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Research paper

Handling simulation failures of a computationally expensive multiobjective optimization problem in pump design

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ABSTRACT

Solving real-world optimization problems in engineering and design involves various practical challenges. They include simultaneously optimizing multiple conflicting objective functions that may involve computationally expensive simulations. Failed simulations introduce another practical challenge, as it is not always possible to set constraints a priori to avoid failed simulations. Failed simulations are typically ignored during optimization, which leads to wasting computation resources. When the optimization problem has multiple objective functions, failed simulations can also be misleading for the decision maker while choosing the most preferred solution. Utilizing data collected from previous simulations and enabling the optimization algorithm to avoid failed simulations can reduce the computational requirements. We consider data-driven multiobjective optimization of the diffusor of an axial pump and propose an approach to reduce the number of solutions that fail in expensive computational fluid dynamics simulations. The proposed approach utilizes Kriging surrogate models to approximate the objective functions and is inexpensive to evaluate. We utilize a probabilistic selection approach with constraints in a multiobjective evolutionary algorithm to find solutions with better objective function values, lower uncertainty, and lower probability of failing. Finally, a domain expert chooses the most preferred solution using one's preferences. Numerical tests show significant improvement in the ratio of feasible solutions to all the available solutions without special treatment of failed simulations. The solutions also have a higher quality (hypervolume) and accuracy than the other tested approaches. The proposed approach provides an efficient way of reducing the number of failed simulations and utilizing offline data in multiobjective design optimization.

1. Introduction

Solving real-world optimization problems poses multiple challenges. In many optimization problems, there is no single objective function to be optimized, but multiple objective functions need to be considered. Typically, the objective functions are conflicting and need to be optimized simultaneously. This means that multiobjective optimization methods must be applied (Coello et al., 2007; Hwang and Masud, 1979; Miettinen, 1999; Steuer, 1986). Another challenge in solving real-world optimization problems is that evaluations of objective function values may be based on computationally expensive simulations, which puts a limit on the number of evaluations performed in the optimization process. In such situations, surrogate models may be used to approximate the underlying objective functions to speed up calculations (Chugh et al., 2017; Tabatabaei et al., 2019; Qing et al., 2023; Daulton et al., 2020).

Besides the general challenges of real-world surrogate-assisted multiobjective optimization, we focus here on how to cope with situations when numerical simulations fail. This can happen when evaluations of objective functions are unsuccessful for some combination of design variables. Simulation failures can occur for different reasons, such as geometry or mesh creation errors when solving underlying partial differential equations. Simulation failures can be difficult to avoid because the infeasible region in the design space is not always known a priori. While the designs leading to unsuccessful function evaluations can be ignored when building the surrogate approximations of the objective functions, using the classification information about feasible and infeasible solutions can improve the quality of surrogates and increase the

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possibility of finding optimal solutions in the feasible region. It can also avoid wasting computing resources in failed simulations.

We demonstrate these challenges on a hydraulic design of a pump stator, where a pump shape is to be found that meets the desired performance goal — typically meeting a specified head for a given flow rate called *design point*, with good efficiency and other characteristics in a specified working range (of flow rates). As the pump performance depends on the character of flow in its interior parts, and the fluid dynamics are complex, a hydraulic design problem cannot be solved directly. Instead, a starting design (based on "engineering methods") is usually created and further improved by evaluating its performance using computational fluid dynamics (CFD) simulations. This is a very complex and computationally expensive optimization problem that human experts typically try to approach as a semi-intuitive, iterative process: *analyze results, change design, perform simulations, analyze results, etc*. However, the design creation and evaluation can be seamlessly connected with an optimizer, fully utilizing the potential of multiobjective optimization.

The design of the pump considered has 22 geometry parameters and three objective functions defined as the efficiency of the pump at three different flow rates (to ensure a good performance and peak efficiency at the whole working range). The three objective functions are conflicting, because it is impossible to construct a pump with a high efficiency at suboptimal, optimal and high flow rates simultaneously. The evaluation of the objective function values is based on numerical CFD simulations that are computationally very expensive. In fact, one simulation run takes between 16 and 20 h. Taking the extreme computation cost into account, we can consider the pump design problem from the perspective of offline data-driven optimization (Jin et al., 2019), where no additional simulations are accessible during the optimization process. In such a case, we need to utilize the already available and evaluated data as efficiently as possible to improve the pump design.

The occurrence of simulation failures complicates the optimization of the pump design problem. This situation happens when a combination of geometric parameters leads to a nonviable geometry shape, and the corresponding geometry or mesh generation fails. Therefore, we need to incorporate information about failed and successful simulations into the solution process to avoid infeasible solutions. Otherwise, the limited computation resources are wasted by generating solutions that cannot be used. In extreme cases, this can lead to only few or even no feasible solutions obtained by the optimization.

Handling infeasible solutions in surrogate-assisted optimization, including Bayesian optimization, has been an active research topic over the last few decades Wauters (2024), Ungredda (2022). One approach for constraint handling is to maximize the probability of feasibility (Schonlau et al., 1998), where, first, a surrogate for each computationally expensive constraint function is built, and the resulting probabilistic models are used by the optimization algorithm (similar to an infill criterion in Bayesian optimization). The first such work on constraint handling was proposed in Schonlau et al. (1998) for single-objective optimization problems, where the authors used the expected improvement (Jones et al., 1998) and the probability of feasibility to find potentially feasible solutions. Later, the approach was applied in many works, including Gardner et al. (2014), Parr et al. (2012), Sasena et al. (2002). A review can be found in Gelbart (2015). All these works combine expected improvement and the probability of feasibility in one function by taking the product of the two. The same idea can also be applied to multiobjective optimization problems. For instance, the works in Daulton et al. (2020), Feliot et al. (2016), Singh et al. (2014) used the expected hypervolume improvement (Emmerich et al., 2006) and the probability of feasibility to find a feasible set of design vectors. The use of such probabilistic models allows the algorithm to search for feasible solutions close to optimal ones. A robust multiobjective Bayesian optimization technique was proposed in Wauters (2024) that has the ability to reduce the number of failed designs.

The primary research gap in the previously proposed approaches for handling constraints is that they were not designed to solve offline data-driven optimization problems. As mentioned in Mazumdar et al. (2022), solving offline data-driven multiobjective optimization has its own challenges due to the uncertainty in the surrogates' prediction and the inability to run any further simulations during the optimization process. Motivated by the works in constraint handling, we propose an approach that uses the probability of the selection criterion (Mazumdar et al., 2022) and the probability of feasibility to handle failed simulations in computationally expensive problems in an offline setting.

In particular, we use Kriging-assisted probabilistic reference vector guided evolutionary algorithm (KP-RVEA) (Mazumdar et al., 2022) as a multiobjective optimization method, and refer to the proposed approach with a modified selection criterion based on constraint handling as CKP-RVEA.

We demonstrate with numerical results that the proposed CKP-RVEA approach produced more feasible solutions compared to generic (Jin et al., 2019) and probabilistic selection (Mazumdar et al., 2022) approaches while solving the pump design optimization problem. After simulations, the solutions had a higher hypervolume and accuracy compared to the other tested approaches. Finally, a domain expert (also called a decision maker) was satisfied with the solutions and successfully found the most preferred design based on visualizations.

To summarize, the contributions of this paper are two-fold. We propose the approach called CKP-RVEA for probabilistic constraint handling in offline data-driven multiobjective optimization and demonstrate that it:

1. can successfully solve a real-world optimal pump design problem with multiple objective functions involving computationally very expensive simulations, which limit the number of function evaluations,
2. profits from the feasibility classification incorporated in the modified probabilistic selection criterion, successfully detects the feasible region and, thus, reduces the number of failed simulations in the solution process.

