Optimization Techniques for Chlorine Dosage Scheduling in Water Distribution Networks: A Comparative Analysis

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ABSTRACT

A sufficient dose of disinfectant needs to be applied to maintain a minimum residual throughout drinking water distribution systems (WDSs). Yet, excessive dosing of chlorine-based disinfectants leads to the formation of hazardous disinfection byproducts. Several frameworks have been proposed in previous literature to optimize chlorine dosing schedules by minimizing the total dose while maintaining evenly distributed residuals throughout the WDS. Many of these studies relied on evolutionary algorithms (EAs), such as the genetic algorithm (GA) and particle swarm optimization (PSO). EAs are known to require numerous evaluations of computationally expensive water quality (WQ) models and typically feature many parameters that require careful tuning. Recently, Bayesian optimization (BO) has been proposed as an alternative to EAs for the optimization of water quality in WDSs. To speed up convergence, BO builds a probabilistic surrogate model (e.g., Gaussian process) in place of the original black-box model and then leverages the predictions to explicitly control the exploration/exploitation trade-off. Yet, it is still unclear how BO's performance compares against EA's for the optimization of WDSs. This study aims to fill this knowledge gap by conducting a systematic comparison between the performance of BO, GA, and PSO for the optimization of chlorine dosage schedules. To that end, a comprehensive sensitivity analysis is conducted on each optimization approach to understand how different optimization parameters influence their performance. The results revealed that BO requires significantly fewer evaluations than GA and PSO to converge to high-quality solutions. On the other hand, GA displayed lower sensitivity to the change in the optimization parameters compared to BO and PSO.

INTRODUCTION

Reliable supply of safe drinking water is faced with a multitude of challenges, one of which is the deterioration of water quality (WQ) in drinking water distribution systems (WDSs). The latter takes place as a result of a number of physical, chemical, and microbiological processes that occur in the pipes transporting water from treatment to consumption locations. To suppress the growth of microbiological species in the WDS and prevent microbial recontamination of the treated drinking water, chlorine disinfectant residuals need to be maintained at all points throughout the distribution network. This requires careful adjustment of disinfectant injection

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into the WDS to ensure that the applied chlorine dose can sufficiently overcome the decay of chlorine by side reactions within the bulk flow and at the pipe walls.

Optimizing the dosage scheduling (i.e., the injection rates) of chlorine sources in WDSs has been attempted by numerous studies, in which a wide range of optimization methods, including both linear and nonlinear optimization techniques, were implemented. Among these techniques, evolutionary optimization algorithms, such as the Genetic Algorithm (GA) and Particle Swarm Optimization (PSO), were widely implemented. For instance, Munavalli and Kumar (2003) used GA to determine the chlorine dosage at the sources subject to minimum and maximum constraints on chlorine concentrations at all monitoring nodes. Ostfeld and Salomons (2006) used GA to optimize the scheduling of pumping units in conjunction with the design and operation of booster chlorination stations by minimizing the costs of pumping and the chlorine booster design and operation. Ayvaz and Kentel (2014) developed a hybrid GA–linear programming optimization approach to determine the best booster station network for a WDS by minimizing total chlorine injection dosage and the number of booster stations while maintaining residual chlorine concentrations within desired limits. Ohar and Ostfeld (2014) developed a GA-based framework to set the required chlorination dose of the boosters for delivering water at acceptable residual chlorine and disinfection byproduct concentrations for minimizing the overall cost of booster placement, construction, and operation. Kang and Lansey (2010) implemented GA to find optimal valve operation and booster disinfection scheduling to minimize chlorine injection mass at sources or to minimize excessive chlorine concentrations at withdrawal points while maintaining minimum chlorine concentrations and pressures throughout the system. Wang et al. (2010) proposed a hybrid PSO-GA framework for optimizing the locations of booster chlorination stations. Goyal and Patel (2018) implemented PSO to optimize the location of booster stations while minimizing the total mass rate of chlorine injection.

Despite their popularity, evolutionary optimization techniques are known to be computationally expensive since they typically involve conducting numerous evaluations of the objective function(s). The latter usually includes running a black-box model, such as EPANET, in which the partial differential equation(s) governing the transport and decay of chlorine, and potentially other species, in the distribution system are numerically solved. The high computational cost involved in evaluating such black-box numerical models limits the applicability of evolutionary optimization algorithms to real-time WQ regulation applications.

