

Multi-objective Bayesian Optimisation and Applications



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A thesis submitted for the degree of
Doctor of Philosophy
Trinity 1998

Abstract

Bayesian optimisation has become a powerful framework for global optimisation of black-box functions that are expensive to evaluate and possibly noisy. In addition to expensive evaluation of objective functions, many real-world optimisation problems deal with similarly expensive black-box constraints. However, there are few studies regarding the role of constraints in multi-objective Bayesian optimisation. In this report, we extend the Expected Hypervolume Improvement by introducing expectation of constraints satisfaction and merging them into a new acquisition function called Expected Hypervolume Improvement with Constraints (EHVIC). We analyse the performance of our algorithm by estimating the feasible region dominated by Pareto front using 4 benchmark functions. The proposed method is also evaluated on a real-world problem of Alloy Design. We demonstrate that EHVIC is an effective algorithm that provides a promising performance by comparing to a well-known related method. As another potential aim of the further research we have also introduced an objective ranking multi-objective optimisation method.

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Chapter 1

Introduction

Bayesian optimisation is considered to be the specific case of model-based optimisation methods which is structured based on the Bayesian formulations. Like the most cases of Bayesian approaches, there is a prior distribution over a function, a likelihood function, and a posterior distribution over the unknown functions given data [1]. Bayesian optimisation aims to solve a difficult though concise problem:

$$\min_{x \in \mathcal{X}} f(x) \quad (1.1)$$

However $f(x)$ is considered to have following features [1]:

1. **Expensive to Evaluate:** Evaluation of $f(x)$ is highly expensive. Such as most of engineering problems like making alloys [2], designing a pharmaceutical drug, optimising machine learning algorithms [3] and many other engineering problems.
2. **Black-box:** The exact formulation of $f(x)$ function or the derivatives of $f(x)$ is not available. Like the most of the engineering problems that we have already mentioned.
3. **Noisy Evaluations:** The value of $f(x)$ for a specific x usually corrupted with a noise. So for the same values of x , $f(x)$ would result in different values.
4. **Global and non-convex:** Bayesian optimization of $f(x)$ is a global optimisation problem for a non-convex function in the \mathcal{X} domain.

While traditional numerical methods have proved ineffective for solving some optimisation problems, Bayesian optimisation has proved to be effective in variety of

optimisation problems dealing with black-box objective functions, expensive to evaluate. There have been number of studies on the use of Bayesian optimisation on hyperparameter tuning in machine learning and big data [4], expensive multi-objective optimisation for Robotics [5], and experimentation optimisation in product design such as short polymer fiber materials [6].

Practical problems are often involved in several non-commensurable objectives. In other words, the real-world problems consist of multiple, conflicting black-box objectives. In Multi-Objective Optimisation (MOO) potential solutions are assessed by their performance in more than one objective [7]. In MOO, based on definition of Pareto optimality, we wish to return a Pareto front that represents the best trade-off possible considering all criteria [8]. More generally, MOO includes M objective functions f_1, f_2, \dots, f_M which are usually modelled by Gaussian Process (GP) [9]. Formally:

$$\begin{aligned} & \underset{\mathbf{x}}{\text{minimize}} \quad \mathbf{y} = \mathbf{Z}(\mathbf{x}) = \{f_1(\mathbf{x}), f_2(\mathbf{x}), \dots, f_M(\mathbf{x})\} \\ & \text{where:} \quad \mathbf{x} \in \mathcal{X} \subseteq \mathbb{R}^d \\ & \quad \mathbf{y} \in \mathcal{Y} \subseteq \mathbb{R}^M \end{aligned}$$

Generally two categories of solutions are available for solving multi-objective problems. In such scenarios it is customary to seek for a set of Pareto optimal outcomes often called the Pareto front [7]. The first category uses scalarization for transforming a multi-objective problem into single-objective problem. The single-objective problem is then tackled using different evolutionary algorithms such as Genetics Algorithm (GA). So in this case, such solutions are not suited for the highly expensive and black-box $f(x)$ function. But there are studies trying to solve the transformed single-objective problem by Bayesian optimisation or entropy search methods. In this case, researchers try to eliminate the highly expensive costs of evolutionary algorithms. In such studies, there are differnt methods of scalarization in order to solve the multi-objective problems. Tchebycheff Method, k^{th} -Objective Weighted-Constraint, and Pascoletti and Serafini Scalarization are the three most popular approaches for scalarization among researchers [10].

The next category of solutions are focused on the multi-objective structure of the problem. These methods do not transform the multi-objective problems into single-objective space. Instead, these methods tend to use more complex acquisition functions based on Expected Hypervolume Improvement (EHI) or Entropy Search (ES) in order to handle the multidimensionality of the problem. So they provide a set of solutions by optimizing all M objective simultaneously.

1.1 Motivation

Large diversity of optimisation problems take the form described above. Examples include increasing the Pouring Temperature of an alloy to withstand enormously high temperature of molten metals while overall alloy hardness must not increase drastically; or tuning training parameters of an SVM model to maximize the accuracy and minimizing the consumption of resources. In addition to expensive evaluation of objective functions, many optimisation problems deal with similarly expensive black-box constraints. Unknown constraints are part of many black-box multi-objective optimisation problems. For example, when tuning SVM hyperparameters we may want to optimise performance subject to a limit on the number of support vectors (and hence the complexity of evaluating the trained classifier) if the trained machine is to be implemented on limited hardware (such as accessible memory). The goal of optimisation in such cases is to minimize the number of black-box function evaluations to find the global optimum of the function with respect to constraints. Bayesian optimisation has recently been used successfully in this area [11]. Another use of multi-objective with constraints problem arises when there is a priori such as Ranking of the objectives. In many real-world problems, there are more important objectives we would like to have a slight advantage over other objectives. For example, in autonomous flying airplanes, the nature of the problem demands a huge advantage on safety measures of the airplane than the fuel consumption; or in Robotics, one of the current problems researches are working on, is about overheating of motors or power consumption of them. While other objectives such as the accuracy of movements with some constraints are also play a role in this problem. One may like to focus on the safety of motors or the accuracy of the movements. So ranking of the objectives as a priori information could be really useful in many real-world problems.

1.2 Summary of contributions

The main contribution of our first proposed method is to characterize a general formulation for Multi-objective Bayesian optimisation with unknown constraints based on hypervolume calculation. The other related contributions are:

- Formulation of the expected hypervolume improvement with constraints based on the simple but effective expected improvement acquisition function.

- Evaluation of the proposed algorithm based on feasible dominated region on all related benchmark test functions for the first time. We also estimated the volume of the feasible region of the test functions for more accurate evaluation.
- Discussion of the issues involved in the method in terms of the efficiency and size of the problem.

The main contribution of multi-objective Bayesian optimisation with constraints and objective rankings is incorporating the rankings as a feature to multi-objective Bayesian optimisation. The contributions of the proposed model are summarized in the following three aspects:

- We formulated a single-objective constrained Bayesian optimisation problem for mapping a multi-objective Bayesian optimisation with constraints and objective rankings into a more feasible space.
- For evaluation of the proposed algorithm, we will introduce new measurements which should contain both diversity/density and accuracy of the obtained Pareto set.
- It is the first time that multi-objective Bayesian optimisation has been incorporated in ranking or planning problems.

Chapter 2

Literature Review

Bayesian optimisation is a well-known tool for solving a variety of optimisation problems. While traditional numerical methods have proved ineffective for solving some optimisation problems, Bayesian optimisation has proved effective in variety of optimisation problems dealing with blackbox objective functions expensive to evaluate [12]. Bayesian optimization is impacting a wide range of areas, including Robotics [13, 14], environmental monitoring [15], interactive user interface [16], information extraction [17], combinatorial optimisation [18, 19], reinforcement learning [20], sensor networks [21, 22], and automated machine learning algorithms [23, 3, 24, 25].

Fundamentally, Bayesian optimization is a sequential model-based approach for solving optimisation problems. Bayesian optimisation framework has two main stages. The first one is a probabilistic surrogate model, consist of a prior distribution which encodes our beliefs about the nature of the expensive black-box function [26]. The second stage is constructing a proper acquisition function which can accurately model the behavior of the black-box function. Equipped with these probabilistic models, acquisition functions will be sequentially induced in order to leverage the uncertainty in the posterior for leading the exploration [26]. After observing the output value of each selected point in that iteration, the prior understanding of the black-box function and the acquisition function will be updated subsequently. Algorithm 1 illustrates the procedure of Bayesian optimisation.

But as we have mentioned before, many real-world optimisation problems are dealing with unknown constraints. In the next section we are investigating the role of unknown constraints in single-objective Bayesian optimisation.

Algorithm 1 Bayesian optimisation Algorithm

```
1: for  $n = 1, 2, \dots$ , do
2:   Optimise acquisition function  $\alpha$ ,  $\mathbf{x}_{t+1} = \operatorname{argmax}_{\mathbf{x} \in \mathcal{X}} \alpha(\mathbf{x}; \mathcal{D}_n)$ 
3:   Evaluate  $\mathbf{x}_{t+1}$ , obtain  $y_{t+1}$ 
4:   Augment data to the observation set,  $\mathcal{D}_{n+1} = \{\mathcal{D}_n, (\mathbf{x}_{n+1}, y_{n+1})\}$ 
5:   Update the prior model based on the new observed point.
6: end for
```

2.1 Constrained single-objective Bayesian optimisation

Consider an SVM model; when tuning SVM hyperparameters, we may want to optimise performance on limited hardware (such as accessible memory). So, in addition to expensive evaluations of the objective function, we may face with similarly expensive evaluations of constraint functions. The only single-objective Bayesian optimisation with constraints method is proposed by [27]. In this paper, the authors have extended Bayesian optimization to incorporate inequality constraints. The aim of this method is:

$$\min_{c(\mathbf{x}) \leq \lambda} f(\mathbf{x}) \quad (2.1)$$

where $f(\mathbf{x})$ and $c(\mathbf{x})$ are both expensive and black-box functions. Authors defined a new *Constrained Improvement* in order to form the acquisition function. Constrained improvement is defined as:

$$I_C(\hat{\mathbf{x}}) = \Delta(\hat{\mathbf{x}}) \max\{0, f(\mathbf{x}^+) - f(\hat{\mathbf{x}})\} = \Delta(\hat{\mathbf{x}}) I(\hat{\mathbf{x}}) \quad (2.2)$$

In equation 3.17, $\Delta(\hat{\mathbf{x}})$ is defined to be $\Delta(\hat{\mathbf{x}}) \in \{0, 1\}$ which is a feasibility indicator function that returns 1 when $c(\hat{\mathbf{x}}) \leq \lambda$ and 0 otherwise. Also x^+ denotes a feasible point with lowest function value observed in time τ . Due to dealing with black-box functions for both objectives and constraints, the authors use Bayesian formalism to model each with a GP $\hat{c}(\mathbf{x}) \sim \mathcal{N}(\hat{\mu}_c(\mathbf{x}), \hat{\Sigma}_c(\mathbf{x}))$ and $\hat{f}(\mathbf{x}) \sim \mathcal{N}(\hat{\mu}_f(\mathbf{x}), \hat{\Sigma}_f(\mathbf{x}))$. Due to the marginal Gaussianity of $\hat{c}(\mathbf{x})$, the expected constrained improvement acquisition function is defined as:

$$\begin{aligned} EI_C(\hat{x}) &= \mathbb{E}[I_C(\hat{\mathbf{x}})|\hat{\mathbf{x}}] = \mathbb{E}[\Delta(\hat{\mathbf{x}})I(\hat{\mathbf{x}})|\hat{\mathbf{x}}] \\ &= \mathbb{E}[\Delta(\hat{\mathbf{x}})|\hat{\mathbf{x}}]\mathbb{E}[I(\hat{\mathbf{x}})|\hat{\mathbf{x}}] \\ &= PF(\hat{\mathbf{x}})\mathbb{E}[I(\hat{\mathbf{x}})] \end{aligned} \quad (2.3)$$

which the $\text{PF}(\hat{\mathbf{x}})$ is defined as a simple univariate Gaussian cumulative distribution function $\text{PF}(\hat{\mathbf{x}}) = \Pr[c(\hat{\mathbf{x}}) \leq \lambda] = \int_{-\infty}^{\lambda} p(c(\hat{\mathbf{x}})|\hat{\mathbf{x}}, \tau_c) dc(\hat{\mathbf{x}})$. Thus the expected constrained improvement acquisition function $\text{EI}_C(\hat{\mathbf{x}})$ is the expected improvement of $\hat{\mathbf{x}}$ over the best feasible point observed so far. It is also possible to extend the constraint function to the set of independent constraint functions $c(\mathbf{x}) = [c_1(\mathbf{x}), c_2(\mathbf{x}), \dots, c_k(\mathbf{x})]$ [27]. In this case, $\text{PF}(\hat{\mathbf{x}})$ is multiplication of k constraints as $\Pr[c(\mathbf{x})_i \leq \lambda_i]_{i=1\dots k}$. The authors evaluated their proposed model on one simulation function and two real-world problem of Locality Sensitive Hashing and SVM compression. The proposed method proved to be robust in the case of constraints existence.

