00%	F1	0.00%	0.00%	0.00%
F2	5.71%	59.70%	50.71%	F2	6589.66%	7861.45%	585.31%
F3	10.22%	27.81%	16.80%	F3	26.95%	56.09%	23.06%
F4	5.01%	18.19%	12.62%	F4	29.90%	63.32%	26.56%
F5	0.00%	0.00%	0.00%	F5	0.00%	0.00%	0.00%
F6	1.52%	3.45%	1.89%	F6	31.23%	105.48%	58.40%
F7	0.08%	0.18%	0.10%	F7	0.05%	0.09%	0.05%
F8	0.07%	1.75%	1.68%	F8	4.33%	5.16%	0.84%
F9	0.12%	3.66%	3.54%	F9	5.76%	11.17%	5.25%
F10	15.30%	1282.36%	1133.40%	F10	454.52%	4275.66%	1253.11%
F11	8.50%	719.52%	656.81%	F11	22.84%	2774.84%	2255.78%
F12	1645.98%	2907234.96%	1209546.08%	F12	526280.42%	27772809.81%	11673.63%
F13	0.96%	1.78%	0.81%	F13	27.39%	12.98%	-11.03%
F14	0.01%	0.02%	0.02%	F14	0.01%	0.03%	0.01%
F15	5.26%	23.30%	17.33%	F15	22.63%	64.67%	34.49%
F16	0.74%	26.55%	25.71%	F16	3.20%	14.22%	10.55%
F17	0.52%	4.43%	3.89%	F17	0.91%	1.20%	0.30%
F18	0.76%	11.46%	10.62%	F18	2.40%	3.50%	1.08%
F19	0.25%	10.95%	10.68%	F19	2.90%	14.37%	11.13%
F20	1.64%	5.11%	3.41%	F20	2.78%	6.00%	3.13%
F21	0.07%	0.14%	0.07%	F21	0.70%	0.84%	0.13%
F22	0.46%	0.75%	0.29%	F22	3.62%	3.87%	0.24%
F23	4.48%	50.64%	44.24%	F23	3.10%	24.36%	20.63%
F24	5.11%	27.33%	21.20%	F24	20.30%	49.25%	24.22%

Table 2: Noise-free results

The first two columns in the table show the loss rate of the output methods **obs**,**obs_M** relative to the global optimal value of each test function. The third columns is the relative loss rates of these two output methods(If positive, **obs** is better than **total_M**). For two-dimensional problems, the predictive method **total_M** is significantly less efficient in optimization than **obs** when applied to the functions F2, F10, F11, and F12. A review of Table 1 reveals a common feature of these functions: their conditioning levels are significantly high, exceeding 10^6. The standard deviation of each of these functions are very large, resulting in high noise levels. This high noise level can easily mask the original structural characteristics of the objective function, making it difficult to build a suitable model for the Gaussian process to predict. By examining Table 2, it can be seen that the loss rate of **obs** is likewise relatively high on these four functions compared to the others, which further suggests that the surrogate model struggles due to high conditioning levels. Therefore, it can be concluded that for noiseless problems, low accuracy in surrogate model modeling can greatly increase the loss rate of predictive output methods, in which case observational output method **obs** is more plausible.

For simpler functions, the results in the third column show that the loss ratio of **total_M** relative to **obs** is mostly above 10%. For more complex functions such as F10, F12, etc., the gap between the optimization results will increase further. Therefore, for noise-free problems, we should indeed directly use the observation-based bayesian optimization result output method (The loss rate of **total_M** relative to **obs** in all test functions is greater than 0). For 4D problems, the conclution remains same, however, after increasing the dimension, we find that the relative loss rate of these two output methods begins to decrease on many functions.This will be discussed later in the article.

4.2 Experimental results for the 2D noisy problem

In the previous section, we briefly compared the optimization results of the observative and predictive outputs on 24 noise-free functions. In this section, we will select some functions and add noise to them as new optimization problems. To ensure the consistency of the conclusions, we will use EI as the acquisition function for the observable output method (**obs**), and EIM for the predictive output method (**obs_M**, **total_M**). It was noted that in the noisy problems, **obs** is no longer exactly the same as **obs_M**, as the observed value will not be accurate.(See Section 3.2 for details on noise settings). We will use the Instant Regret as the vertical axis of the figures, and the number of iterations of BO as the horizontal axis to generate curves for analysis. For example, in each iteration of BO, **obs** selects a point as the output result. We subtract the optimal value of the function from the value of the real function corresponding to the selected point to get the instantant regret value of **obs** at the corresponding round. **obs_M** and **total_M** can do the same for similar curves. For comparison, we add a curve corresponding to a completely randomized output method, which randomly selects a point in the search space as the output for each round of iteration.