Bayesian Optimization (BO) has been recently gaining significant popularity due to its high efficiency in optimizing computationally expensive black-box functions (Gelbart et al., 2014; Wu et al., 2017). Instead of directly optimizing the black-box objective function, BO builds a probabilistic model of the objective function (known as the surrogate model) that is sequentially updated by sampling the underlying numerical model. The sequential sampling process aims to balance exploration and exploitation, which is done by using an explicit acquisition function that guides the search towards the most promising solutions with potentially high values of the objective function and/or high uncertainty.

In a recent study, we proposed a novel framework for implementing BO for the optimization of booster chlorination scheduling in WDSs (Moeini et al., 2022). The framework showed robust performance and fast convergence, yet the results revealed substantial variability in the performance of different BO methods. More importantly, it remains unclear how the performance of BO compares to the more popular evolutionary algorithms. The objectives of this study are (1) to conduct a systematic comparison between the performance of BO against popular EAs, namely GA and PSO, for the optimization of chlorine dosage scheduling in WDSs,

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and (2) to perform a comprehensive sensitivity analysis on each of the three optimization approaches to understand how different optimization parameters influence their performance and to select the best parameters for each optimization technique.

METHODOLOGY

In this study, we developed a simulation-optimization framework that integrates water quality simulation using EPANET, with either one of the three optimization techniques (BO, GA, and PSO) to optimize the scheduling of chlorine dosing stations in WDSs.

Optimization Model Formulation

The objective of the optimization process is to minimize the total cost of chlorine injection while simultaneously ensuring that the chlorine concentrations remain within an acceptable range at all consumption nodes in the WDS. The objective function is computed as the total cost of chlorine injection, which includes the operational cost of booster chlorine injection (BCI) as well as the capital cost of the booster system design (BCD) (Abokifa et al., 2019; Ostfeld and Salomons, 2006):

$$BCI = \lambda \sum_{b=1}^{n_b} \sum_{i=1}^{n_i} C_{b,i} \times \Delta t_i \tag{1}$$

$$BCD = DRV(AI, BLD) \left[\sum_{b=1}^{n_b} \alpha (C_b^{max})^{\beta} + \gamma V_b \right] \tag{2}$$

Where $C_{b,i}$ is the chlorine mass injection rate of booster "b" during injection event "i" ($kgCl/min$); n_b is the number of chlorine boosters in the WDS; n_i is the number of injection events in one day ($events/day$); Δt_i is the length of the injection event "i" in minutes ($min/event$); λ is the chlorine injection cost per unit mass of chlorine ($\$/kgCl$); DRV is the daily return value coefficient (day^{-1}), which is a function of the annual interest rate AI (%) and booster design lifetime BLD (years); C_b^{max} is the maximum injection rate booster station b can produce ($mgCl/min$); V_b is the total injected mass of chlorine by booster station b ($mgCl$); and α, β, and γ are empirical booster chlorination capital cost coefficients.

To maintain chlorine concentrations between a minimum (c^{min}) and maximum (c^{max}) concentration at all network junctions at all times, a penalty function (PEN) is constructed to account for violations of the upper and lower concentration bounds:

$$PEN = \delta \times \sum_{j=1}^{n_j} \left(\sum_{t=1}^{n_t} \max\left(c_{t,j} - c^{max}, 0\right) + \sum_{t=1}^{n_t} \max(c^{min} - c_{t,j}, 0) \right) \tag{3}$$

where, δ is a constraint violation penalty coefficient; and $c_{j,t}$ is the residual concentration at junction "j" during time-step "t" (mg/L). The objective function to be minimized is the summation of the cost and penalty terms:

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$$OBJ = BCI + BCD + PEN \quad (4)$$

Water Quality Simulation

In this study, chlorine transport and decay in the WDS were simulated using EPANET's water quality module, which features the dynamic 1-D advection-reaction equation with first-order decay kinetics through the bulk flow and at the pipe wall (Rossman et al., 1994):

$$\frac{\partial c}{\partial t} = -u\frac{\partial c}{\partial x} - \left(k_b + \frac{k_w k_f}{r_h(k_w + k_f)}\right)c \quad (5)$$

where c is the chlorine concentration (mg/L); t is the time (s); u is the flow velocity (m/s); x is the distance along the pipe (m); k_b is the bulk decay rate constant (s^{-1}); k_f is the mass-transfer coefficient (m/s); r_h is the hydraulic radius (m); c_w is the pipe wall chlorine concentration (mg/L). EPANET simulation results were implemented by means of the Water Network Tool for Resilience (WNTR) Python package (Klise et al., 2017).