2.2 Multi-objective optimisation and Bayesian optimisation

There are many studies on the topic of multi-objective optimisation. A quick summary of the most related studies have been illustrated in the Table 2.1.

Table 2.1: Summary of related studies in Multi-objective optimisation.

| Study | Method | Constraints | Ranking |
|---|------------------------------|-------------|---------|
| A Bayesian approach to constrained single- and multi-objective optimization [28] | Bayesian optimisation | ✓ | - |
| Predictive Entropy Search for multi-objective Bayesian optimization with constraints [29] | Bayesian optimisation | ✓ | - |
| Predictive Entropy Search for multi-objective Bayesian optimization [30] | Bayesian optimisation | - | - |
| Pareto frontier learning with expensive correlated objectives [31] | Bayesian optimisation | - | - |
| Pareto front modeling for sensitivity analysis in multi-objective bayesian optimization [8] | Bayesian optimisation | - | - |

| | | | |
|--|---|---|---|
| Active learning of Pareto fronts [32] | Active Learning for Regression Task; Gaussian Processes | ✓ | - |
| A generative kriging surrogate model for constrained and unconstrained multi-objective optimization [33] | Generative surrogate modeling | ✓ | - |
| Multi-objective reinforcement learning with continuous Pareto frontier approximation [34] | gradient-based approach | ✓ | - |
| Active learning for multi-objective optimization [35] | Pareto Active Learning (PAL); Gaussian Processes | - | - |
| Faster computation of expected hypervolume improvement [36] | Expected Hypervolume Improvement | - | - |
| Multi-objective bandits optimizing the generalized Gini index [37] | Generalized Gini Index; Gradient-based algorithm | - | - |

The authors in [28] proposed a new Bayesian optimization approach to solve multi-objective optimization problems with non-linear constraints. The constraints are handled by extended domination rule. Also a new expected improvement formulation is proposed. In particular, the new formulation makes it possible to work around the problems in which no feasible solutions are available from the start. Sequential Monte Carlo sampling techniques are used in the process of computation and optimization of the new expected improvement criterion. The reason for using Sequential Monte Carlo sampling is due to no closed-form expression of expected improvement criterion. The contribution of this article is twofold. The first part of the contribution is about formulation of new sampling criterion that handles multiple objectives and non-linear constraints simultaneously. The second part of the contribution lies in the numerical methods employed to compute and optimize the sampling criterion [28]. There is another study about multi-objective optimisation with constraints based on Bayesian optimisation. The authors in [29] have described an information-based approach which can handle multiple objectives and several constraints. Motivated by the lack

of Entropy-based methods, PESMOC is based on the Predictive Entropy Search for multi-objective Bayesian optimization [30]. At each iteration, PESMOC evaluates the objective functions and the constraints at an input location that is expected to reduce the entropy of the posterior distribution of the Pareto set the most. The proposed method is most useful in practical situations in which the objectives and the constraints are very expensive to evaluate [29].

There are other related studies about multi-objective optimisation. The study conducted in [30] described PESMO, a method for multi-objective Bayesian optimization. PESMO evaluates the objective functions at the input location that is most expected to reduce the entropy of posterior estimate of the Pareto set. The structure of acquisition function of PESMO can be understood as a sum of K individual acquisition functions, one per each of the K objectives. This triggers a decoupled evaluation scenario, in which the most promising objective is calculated by maximizing the individual acquisition functions. The other study in multi-objective Bayesian optimisation is proposed by [31]. The authors focus on modelling correlations amongst objectives in multi-objective Pareto optimization problems. To overcome the problem of intractable integrals in the proposed method, they have designed a novel approximation which leads to an analytic and differentiable approximation to the expected increase in Pareto hypervolume acquisition function. Another related study has been conducted in [8]. The authors showed that by computation of arbitrarily dense and continuous Pareto front, they can approximate the real Pareto front better in presence of measurement noise. These are useful tools to assist the user while making final decision among the Pareto points. An study based on Active learning is proposed in [32]. Active learning of Pareto fronts framework adopts a different strategy. Pareto-optimal objective vectors are generated by combining the active learning paradigm with the solution of a scalarized optimization problem. The proposed model was iteratively refined until the information gain obtained by the new candidate training examples became negligible. In another related study, a generative surrogate modeling procedure proposed in [33]. In this work, the authors have proposed a generative surrogate modeling procedure for multi-objective optimization. The main idea is “finding a particular Pareto-optimal solution helps in modeling and finding another neighboring Pareto-optimal solution”. The authors in [34] have proposed PMGA, a novel gradient-based approach to learn a continuous approximation of the Pareto frontier in multi-objective Markov Decision Problems (MOMDPs). The idea is to define a parametric function that describes a manifold in the policy-parameter space. The authors have presented different alternatives, discussed about the advantages and

disadvantages of the model and shown their properties through an empirical analysis. The presented model in [35], uses a Gaussian processes to predict the objective functions and to guide the sampling process in order to improve the prediction of the Pareto optimal set. it can be intuitively parameterized to achieve the desired level of accuracy at the lowest possible cost of evaluation. The authors presented an extensive theoretical analysis including bounds for the required number of evaluations to achieve the final accuracy. There is an study in which the authors use Gini index in the process of optimisation [37]. They introduced a new problem in the context of multi-objective multi-armed bandit (MOMAB). Contrary to most previously proposed approaches that tried to search for the Pareto front, instead they aim for a fair solution. To incorporate the fairness into the formulations, they have used the Generalized Gini Index (GGI), a well-known criterion developed in economics [37].

2.3 Multi-objective Bayesian optimisation with constraints

The goal of optimisation in such cases is to minimize the number of black-box function evaluations to find the global optimum of the function with respect to constraints. Bayesian optimisation with inequality constraints [27] and predictive entropy search for Bayesian optimization with unknown constraints [29] are two major studies investigating the role of inequality black-box expensive constraints in single-objective Bayesian optimisation. There are also two recent studies on multi-objective Bayesian optimisation with constraints. For example, in [28] authors proposed a Bayesian multi-objective optimisation (BMOO) approach to solve the single-objective and multi-objective optimisation with non-linear constraints which is in the same context with the proposed problem in this paper. The method handles the constraints using an extended Pareto domination rule that takes both objectives and constraints into account. The authors evaluated their method on the benchmark test functions with respect to hypervolume improvement. They proposed approach is inspired from [38] which relies on highly complex data models. BMOO uses Sequential Monte-Carlo (SMC) in order to compute the integral over the expected improvement formulation. In [29], the authors proposed a method based on predictive entropy search. The authors generated 100 synthetic optimization problems obtained by sampling the objectives and the constraints from their respective GP prior and they did not use benchmark test functions to evaluate their method. This method is generally

categorized as information-based methods while our proposed problem is based on hypervolume improvement approaches

2.4 Evolutionary algorithms and Multi-objective problems with constraints

Generally evolutionary algorithms and Surrogate-assisted evolutionary computation are not designed to work on limited budget of evaluation. But we are covering the overall review of the most related ones. Table 5.1 illustrates the related studies about such evolutionary methods.

Table 2.2: Summary of related studies in Evolutionary Multi-objective optimisation.

| Study | Method | Constraints | Ranking |
|---|-------------------------------------|-------------|---------|
| A surrogate-assisted evolution strategy for constrained multi-objective optimization [39] | Surrogate-assisted evolution | ✓ | - |
| A simple and fast hypervolume indicator-based multi-objective evolutionary algorithm [40] | Evolutionary Algorithm; Hypervolume | - | - |
| Multi-objective evolutionary algorithm for a quick computation of Pareto-optimal solutions [40] | Evolutionary Algorithm | ✓ | - |
| A fast and elitist multiobjective genetic algorithm: NSGA-II [41] | Evolutionary Algorithm | ✓ | - |
| SPEA2: Improving the strength Pareto evolutionary algorithm [42] | Evolutionary Algorithm | ✓ | - |

A surrogate-assisted evolution strategy is proposed in [39]. They have developed a surrogate-assisted multi-objective evolution strategy (SMES) for computationally expensive constrained multiobjective optimization. The main limitation of the present work is that, as with most evolutionary algorithms, there is no theoretical guarantee that the proposed surrogate-assisted ES will converge to the Pareto front. Moreover, the proposed approximations could be inaccurate when the computational budget is severely limited due to the computational expense of the simulations. The authors in [40] proposed a way for finding high quality of solutions in indicator-based multi-

objective evolutionary algorithms (MOEAs). Hypervolume is a critical performance factor playing a role in solution selection. In this paper, a simple and fast hypervolume indicator-based MOEA (FV-MOEA) is proposed to quickly update exact HV contributions for different solutions. The core idea of FV-MOEA is that the HV contribution of a solution is only associated with parts of the solutions rather than the full solution set. The authors in [40] introduced a new method called ϵ -MOEA. They have proven that ϵ -MOEA has two main advantages: 1. It has helped in reducing the cardinality of Pareto-optimal region and 2. It has also ensured that no two obtained solutions are within an ϵ_i from each other in the $i - th$ objective. Also, NSGA-II [41] is one of the most famous evolutionary multi-objective algorithm. The authors have proposed a computationally fast and elitist MOEA based on a nondominated sorting approach. The authors believe the proposed method has less computational complexity of nondominated sorting, more elite, and lack of need for specifying the sharing parameter. The last study is about SPEA2 [42]. The authors name many advantages over the similar strategies:

- SPEA2 performs better than SPEA on all problem sets.
- PESA has fastest convergence power, probably due to its higher elitism intensity, but has difficulties on some problems regarding the boundary solutions because it does not always keep the boundary solutions.
- In higher dimensional objective spaces, SPEA2 seems to have advantages over NSGA-II.

2.5 Multi-objective problems with constraints and objective rankings

As we have already explained in section 1.1, there are many real-world problems, requiring handling the importance of the objectives. In other words, objective ranking. This information could either be used as priori or as an output of the algorithm. There are not any specific studies on this problem. However, there is an study [43] about the ranking of the solutions based on the objectives. The authors studied on an alternative dominance relation to Pareto-dominance. Based on each separate objective, ranking set of solutions will be calculated and an aggregation function is used to calculate a scalar fitness value for each solution. The authors called this relation as *ranking-dominance* and it can be used to sort a set of solutions even for many

objectives when Pareto-dominance relation is not able to distinguish solutions from one another.

Later in this proposal, we will explain our presented idea based on Bayesian optimisation for this particular problem and will present the corresponding results.

Chapter 3

Background

This chapter describes the background and related work on which this proposal builds. We will start from Gaussian process as a power tool for placing the prior belief and compute the uncertainty over the function space. Then we will cover the Bayesian optimisation and the acquisition functions. Finally we will explain about multi-objective Bayesian optimisation and expected hypervolume improvement.