The rest of the paper is arranged as follows. We describe the pump design problem, key ideas of simulation-based optimization, offline data-driven multiobjective optimization, and probabilistic evolutionary algorithm in Section 2. Section 3 presents the proposed probabilistic selection approach for handling failed simulations. We solve the pump design optimization problem, analyze the results, and illustrate the decision-making process in Section 4. Finally, we conclude our work and discuss future research directions in Section 5.

2. Background

This section is devoted to the description of the pump design problem and the basic concepts needed for the rest of the paper. We also provide a brief summary of the reference vector-guided evolutionary algorithm called RVEA and a probabilistic approach embedded in the selection criterion of RVEA.

2.1. Description of the pump design problem

Hydrodynamic pumps (Gülich, 2020) serve for energy conversion between the mechanical and kinetic energy of a moving fluid. They find applications in several areas, such as the water and petroleum industry. Large pumps for industrial applications, with (tens of) MWs of power, are tailored exactly to customers' needs. A good practice is to create a starting design utilizing engineering methods (i.e., a combination of simplified design formulas and real-world performance data of already existing designs), followed by expert-supervised iteration and/or optimization processes based on numerical simulations. Such a process, called hydraulic design, is very complex and involves a combination

Table 1
Design variables with their lower and upper bounds and descriptions.

Index	lb	ub	Units	Description
1	20	30	degree	Beta angle - hub - leading edge
2	0.22	0.72		Beta angle - hub - relative value at 25%
3	0.22	0.76		Beta angle - hub - relative value at 50%
4	0.25	0.78		Beta angle - hub - relative value at 75%
5	−5	0	degree	Beta angle - hub - value at 95% - difference to trailing edge value
6	85	90	degree	Beta angle - hub - trailing edge
7	355	380	mm	Outlet diameter - hub
8	450	600	mm	Meridional length - hub
9	15	45	mm	Leading edge position - hub - distance from the inlet
10	15	50	mm	Trailing edge position - hub - distance to the outlet
11	−10	10	degree	Sweep angle (defined at the shroud)
12	16	26	degree	Beta angle - shroud - leading edge
13	0.25	0.76		Beta angle - shroud - relative value at 25%
14	0.22	0.7		Beta angle - shroud - relative value at 50%
15	0.25	0.76		Beta angle - shroud - relative value at 75%
16	−5	0	degree	Beta angle - shroud - value at 95% - difference to trailing edge value
17	85	90	degree	Beta angle - shroud - trailing edge
18	450	600	mm	Meridional length - shroud
19	15	60	mm	Leading edge position - shroud - distance from the inlet
20	15	50	mm	Trailing edge position - shroud - distance to the outlet
21	27	35	degree	Outflow angle - hub
22	−15	5	degree	Outflow angle - shroud - relative to the hub angle

of different tools and approaches, computationally demanding simulations, and careful balancing of many conflicting objective functions. The basics of hydraulic design are described in Gülich (2020, Chapter 7.6). A similar approach to creating the parametric model of the pump was used in De Donno et al. (2019), Bellary et al. (2015).

The pump considered here is a diagonal pump with an axial diffuser designed for a specific speed ns = 200 (Gülich, 2020, Chapter 2.3). Due to the computation cost of numerical simulations (tens of hours to days) and a high number of design variables necessary for describing the shape, it is not possible to optimize the complete pump in an acceptable time. This, and the prior knowledge of what to expect from the stator design, is the reason why we restrict the optimization to the pump stator. Due to this, the geometry and the formulations of objective functions to be optimized can be safely simplified, and some (important) aspects of the pump performance (such as cavitation characteristics) can be neglected. The CFD model of the stator is shown in Fig. 1. Its geometry is described by 22 geometry parameters that represent meridional shapes and blade positions, angles, and thickness in a CFD model. They are the design variables of the problem considered. Their descriptions and their lower and upper bounds are listed in Table 1.

The goal of shape optimization is to improve the pump performance and to find a design that is as efficient as possible. Typically, a pump is not operated at a single flow rate. Instead, high efficiency in the whole working range of flow rates is required. However, it is not possible in practice to design a pump with a high efficiency at all considered flow rates. Instead, the problem is considered as a multiobjective optimization problem. Based on the CFD performance results of the starting pump design, we have selected three pump efficiencies at 76%, 100%, and 120% of the pump's optimal flow rate (the so-called design point) to be optimized, and thus, the problem has three objective functions. Three different flow rates for the optimization represent a good balance in computation costs and pump performance in the whole working range.

We use the commercial software ANSYS CFX (Anon, 2013; Trev, 2012) and related tools combined with custom-made scripts and codes to solve the problem. The solution process starts with a parametric geometry model created with ANSYS DesignModeler and BladeModeler tools. Next, the computation meshes are created with TurboGrid and ANSYS Meshing. With Python codes and ANSYS scripts, the simulation models are updated and run on an HPC cluster. The simulations are set as transient, i.e., with rotating impeller blades. This means that the position of the impeller blades with respect to the stator blades is changing during the impeller rotation, and so is the performance.

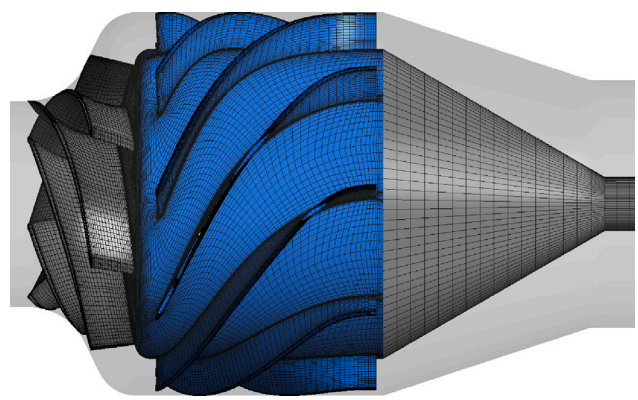

Fig. 1. CFD model of the pump with mesh details. The optimized stator part is in blue.

It is thus necessary to evaluate the objective function values through time series data obtained by CFD simulations. We consider the moving average efficiency values over the last two impeller rotations, as it is a general engineering practice for transient simulations. For most simulations, it means running between 10 to 20 impeller rotations before the averaged objective function values are reasonably stable. The simulation time is between 16 and 20 h on a 16-core HPC cluster node. A more detailed description of the stator problem is given in Krátký (2020).

2.2. Basics of multiobjective optimization

As said, the shape optimization of the pump design is an example of a multiobjective optimization problem with computationally very expensive objective functions. The optimization process can be assisted by surrogate models that are computationally inexpensive to evaluate. This type of optimization is referred to as data-driven optimization (Jin et al., 2019; Wang et al., 2019) as the surrogates are built using simulation data that has been previously acquired. When the time taken to run each simulation is long, running new simulations can be too costly while performing the optimization. The optimization process can be performed using only available data in such cases. This type of data-driven optimization is often regarded as 'offline' optimization (Jin et al., 2019; Wang et al., 2019).

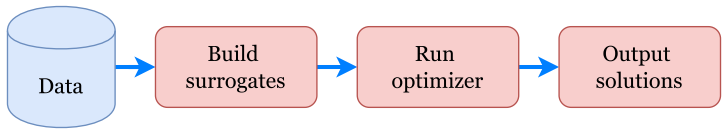

Fig. 2. A generic approach for offline data-driven multiobjective optimization.