Sensitivity Analysis of Optimization Parameters

The developed simulation-optimization framework is implemented to conduct a systematic sensitivity analysis of the parameters of each of the three optimization methods to understand the influence of the different optimization parameters on the performance of each of the optimization techniques and to select the best parameters for each optimization technique.

Bayesian Optimization (BO)

BO builds a probabilistic model to act as a surrogate for the objective function in the optimization process. The surrogate model is constructed and sequentially updated by sampling the underlying numerical model with each iteration. At each iteration, the surrogate model provides predictions on the mean and variance of the objective function, which are then propagated into an acquisition function that guides the search toward the most promising solutions. The acquisition function is optimized to balance exploration (i.e., sampling areas with the highest uncertainty) and exploitation (i.e., sampling areas with the fittest solutions). In this study, we tested the sensitivity of BO to the choice of the acquisition function as well as the choice of the covariance kernel of the Gaussian Process (GP) surrogate model. Three different acquisition functions were tested, namely expected improvement (EI), probability of improvement (PI), and upper confidence bound (UCB). Each acquisition function provides a different formulation for the trade-off between exploration and exploitation. Furthermore, four different GP covariance kernels were tested, namely Matérn (MA), squared-exponential (SE), gamma-exponential (GE), and rational quadratic (RQ). The covariance kernel function controls the statistical relationship between any two points in the solution space.

Genetic Algorithm (GA)

GA is a metaheuristic, population-based evolutionary optimization method inspired by the Darwinian evolutionary theory. In this study, we tested the sensitivity of GA to three of the most important parameters that control its performance, namely population size, mutation probability,

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and crossover probability. Typically, the larger and more diverse the population, the better the range of potential candidate solutions the GA can explore. Yet, a larger population generally leads to slower iterations. Thus, the population size needs to be carefully selected to produce the best performance at the lowest computational cost. Mutation is the process in which GA applies random changes to the individual solutions in the current generation to add to the diversity of the following population. Crossover is the process through which GA extracts the best genes from different individuals and recombines them into potentially superior children. The rates of cross-over and mutation need to be adjusted to maximize the likelihood that the algorithm will generate individuals with better fitness values for every new generation.

Particle Swarm Optimization (PSO)

PSO is a population-based stochastic algorithm that simulates the optimization process by mimicking the navigation of entities (swarm theory), such as a flock of birds or fishes (Kennedy and Eberhart, 1995). PSO utilizes the velocity vector to update the particles' location based on the social behavior of each individual in the swarm and knowledge obtained by considering the swarm as a whole. In this study, we tested the sensitivity of the PSO results to three of the most important parameters, namely the cognitive parameter, social parameter, and inertia parameter. The inertia parameter regulates the balance between exploration and exploitation. The cognitive parameter controls the confidence of each particle in learning from its own experience (i.e., distance from the best position obtained in previous steps). The social parameter represents how much confidence each particle has in learning from the social interaction with the rest of the swarm (i.e., the best position obtained with respect to other particles).

Case Study WDS

The Net 2 benchmark WDS was adopted to conduct the analyses in this study (Fig. 1). The network comprises of 46 links, 41 nodes, one pumping station, and one reservoir (i.e., source). Chlorine is assumed to follow first-order decay kinetics at both the pipe wall ($k_w = -0.55\, m/day^{-1}$) and in the bulk flow ($k_b = -0.3\, day^{-1}$) (Rossman et al., 1994). A 7-day simulation is implemented in this study, and the last 24 hours of chlorine residual concentrations are used to compare the performance of the optimization methods, consistent with previous studies (Abokifa et al., 2019; Ostfeld and Salomons, 2006). The chlorine concentration is limited to minimum and maximum bounds of $0.2\ mg/L$ and $4\ mg/L$, respectively (Abokifa et al., 2019; US EPA, 1998).

RESULTS AND DISCUSSION

The developed framework was used to first conduct an independent sensitivity analysis for each of the three optimization techniques to better understand the influence of the key parameters on the performance of each technique and to find the parameter settings that would produce the best performance. Then, the three optimized techniques were compared to understand how their performance compares in optimizing the scheduling of chlorine dosage in WDSs.