3.1 Gaussian processes

A Gaussian process is a collection of random variables $\{f(\mathbf{x}) : \mathbf{x} \in \mathcal{X}\}$ in which any finite collection of random variables has a multivariate Gaussian distribution [9]. GPs are determined by using a mean function $\mu(\mathbf{x}) : \mathcal{X} \rightarrow \mathbb{R}$ and a covariance function $k(\mathbf{x}) : \mathcal{X} \times \mathcal{X} \rightarrow \mathbb{R}^+$:

$$f(\mathbf{x}) \sim \mathcal{GP}(\mu(\mathbf{x}), k(\mathbf{x}, \mathbf{x}')). \quad (3.1)$$

The particular choice of covariance function determines the properties of sample functions drawn from the GP prior. Popular kernels for covariance function are Squared Exponential, Matern, Periodic, and Linear [44]. Without loss of generality, the prior mean function generally assumed to be zero in Gaussian process. Let us assume that we already made t observations on the points $\mathbf{x}_{1..t} = \{\mathbf{x}_1, \dots, \mathbf{x}_t\}$. The obtained evaluated results of these t observations are $f(\mathbf{x}_{1..t}) = \{f(\mathbf{x}_1), \dots, f(\mathbf{x}_t)\}$. Based on the defined properties of Gaussian process, the function values $f(\mathbf{x}_{1..t})$ jointly follow a multivariate Gaussian distribution $f(\mathbf{x}_{1..t}) \sim \mathcal{N}(0, K)$ [6]. Where K is a positive definite kernel matrix:

$$K = \begin{bmatrix} k(\mathbf{x}_1, \mathbf{x}_1) & \dots & k(\mathbf{x}_1, \mathbf{x}_t) \\ \vdots & \ddots & \\ k(\mathbf{x}_t, \mathbf{x}_1) & \dots & k(\mathbf{x}_t, \mathbf{x}_t) \end{bmatrix}.$$

3.1.1 Computing the posterior

The posterior can be similarly derived the way how the update equations for the Kalman filter was derived. First we need to find the joint distribution of $[f(\mathbf{x}_{t+1}), f(\mathbf{x}_1), f(\mathbf{x}_2), \dots, f(\mathbf{x}_t)]$. Considering t observations of the objective function, for a new point \mathbf{x}_{t+1} , $P(f(\mathbf{x}_{t+1})|\mathbf{x}_{1..t}, f(\mathbf{x}_{1..t})) = \mathcal{N}(\mu_t(\mathbf{x}_{t+1}), \sigma_t^2(\mathbf{x}_{t+1}))$:

$$\begin{bmatrix} f(\mathbf{x}_{t+1}) \\ f(\mathbf{x}_1) \\ f(\mathbf{x}_2) \\ \vdots \\ f(\mathbf{x}_t) \end{bmatrix} \sim \mathcal{N}\left(\begin{bmatrix} 0 \\ 0 \\ \vdots \\ 0 \end{bmatrix}, \begin{bmatrix} k(\mathbf{x}_{t+1}, \mathbf{x}_{t+1}) & k(\mathbf{x}_{t+1}, \mathbf{x})^T \\ k(\mathbf{x}_{t+1}, \mathbf{x}) & K_{\mathbf{xx}} \end{bmatrix} \right) \quad (3.2)$$

Where posterior mean and variance are calculated as:

$$\mu_t(\mathbf{x}_{t+1}) = k^T K^{-1} f(\mathbf{x}_{1..t}), \quad (3.3)$$

$$\sigma_t^2(\mathbf{x}_{t+1}) = k(\mathbf{x}_{t+1}, \mathbf{x}_{t+1}) - k^T K^{-1} k. \quad (3.4)$$

k in equation 3.16 and 3.17, is a kernel vector such that $k = [k(\mathbf{x}_{t+1}, \mathbf{x}_1), \dots, k(\mathbf{x}_{t+1}, \mathbf{x}_t)]^T$. After modelling the observations with GP, it is required to find the best possible point for next iteration of optimisation (\mathbf{x}_{t+1}). Figure 7.2 illustrates an example on Gaussian processes fitting process.

3.1.2 A few basic kernels

In this section we will briefly mention to some basic kernels for Gaussian processes. Figure 3.2 illustrates different kernels.

3.1.2.1 Linear Kernel

We are simply doing Bayesian linear regression when working with linear kernel.

$$k_{lin} = \sigma_f^2(x - c)(x' - c) \quad (3.5)$$

3.1.2.2 Matern32 Kernel

The Matern kernel is likely the second most popular kernel. Many believe the smoothness of the squared exponential kernel is unrealistic for modelling physical processes [9].

$$\sigma_f^2 \left(1 + \frac{\sqrt{3}(x - x')}{\sigma_l} \right) \exp\left(-\frac{\sqrt{3}(x - x')}{\sigma_l}\right) \quad (3.6)$$

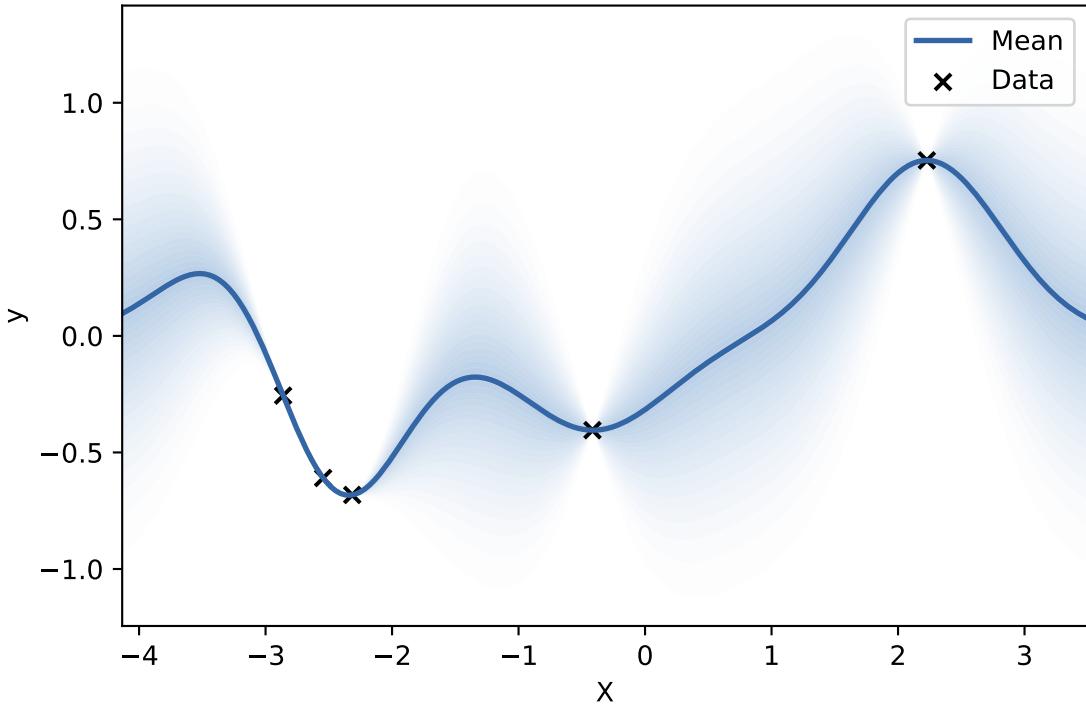


Figure 3.1: Gaussian process fitted at five points, blue line indicates the mean function, the black points indicates the observations.

3.1.2.3 Squared Exponential Kernel

The squared exponential (SE) kernel, also called the Gaussian, radial, basis function (RBF) or exponentiated quadratic kernel, is probably the most widely-used kernel in Gaussian processes.

$$k_{SE} = \sigma^2 \exp\left(-\frac{(x - x')^2}{2l^2}\right) \quad (3.7)$$

3.1.2.4 Periodic Kernel

This kernel is mostly useful in combination with other covariance functions.

$$k_{periodic}(x, x') = \exp\left(\frac{-2\sin^2(\pi(x - x')/2)}{l^2}\right) \quad (3.8)$$

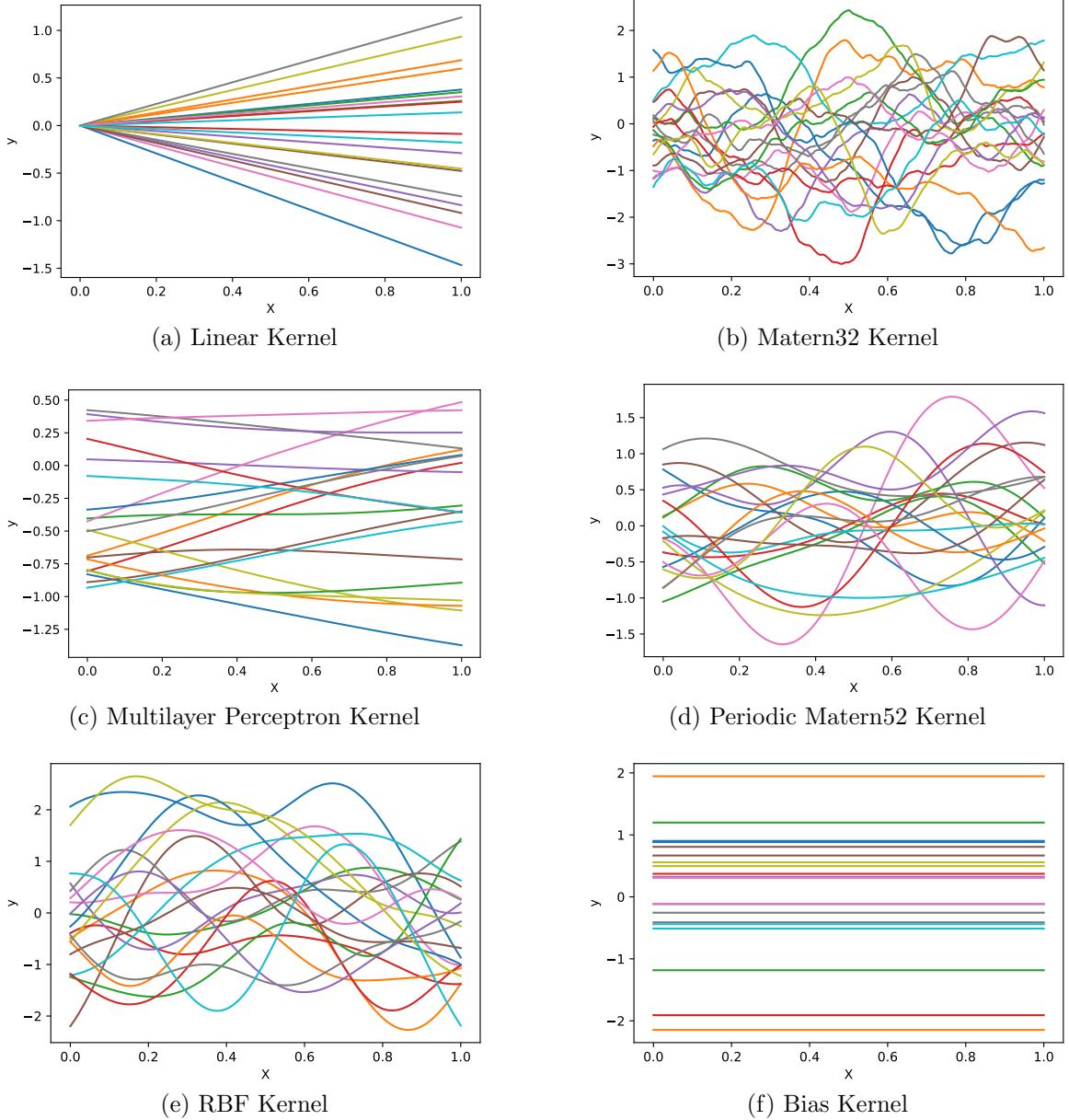


Figure 3.2: Comparison of different kernels in Gaussian processes.

3.2 Bayesian optimisation

In Bayesian optimisation, we use GP to define a prior. The sequential nature of the Bayesian optimization leads the sampling of the continuous search space [45]. In order to optimise the expensive functions, Bayesian optimisation uses a surrogate function called acquisition functions. Acquisition function denoted by $\alpha : \mathcal{X} \rightarrow \mathbb{R}^+$, determines the point in \mathcal{X} that should be evaluated next:

$$\mathbf{x}_{t+1} = \operatorname{argmax}_{\mathbf{x} \in \mathcal{X}} \alpha(\mathbf{x}). \quad (3.9)$$

Acquisition functions depend on the both previous observations and the GP hyperparameters and kernel functions [3]. For explaining the exact mechanism for selecting the sequence of query points, we need to first explain the acquisition function. The standard Bayesian optimisation algorithm is illustrated in Algorithm 1 (section 2).