A multiobjective optimization problem (MOP) with $K \geq 2$ objective functions in the feasible region in the design space, $\Omega \in \Re^N$ is:

$$\begin{aligned} &\text{minimize} \quad f_1(\mathbf{x}), \dots, f_K(\mathbf{x}) \\ &\text{subject to} \quad \mathbf{x} \in \Omega. \end{aligned} \tag{1}$$

Objective vector $\mathbf{f}(\mathbf{x}) = (f_1(\mathbf{x}), \dots, f_K(\mathbf{x}))$ is to represent every feasible design vector $\mathbf{x}$ that consists of n design variables. A solution $\mathbf{x}^1 \in \Omega$ is considered to dominate another solution $\mathbf{x}^2 \in \Omega$ if $f_i(\mathbf{x}^1) \leq f_i(\mathbf{x}^2)$ for all $i = 1, \dots, K$ and at least one of the inequalities $f_j(\mathbf{x}^1) < f_j(\mathbf{x}^2)$ for $j = 1, \dots, K$ is satisfied. A solution of a MOP is considered nondominated if it is not dominated by any other feasible solution. The solutions of (1) that are nondominated in the entire set Ω are known as Pareto optimal solutions. Although multiobjective evolutionary algorithms (MOEAs) provide a set of mutually nondominated solutions, they may not guarantee Pareto optimality due to their heuristic nature. They are applicable for problems where mathematical properties (like convexity) cannot be verified, and that is why we use them here.

For data-driven optimization, data of feasible design vectors and the corresponding objective vectors must be produced by calling the *underlying*, that is, the original, objective functions. Fig. 2 presents a general method for addressing an offline data-driven multiobjective optimization problem (MOP). The process starts with the given dataset, and computationally inexpensive surrogate models are constructed using this data. Subsequently, a multiobjective optimization algorithm is employed to solve a modified problem with the surrogates as objective functions (when all objective functions are computationally costly).

Certain surrogates such as Kriging (also known as Gaussian process regression) (Rasmussen and Williams, 2006) also provide information about the uncertainty in the prediction, which we can refer to as the accuracy of the surrogate. However, it should be noted that the above-mentioned generic approach does not utilize uncertainty information in the optimization process.

2.3. Probabilistic approach for RVEA

As mentioned in Section 2.1, optimizing the pump design is a data-driven multiobjective optimization problem. Because of the very long simulation times, we mainly focus on optimizing the problem without performing further simulations, that is, in an offline configuration. While solving an offline MOP using the generic approach (described in the previous section), the optimization process does not consider the uncertainty in the prediction of the surrogates. As shown in Mazumdar et al. (2022), using only the mean prediction leads to solutions with a lower accuracy compared to the corresponding underlying (real) objective function values. Applying a probabilistic approach enables incorporating uncertainties related to the quality of the surrogates. It is also promising for incorporating additional "classification" information that can help guide the optimization process and increase its efficiency. Because of the complexity of physical phenomena in the pump operation, creating a complex multi-physical model and obtaining exact numerical predictions for all required objective functions is often very problematic. Instead, simplified simulations are used, and the quality of the design can be estimated by some alternative approaches. Considering this additional information when using standard surrogate models is challenging. However, with a probabilistic approach, it can be added as a part of the selection process.

The probabilistic selection approaches for MOEAs, proposed in Mazumdar et al. (2022), are specifically designed to utilize the uncertainty information from Kriging surrogates in the selection process of the evolutionary algorithm. In the reported study, the probabilistic selection approaches produced solutions with a better hypervolume and accuracy compared to their generic counterparts. These approaches are quite flexible and can be embedded in the selection criterion for different MOEAs. In Mazumdar et al. (2022), the approaches were introduced in a general form without fixing the MOEA.

In this paper, we utilize probabilistic selection with RVEA (KP-RVEA) (Cheng et al., 2016) as the MOEA since it had superior performance in both hypervolume and accuracy in Mazumdar et al. (2022). We extend it to handle infeasible solutions and solve the pump optimization problem later. In what follows, we discuss RVEA and KP-RVEA in brief.

2.3.1. RVEA

RVEA (Cheng et al., 2016) is a so-called decomposition-based MOEA that can handle MOPs with a large number of objective functions. It uses reference vectors to decompose the MOP into several sub-problems determined by a set of N uniformly distributed unit reference vectors $\mathbf{v_j}$, $j = 1, \dots, N$. First, objective vectors are translated to have the best objective function values located in the origin. Next, N uniformly distributed reference vectors are generated, and each individual in a population is assigned to the closest reference vector. The spatial distance is measured by the angle $\theta_{i,j}$ between the (translated) objective vector $\mathbf{f}_i'$ and the reference vector $\mathbf{v_j}$. In this way, the population is partitioned into N subpopulations. RVEA selects one individual from each subpopulation with the minimum angle penalized distance (APD). APD dynamically balances the convergence and diversity of the solutions and is defined as:

$$d_{i,j} = (1 + P(\theta_{i,j}))\|\mathbf{f}_i'\|. \tag{2}$$

Here $P(\theta_{i,j}) = K\left(t/t_{max}\right)^{\alpha} \theta_{i,j}/\gamma_{\mathbf{v}_j}$ is the penalty function dependent on $\theta_{i,j}$, $\gamma_{\mathbf{v}_j}$ is the smallest angle between the reference vector $\mathbf{v}_j$ and the other reference vectors and $\|\cdot\|$ denotes the Euclidean norm of a vector. In addition, the variables t and t_{max} represent the generation counter and the maximum number of generations, respectively. Meanwhile, α regulates the rate of alteration for $P(\theta_{i,j})$. For more details, we refer the reader to Cheng et al. (2016).

2.3.2. Kriging assisted probabilistic RVEA

For computationally expensive MOPs, such as the pump design problem or purely offline data-driven MOPs, it is necessary to use surrogate models in MOEAs to approximate the underlying objective functions. We apply Kriging models as surrogates since they provide information about the uncertainty in the prediction of objective function values. The proposed approach uses a provided dataset to build Kriging surrogates for each computationally expensive objective function. However, the uncertainty in the Kriging model causes the possibility of making a wrong decision in selecting a worse solution over a better one because we cannot identify for certain which solution is superior. To utilize the uncertainty information from Kriging surrogates, a probabilistic selection approach can be embedded an MOEA like RVEA. In this paper, we refer to the probabilistic selection embedded in RVEA with Kriging surrogates as KP-RVEA (Mazumdar et al., 2022). KP-RVEA uses the uncertainty in the prediction provided by Kriging surrogates in the APD selection criterion of RVEA. In particular, KP-RVEA estimates the probability of a wrong selection of a solution with inferior APD and selects the solutions with the lowest probability of making a wrong decision.