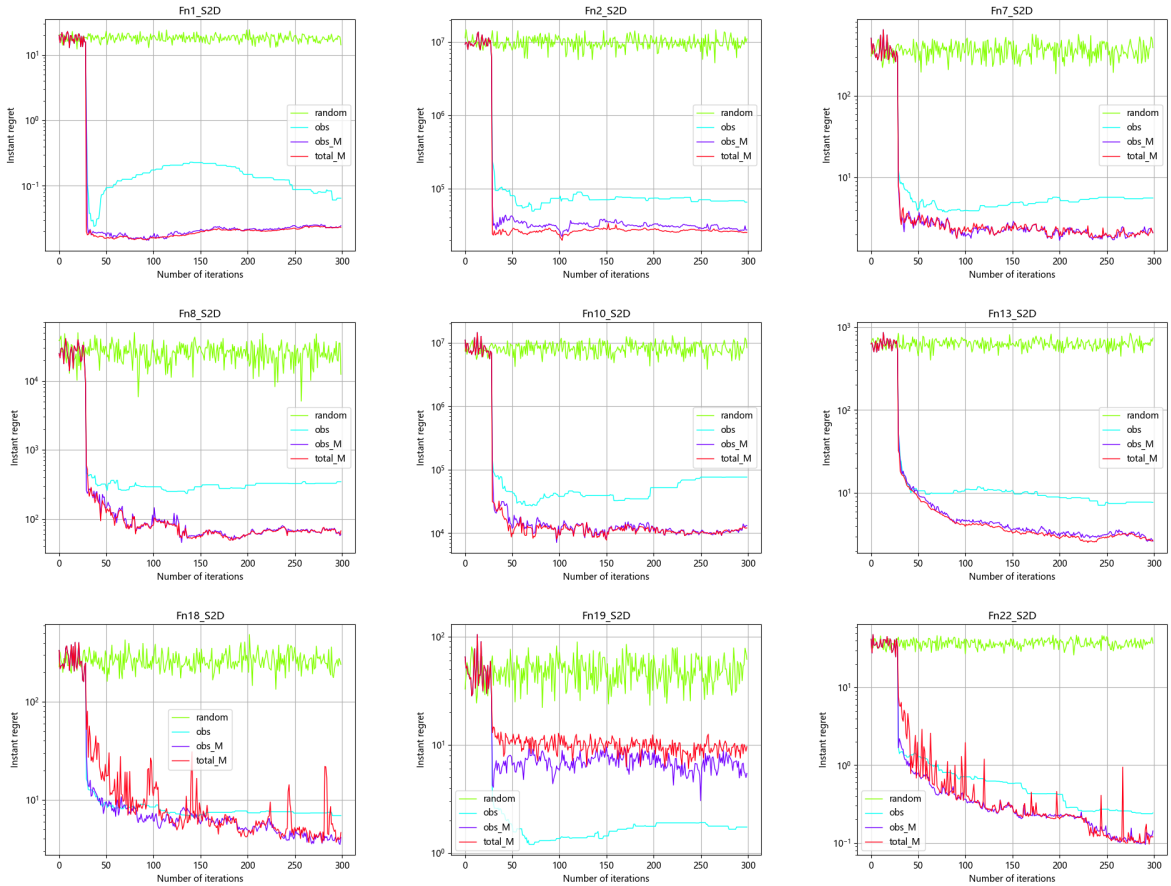


Figure 2: 2D optimization results(small noise)

Since the random seeds used in the initialization are identical, all experiments start with the exact same 20 initial points. Therefore, the curves corresponding to each output method for the first 20 rounds of iterations are exactly overlapped. After that, the Instant Regret curves for different output methods begin to show differences. We can arbitrarily take vertical intercepts of the curves to compare the advantages and disadvantages of the four output methods

in a particular round. For example, we can take a vertical intercept of the curve at round 200 on the horizontal axis and compare the average instant regret value of the four curves at round 200. The closer this value is to 0, the closer the output is to the true optimum. Since the budget of an optimization problem is often not fixed, we are more interested in the overall position and trend of these curves, rather than only comparing the average Instant Regret value after 300 rounds when the budget is exhausted.

Let's start with two predictive output methods. From Figure2, there is little difference between **obs_M** and **total_M** in the final optimization results, but the output of **total_M** shows great instability in some functions. For example, for the function Fn18, the output of **total_M** in turns 280-290 fluctuates greatly. Considering that our budget is actually arbitrary, if the budget happens to be between 280-290, the final output returned by **total_M** will be very poor. Compared with **total_M**, the output value of **obs_M** is more stable. Therefore, for two-dimensional problems with small noise, we recommend using **obs_M** instead of **total_M** if you prefer a predictive output method.