3.3 Acquisition function

Whereas in experimental design and decision theory, the function α is called expected utility, in Bayesian optimisation it is often called Acquisition function. While optimising the expensive black-box function, one could simply select arbitrary points, however that would be wasteful. Instead, there is a proper mechanism that utilizes the posterior model on selection strategies and guiding the sequential search. One of the most import features of acquisition functions must be *the balance in the exploration of the search and exploitation of current promising area* [26]. Based on this criteria, three types of acquisition functions are introduced. The first category is *Improvement-Based Acquisition Functions*, the second one is based on *Optimistic Policies*[26] and the third on is based on *Information-Based Policies*.

3.3.1 Improvement-Based

Improvement-Based acquisition functions are in favor of points which are likely to make an improvement on the observations. The most naive strategy based on this idea is Probability of Improvement (PI) acquisition function. PI is formulated as follow:

$$\alpha_{PI}(\mathbf{x}; \mathcal{D}_t) = \Phi\left(\frac{\mu_t(\mathbf{x}) - f(\mathbf{x}^+)}{\sigma_t(\mathbf{x})}\right) \quad (3.10)$$

where $\Phi(\cdot)$ is the standard normal cumulative distribution function. Current best observation after t observations is \mathbf{x}^+ , where $\mathbf{x}^+ = \operatorname{argmax}_{\mathbf{x}_i \in \mathcal{X}_{1..t}} \alpha(\mathbf{x}_i)$. Although PI could

be a good solution in some scenarios but it is clear that it can excessively focus on exploitation.

Expected Improvement (EI) is one of the most widely-use acquisition function in this area. Whereas PI can lead to an overly greedy optimisation [26], it works reasonably as a part of EI. Then $\alpha_{EI}(\mathbf{x})$ is defined as:

$$\alpha_{EI}(\mathbf{x}) = \begin{cases} (\mu(\mathbf{x}) - f(\mathbf{x}^+))\Phi(Z(\mathbf{x})) + \sigma(\mathbf{x})\phi(Z(\mathbf{x})), & \text{if } \sigma(\mathbf{x}) > 0 \\ 0, & \text{if } \sigma(\mathbf{x}) = 0 \end{cases} \quad (3.11)$$

Where $\phi(\cdot)$ is PDF of normal distribution. $Z(\mathbf{x})$ is also defined as:

$$Z(\mathbf{x}) = \begin{cases} \frac{(\mu(\mathbf{x}) - f(\mathbf{x}^+))}{\sigma(\mathbf{x})}, & \text{if } \sigma(\mathbf{x}) > 0 \\ 0, & \text{if } \sigma(\mathbf{x}) = 0 \end{cases} \quad (3.12)$$

3.3.2 Optimistic policy

The major guideline behind this category of acquisition functions is to be optimistic in the face of uncertainty. In a bandit task, there are multiple options as arms. These arms have unknown probability of generating a reward and the aim of the agent is to select the best arm in order to maximise the overall reward. Let us consider the current situation of iteratively point selection as arms of a multi-armed bandit problem. Consequently the evaluation value of these points represents the reward of the arm. What distinguishes the current situation from the basic bandit problem is the fact that the rewards of the arms are correlated in dependency of the underlying covariance kernel [46]. As a result of viewing this problem in a multi-arm bandit setting, the popular strategy called upper confidence bound (UCB) can be used in this context.

$$\alpha_{UCB}(\mathbf{x}; \mathcal{D}_t) = \mu_t(\mathbf{x}) + \beta_t \sigma_t(\mathbf{x}) \quad (3.13)$$

There are theoretically motivated guidelines for setting the hyperparameter β_t [22].

3.3.3 Information-Based policy

Information-Based acquisition functions consider the posterior distribution over the unknown minimizer x^* , $p_*(\mathbf{x}|\mathcal{D})$. The Entropy Search selects a point which is most likely offer a great deal of information about the unknown \mathbf{x}^* [47]. The goal of entropy search is to reduce the uncertainty in the location of \mathbf{x}^* by selecting the point that is expected to cause the highest reduction in entropy of the distribution $p_*(\mathbf{x}|\mathcal{D})$ [26]:

$$\alpha_{ES}(\mathbf{x}; \mathcal{D}_t) = H(\mathbf{x}^*|\mathcal{D}_t) - \mathbb{E}_{y|\mathcal{D}_{n,\mathbf{x}}} H(\mathbf{x}^*|\mathcal{D}_t \cup \{(\mathbf{x}, y)\}) \quad (3.14)$$

In equation 3.14, $H(\mathbf{x}^*|\mathcal{D}_t)$ denotes the differential entropy of the posterior distribution $p_*(\mathbf{x}|\mathcal{D})$. It is noteworthy to mention that the expectation is over the distribution of the random variable $y \sim \mathcal{N}(\mu_t(\mathbf{x}), \sigma_t^2(\mathbf{x}))$. Since Mutual Information is symmetric, entropy is defined to be symmetric too [47]. Thus Predictive Entropy Search (PES) removes the need for discretization and approximates the acquisition function. Therefore α_{PES} is defined as:

$$\alpha_{PES}(\mathbf{x}; \mathcal{D}_t) = H(y|\mathcal{D}_t, \mathbf{x}) - \mathbb{E}_{\mathbf{x}^*|\mathcal{D}_t}[H(y|\mathcal{D}_t), \mathbf{x}, \mathbf{x}^*)] \quad (3.15)$$

3.4 Multi-objective Bayesian optimisation

In single-objective problems, the optimiser looks for the best single answer. For example, selection of a single best design, selection of the best set of parameters for a machine learning method regarding the final accuracy. However, in many real-world problems, it is very common to deal with multiple competing objectives. Competition arises through incommensurability of objectives in real-world systems, usually bounded by physical laws [48]. Consider a Robotic for an example. in Robotics, one of the current problems researches are working on, is about overheating of motors or power consumption of them. While other objectives such as the accuracy of movements with some constraints are also play a role in this problem. For the multi-objective problem, the optimization task involves identification of those solutions that are *Pareto optimal*. A solution is said to be Pareto optimal if none of the objectives can be improved without degrading in at least one other objective [48]. Consider Figure 3.3 as an example. There may exist many or even an infinite number of points that structures a Pareto optimal set where each point represents a specific solution. Rather than locating the potentially infinite number of Pareto optimal solutions, a theoretical boundary of Pareto optimality can be drawn called a Pareto frontier [48]. All points that fall on the frontier are Pareto optimal.

So in multi-objective optimisation problems, we are dealing with Pareto points and not just single solution. Now the main question is: “How to calculate the expected improvement of the selected points in more than one dimension?”. In the next section we are going to explain expected hypervolume improvement for calculating the expected improvement in this context.

3.4.1 Expected Hypervolume Improvement (EHVI)

In this study we are particularly interested in the EHVI with a closed form expression introduced in [49]. Our aim is to jointly minimize $m > 1$ objective functions $f_m :$

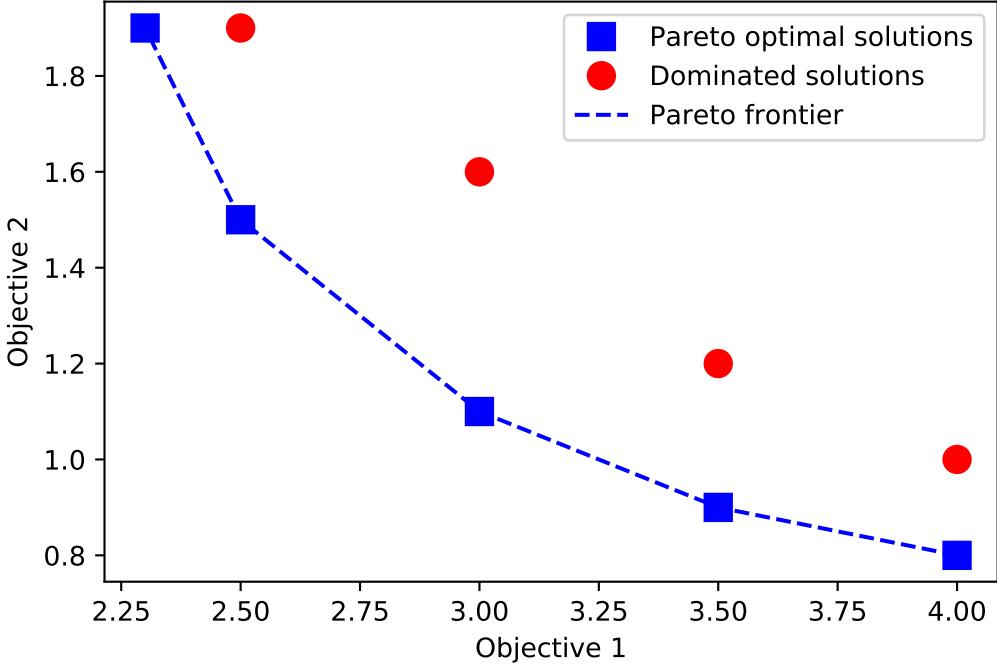


Figure 3.3: Illustration of Pareto optimal solutions, dominated solutions, and Pareto frontier.

$\mathcal{X} \rightarrow \mathbb{R}$ for $m = 1, \dots, M$. A point $\mathbf{y} \in \mathbb{R}^M$, is said to dominate a point $\mathbf{y}' \in \mathbb{R}^M$, iff $\forall i \in \{1, \dots, M\} : y_i \leq y'_i$ and $\mathbf{y} \neq \mathbf{y}'$; written as $\mathbf{y} \preceq \mathbf{y}'$. For a set of points $\mathcal{Y} = \{\mathbf{y}_1, \mathbf{y}_2, \dots, \mathbf{y}_N\}$, Pareto efficient points $P(\mathcal{Y})$, $P(\mathcal{Y}) \subset \mathcal{Y}$ is defined as $P(\mathcal{Y}) = \{\mathbf{y}_i \in \mathcal{Y} : \mathbf{y}_j \not\preceq \mathbf{y}_i, \forall \mathbf{y}_j \in \mathcal{Y} \setminus \{\mathbf{y}_i\}\}$ [31]. A point is Pareto efficient if there is no other point that can improve any one objective without making at least one other objective worse.

One of the most popular indicators for multi-objective optimisation is hypervolume, otherwise known as The S-metric or Lebesgue measure [50]. We denote the Lebesgue measure of a set U by $Vol(U)$. The S-metric or Lebesgue measure for $P(\mathcal{Y}) = \{\mathbf{y}_1, \mathbf{y}_2, \dots, \mathbf{y}_P\}$ is defined to be:

$$S(P(\mathcal{Y}), \mathbf{y}^{ref}) = Vol(\{\mathbf{y} \in \mathbb{R}^M | P(\mathcal{Y}) \preceq \mathbf{y} \preceq \mathbf{y}^{ref}\}), \quad (3.16)$$

where \mathbf{y}^{ref} is a reference point in \mathbb{R}^M which is always dominated by all elements of $P(\mathcal{Y})$. By considering equation 3.16, the improvement in hypervolume is defined to be $I(\mathbf{y}, P(\mathcal{Y})) = S(P(\mathcal{Y}) \cup \{\mathbf{y}\}) - S(P(\mathcal{Y}))$, Therefore the expected hypervolume

improvement EHVI(\mathbf{x}) is:

$$\text{EHVI}(\mathbf{x}) = \int_{\mathbf{y} \in \mathbb{R}^M} I(\mathbf{y}, P(\mathcal{Y})) \times P_{f_{\mathbf{x}}}(\mathbf{y}) d(\mathbf{y}), \quad (3.17)$$

where the $P_{f_{\mathbf{x}}}(\mathbf{y})$ is a probability density function of a predictive distribution of objective function vectors.