Algorithm 1: KP-RVEA

Input: Offline data of size N_D; N = number of reference vectors; $G_{\max}$ = maximum number of generations; S = number of Monte-Carlo samples
Output: Solutions

1 Build Kriging surrogates using the offline data
2 Initialize $G = 0$
3 Create a set of N uniformly distributed unit reference vectors V_0
4 Find the neighborhood for each unit reference vector
5 **while** $G < G_{max}$ **do**
6 Apply crossover and mutation on the current population to generate offspring
7 Use the Kriging surrogates to evaluate the individuals and combine the parents and offspring
8 Update $G = G + 1$
9 Draw S samples using Monte-Carlo from Kriging surrogates' predictive distribution
10 Assign each individual to a subpopulation by probabilistic ranking of angles $\theta_{i,j}$
11 Select an individual from each subpopulation using probabilistic ranks of APD
12 end

Algorithm 1 shows the working of KP-RVEA. First, S samples are drawn from the posterior predictive distribution of objective function values of the Kriging surrogates for all the individuals in the population. Each of these samples is assigned to a subpopulation with its closest reference vector measured by angles between them and the reference vectors (step 10 of Algorithm 1). Next, each individual is assigned to a specific subpopulation if it has the highest number of samples assigned to that reference vector. Then, from each subpopulation, one individual is selected based on the probabilistic ranking of APD (step 11 of Algorithm 1). The probabilistic selection criterion utilizes APD values (2) of the samples for each individual to estimate the probability density function of APD using kernel density estimation (KDE) (Silverman, 1986). In each subpopulation, the individual with the lowest probability rank $R_{i,j}$ is selected for the next generation. The rank is:

$$R_{i,j} = \sum_{n=1}^{|P_j|} Pr_{\text{wrong}}(d_{n,j} > d_{i,j}) - 0.5, \tag{3}$$

where $Pr_{wrong}(d_{n,j} > d_{i,j})$ is the probability of a wrong selection of the ith individual over the nth individual based on their APD values and $|P_j|$ is the size of the corresponding subpopulation. In this way, such an individual is selected that has the smallest probability of having higher values of APD over the other individuals in the subpopulation. The selected individuals form the next generation and are used to generate $|P_{\text{offspring}}|$ offspring with the crossover and mutation operators. The algorithm is terminated when the maximum number of function evaluations is met, i.e., $G \geq G_{\max}$. For more details, see Mazumdar et al. (2022).

3. The proposed CKP-RVEA approach for probabilistic handling of failed simulations

The KP-RVEA approach introduced in Section 2.3.2 is suitable for solving offline data-driven MOPs. However, it cannot handle infeasible or failed simulations while solving problems like the pump design optimization problem. In this section, we describe the proposed probabilistic approach to handle infeasible solutions and illustrate with examples how it works.

3.1. The proposed approach

As mentioned, solving an offline data-driven MOP using probabilistic selection approaches is advantageous since it has proved to produce solutions with a higher hypervolume and accuracy (Mazumdar et al., 2022). However, they cannot handle constraints and hence, in their current form, they are unsuitable for solving the pump design optimization problem. To tackle this problem, we modify and extend the probabilistic selection criterion to incorporate a probabilistic constraint handling strategy.

We refer to the new approach for constraint handling in probabilistic RVEA with Kriging surrogates as CKP-RVEA. The overall flowchart of the proposed CKP-RVEA approach is shown in Fig. 3. The provided initial dataset consists of the design variable and objective function values. In addition, a separate dataset is provided that includes the design variable values for the simulations whose CFD design generation failed. From these two datasets, we create a classification dataset consisting of design variable values (as features) and the status of the CFD simulation (as output). In what follows, we use labels or classes '0' for failed simulations and '1' for successful simulations. Next, we build a Kriging model for classification using the compiled dataset consisting of design variable values and simulation status. The posterior predictive distribution Pr_{failed} of the Kriging classification model provides us with the probability of a simulation failing. The MOEA is initialized with its initial population and uniformly distributed set of reference vectors. The new offspring individuals are generated by crossover and mutation operators and the individuals are ranked by their probability of APD selection. The ranks of the individuals are modified by their probability of constraint violation and individuals with the best ranks are selected from each sub-population. The evolution process is continued until the generation counter G reaches the maximum number of generations ($G_{\max}$). The solutions are later shown to the DM with decision support tools to choose the most preferred solution(s). In what follows, we demonstrate how to utilize the classification probability in the probabilistic selection approach of our MOEA.

In Algorithm 2, we present the proposed CKP-RVEA approach with algorithmic terms. We extend KP-RVEA to handle failed simulations based on the constraint handling approach proposed in Jain and Deb (2014). The concept is to utilize the probability of failed simulations of the Kriging model for classification in the selection criterion of RVEA. The approach is similar to the probability of feasibility as proposed previously in Schonlau et al. (1998). We define a set SI as the index set of the individuals that have the probability of failure, $P_{\text{failed}} > 0.5$. If all the individuals in the jth subpopulation (consisting of $|\overline{P_j}|$ individuals) are in the set SI, we select the individual with the lowest probability of failure, or P_{failed}. If some individuals have $P_{\text{failed}} \leq 0.5$, then we select the individual with the lowest $R^{\text{failed}}_{i,j} = Pr_{\text{failed}}(\mathbf{x_i})\dot{R}'_{i,j}$. This ensures that only individuals with low probabilistic ranks and a low probability of failure are selected from each subpopulation.

3.2. A simple example

As an example, we solve a modified, that is, constrained bi-objective DTLZ2 (Deb et al., 2002) test problem with two design variables in an offline setting to study the behavior of the proposed approach. To emulate the characteristics of failed simulations, we artificially created a bounding box in the design space of the problem. The modified MOP does not provide any solutions (or is infeasible) when evaluated with a design point that is within the bounding box. This can be better understood from Fig. 4(d)–(f), where the infeasible region is defined in the design space by the bounding box. The light blue and pink points denote whether the simulations are feasible or infeasible, respectively. We start with 100 simulations produced by Latin hypercube sampling (LHS). We then build Kriging surrogates for each objective function and utilize three different approaches to solve the MOP: generic RVEA, KP-RVEA, and CKP-RVEA. The generic RVEA approach is identical

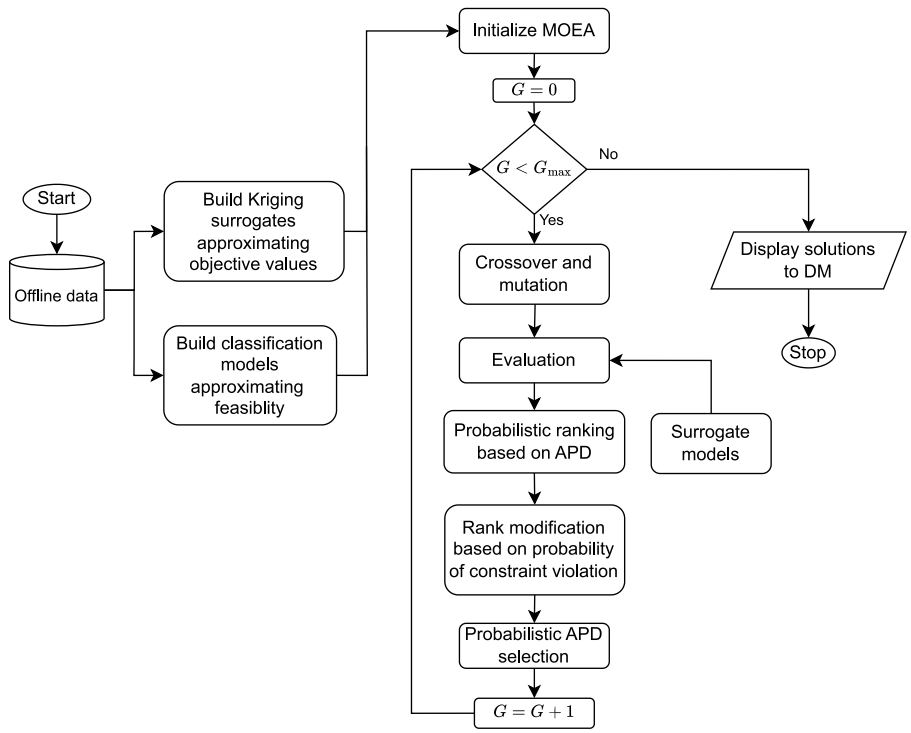

Fig. 3. Flowchart of the proposed CKP-RVEA approach.