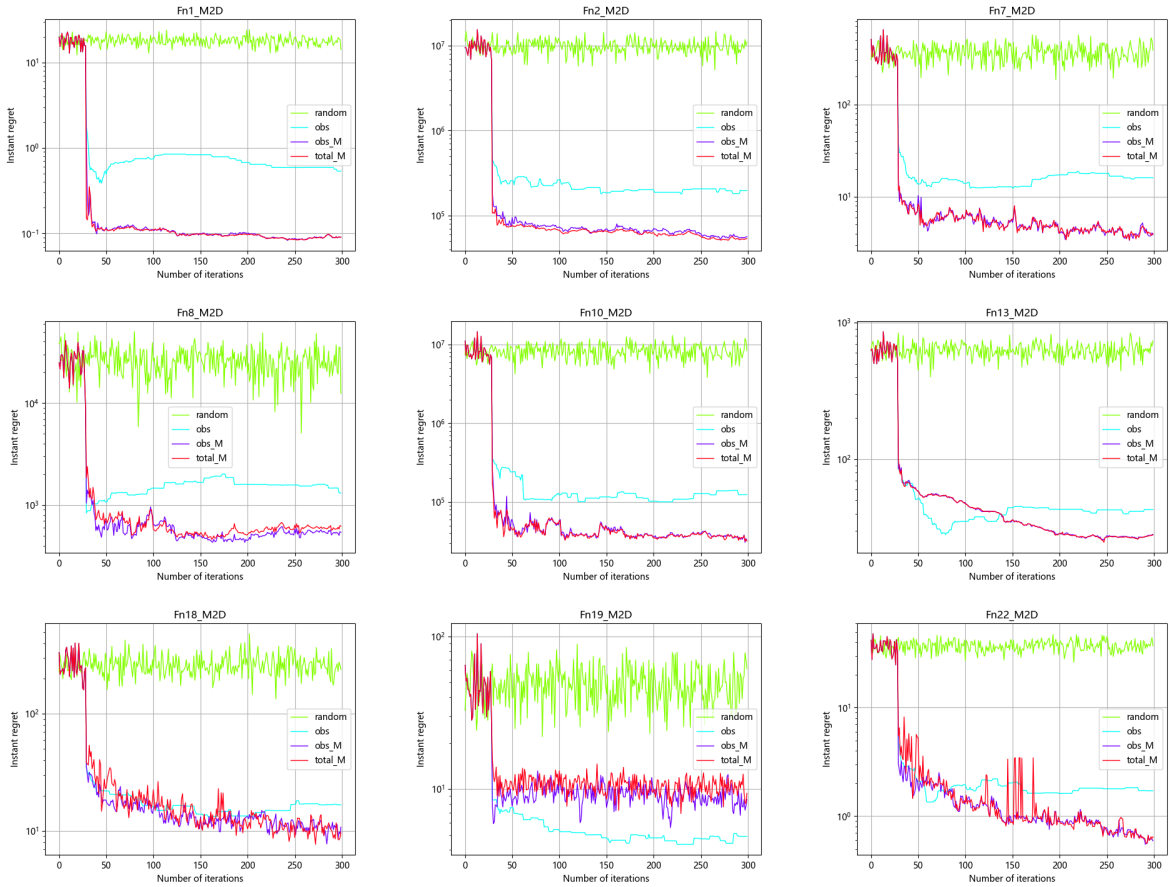


Figure 3: 2D optimization results(Medium noise)

As for the observational output method **obs**, we can see from Figure2 that the final output result of obs is much worse than **obs_M** on most of the test functions, and its curve will always be above the curve of **obs_M** after fewer rounds of iterations. This means that for any arbitrary given budget, the final output of obs is worse than **obs_M**. However, in terms of optimization of the test function Fn19 , we find that obs has a clear advantage over other output methods. We further observe the distribution characteristics of the output points for the three output methods on the function. We find that most of the points output by **obs_M** and **total_M** are concentrated in an area where the function's value is generally high. Even if a small number of points visit the area where the true optimum is located in some experiments, they do not linger in that area for long. In contrast, when **obs** accesses the region with a low function value, where the true optimal value is located, its subsequent output points tend to stay in this region. This indicates that the GP model has made a significant misjudgment in predicting the value of function Fn19, and the effectiveness of the **obs** point selection method is not influenced by the model's quality but is only related to the noise level. The performance of **obs_M** and **total_M**, however, is more dependent on the model's predictive accuracy. For Fn19, its small standard

deviation results in a relatively low absolute noise value. However, its highly multimodal characteristics severely impact the modeling accuracy of the GP, leading to better output results from **obs** compared to the other two output methods.

Therefore, when the model's prediction accuracy is poor, we indeed need to consider whether it might be better to use **obs**. However, we believe that this discussion is not very meaningful in essence. For an optimization problem, if we can anticipate that the model's predictive performance will be poor, our primary focus should be on improving the model itself rather than debating which output method to choose. For most problems with small noise, when the model is capable of making reasonable predictions, we still recommend to use **obs_M**.

Figure3 illustrates the optimization results for medium noise levels. It can be seen that with increased noise, the gap between the observational output method **obs** and the predictive output method widens further for most of the test functions. Overall, the conclusions for the choice of output methods are generally consistent with those under small noise. That is, for most problems with small noise, the use of the **obs_M** output method is the best choice. The use of **obs** only needs to be considered if one is convinced that BO's surrogate has low predict accuracy; however, in such cases, replacing the model may be the better choice. If we increase the noise level further (see Appendix B for details), the above conclusions still hold true, and when noise level is too high, the advantage of **obs** in Fn19 even ceases to exist.