The EHVI can be computed by piecewise integration over a set of cells. These cells are formed by horizontal and vertical lines through the set of Pareto efficient points (P) and \mathbf{y}^{ref} (see figure 3.4). The cuboidal set of interest considered to be the space: $S \equiv \{\mathbf{y} \in \mathbb{R}^M : \mathbf{y} \preceq \mathbf{y}^{ref}\}$. Let us assume $b_i^{(1)}, b_i^{(2)}, \dots, b_i^{(p)}$ are the sorted list of $i - th$ coordinate for $P(\mathcal{Y})$. For simplicity, let $b_i^{(0)} = -\infty$, $b_i^{(p+1)} = \mathbf{y}^{ref}$ and also $b_i^{(p+2)} = \infty$. As a result of this partitioning, for each $(i_1, i_2, \dots, i_M) \in \{0, \dots, p\}^M$, a grid cell $S(i_1, \dots, i_M)$ is defined by $(b_1^{(i_1)}, b_1^{(i_1+1)}) \times (b_2^{(i_2)}, b_2^{(i_2+1)}) \times \dots \times (b_M^{(i_M)}, b_M^{(i_M+1)})$. For each given cell $S(i_1, \dots, i_M)$, we define $\mathbf{l}(i_1, \dots, i_M) = (b_1^{(i_1)}, \dots, b_M^{(i_M)})^T$ as the lower bound and $\mathbf{u}(i_1, \dots, i_M) = (b_1^{(i_1+1)}, \dots, b_M^{(i_M+1)})^T$ as the upper bound [49].

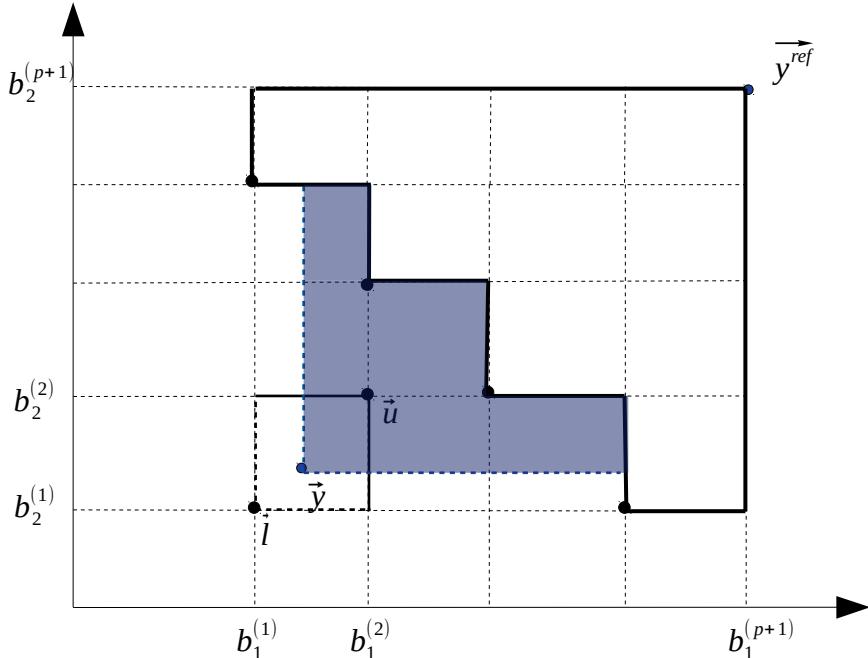


Figure 3.4: Sample bi-objective case with partitioned cells. The black points are in set of $P(\mathcal{Y})$ and dominated the \mathbf{y}^{ref} . Also the upper (\mathbf{u}) bound and lower bound (\mathbf{l}) for a sample point \mathbf{y} in a cell is illustrated. The $b_1^{(i)}$ and $b_2^{(i)}$, $\{i = 1, \dots, p + 1\}$ are representative of first and second coordinate.

The EHVI can be computed using piecewise integration over a set of cells defined by $P(\mathcal{Y})$ as shown in Fig. 1 (see [49] for details). We denote this set of cells S .

After partitioning the integration space into grid cells, it can be inferred that the expected improvement integral is the sum of improvement integral over the set of non-dominated cells. Non-dominated cells are the one whose points are not dominated by any member of Pareto efficient set [31]: $S^+ = \{s \in S : \forall \mathbf{y} \in s, \mathbf{y}' \in P(\mathcal{Y}), \mathbf{y}' \not\leq \mathbf{y}\}$. So the expected hypervolume improvement over the cells is defined to be:

$$\text{EHVI}(\mathbf{x}) = \sum_{s \in S^+} \int_{\mathbf{y} \in s} I(\mathbf{y}, P(\mathcal{Y})) P_{f_\mathbf{x}}(\mathbf{y}) d\mathbf{y} \quad (3.18)$$

as f_1, \dots, f_M are assumed to be generated from independent GPs, the EHVI can be computed analytically [49].

Chapter 4

Aims and Approaches

In this chapter we will elaborate on further details about aims and approaches regarding the multi-objective Bayesian optimisation problem. In the first approach, we incorporated the unknown constraints into multi-objective Bayesian optimisation and hypervolume improvement. This study resulted in a publication in ICPR 2018 conference. The second aim is about the need for utilizing objective rankings in many problems in multi-objective Bayesian optimisation.

4.1 Expected Hypervolume Improvement with Constraints (EHVIC)

As it was illustrated in literature review (see section 2) there are few studies regarding the role of constraints in multi-objective Bayesian optimisation. This article provides an extension on the well-known expected improvement acquisition function in order to handle the independent constraints and multi-objective functions. We call our method expected hypervolume improvement with constraints (EHVIC) since it is generally based on hypervolume expected improvement. The contributions of our approach are:

- Formulation of the expected hypervolume improvement with constraints based on the simple but effective expected improvement acquisition function.
- Evaluation of the proposed algorithm based on feasible dominated region on 6 benchmark test functions for the first time. We also estimated the volume of the feasible region of the test functions for more accurate evaluation.
- Discussion of the issues involved in the method in terms of the efficiency and size of the problem.

In MOO potential solutions are assessed by their performance in more than one objective [7]. In MOO, based on definition of Pareto optimality, we wish to return a Pareto front that represents the best trade-off possible considering all criteria [8]. More generally, MOO with constraints (MOOC) includes M objective functions and a set of K constraints. We assume that f_1, f_2, \dots, f_M and c_1, c_2, \dots, c_K are drawn independently from Gaussian Process (GP) [9] as $f_i \sim \text{GP}(\mu_i^f, \sigma_i^f)$ and $c_i \sim \text{GP}(\mu_i^c, \sigma_i^c)$. Formally:

$$\begin{aligned} & \underset{\mathbf{x}}{\text{minimize}} \quad \mathbf{y} = \mathbf{Z}(\mathbf{x}) = \{f_1(\mathbf{x}), f_2(\mathbf{x}), \dots, f_M(\mathbf{x})\} \\ & \text{subject to} \quad \mathbf{C}(\mathbf{x}) = \{c_1(\mathbf{x}), c_2(\mathbf{x}), \dots, c_K(\mathbf{x})\} \leq 0, \\ & \text{where:} \quad \mathbf{x} \in \mathcal{X} \subseteq \mathbb{R}^d \\ & \quad \mathbf{y} \in \mathcal{Y} \subseteq \mathbb{R}^M \end{aligned}$$

We assume that both the objectives and constraints are expensive to evaluate and that observations of same are noisy. We accumulate the observations of objective functions to $D_{z_{\{1:t\}}} = \{\mathbf{x}_{1:t}, Z(\mathbf{x})_{1:t}\}$ and as for constraint function to $D_{c_{\{1:t\}}} = \{\mathbf{x}_{1:t}, C(\mathbf{x})_{1:t}\}$. In the single-objective case, Expected Improvement with Constraints (EIC) or constrained acquisition function is a popular acquisition function that estimates the expected change in the objective function while satisfying constraints [1]. There are a few studies in single-objective Bayesian optimisation, using EIC or related extensions to handle inequality constraints [27]. There are others frameworks such as information-based search [51], and predictive entropy search for Bayesian optimization with unknown constraints [47]. EHVIC is the analogue of the EIC-based methods in multi-objective case with constraints.

4.1.1 Proposed method

In EHVIC, the improvement is defined only when all the constraints are satisfied. Since we are not certain about the values of the constraints, we need to extend our model to include this uncertainty. Because $f_{1..M}(\mathbf{x})$ and $c_{1..K}(\mathbf{x})$ are both black-box function and expensive to evaluate, we need to use the Bayesian formalism to model each of $f_{1..M}(\mathbf{x})$ and $c_{1..K}(\mathbf{x})$, given \mathbf{x} . We consider $D_{z_{\{1:t\}}}$ and $D_{c_{\{1:t\}}}$ as set of observations for objective functions and constraint functions. During the Bayesian optimisation, by picking a candidate point like \mathbf{x} , we can evaluate $Z(\mathbf{x})$ and $C(\mathbf{x})$ and add the point to $D_{z_{\{1:t\}}}$ and $D_{c_{\{1:t\}}}$ respectively. To consider the most general case, we assume that the constraints and the objective functions are independent. So the Gaussian process posterior is used to independently update $c_i(\mathbf{x}) \sim \mathcal{N}(\mu_i^c(\mathbf{x}), \sigma_i^c(\mathbf{x}))$; $i = 1, \dots, K$

for constraint functions and $f_i(\mathbf{x}) \sim \mathcal{N}(\mu_i^f(\mathbf{x}), \sigma_i^f(\mathbf{x}))$; $i = 1, \dots, M$ for objective functions.

The proposed acquisition function is made of two main parts, namely the hyper-volume improvement with respect to the objective functions as explained in section 2, and the expectation of constraints satisfaction $\Delta(s)$. We define $\Delta(s)$ for each given cell s as:

$$\begin{aligned}\Delta(s) &= \int_{\mathbf{x}|\mathbf{y} \in s} Pr(c(\mathbf{x}) \leq 0) d\mathbf{x} \\ &= \int_{\mathbf{x}|\mathbf{y} \in s} \int_{-\infty}^0 p(c(\mathbf{x})|\mathbf{x}, D_{c_{\{1:t\}}}) dc(\mathbf{x}) d(\mathbf{x})\end{aligned}\quad (4.1)$$

Since the expectation of satisfaction for constraints is defined on each cell, the integral bound is on the inputs \mathbf{x} whose corresponding objective values satisfies $\mathbf{y} \in s$ that is $\mathbf{x} = \{\mathbf{x} \in \mathcal{X} : \mathbf{y} \in s\}$. Due to marginal Gaussianity of $c(\mathbf{x})$ and the independence of constraints, the value of $\int_{-\infty}^0 p(c(\mathbf{x})|\mathbf{x}, D_{c_{\{1:t\}}}) dc(\mathbf{x})$ is equal to product of K Gaussian univariate cumulative distribution functions on constraint functions. The required integral is intractable without making further approximations. To solve this integral, we approximate it using a set of samples from the posterior distribution of the objective functions. The input points of each sample are selected if the posterior sample satisfies the interval criteria $(\mathbf{x}|\mathbf{y} \in s)$. Then, the well-known Monte-Carlo sampling method in [52] is used to estimate the value of $\Delta(s)$. Thus the EHVIC acquisition function results as following equation:

$$EHVIC(\mathbf{x}) = \sum_{s \in S^+} \left\{ \Delta(s) \times \underbrace{\int_{\mathbf{y} \in s} I(\mathbf{y}, P(\mathcal{Y})) \times P_{f_{\mathbf{x}}}(\mathbf{y}) d\mathbf{y}}_{\text{EHVI calculation for given cell } s} \right\} \quad (4.2)$$

It is noteworthy to mention that, while infeasible points may be selected in our experiment, they are never considered for calculation of Pareto set, though they help to shape the Gaussian processes posteriors. By allowing the Gaussian Process to discern the regions which are more likely to be feasible, the number of evaluations that is required to find the first feasible point, will be reduced. Algorithm 2 illustrates the EHVIC method.

It is worth noting that the stopping criteria in Algorithm 2 is usually related to resources, such as the number of maximum black-box function evaluation, the value of similarity to the best estimated Pareto front, etc.. Moreover, volume of the region dominated by the Pareto front can be used as stopping point and also as an evaluation factor [28].