Algorithm 2: CKP-RVEA – Handing failed simulations with probabilistic RVEA

for $j = 1$ *to* N **do**
  $SI = \emptyset$
  for $i = 1$ *to* $|\overline{P_j}|$ **do**
    if $Pr_{failed}(\mathbf{x_i}) > 0.5$ **then**
      $SI = S_i \cup \{i\}$
  if $|SI| == |\overline{P_j}|$ **then**
    $k = \text{argmin}_{i \in \{1,\ldots,|\bar{P}_j|\}} \; Pr_{\text{failed}}(\mathbf{x_i})$
  else
    $R^{\text{failed}}_{i,j} = Pr_{\text{failed}}(\mathbf{x_i})\dot{R}'_{i,j}$
    $k = \text{argmin}_{i \in \{1,\ldots,|\bar{P}_j|\}, i \notin SI} \; R^{\text{failed}}_{i,j}$
  $P_{\text{next gen}} = P \cup I_k$
end

to the generic approach described in Section 2.2 and utilizes RVEA as the optimizer. Generic RVEA and KP-RVEA are considered in the demonstration to measure the effectiveness of the CKP-RVEA approach proposed in this paper. Generic RVEA and KP-RVEA do not have any constraint handling mechanisms, and thus, the solutions they produce can lie in infeasible regions.

In Fig. 4, we show the final solutions obtained by the three different approaches. The first three subfigures represent the objective space and the others the design space. The black bounding box in the latter is the infeasible region. The solutions obtained by the three approaches are shown by the dark blue and red points representing the feasible and infeasible ones, respectively. It can be observed that the solutions produced by CPK-RVEA are all blue and, hence, feasible. However, both generic RVEA and PK-RVEA produced solutions that are infeasible or red in color. We can observe similar characteristics in the solutions in the design space. No solutions produced by CKP-RVEA are within the infeasible region (or the bounding box) in the design space.

Generic RVEA and KP-RVEA do not consider the probability of feasibility while selecting an individual. The probability of feasibility predicted by the Kriging classification model in CKP-RVEA provides valuable information in the selection process. Hence, the CKP-RVEA approach produces more feasible solutions and avoids the infeasible regions in the design space. This is beneficial from the perspective of running computationally expensive simulations (as only the feasible solutions matter) without wasting resources on infeasible solutions.

In an offline data-driven problem setting, the DM has to make decisions based on the objective function values approximated by the surrogate models. Making decisions based on the solutions produced by generic RVEA and KP-RVEA could be misleading as some solutions are infeasible and thus cannot be implemented in the real world. The CKP-RVEA approach avoids the infeasible regions of the MOP, and only feasible nondominated solutions are shown to the DM.

4. Case study: Solving the pump design problem

The CKP-RVEA approach was implemented in Python using the DESDEO software framework (Misitano et al., 2021) (https://desdeo.it.jyu.fi).[1] In what follows, we apply the proposed CKP-RVEA approach to solve the pump design optimization problem.

4.1. Optimization settings

The initial dataset for the offline pump design optimization problem consisted of 472 simulation results. Latin hypercube sampling was used to generate the data. This data set was already available and was evaluated prior to optimization with a numerical CFD solver. Out of the simulation data, 390 simulations were successfully generated after evaluation and 82 simulations failed and did not produce any geometry, i.e., they were failed simulation. Two data files were compiled, one consisting of the objective function and design variable values. The other file consisted of the design variable values and a corresponding

[1] Source code available at https://github.com/amrzr/CKP-RVEA

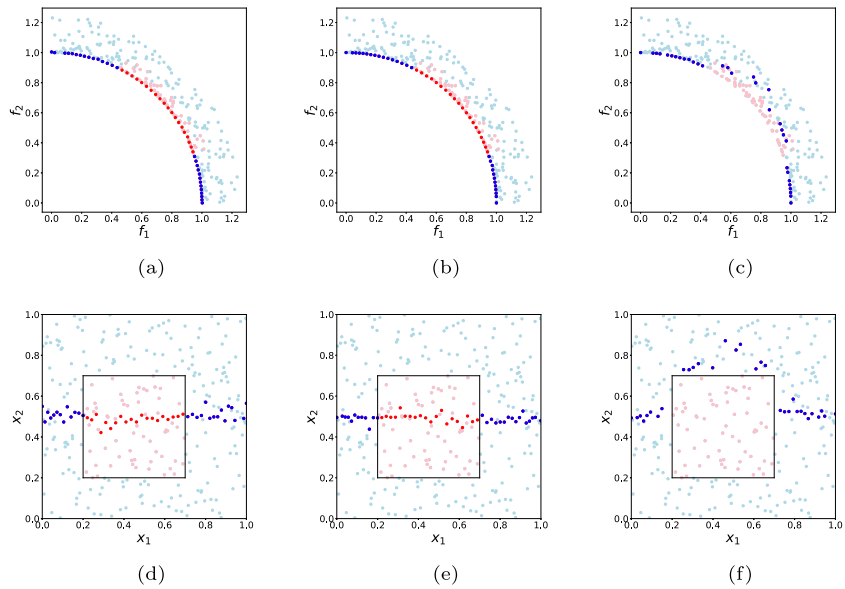

Fig. 4. The solutions of solving the bi-objective constrained DTLZ2 test problem with two design variables with generic RVEA, KP-RVEA, and CKP-RVEA. Figures (a)–(c) show the objective space, and (d)–(e) the design space. The light blue and pink points represent feasible and infeasible samples, respectively, for 100 design points. The dark blue and red points represent the final solutions obtained by the three approaches. The black bounding box denotes the infeasible region in the design space.

value of '0' or '1' to indicate whether it was infeasible or feasible, respectively.

All the objective functions of the problem were to be maximized. However, for the purpose of representation, we transformed them to be minimized simply by multiplying the objective function values by -1. As in the previous section, we tested generic RVEA, KP-RVEA, and CKP-RVEA. The parameters used for RVEA for all three approaches were kept the same (standard parameter settings) as per the recommendation in Cheng et al. (2016). We used a Kriging surrogate model for each objective function with a Matern 5/2 kernel and automatic relevance determination enabled as proposed in Mazumdar et al. (2022). All the approaches were run for a maximum of 5000 generations. For KP-RVEA and CKP-RVEA, we used S = 1000 as the number of Monte-Carlo samples drawn from the predicted distribution of Kriging surrogates. The approaches use these samples for the probabilistic selection process.

4.2. Pump design optimization results

We first solve the pump design problem with the generic RVEA approach that uses neither uncertainty nor classification of feasibility information. The optimization is performed on surrogates based on all the provided data of 390 successful simulations resulting with 57 nondominated solutions. After solving the surrogate problem, the solutions are evaluated with computationally expensive numerical simulations. Note that in practice, while solving an offline data-driven MOP, we may not be able to evaluate the solutions with the underlying objective functions. Here, we evaluate the designs found (using surrogates in optimization) using underlying objective functions to examine the efficiency of different approaches and the quality of the produced solutions. As a result of the optimization with the generic approach, only two nondominated were successfully generated, and the rest were infeasible. Therefore, the generic selection strategy needed to be revised.

We then applied the probabilistic approach KP-RVEA that incorporates uncertainty information to improve the accuracy of the surrogate models. In this case, 40 nondominated solutions were generated. However, only eight solutions could be successfully evaluated by running CFD simulations, and 32 solutions failed.

The simulation failures with most of the solutions generated by the generic and probabilistic approaches showed that a modification in the selection criteria is needed. This shows that a classification model was to be incorporated into the selection process to improve the quality of the solutions. We then applied the proposed approach CKP-RVEA with the new selection strategy and obtained 47 solutions to the surrogate problem. From there, the number of failed simulations was reduced to 11, and 36 simulation designs were successfully generated. These experimental results showed that the proposed probabilistic failure handling approach with modified selection criteria was considerably better in producing feasible solutions and effectively utilized the classification information from the Kriging surrogates.