Bayesian Optimization

BO comprises of two main components, namely the surrogate function and the acquisition function. Twelve different combinations of these two functions were tested and the optimization

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results are depicted in Fig. 2. The results revealed that the performance of BO appears to be more sensitive to the choice of the acquisition function than that of the covariance kernel. This can be seen by comparing the variability in the final objective function values produced by the different BO methods in Fig. 2-b, d, and f. For instance, Fig. 2-d shows that the final value of the objective function is the same for all four covariance kernels when used in conjunction with the PI acquisition function. On the other hand, the performance of the MA kernel varies significantly when combined with each of the three different acquisition functions (EI, PI, and UCB). These results indicate that the influence of the acquisition function on the performance of BO is more profound than that of the choice of the surrogate model covariance kernel.

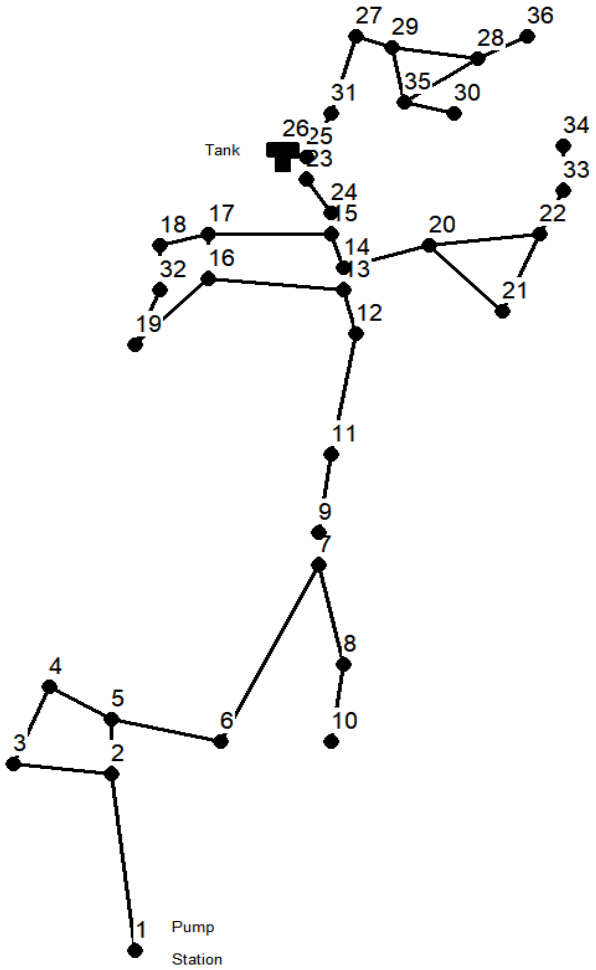

Fig 1. Net 2 benchmark WDS

Generally, the UCB acquisition function showed the best performance among all three acquisition functions tested in this study, followed by EI. This can be seen from the convergence profiles of the different BO methods as shown in Fig. 2-a, c, and d. As can be seen in the figures, UCB achieved faster convergence when combined with all four covariance kernels compared to the other acquisition functions tested in this study. Overall, the combination of the UCB acquisition function with both the RQ and SE covariance kernels produced the best performance for BO.