4.3 Experimental results for the 4D noisy problem

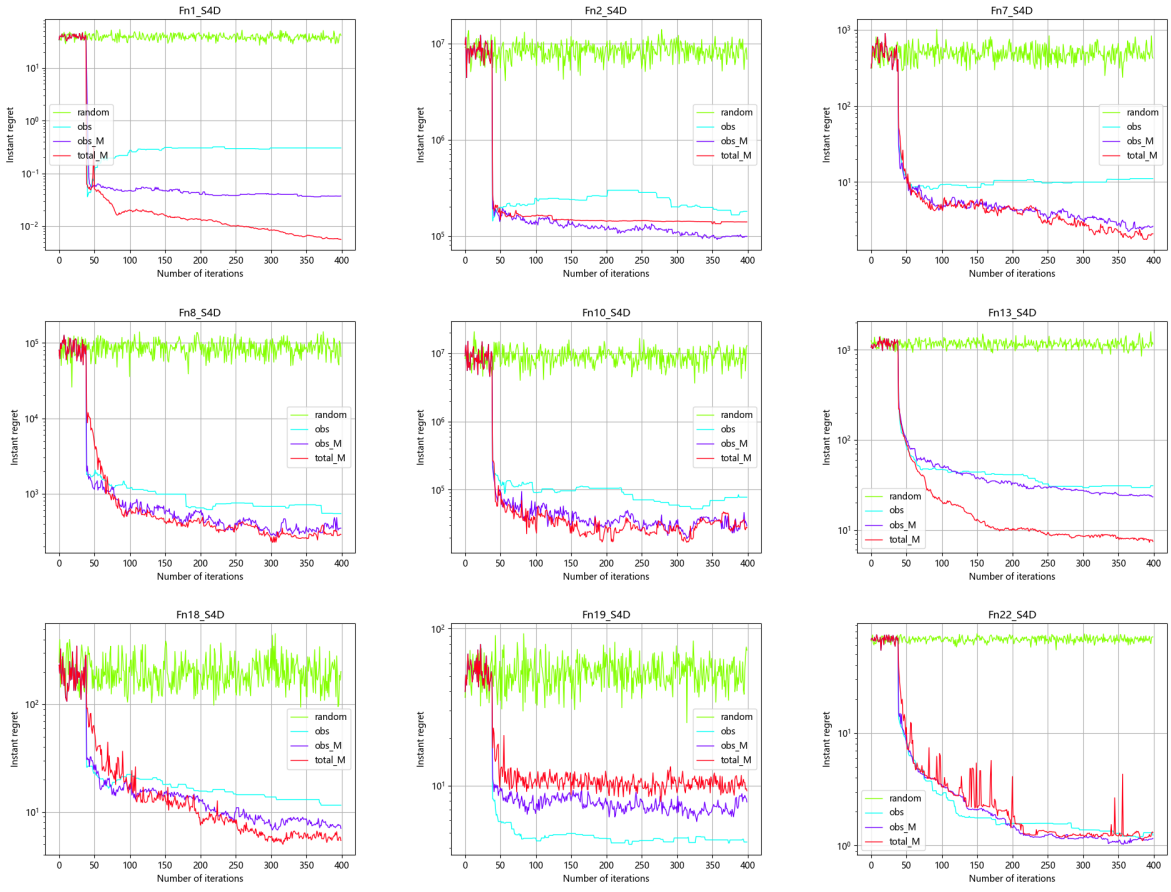


Figure 4: 4D optimization results(small noise)

In this section we increase the dimensionality of the optimisation problem from 2 to 4, thereby expanding the search space geometrically. Figure 4 shows the optimization results for a low noise level problem. we can clearly see that the output method **total_M** starts to become more competitive. For example, on function Fn1, which is the simplest and least difficult to optimize, textbftotal_M yields significantly better results than the other output methods. The same is true for function Fn13. There is also a small advantage over **obs_M** on functions Fn7 and Fn18.

This is mainly due to the fact that **obs_M** can only select among the observed points. Despite increasing the maximum number of iterations to 400 for the four-dimensional problem, 400 points are still too few for a four-dimensional search space. As discussed earlier, both EI and EIM acquisition functions must balance exploitation and exploration tasks. This reduces the proportion of the 400 points that are focused on exploitation. In contrast, **total_M** can focus entirely on exploitation without being limited to observed points, making it more likely to find local optimal points.

For higher-dimensional problems, the vast search space makes finding the global optimal solution extremely difficult, so finding a local optimal solution may be a better choice. However, it is worth noting that increasing the dimensionality does not solve the instability problem of **total_M**. For example, on Fn22 **total_M** still exhibits large fluctuations, indicating that it may still produce poor optimization results in some experiments. While **total_M** is competitive in higher-dimensional optimization problems, it still carries the risk of instability. Therefore, its use should be approached with caution. In contrast, **obs_M** remains relatively stable, outperforming **obs** on all test problems except Fn19 and performing comparably to or better than **total_M** on most problems. Overall, **obs_M** continues to be the most reasonable choice for four-dimensional problems with low noise levels.

4.4 Other complementary experiments

We have added three sets of complementary experiments to Appendices. The experiments in Appendix A demonstrate the output of the three methods under more extreme conditions. In fact, even in experiments with medium noise levels in 2D, we observed that for some functions, the quality of the points selected by EI and EIM is not even as good as that of completely random selection. This suggests that the GP model has been somewhat compromised on these functions. Under more extreme conditions, such as 2D high noise levels and 4D medium noise levels, the GP model may degrade further and even fail completely. Due to space constraints, we have included a discussion of the results from these experiments in the appendix.

The experiments in Appendix B were performed under conditions of moderate noise levels in two dimensions. Unlike Section 4.2, all the output methods in the experiments in Appendix B use EI, with no EIM used in the optimization process. The purpose of this experiment is to demonstrate that the gap between **obs** and **obs_M** or **total_M** is not primarily caused by differences in acquisition functions. In fact, in Appendix B, you can see that even when the same acquisition function is used, the results remain consistent.

It is also worth mentioning that the form of the noise can likewise influence the choice of output methods. Our experiments above only discuss homogeneous noise, and the conclusions may change when the noise becomes non-homogeneous. We briefly discuss this scenario in Appendix C and give the corresponding experimental results.

5 Conclusion

In the previous section we conducted numerical experiments on optimisation test problems without noise and with different noise levels and dimensions. The main conclusions are summarised as follows:

- For the noise-free problem, directly using the observation-based output method **obs** is the most reasonable choice.
- For the noisy problem, using the predictive-based output is superior to the observation-based output in most of the cases, even when the noise level is low(5% sd). Considering that the output results of **total_M** are not stable, the use of **obs_M** is the most reasonable choice.
- For more complex problems, when the BO's surrogate model has low prediction accuracy, the predictive-based output method should be used with caution, since the model's prediction of the objective function is less credible. In this case, the choice of observation-based output will often give better output results, but in practice it is meaningless. If we can be sure that the model is less predictive, then we should consider replacing the model rather than discussing what output method to use.
- When the optimisation problem is of high dimensionality, the use of **total_M** can be considered, but it still carries the risk of unstable output results.