Table 2
Performance of the different approaches in solving the pump design optimization problem in terms of the ratio of feasible solutions, hypervolume and root mean squared error (RMSE) indicators.

	Feasibility ratio	Hypervolume	RMSE
Generic RVEA	3.60%	6.58e+5	9.54
KP-RVEA	20.50%	6.77e+5	10.03
CKP-RVEA	78.30%	7.13e+5	7.89

A comparison of the three optimization approaches in terms of various indicators is shown in Table 2. We use the ratio of feasible solutions to the total number of solutions to measure the performance in producing feasible solutions. The hypervolume indicator measures the convergence and diversity of the solutions. The hypervolume was computed after evaluating the solutions with the simulator. The negative of the evaluated objective values was used to compute the hypervolume with the reference point of $(0, 0, 0)$. The multivariate root mean squared error (RMSE) indicator shows the accuracy of the solutions found in the surrogate objective space compared to when they were evaluated with underlying objective functions. In this paper, we used the multivariate RMSE formulation described in Mazumdar et al. (2022). It should be noted that both hypervolume and RMSE indicators were computed on feasible solutions.

It can be observed that the proposed CKP-RVEA approach produced solutions with a better feasibility ratio, hypervolume, and accuracy. This is primarily because the other approaches did not have any mechanism to avoid the regions in the design space that have a high probability of producing failed simulations. CKP-RVEA tackled this challenge with the probabilistic constraint handling and selection strategy to produce more feasible solutions. As more feasible solutions

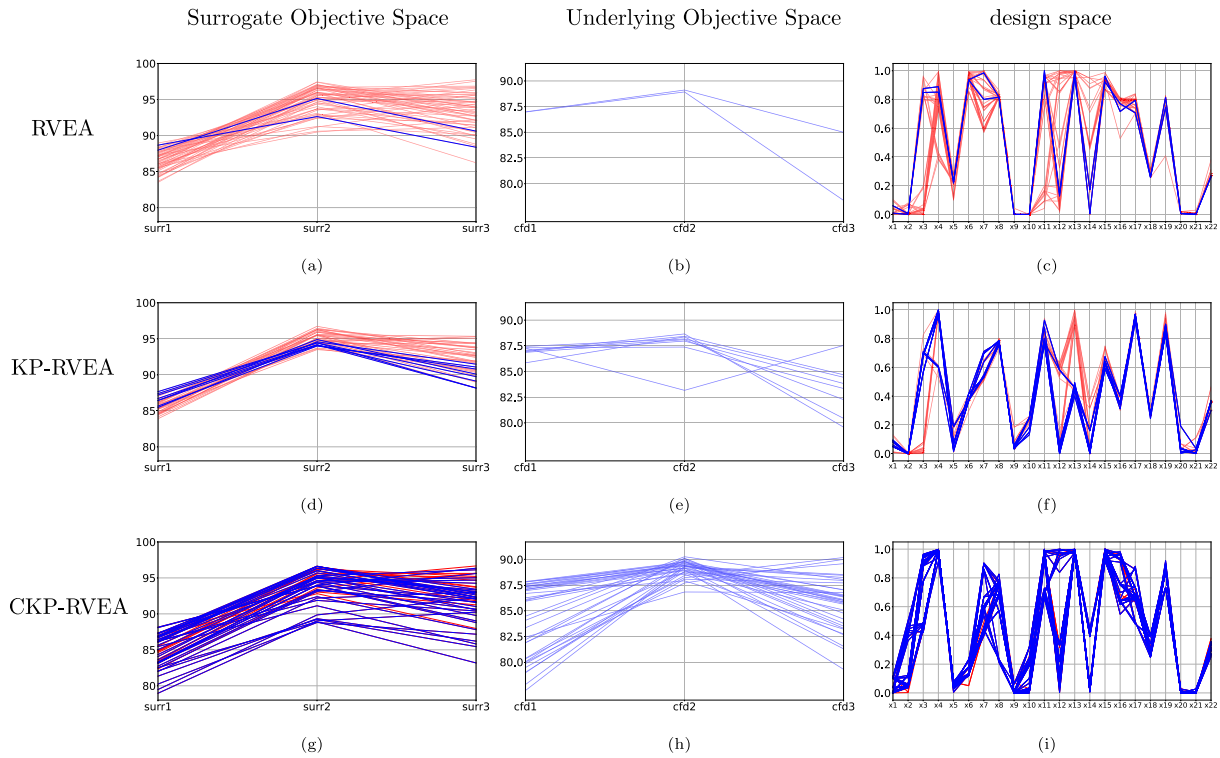

Fig. 5. Solutions obtained by generic RVEA, KP-RVEA, and CKP-RVEA shown in the first, second, and third rows, respectively. The first column shows the solutions in the surrogate objective space. The second column shows the underlying objective function values (after CFD simulations). The last column shows the design variable values of the solutions found by the approaches.

existed, the overall hypervolume was greatly improved over generic RVEA and KP-RVEA.

Fig. 5 shows the solutions found by generic RVEA, KP-RVEA, and CKP-RVEA in the first, second, and third rows, respectively. The first column shows the solutions in the surrogate objective space while the second column shows the objective values of the solutions after the CFD simulations. The last column shows the design variable values of the solutions found by the approaches. The solutions in red represent the ones that failed the CFD simulations and the blue ones are feasible. It can be observed that the number of failed simulations is relatively high with generic RVEA and KP-RVEA compared to CKP-RVEA. The working of the proposed CKP-RVEA approach can also be analyzed by observing the solutions in the design space. It can be observed that these solutions avoid lower values and higher values of design variables x_3 and x_6, respectively, which boosts its feasibility ratio. Overall, avoiding the failed simulations improved the optimization process and saved significant resources. While the failures can be ignored when building the surrogates (as long as there is at least one new set of objective functions to make the update), it means wasting computation resources. In addition, a high failure rate can also make decision-making difficult, as the selected designs are likely to fail.

4.3. Decision making

While solving an offline data-driven MOP, decisions are made by observing the solutions obtained by utilizing the surrogates as objective functions. Hence, the solutions are approximations, and the decisions are made on uncertain objective function values. The proposed CKP-RVEA approach presents a set of solutions to the DM that are approximated by Kriging surrogates and have uncertainty in the prediction (as standard deviation). The DM, a domain expert in pump design optimization, was interested in observing the worst-case objective function values instead of the predicted mean objective function values for making decisions. Hence, we presented him with two types of scatter plot matrices, as shown in Fig. 6. The first type showed the pairwise objective-wise predicted mean objective function values. The second type showed the 95% upper confidence bound of the predicted objective function values. It should also be remembered that all the objective functions here were minimized, and the DM was comfortable making decisions in such a setup. The visualizations were interactive and indicated the objective function values and the upper confidence bounds of the solutions when the DM hovered and clicked on a specific solution of interest. The solutions were color-coded based on the average uncertainty in the solutions (darker is lower uncertainty). Figs. 6 (a)–(c) show the three solutions that were chosen by the DM as the most preferred ones.

The three chosen solutions displayed the best combination of high mean objective function values (of predicted efficiencies) and reasonably low uncertainty of these predictions, represented by the uncertainty intervals. As the intention was to improve the f_1 value, and according to prior knowledge f_3 is mildly correlated with f_2, during the selection, more attention was paid to f_1 and f_2. The selected solutions were then validated using the underlying CFD simulations. Selecting three solutions was seen as a reasonable compromise between the computation cost and increasing the chance of selecting the best possible solution.