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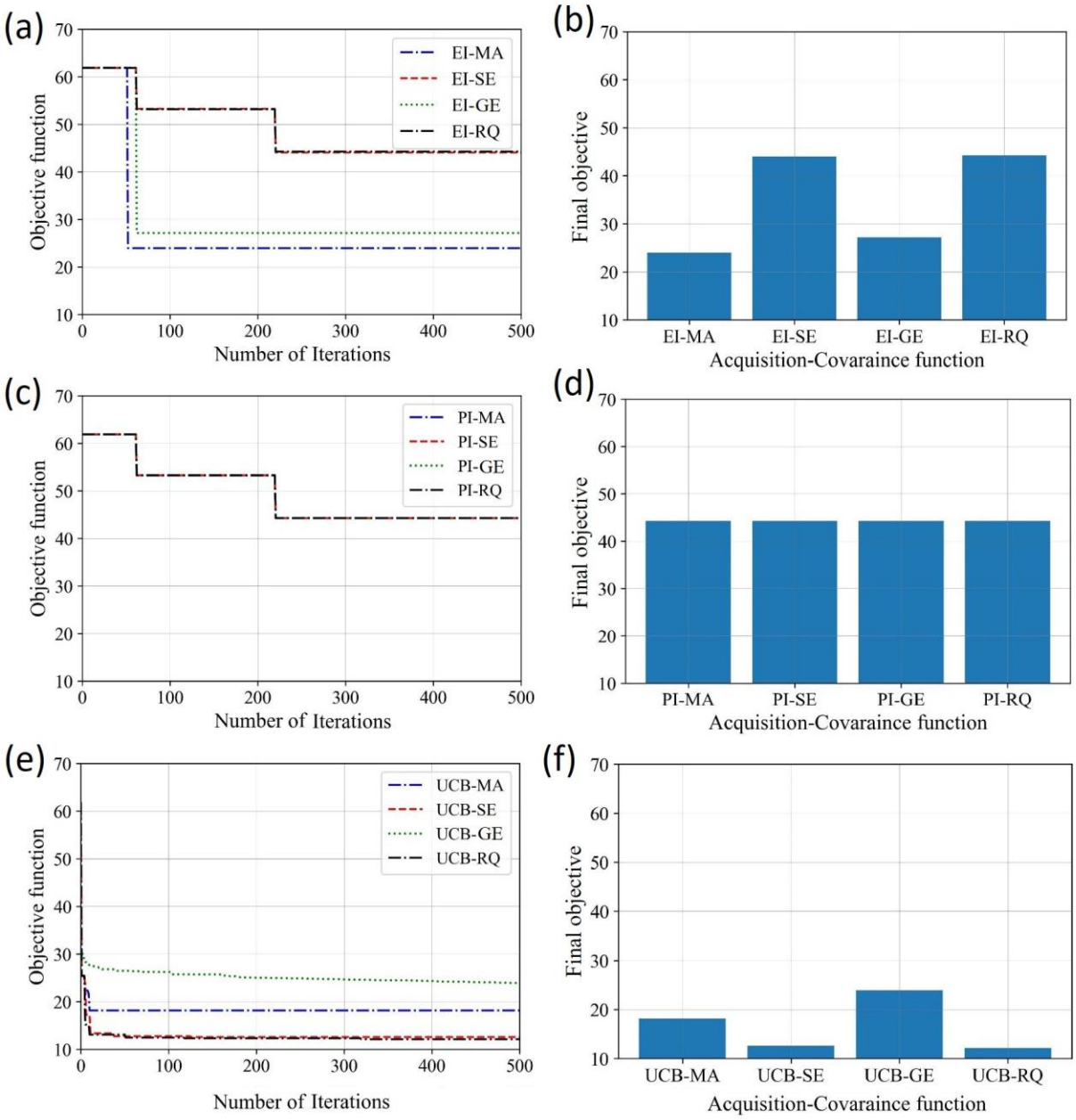

Fig 2. Performance of different Bayesian Optimization (BO) acquisition functions and covariance kernels.

Genetic Algorithm

Sensitivity of the performance of GA to the population size, mutation probability, and crossover probability was examined. The framework was evaluated using a range of different values for the population size (25, 50, 100, 125, and 150), mutation rate (0.1, 0.15, 0.2, 0.25, and 0.3), and crossover probability rate (0.1, 0.15, 0.2, 0.25, and 0.3). The results are depicted in Fig. 3. Generally, the results revealed that GA is less sensitive to the variability in optimization

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parameters compared to the sensitivity of BO. This can be seen from the lower variability in the final objective obtained for GA using different parameters (Fig. 3-b, d, and f) compared to BO (Fig. 2-b, d, and f). Surprisingly, no particular relationship was observed between the population size and the performance of GA. Yet, a population size of 100 was found to produce the best performance in terms of both the final objective (Fig. 3-a) and convergence speed (Fig. 3-b). The results also revealed that the performance of GA generally improved with decreasing the mutation rate. This can be seen from the consistent increase in convergence speed (Fig. 3-c) and decrease in the final objective (Fig. 3-d) with decreasing the mutation rate from 0.3 to 0.1. Moreover, GA showed little variability with the different values of the crossover rate (Fig. 3-e, and f) and was found to be significantly less sensitive toward the crossover rate compared to the mutation rate.