Taking all these points together, it seems that using **obs_M** is a relatively reasonable choice in almost all situations. Firstly, when there is no noise or very little noise in the objective function, our experiments show that the output of **obs** is much better than that of **total_M**. In fact, the outputs of **obs_M** and **obs** are essentially the same in this case since both select from observed points, and in the absence of noise or with very little noise, the observed values and the predicted mean of the model are nearly identical.

After increasing the noise level, **obs_M** and **total_M** generally outperform **obs**, with **obs_M** avoiding the instability problem that plagues **total_M**. Excluding situations where the objective function is too complex, leading to poor model predictions (where discussing the output method becomes less meaningful), our experiments consistently show that using **obs_M** as the output method is always a suitable choice. Therefore, we can conclude that using **obs_M** as the output method is a reasonable choice for most optimization problems.

References

Chen Wei Zhang Yichi, Apley Daniel W. Bayesian optimization for materials design with mixed quantitative and qualitative variables. *Scientific Reports*, 10:4924, 2020. doi:10.1038/s41598-020-60652-9. URL `https://doi.org/10.1038/s41598-020-60652-9`.

Ruben Martinez-Cantin. Bayesian optimization with adaptive kernels for robot control. In *2017 IEEE International Conference on Robotics and Automation (ICRA)*, pages 3350–3356, 2017. doi:10.1109/ICRA.2017.7989380.

Jasper Snoek, Hugo Larochelle, and Ryan P. Adams. Practical bayesian optimization of machine learning algorithms, 2012. URL `https://arxiv.org/abs/1206.2944`.

Carl Edward Rasmussen and Christopher K. I. Williams. *Gaussian Processes for Machine Learning*. The MIT Press, 11 2005. ISBN 9780262256834. doi:10.7551/mitpress/3206.001.0001. URL `https://doi.org/10.7551/mitpress/3206.001.0001`.

Bobak Shahriari, Kevin Swersky, Ziyu Wang, Ryan P. Adams, and Nando de Freitas. Taking the human out of the loop: A review of bayesian optimization. *Proceedings of the IEEE*, 104(1):148–175, 2016. doi:10.1109/JPROC.2015.2494218.

Peter I. Frazier. *Bayesian Optimization*, chapter 11, pages 255–278. 2018. doi:10.1287/educ.2018.0188. URL `https://pubsonline.informs.org/doi/abs/10.1287/educ.2018.0188`.

Roman Garnett. *Bayesian Optimization*. Cambridge University Press, 2023.

Donald R. Jones, Matthias Schonlau, and William J. Welch. Efficient global optimization of expensive black-box functions. *J. of Global Optimization*, 13(4):455–492, dec 1998. ISSN 0925-5001. doi:10.1023/A:1008306431147. URL `https://doi.org/10.1023/A:1008306431147`.

Nikolaus Hansen, Anne Auger, Steffen Finck, and Raymond Ros. Real-parameter black-box optimization benchmarking bbob-2010 : Experimental setup. 2010. URL `https://api.semanticscholar.org/CorpusID:260830254`.

Niranjan Srinivas, Andreas Krause, Sham M. Kakade, and Matthias Seeger. Gaussian Process Optimization in the Bandit Setting: No Regret and Experimental Design. *arXiv e-prints*, art. arXiv:0912.3995, December 2009. doi:10.48550/arXiv.0912.3995.

William R. Thompson. On the likelihood that one unknown probability exceeds another in view of the evidence of two samples. *Biometrika*, 25(3/4):285–294, 1933. ISSN 00063444. URL `http://www.jstor.org/stable/2332286`.

Philipp Hennig and Christian J. Schuler. Entropy search for information-efficient global optimization. *J. Mach. Learn. Res.*, 13(null):1809–1837, jun 2012. ISSN 1532-4435.

D. Huang, Theodore Allen, William Notz, and Ning Zheng. Global optimization of stochastic blackbox systems via sequential kriging meta-models. *Journal of Global Optimization*, 34:441–466, 03 2006. doi:10.1007/s10898-005-2454-3.

Alexander I. J. Forrester, Andy J. Keane, and Neil W. Bressloff. Design and analysis of "noisy" computer experiments. *AIAA Journal*, 44(10):2331–2339, 2006. doi:10.2514/1.20068. URL `https://doi.org/10.2514/1.20068`.

Victor Picheny, David Ginsbourger, Yann Richet, and Grégory Caplin. Quantile-based optimization of noisy computer experiments with tunable precision. *Technometrics*, 55, 03 2012. doi:10.1080/00401706.2012.707580.

Victor Picheny, Tobias Wagner, and David Ginsbourger. A benchmark of kriging-based infill criteria for noisy optimization. *Structural and Multidisciplinary Optimization*, 48, 09 2013. doi:10.1007/s00158-013-0919-4.

Jakob Bossek, Carola Doerr, and Pascal Kerschke. Initial Design Strategies and their Effects on Sequential Model-Based Optimization. *arXiv e-prints*, art. arXiv:2003.13826, March 2020. doi:10.48550/arXiv.2003.13826.