Algorithm 2 Expected Hypervolume Improvement with Constraints (EHVIC) Algorithm

Require:

```
1:  $Z(\mathbf{x}) = \{f_1(\mathbf{x}), f_2(\mathbf{x}), \dots, f_M(\mathbf{x})\}$ 
2:  $C(\mathbf{x}) = \{c_1(\mathbf{x}), c_2(\mathbf{x}), \dots, c_K(\mathbf{x})\}$ 
3: Generate the initial design  $\mathcal{X}$ ,  $\mathcal{Y}$ ,  $D_{z_{\{1:t\}}}$  and  $D_{c_{\{1:t\}}}$ 
4: Calculate the initial values of Pareto set  $P_t = P(\mathcal{Y})$ 
5: procedure EHVIC( $\mathbf{x}$ )
6:   while !(Stopping Criteria) do
7:     Fit the independent GP models based on  $D_{z_{\{1:t\}}}$  and  $D_{c_{\{1:t\}}}$ 
8:     Compute  $\Delta(s)$  and  $\text{EHVI}(\mathbf{x})$  for  $\forall s \in S^+$ 
9:     Find the  $\mathbf{x}_{t+1} = \underset{\mathbf{x} \in \mathcal{X}}{\operatorname{argmax}} \text{EHVIC}(\mathbf{x})$ 
10:    Evaluate the  $Z(\mathbf{x}_{t+1})$  and  $C(\mathbf{x}_{t+1})$ 
11:    Add  $\{\mathbf{x}_{t+1}, Z(\mathbf{x}_{t+1})\}$  and  $\{\mathbf{x}_{t+1}, C(\mathbf{x}_{t+1})\}$  to  $D_{z_{\{1:t\}}}$  and  $D_{c_{\{1:t\}}}$ 
12:   end while
13:   Update  $P_t = P(\mathcal{Y} \cup \mathbf{y}_{t+1})$ 
14: end procedure
```

4.2 Multi-objective optimisation with objective ranking

Objective ranking based on importance of the objectives is an extremely valuable information in many-objective problems. Performing multi-objective optimisation while facing with a ranking for objectives can dramatically influence on final solution set of the problem. For example, while buying a car, many features are available. But one may like to buy a “safer” rather than having an efficient car in terms of fuel consumption or beauty. In such scenarios, one or many objectives are preferred over the other objectives. There are two ways to express this importance. The first one is to exactly indicate the values of the rankings. For example for the car problem, safety is 10 out of 10, and beauty is 6 out of 10. However the other way is expressing the preference over another objective. In this study we will focus on the second scenario since we believe in many real-world problems the exact values of importance or ranking is not easy to calculate.

4.2.1 Proposed method

Assuming the same context as the one in section 4.1. Let us define the problem as follows:

$$\begin{aligned}
 & \underset{\mathbf{x}}{\text{minimize}} \quad \mathbf{y} = \mathbf{Z}(\mathbf{x}) = \{f_1(\mathbf{x}), f_2(\mathbf{x}), \dots, f_M(\mathbf{x})\} \\
 & \text{subject to} \quad \mathbf{R} = \{\mathbf{R}_1, \mathbf{R}_2, \dots, \mathbf{R}_N\} \\
 & \text{where:} \quad \mathbf{x} \in \mathcal{X} \subseteq \mathbb{R}^d \\
 & \quad \mathbf{y} \in \mathcal{Y} \subseteq \mathbb{R}^M \\
 & \quad \mathbf{R}_i = [r_1^i, \dots, r_M^i] \in \mathcal{R} \subseteq \mathbb{R}^+
 \end{aligned} \tag{4.3}$$

It is noteworthy to mention that the exact values of the $r_1^i \dots r_M^i$ is not available initially, but without loss of generality we assume that we know $r_1 \geq r_2 \geq \dots \geq r_M$ and $\sum_{i=1}^M r_i = 1$. Our proposed method for solving this problem is based on the idea of scalarization. By mapping this problem into a single-objective Bayesian optimisation problem with constraints, we can overcome the difficulty of handling objective rankings in multi-dimensional space. The proposed method is formulated as follows:

$$\begin{aligned}
 & \underset{\mathbf{x}}{\text{minimize}} \quad \mathbf{y} = \mathbf{Z}(\mathbf{x}, \mathbf{R}_{N+1}) = f_1(\mathbf{x})r_1 + \dots + f_M(\mathbf{x})r_M + \frac{1}{D(\mathbf{R}_{N+1}, \mathbf{R})} \\
 & \text{subject to} \quad r_1 \geq r_2 \geq \dots \geq r_M \\
 & \text{where:} \quad \mathbf{x} \in \mathcal{X} \subseteq \mathbb{R}^d \\
 & \quad \mathbf{y} \in \mathcal{Y} \subseteq \mathbb{R}^M \\
 & \quad \sum_{i=1}^M r_i = 1 \\
 & \quad D(\mathbf{R}_{N+1}, \mathbf{R}) = \min(\|\mathbf{R}_{N+1} - \mathbf{R}_i\|_{i=1 \dots M})
 \end{aligned} \tag{4.4}$$

Equation 4.4 formulates the single-objective problem based on objective rankings. At the first iteration, $N = 1$ and the value of \mathbf{R}_1 will be generated randomly. But in the next upcoming iterations of the optimisation, the objective rankings of Pareto optimal points will be augmented to \mathbf{R} called the ranking set. The reason for this augmentation is to finding diverse pareto optimal points. The value of a new proposed \mathbf{R}_{N+1} should be as far as possible from the other existing ranking sets in the \mathbf{R} while it meets the proposed constraints. If the new proposed ranking \mathbf{R}_{N+1} is too close the current rankings of \mathbf{R} , the high value of $\frac{1}{D(\mathbf{R}_{N+1}, \mathbf{R})}$ will prevent the selection of the point to in the next iteration.

4.3 Multi-objective bayesian optimisation in Robotics

Consider a baby is learning a new behavior, like crawling or grasping, she performs it several times, trying to improve the result of the behavior in each trial while exploring new strategies. In this proposal we will focus on optimising biped locomotion in extremely complex environments such as Poppy Humanoid Robot.

Poppy is a humanoid robotic platform mainly designed to jointly address three central goals of humanoid robotics [53]:

- Study the role of morphology in biped locomotion
- Study full-body compliant physical human-robot interaction
- Robustness and also easy and fast to duplicate to facilitate experimentation

One of the particularly interesting skills is biped locomotion. Poppy uses the bio-inspired trunk developed for the Acroban humanoid robot [54]. In addition, it also includes a novel hip and thigh physical design with regards to the impact on balance control and locomotion. A mesh structure is used in the geometry of limbs which has been optimized to minimize weight. As a result this structure allowed the decrease of motor power and weight, as well as energy consumption. To allow efficient and proper walking gait, Poppy's feet design takes some functional inspiration from the actual human foot such as the proportion, compliance and toes which are key features concerning both the human walking [55] and biped robots with a human-like gait [56].

Figure 4.1 shows Poppy sitting on a chair in our lab.

Robotic algorithms typically rely on various parameters, the choice of which significantly affects the performance [57]. Optimization algorithms, such as Bayesian optimization, have been used to automate this process. One of the key challenges in Humanoid robots is finding gait parameters that optimize a desired performance metric while walking on even surface. For this purpose we need to design an extremely fast multi-objective Bayesian optimisation, capable of handling large set of parameters (at least 50). Also in this problem we are facing with constraints such as overheating. In Order to overcome the possible difficulties in the proposed problem, we will introduce a direct policy search combined with a multi-objective Bayesian optimisation with constraints because we believe it scales well to high dimensional and continuous state-action spaces [57].

There have been studies such as [58] working on gait optimisation in Robotics, but we believe by solving this problem in an actual humanoid robot (teen size) we

can extend the proposed method in many complex environments in Robotics which need multi-objective optimisation with constraints.



Figure 4.1: Poppy open source robot, sitting on a chair!.

Chapter 5

Experiments

This chapter evalautes the performance of the proposed algorithms in section 4.1.

5.1 EHVIC

In this section, we evaluate the performance of EHVIC on a suite of benchmark test functions for multi-objective optimisation with constraints. All test problems are minimization problems. To the best of our knowledge, there is only one study, BMOO [28] based on hypervolume improvement and Bayesian approaches that investigates the role of black-box constraints on multi-objective optimisation. The other studies are based on genetic or evolutionary algorithms such as NSGAII [41], SPEA2 [42] and Surrogate-assisted evolutionary computation [59] which are not designed to work on limited budget of function evaluations [28]. However, we still compared the performance of the proposed method with NSGAII to demonstrate the efficiency of our method for expensive functions. The BMOO method introduced by [28] used the volume of the region dominated by the Pareto front relative to a reference point as the evaluation factor expressing the quality and diversity of Pareto front. According to our experiments the volume of the feasible region should be considered to better quantify the quality of the obtained Pareto set. The reason to use the volume of the feasible region is illustrated in Fig. 5.1 based on BNH function introduced in Table 5.1. The shaded region in Fig. 5.1 is the dominated area based on the true Pareto set (Black dots). The darker shaded area is the feasible dominated region. Note that the sample Pareto set in Fig. 5.1 dominated almost 80% of the dominated region. Though the sample Pareto set just dominated 60% of the feasible dominated region. Considering this fact, we believe constraints should not be ignored while evaluating the quality of the obtained Pareto front. So feasible dominated region is a more ac-

curate criterion to be used while handling both objective and constraint functions.

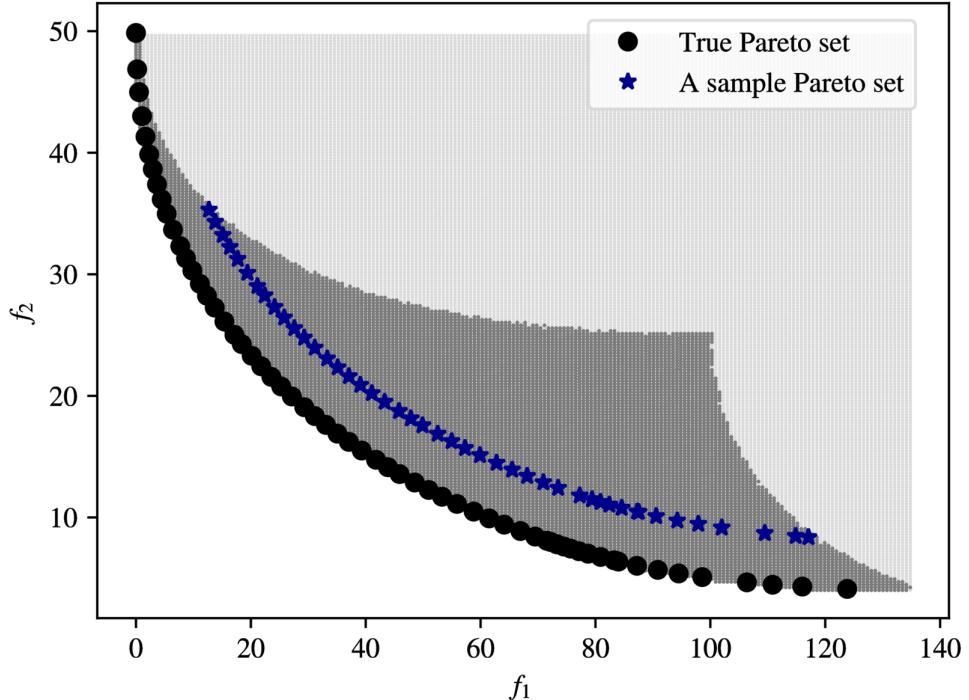


Figure 5.1: Comparison of feasible dominated region with the whole dominated region for evaluation of a sample Pareto set. Although the sample Pareto set covered more than 80% of the dominated region, but almost 40% of the feasible dominated region has not been dominated by the sample Pareto set.

All simulations and obtained results were written in Python. The objectives and constraint functions are modeled by independent GPs. We applied the standard approach to set all GP hyper-parameters with maximum likelihood estimation [9]. The maximum number of function evaluation is set to be 200 for $M = 2$ and the algorithm is initialized with $5d = 10$ ($d = 2$) function evaluations. Note that, if no feasible solution is found in this initial random set then the acquisition function keeps exploring so that it can discern the feasible region.

For hypervolume based comparison, fast method to calculate multi-objective probability of improvement and expected improvement is implemented [7]. The amount of volume dominated in feasible region by Pareto front for each function is estimated by approximating the true Pareto front and estimating the volume of the feasible region by extracting the feasible cells.

| Function | Target 90% | Target 95% | Target 99% |
|----------|--------------|--------------|----------------|
| BNH | 11.3 (0.82) | 37.5 (1.74) | 64.7 (13.69) |
| SRN | 25.7 (6.70) | 48.31 (9.27) | 82.04 (6.88) |
| TNK | 45.57 (9.21) | 71.40 (5.10) | 105.7 (23.52) |
| OSY | 61.8 (11.35) | 97.1 (13.89) | ≥ 200 (-) |

Table 5.1: Experimental results on benchmark test functions. The average number of function evaluations over 10 independent runs in order to dominate 90%, 95% and 99% of the target volume (V). The corresponding standard deviation for each of the iteration numbers are written in parentheses. We use “ \geq ” sign when the Pareto front approximation is beyond the function evaluation limits.