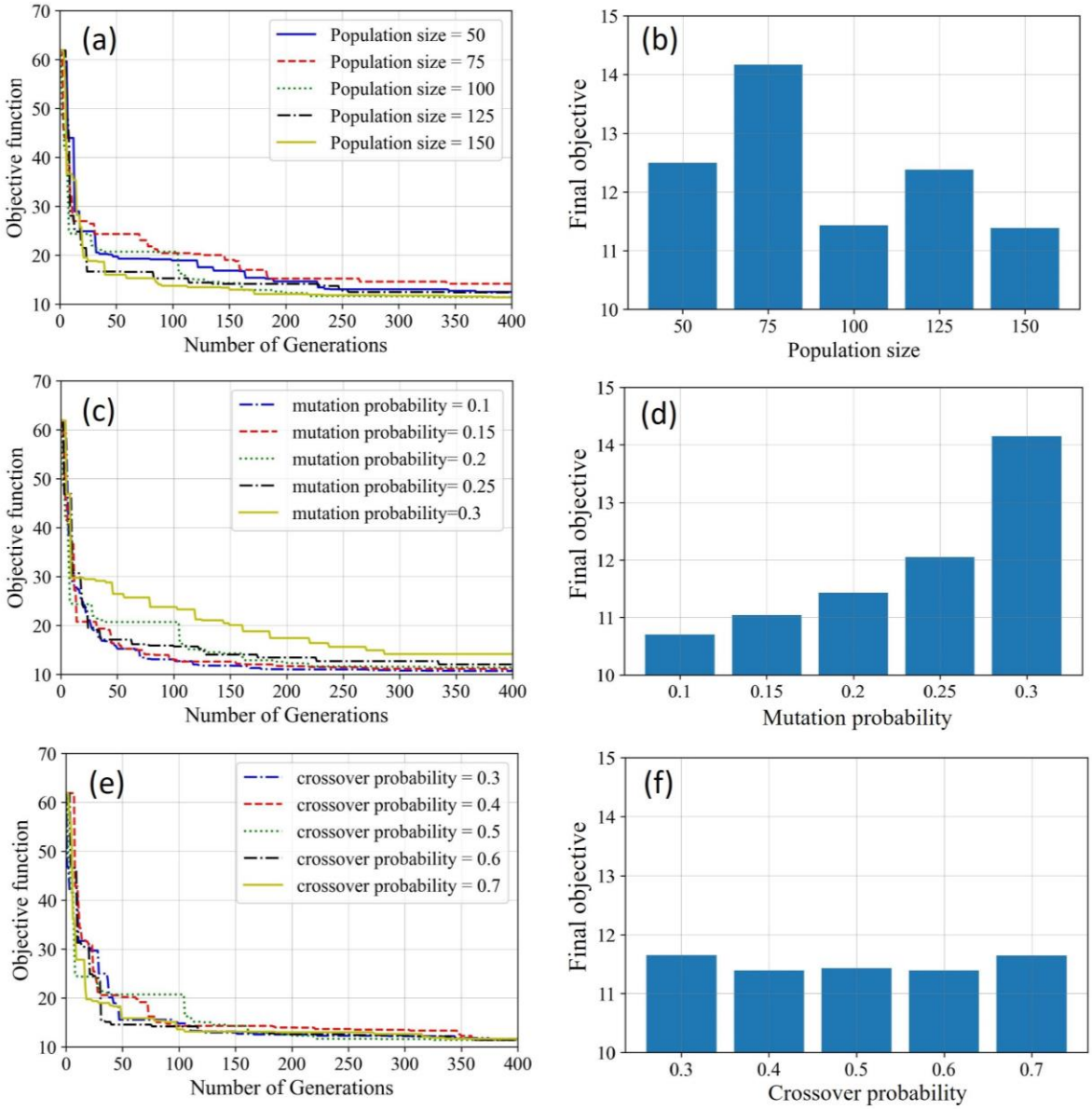

Fig 3. Sensitivity analysis of different Genetic Algorithm (GA) parameters.

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Particle Swarm Optimization

The sensitivity of PSO towards three key parameters was investigated, namely, the cognitive, social and inertia parameters, and the results are displayed in Fig. 4. Overall, PSO showed little sensitivity towards both the cognitive and social parameters. Nevertheless, a clear trend was observed for both parameters, where the final value of the objective function was found to decrease as both parameters increased from 0.3 to 0.5, after which the performance of PSO started to consistently decrease (Fig. 4-b, and d). On the other hand, PSO showed significant sensitivity to the choice of the inertia parameter, and the performance of PSO appeared to consistently decrease as the value of the inertia parameter increased from 0.3 to 0.7 as evidenced by the decrease in the final objective (Fig. 4-f) and increase in convergence speed (Fig. 4-e).