Appendix

A Experiment under extreme conditions

A.1 2-dimensional experiments

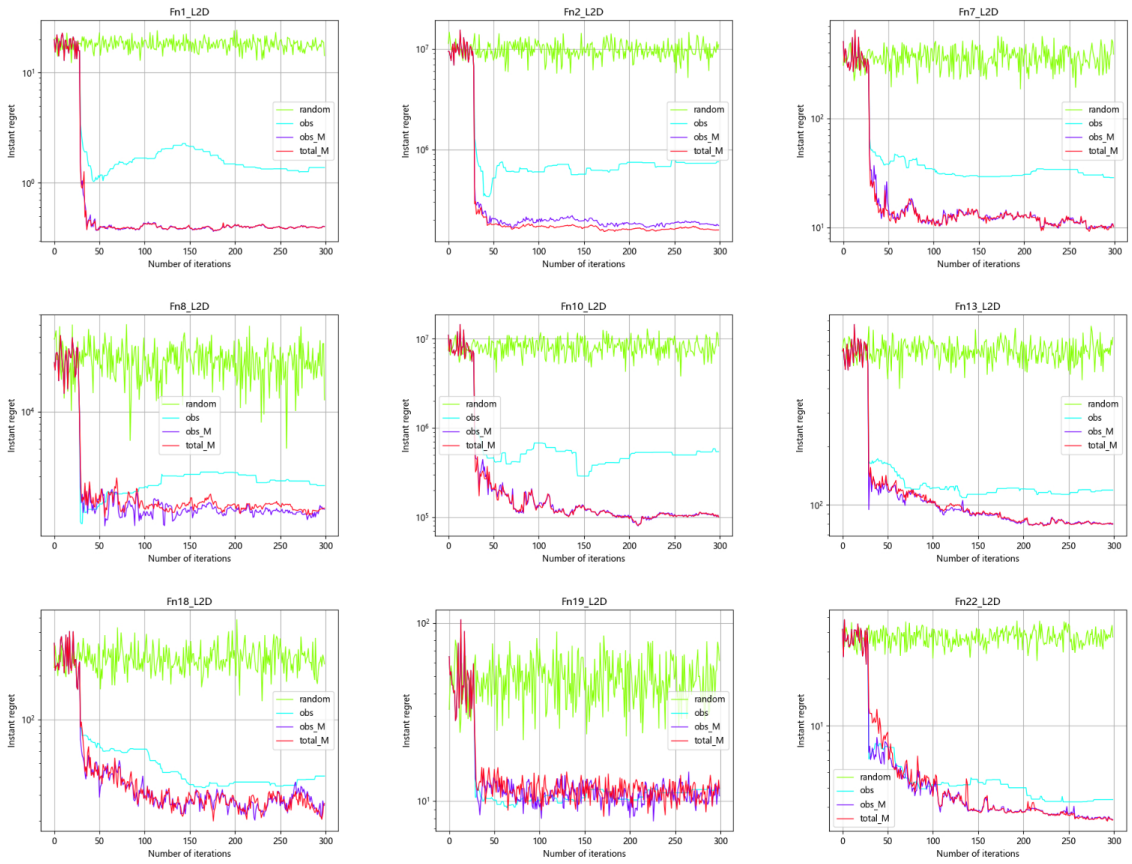


Figure 5: 2D optimization results(Large noise)

In experiments with high noise levels in two dimensions, the GP model often becomes ineffective for most functions. The points selected by EI and EIM based on model predictions are no longer as good as if they had been chosen completely at random within the search space. In this scenario, the degradation of the model's predictive power seriously affects the output results of **obs_M** and **total_M**. Simultaneously, larger noise levels can also directly interfere with the effectiveness of **obs**. Overall, the extreme noise level causes significant disturbances in all three output methods. In this case, we find that the relative performance of the three output methods remains consistent with the results in Section 4.2: **obs** still lags behind the other two methods, except for Fn19. Compared to the other two output methods, **obs** is more directly impacted by extreme noise, which results in the loss of its original advantage on the Fn19 function. **obs_M** and **total_M** do not differ much in this set of experiments, and **total_M** does not exhibit significant instability. However, This is in fact a matter of probability. Considering that **total_M** selects output points from the entire search space based on the model's predictions, the risk of selecting extreme points still remains. It is not the case that its performance can be stabilized by increasing the noise level.