In Fig. 7, we show the solutions as seen by the DM in the surrogate objective space in blue. The solutions chosen by the DM are shown in red; the exact solutions after the simulations are shown in green. The arrows show the mapping of these solutions representing their movement in the objective space when they were evaluated. As can be observed, the underlying objective function values were worse than the surrogate objective values. This behavior is expected in an offline data-driven multiobjective optimization problem as the surrogates have approximation errors, and the approximation error cannot be improved with new solutions.

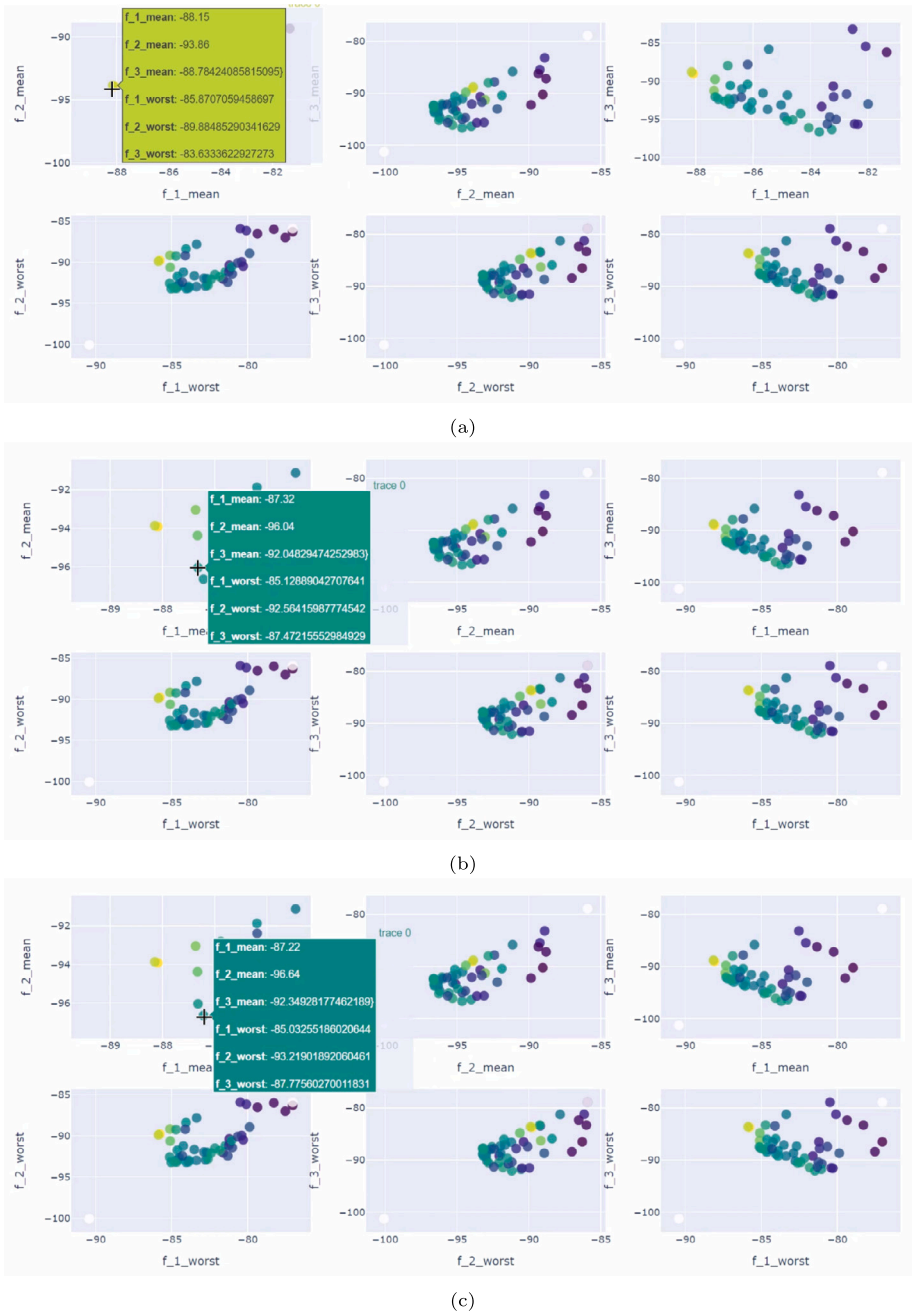

Fig. 6. The three solutions chosen by the DM visualized using scatter plot matrices. The top and bottom rows of each sub-figure show the mean objective function values and the upper confidence bound (95%) of the objective function values, respectively. The solutions are color-graded by their normalized average uncertainties (darker represents lower uncertainty). Note that all the objective functions are minimized in this plot for representation.

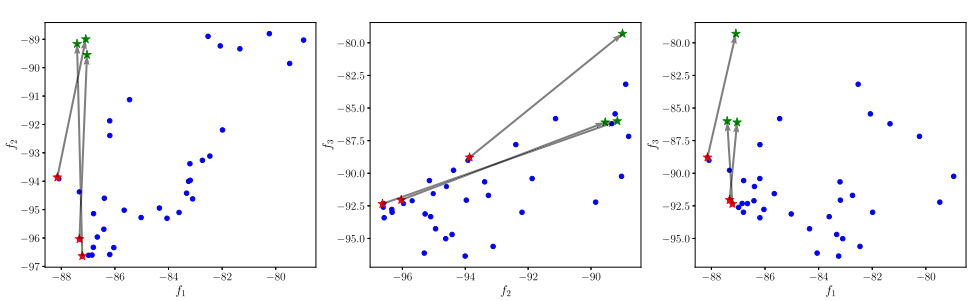

Fig. 7. Scatter plot matrices showing solutions found by CPK-RVEA in the surrogate objective space for the pump design optimization problem (shown in blue). The solutions chosen by the DM are shown in red and the respective solutions after the CFD simulations are shown in green, mapped with arrows. The arrows denote the differences between the surrogate and the simulated objective function values, respectively. Note that all the objective functions are minimized in this plot for representation.

5. Conclusions

One of the practical challenges of real-world optimization problems involving computationally expensive simulations is failed simulations (e.g., in problems involving computational fluid dynamics simulations). In other words, a feasible design vector may not always have corresponding objective function values. A complicating fact is that knowledge about the failed (or an infeasible) region is unavailable a priori. This paper simultaneously addressed the challenges of utilizing existing data and handling failed simulations in solving computationally expensive multiobjective optimization problems. We proposed a new approach called CKP-RVEA utilizing a probabilistic selection criterion and Kriging surrogate models in an evolutionary multiobjective optimization method. We built a probabilistic classification model on the existing data set to handle the failed simulations and adapted the selection criterion. The proposed approach with the modified selection criterion was applied to solve a computationally very expensive pump design problem. The results and a comparison with approaches that do not use any classification models to deal with failures showed the potential of the proposed approach. This approach also proved to be beneficial to the DM as a domain expert by providing decision-support and clearly more feasible solutions than the counterparts.

The proposed approach is designed to solve multiobjective optimization problems in an offline setting. This is challenging to the DM as the actual simulated objective function values can vary from what they observed during the decision-making phase, where surrogate models are applied. The proposed approach aims to reduce the number of failed simulations. However, it is not guaranteed to produce solutions that do not fail.