For finding feasible cells, Monte-Carlo method is used with same configuration as explained in section 4.1. All objective functions and constraint functions are scaled down to $[0, 1]$ space while performing EHVIC. The experimental results are obtained by 10 independent runs of the method. We have used four benchmark multi-objective functions with constraints as the test problems. A summary of the selected benchmark functions can be found in Table 5.1.

Fig. 5.2 shows the obtained set of Pareto front after 128 iteration of the proposed algorithm. The figure shows that EHVIC is able to uniformly maintain solutions in feasible regions for multi-objective functions.

Considering Γ as the estimate of the percentage of the feasible volume to that of the whole search space, it is important to note that smaller values of Γ result in more computations to shape the feasible region based on independent GPs on black-box constraints. Also in this case, the number of expected particles in the feasible cells such s for calculation of $\Delta(s)$ is typically small. As a result, the Pareto set on such test functions might not be accurate compared to other forms of test scenarios (see Fig. 5.2(d) as an example).

Table 5.1 shows the average number of iterations with the corresponding standard deviation required to dominate 90%, 95% and 99% of the target volume (V) for each benchmark function. The BNH test function with the highest value of Γ requires less number of iterations to dominate V and OSY with the lowest value of Γ needs significantly more iterations to dominate 95% of V . However Γ is not the only determining factor. Another important factor is the ability of the GP to accurately model the function.

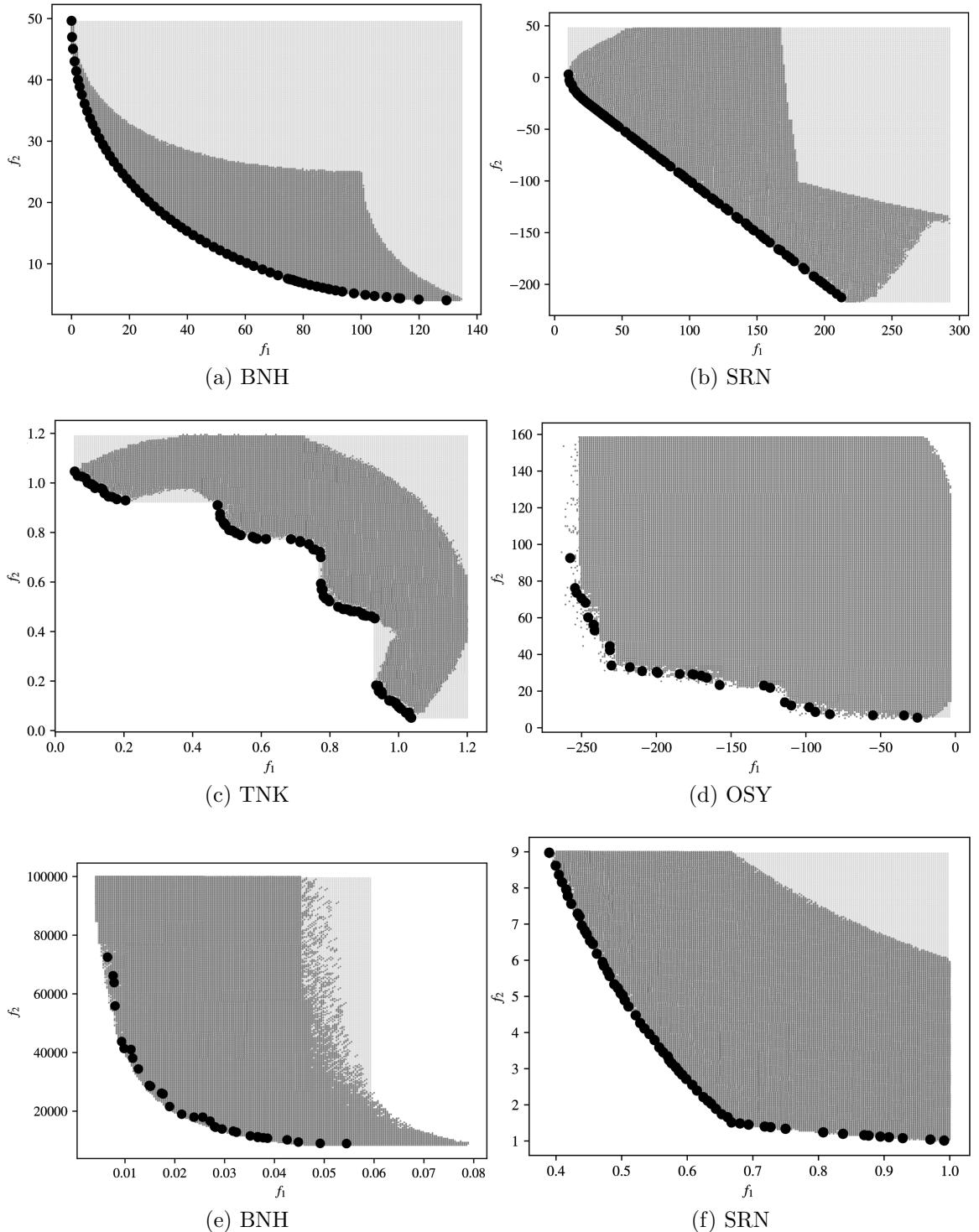


Figure 5.2: Result of EHVIC algorithm on test problems explained in Table 5.1 for 128 evaluations of test functions. Black dots represent non-dominated solutions while the area in gray is the feasible region for each test function.

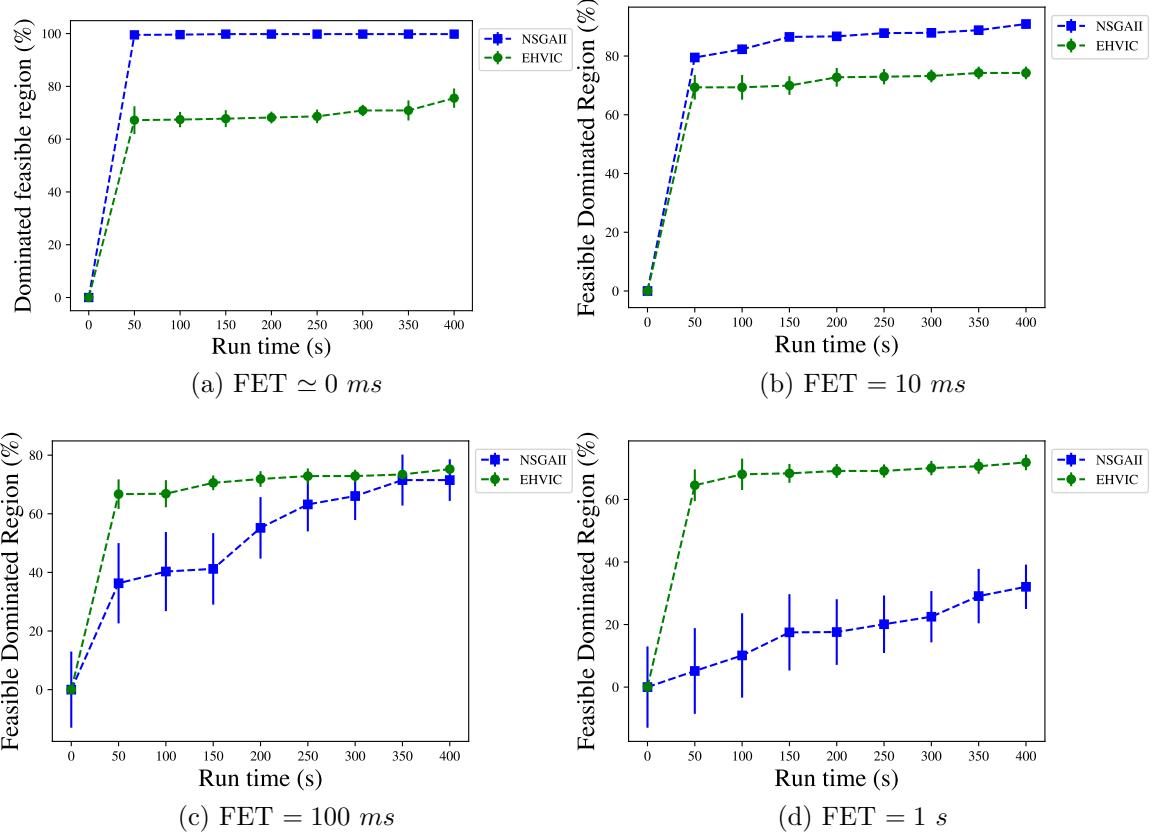


Figure 5.3: Comparing NSGAII method with EHVIC on the TNK function (see Table 5.1). Optimising the TNK function subject to constraints. (a) FET $\simeq 0$ ms, (b) FET = 10 ms, (c) FET = 100 ms, and (d) FET = 1 s. Experiments for each algorithm are repeated 10 times, the mean performance and standard deviation are plotted.

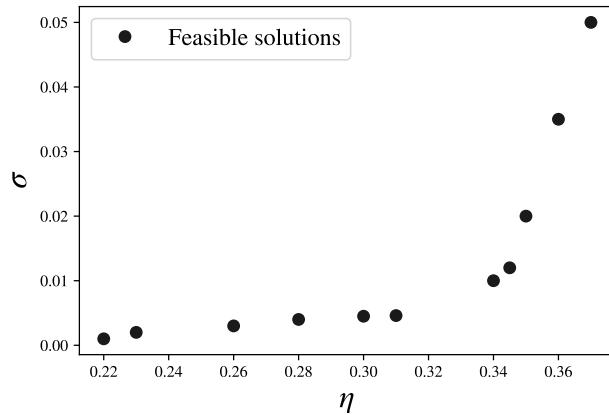


Figure 5.4: Set of solutions obtained by EHVIC for maximizing η and minimizing σ in compositions. Each point represents a feasible solution.