A.2 4-dimensional experiments

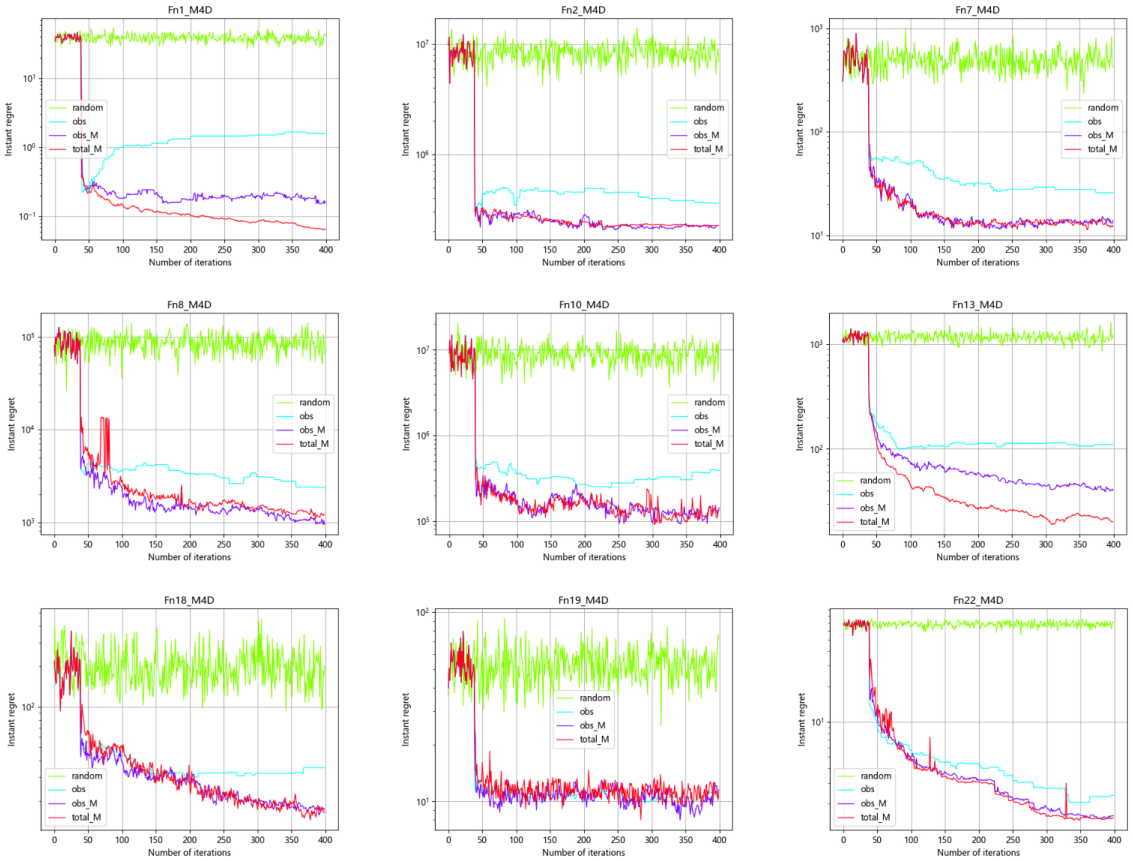


Figure 6: 4D optimization results(Medium noise)

In the four-dimensional experiment with medium noise levels,we get basically the same conclusion as the two-dimensional experiment mentioned above. We observe that the advantage of **obs** in Fn19 also disappears, and **total_M** shows some instability again in Fn8 and Fn22. Based on the above experimental results, we can conclude that even under extreme optimization conditions, **obs_M** is still the most reliable choice.

B Experiment using EI only

B.1 2-dimensional experiments

This set of experiments was performed in two dimensions with moderate noise levels, with the acquisition function for all output methods uniformly set to EI. It is worth mentioning that when the acquisition function is the same, **obs** and **obs_M** actually select output points from exactly the same set of observed points for each experiment. It can be seen that after unifying the acquisition functions, we still get almost exactly the same conclusions as in 4.2: **obs** performs poorly on most of the functions, and **total_M** still suffers from instability. This set of experimental results is mainly used to demonstrate that the gap between **obs** and the other two methods is not mainly caused by the difference between EI and EIM.

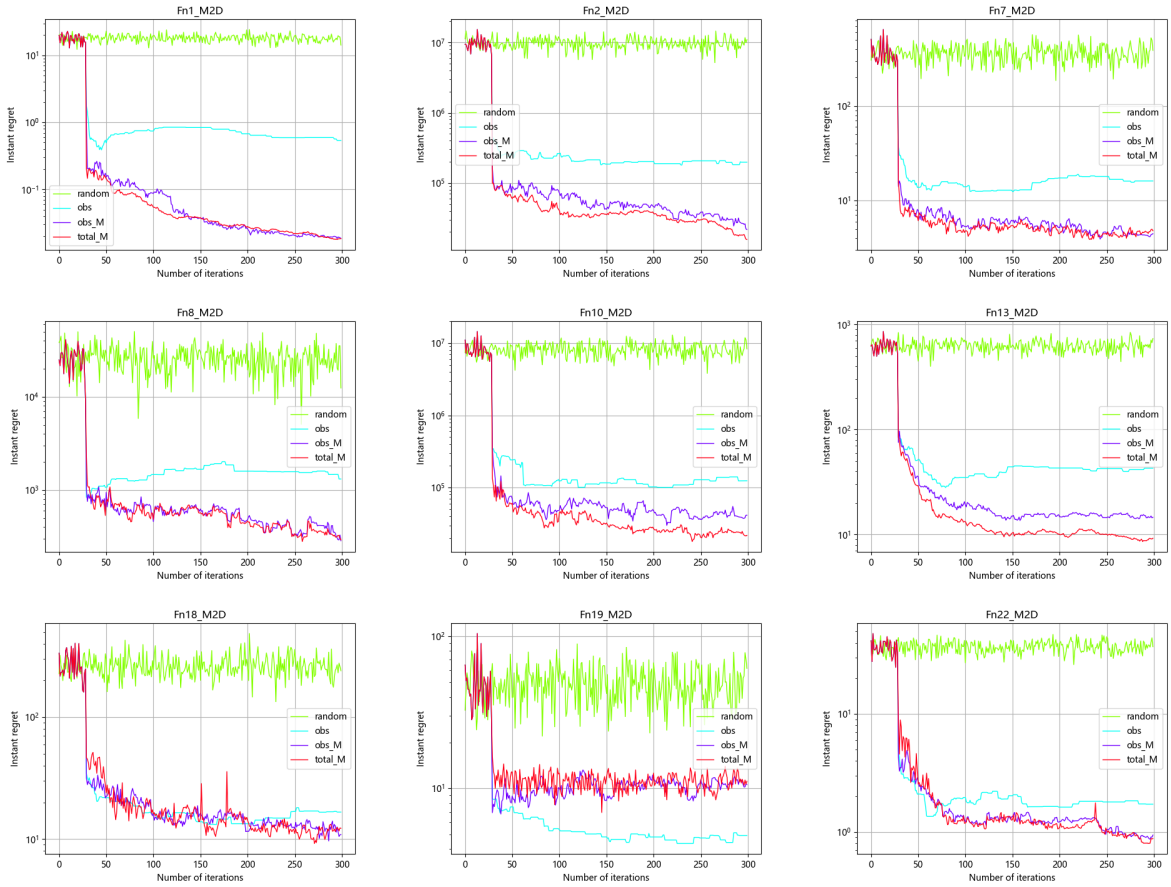


Figure 7: 2D optimization results((Medium noise, with only EI)