The proposed probabilistic feasibility handling is not just limited to offline data-driven optimization problems. Testing the approach for solving online problems will be a future work. We also plan to perform a detailed sensitivity analysis on various benchmarks in the future. Another future research direction is to modify the proposed approach such that a DM can interactively guide the solution process with preference information. The computation resources requirements can be further reduced by using an interactive multiobjective optimization method, where only solutions that are of interest to the DM are generated. Another interesting research direction is an automatic selection of surrogate models based on their approximation accuracy.

CRediT authorship contribution statement

Atanu Mazumdar: Conceptualization, Formal analysis, Investigation, Methodology, Validation, Visualization, Writing – original draft, Writing – review & editing. **Jana Burkotová:** Conceptualization, Data curation, Formal analysis, Resources, Validation, Visualization, Writing – original draft, Writing – review & editing. **Tomáš Krátký:** Conceptualization, Data curation, Formal analysis, Resources, Validation, Writing – original draft, Writing – review & editing. **Tinkle Chugh:** Conceptualization, Methodology, Resources, Supervision, Writing – original draft, Writing – review & editing. **Kaisa Miettinen:** Methodology, Project administration, Resources, Supervision, Writing – review & editing.

Declaration of competing interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

Data availability

https://github.com/amrzr/CKP-RVEA.

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References

Anon, 2013. ANSYS ICEM CFD Tutorial Manual. ANSYS Inc.
Bellary, S.A.I., Samad, A., Couckuyt, I., Dhaene, T., 2015. A comparative study of kriging variants for the optimization of a turbomachinery system. Eng. Comput. 32.
Cheng, R., Jin, Y., Olhofer, M., Sendhoff, B., 2016. A reference vector guided evolutionary algorithm for many-objective optimization. IEEE Trans. Evol. Comput. 20, 773–791.
Chugh, T., Sindhya, K., Hakanen, J., Miettinen, K., 2017. A survey on handling computationally expensive multiobjective optimization problems with evolutionary algorithms. Soft Comput. 23, 3137–3166.
Coello, C., Lamont, G., Veldhuizen, D., 2007. Evolutionary Algorithms for Solving Multi-Objective Problems, second ed. Springer, New York.
Daulton, S., Balandat, M., Bakshy, E., 2020. Differentiable expected hypervolume improvement for parallel multi-objective Bayesian optimization. In: Larochelle, H., Ranzato, M., Hadsell, R., Balcan, M.F., Lin, H. (Eds.), Advances in Neural Information Processing Systems. Curran Associates, Inc., pp. 9851–9864.
De Donno, R., Ghidoni, A., Noventa, G., Rebay, S., 2019. Shape optimization of the ERCOFTAC centrifugal pump impeller using open-source software. Optim. Eng. 20.
Deb, K., Thiele, L., Laumanns, M., Zitzler, E., 2002. Scalable multi-objective optimization test problems. In: Congress on Evolutionary Computation. CEC 2002, IEEE Press, pp. 825–830.
Emmerich, M., Giannakoglou, K., Naujoks, B., 2006. Single- and multiobjective evolutionary optimization assisted by Gaussian random field metamodels. IEEE Trans. Evol. Comput. 10, 421–439.
Feliot, P., Bect, J., Vazquez, E., 2016. A Bayesian approach to constrained single- and multi-objective optimization. J. Global Optim. 67, 97–133.
Gardner, J.R., Kusner, M.J., Xu, Z.E., Weinberger, K.Q., Cunningham, J.P., 2014. Bayesian optimization with inequality constraints. In: International Conference on Machine Learning, vol. 32, JMLR.
Gelbart, M.A., 2015. Constrained Bayesian Optimization and Applications (Ph.D. thesis). Harvard.
Gülich, J.F., 2020. Centrifugal Pumps, fourth ed. Springer Cham.
Hwang, C.-L., Masud, A.S.M., 1979. Multiple Objective Decision Making — Methods and Applications. Springer, Berlin Heidelberg.
Jain, H., Deb, K., 2014. An evolutionary many-objective optimization algorithm using reference-point based nondominated sorting approach, part II: Handling constraints and extending to an adaptive approach. IEEE Trans. Evol. Comput. 18, 602–622.
Jin, Y., Wang, H., Chugh, T., Guo, D., Miettinen, K., 2019. Data-driven evolutionary optimization: An overview and case studies. IEEE Trans. Evol. Comput. 23, 442–458.
Jones, D., Schonlau, M., Welch, W., 1998. Efficient global optimization of expensive black-box functions. J. Global Optim. 13, 455–492.
Krátký, T., 2020. Shape Optimization of Hydraulic Surfaces of the Impeller and Stator Parts of Hydrodynamic Pumps (Ph.D. thesis). Palacký University Olomouc, Faculty of Science.
Mazumdar, A., Chugh, T., Hakanen, J., Miettinen, K., 2022. Probabilistic selection approaches in decomposition-based evolutionary algorithms for offline data-driven multiobjective optimization. IEEE Trans. Evol. Comput. 26, 1182–1191.
Miettinen, K., 1999. Nonlinear Multiobjective Optimization. Kluwer Academic Publishers.
Misitano, G., Saini, B.S., Afsar, B., Shavazipur, B., Miettinen, K., 2021. DESDEO: The modular and open source framework for interactive multiobjective optimization. IEEE Access 9, 148277–148295.
Parr, J.M., Keane, A.J., Forrester, A.I., Holden, C.M., 2012. Infill sampling criteria for surrogate-based optimization with constraint handling. Eng. Optim. 44, 1147–1166.
Qing, J., Moss, H.B., Dhaene, T., Couckuyt, I., 2023. $\{PF\}^2$ES: Parallel feasible Pareto frontier entropy search for multi-objective Bayesian optimization. In: Ruiz, F., Dy, J., van de Meent, J.-W. (Eds.), Proceedings of the 26th International Conference on Artificial Intelligence and Statistics. Proceedings of Machine Learning Research, pp. 2565–2588.

Rasmussen, C.E., Williams, C.K.I., 2006. Gaussian Processes for Machine Learning. MIT Press.

Sasena, M.J., Papalambros, P., Goovaerts, P., 2002. Exploration of metamodeling sampling criteria for constrained global optimization. Eng. Optim. 34, 263–278.

Schonlau, M., Welch, W.J., Jones, D.R., 1998. Global versus local search in constrained optimization of computer models. Lecture Notes-Monogr. Ser. 34, 11–25.

Silverman, B., 1986. Density Estimation for Statistics and Data Analysis. Chapman & Hall/CRC, London, p. 176.

Singh, P., Couckuyt, I., Ferranti, F., Dhaene, T., 2014. A constrained multi-objective surrogate-based optimization algorithm. In: 2014 IEEE Congress on Evolutionary Computation. CEC, IEEE.

Steuer, R., 1986. Multiple Criteria Optimization: Theory, Computation, and Application. Wiley.

Tabatabaei, M., Hartikainen, M., Sindhya, K., Hakanen, J., Miettinen, K., 2019. An interactive surrogate-based method for computationally expensive multiobjective optimisation. J. Oper. Res. Soc. 70, 898–914.

Trev, N., 2012. CFX: Computational Fluid Dynamics, Ansys, HVAC. International Book Market Service Limited.

Ungredda, J., 2022. Efficient Information Collection for Bayesian Optimisation with Constraints, User Preferences and Input Uncertainty (Ph.D. thesis). University of Warwick.

Wang, H., Jin, Y., Sun, C., Doherty, J., 2019. Offline data-driven evolutionary optimization using selective surrogate ensembles. IEEE Trans. Evol. Comput. 23, 203–216.

Wauters, J., 2024. ERGO-II: An improved Bayesian optimization technique for robust design with multiple objectives, failed evaluations and stochastic parameters. J. Mech. Des. 146, 101704.