| Function | D | Bounds | Objectives | Constraints | Γ | V | \mathbf{y}^{ref} |
|---------------|---------|---|---|---|----------|-------|--------------------------|
| BNH | 2, 2, 2 | $x_1 \in [0, 5]$ $x_2 \in [0, 3]$ | $\begin{cases} f_1(x_1, x_2) = 4x_1^2 + 4x_2^2 \\ f_2(x_1, x_2) = (x_1 - 5)^2 + (x_2 - 5)^2 \end{cases}$ | $\begin{cases} c_1(x_1, x_2) = (x_1 - 5)^2 + x_2^2 \leq 25 \\ c_2(x_1, x_2) = (x_1 - 8) + (x_2 + 3)^2 \geq 7.7 \end{cases}$ | 93.6% | 1716 | [140, 50] |
| SRN | 2, 2, 2 | $x_1 \in [-20, 20]$ $x_2 \in [-20, 20]$ | $\begin{cases} f_1(x_1, x_2) = (x_1 - 2)^2 + (x_2 - 1)^2 + 2 \\ f_2(x_1, x_2) = 9x_1 - (x_2 - 1)^2 \end{cases}$ | $\begin{cases} c_1(x_1, x_2) = x_1^2 + x_2^2 \leq 225 \\ c_2(x_1, x_2) = x_1 - 3x_2 \leq -10 \end{cases}$ | 16.1% | 23861 | [200, 50] |
| TNK | 2, 2, 2 | $x_1 \in [0, \pi]$ $x_2 \in [0, \pi]$ | $\begin{cases} f_1(x_1, x_2) = x_1 \\ f_2(x_1, x_2) = x_2 \end{cases}$ | $\begin{cases} c_1(x_1, x_2) = -x_1^2 - x_2^2 + 1 + 0.1\cos(16\arctan(\frac{x_1}{x_2})) \leq 0 \\ c_2(x_1, x_2) = (x_1 - 0.5)^2 + (x_2 - 0.5)^2 \leq 0.5 \end{cases}$ | 5.1% | 0.48 | [1.2, 1.2] |
| TWO-BAR-TRUSS | 3, 2, 1 | $x_1 \in [0, 0.001]$ $x_2 \in [0, 0.001]$ $x_3 \in [1, 3]$ | $\begin{cases} f_1(x_1, x_2) = x_1\sqrt{16+x_3^2} + x_2\sqrt{1+x_3^2} \\ f_2(x_1, x_2) = \max(\sigma_1, \sigma_2) \\ \sigma_1 = 20\frac{\sqrt{16+x_3^2}}{x_1 x_3} \\ \sigma_2 = 80\frac{\sqrt{1+x_3^2}}{x_2 x_3} \end{cases}$ | $\begin{cases} c_1(x_1, x_2) = \max(\sigma_1, \sigma_2) \leq 10^5 \end{cases}$ | 86.3% | 4148 | [0.06, 10 ⁵] |
| CONSTR | 2, 2, 2 | $x_1 \in [0.1, 1]$ $x_2 \in [0, 5]$ | $\begin{cases} f_1(x_1, x_2) = x_1 \\ f_2(x_1, x_2) = \frac{(1+x_2)}{x_1} \end{cases}$ | $\begin{cases} c_1(x_1, x_2) = x_2 + 9x_1 \geq 6 \\ c_2(x_1, x_2) = -x_2 + 9x_1 \geq 1 \end{cases}$ | 52.5% | 2.82 | [1, 9] |
| OSY | 6, 2, 6 | $x_1 \in [0, 10]$ $x_2 \in [0, 10]$ $x_3 \in [1, 5]$ $x_4 \in [0, 6]$ $x_5 \in [1, 5]$ $x_6 \in [0, 10]$ | $\begin{cases} f_1(x_1, x_2) = -[25(x_1 - 2)^2 + (x_2 - 2)^2 + (x_3 - 1)^2 + (x_4 - 4)^4 + (x_5 - 1)^2] \\ f_2(x_1, x_2) = x_1^2 + x_2^2 + x_3^2 + x_4^2 + x_5^2 + x_6^2 \end{cases}$ | $\begin{cases} c_1(x_1, x_2) = x_1 + x_2 - 2 \geq 0 \\ c_2(x_1, x_2) = 6 - x_1 - x_2 \geq 0 \\ c_3(x_1, x_2) = 2 - x_2 + x_1 \geq 0 \\ c_4(x_1, x_2) = 2 - x_1 + 3x_2 \geq 0 \\ c_5(x_1, x_2) = 4 - (x_3 - 3)^2 - x_4 \geq 0 \\ c_6(x_1, x_2) = (x_5 - 3)^2 + x_6 - 4 \geq 0 \end{cases}$ | 3.2% | 16079 | [0, 80] |

Table 5.2: Benchmark functions used for constrained multi-objective optimisation problems. Note that D is the dimension of input space, objective-functions, and constraint functions written as $d_{input}, d_{objectives}, d_{constraints}$. Γ is the estimate of the percentage of the feasible volume to that of the whole search space. V is the representative for the volume of the region dominated by Pareto Front. \mathbf{y}^{ref} is defined same as the BMOO method in [28] for volume calculation of the dominated region.

Fig. 5.3 compares the EHVIC with NSGAI^II when there exists a limited time budget for run time. Also we assume different values of Function Evaluation Time (FET) both for objective functions and constraint functions to simulate expensive evaluation cost of the functions. Fig. 5.3(a),(b) show that NSGAI^II outperforms EHVIC in regard to dominated feasible region when the FET $\simeq 0\text{ ms}$ or FET = 10 ms. As the value of FET increases, NSGAI^II fails to evaluate same number of points at a certain time budget and as a result this affects the performance of NSGAI^II and EHVIC outperforms NSGAI^II (see Fig. 5.3(c)). Finally, significant improvement are made by using EHVIC comparing to NSGAI^II when FET = 1 s (see Fig. 5.3(d)). Although higher values of FET significantly affected the performance of NSGAI^II, but EHVIC has almost the same performance since it is able to reduce the number of redundant evaluations of the objective functions, and making it more efficient.

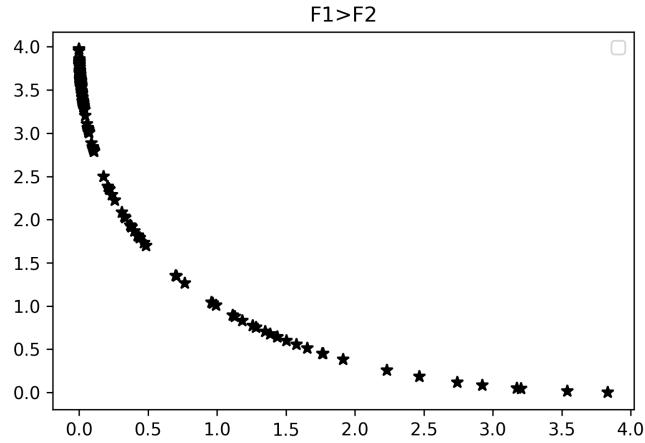
In a practical application we used our method jointly with our metallurgist colleague for alloy optimisation. We seek for the compositions that obtain a set of maximized η hardened Ni alloy with as minimum σ phase as possible at a temperature of 850°C with two hard constraints on the full dissolution of all structural phases at temperature 1100°C and 1200°C. We have a 9-dimensional optimization problem (9 elements as input) and ThermoCalc is used as a thermodynamic phase simulator for this design. Our result in Fig. 5.4 represent that we successfully find a set of Pareto frontiers using EHVIC. The results show the effectiveness of our methods for the real world application of alloy design. The obtained results achieved with 64 experiment evaluations. In future we hope to evaluate these alloys by actually casting them. We have released our implementation as an open-source package available on Github.

5.2 Multi-objective optimisation with objective ranking

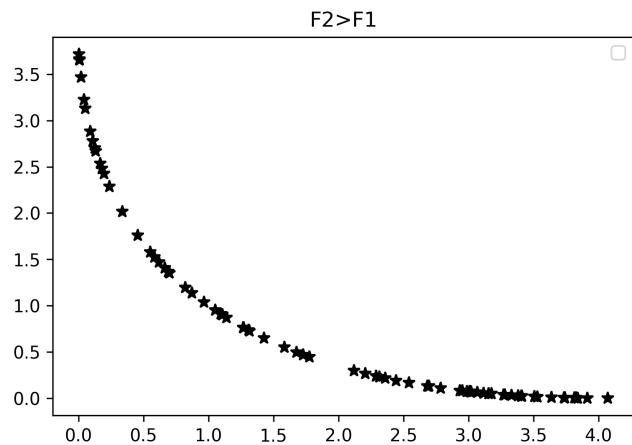
To illustrate the performance of the proposed method, we have used Schaffer function as follows:

$$F = \begin{cases} f_1(x) = x^2 \\ f_2(x) = (x - 2)^2 \end{cases} \quad (5.1)$$

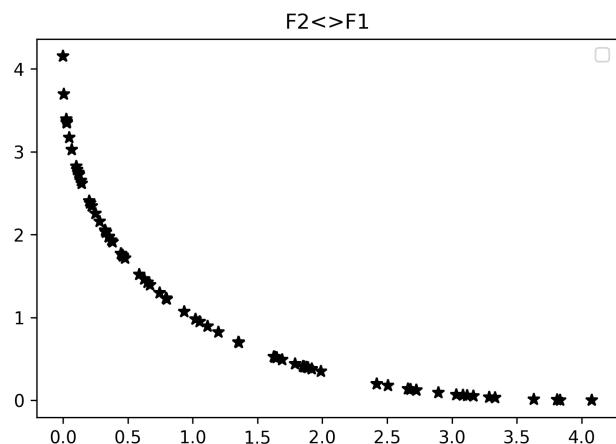
Figure 5.5 illustrates the Pareto optimal set of the minimizing following problem:



(a) $r_1 > r_2$



(b) $r_2 > r_1$



(c) $r_1 \equiv r_2$

Figure 5.5: Evaluating the proposed method with three conditions. (a): Objective f_1 is more important than f_2 . (b): Objective f_2 is more important than objective f_1 . Both objectives are similarly important $r_1 \equiv r_2$. The density of Pareto optimal points in a region indicates the importance of those solution sets with regard to the specific objective.

Chapter 6

Progress Report

During the period of my candidature I conducted a comprehensive research on the following topics:

- PCA (Principal Component Analysis)
- Regression, Ridge and Lasso Regression, and Logistic Regression
- Evolutionary algorithms, Genetic algorithms, Hill climbing with random restart, Nelder-Mead simplicial heuristic, Particle swarm optimization
- Gaussian Processes, Bayesian Optimisation, Acquisition Functions
- Hypervolume Calculation, Expected Hypervolume Improvement
- Shannon Entropy, Information Gain, Stochastic programming
- Multi-objective Optimisation, Pareto Optimality
- Working with GPy, GPyopt, Hypervolume, Spearmint, QT
- Upper Bound Confidence in Multi-objective Context
- Poppy Humanoid Robot
- Electronics (Servo-Electric Grippers)

In the following sections, I will elaborate on the details of the progress.

6.1 EHVIC, first aim

We have tackled the problem of multi-objective optimisation with constraints by proposing a new but simple acquisition function (EHVIC). we extended the expected hypervolume improvement to incorporate with unknown black-box expensive constraints. EHVIC calculates the expected hypervolume improvement and the expectation of constraints satisfaction for all the cells in each iteration and returns the point with the highest value of expected improvement. In contrast to other method proposed for solving this problem, we evaluated our method in regard to the feasible dominated region of the Pareto front. We have also compared the proposed method with NSGAII with different function evaluation time and variety of time budget limitation. Our method proved to outperform the NSGAII when the objective and constraint functions are black-box and expensive to evaluate. As future work on EHVIC, we plan for eliminating the calculation of the cells in each iteration since it is relatively slow in high dimensions. Also we will focus on modeling the correlation among the objective and constraint functions.

6.2 Working with objective rankings, second aim

In this problem, we have formulated a solution to incorporate objective rankings in multi-objective optimisation problems. The proposed solution focuses on utilizing the objective rankings multi-objective scenario. There are many situations in which rankings of individual objects suffice for classification or decision making purposes [60]. To fulfill this task, I conducted a comprehensive literature survey about variety of ranking-based methods. In addition, I have identified the research trend and scientific and technical challenges in this particular problem.

One of the main applications of objective rankings is in Robotics. After successful basic experiments on Poppy Robot, currently we are planning to run many experiments regarding this problem on Poppy. Poppy considers to be a new 3D-printed humanoid robot. Research in humanoid robotics has been thriving in the recent years [53], both due to the predicted importance of humanoid robots for personal and assistive robotics. One of the open

6.3 Publication

During the first year of candidature, we have one accepted paper in ICPR 2018 and one submitted paper to Journal of Electromyography and Kinesiology with collaboration of Nagoya University:

- *Majid Abdolshah , Alistair Shilton, Santu Rana, Sunil Gupta, Svetha Venkatesh, Expected Hypervolume Improvement with Constraints, ICPR 2018, Accepted for oral presentation.*
- *Saeed Abdolshah , Majid Abdolshah, Nader Rajaei, Yasuhiro Akiyama, Yoji Yamada, Shogo Okamoto, Developing an Algorithm to Determine Parameters of Biomechanical Models Based on Bayesian Optimization, submitted to Journal of Electromyography and Kinesiology.*

Chapter 7

Approval and Training

I confirm that I have successfully passed the following trainings:

- Research Induction
- Research Integrity Training

Hi MAJID ABDOLSHAH (mabdolsh),

Congratulations, you have successfully passed the **Research Integrity online training module**.

Please retain this email for your records.

Deakin Research Integrity
research-integrity@deakin.edu.au

Figure 7.1: Certificate of Research Integrity Training.

- Human Research Ethics

Hi MAJID ABDOLSHAH (mabdolsh),

Congratulations, you have successfully passed the Human Research Ethics Training module.

Please retain this email and submit a copy along with your first ethics application to either DUHREC or your Faculty HEAG.

It is your responsibility to ensure that this documentation is supplied of evidence of your successful completion of the training.

You should ensure that you remain familiar with the current ethics guidelines, policies and procedures in order to meet your ethics obligations.

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research-ethics@deakin.edu.au

Figure 7.2: Certificate of Human Research Ethics.

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