Here, we do not immediately proceed to compare the differences in optimization results obtained using different acquisition functions when the output method is the same. This is because the main goal of this paper is not to investigate which acquisition function to use when optimizing a problem with noise. In fact, there are many types of acquisition functions for handling noise, but fundamentally, there is no direct relationship between the choice of result output method in the optimization process and the specific acquisition function used.

C Experiment with non-homogeneous noise

C.1 2-dimensional experiments

The basic settings of the experiments are the same as those in 4.2, with the only difference being that the noise settings are no longer homogeneous variance, but are set as follows:

$$f_{GN}(f, \beta) = f \times exp(\beta \mathcal{N}(0, 1)) \tag{11}$$

where $mathcal N(0, 1)$ represents random sampling from the standard normal distribution, and $beta$ is the parameter that controls the magnitude of the noise, here we set it to 0.1. Note that the value of noise here will be related to the true value of the function. Also similar to 4.2, we give the following image of the experimental results:

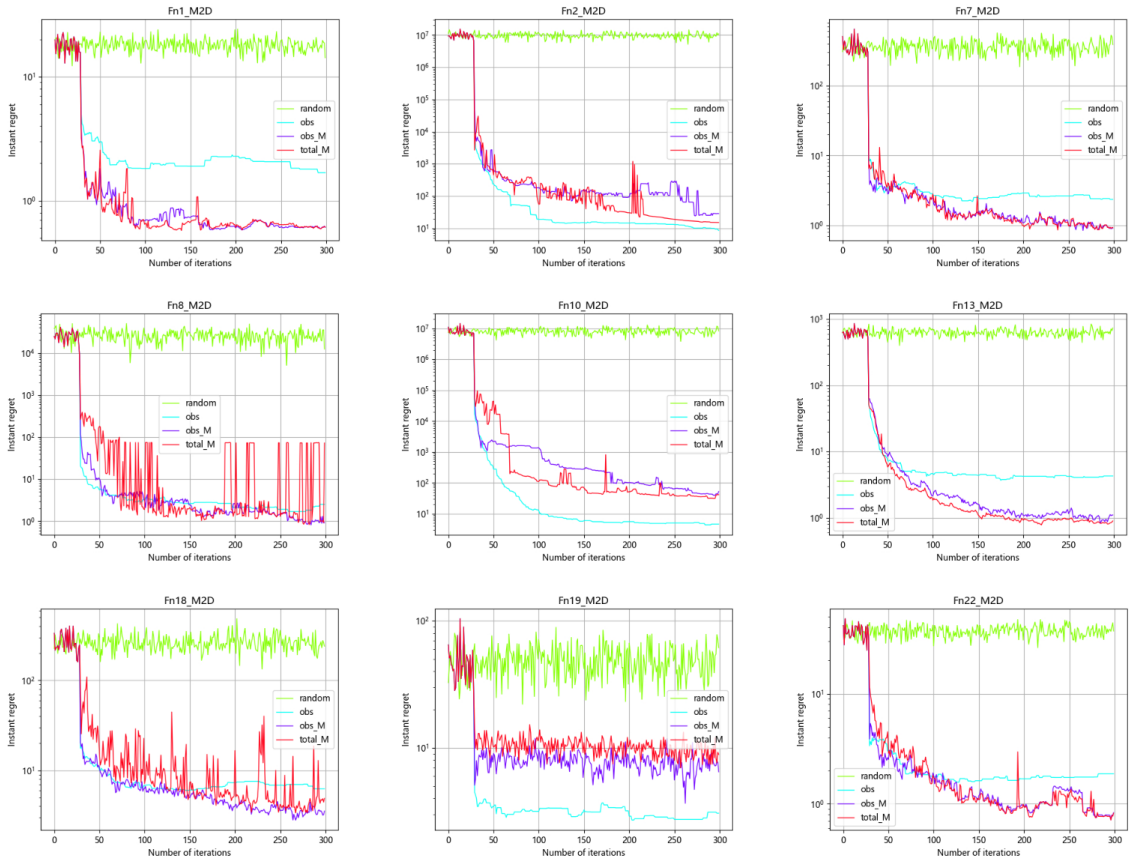


Figure 8: 2D optimization results(Non-homogeneous noise)

The results reflected in the figures are basically similar to those in 4.2, with the only difference being that for functions with large standard deviations (e.g. Fn2, Fn10), the observative output methods in non-homogeneous noise is much better than the predictive output method. This is because when the noise value is positively correlated with the true value of the function, the point with the smaller value of the function corresponds to the less noise, so if we observe that the value of a point is small, it is most likely because the function value corresponding to that point is also small, rather than due to extreme noise. In this case, the observant output method is more reliable than the predictive output methods, even if noise is affected(which is the main difference with the homogeneous variance conclusion).