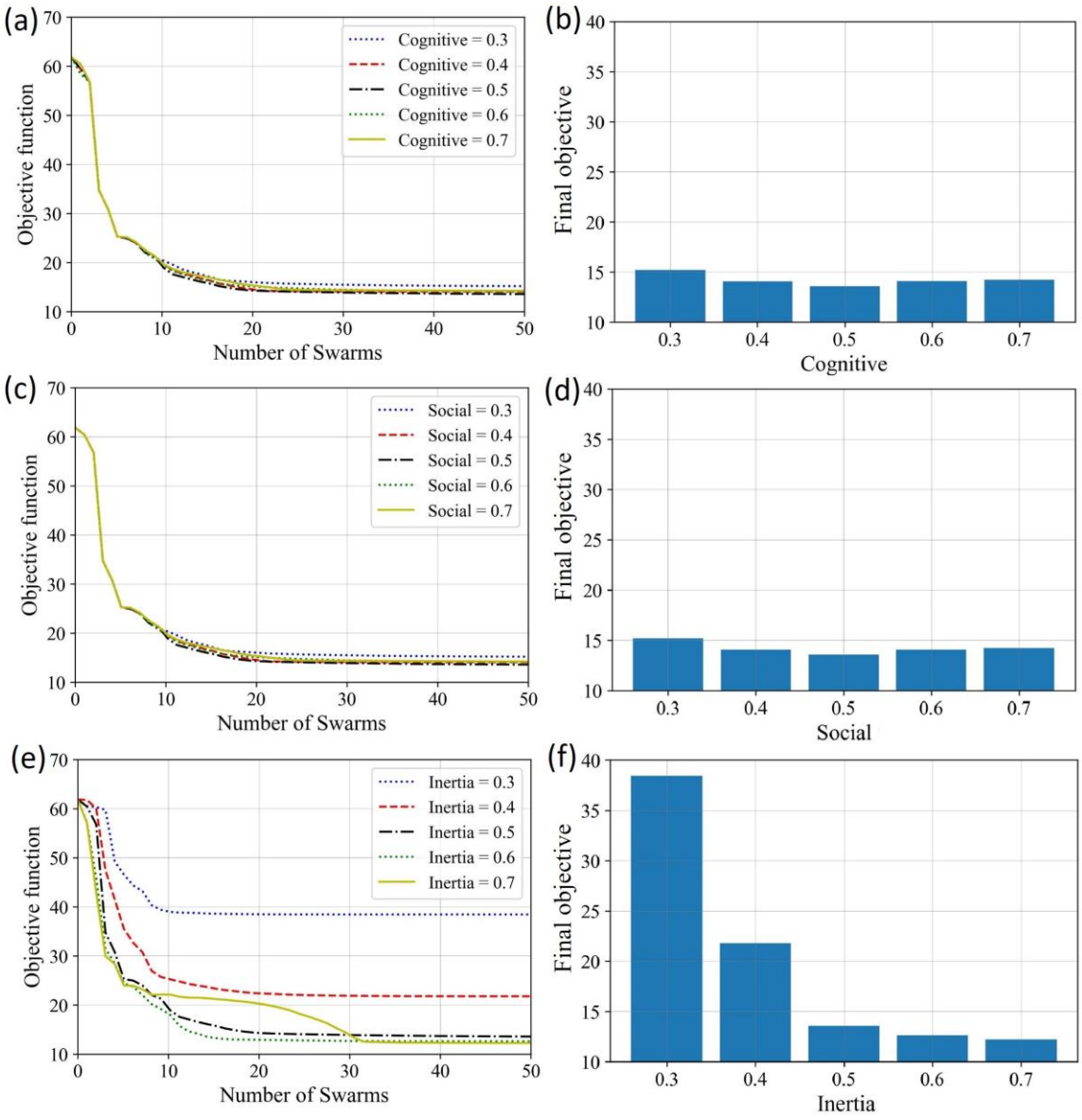

Fig 4. Sensitivity analysis of different Particle Swarm Optimization (PSO) parameters.

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Comparison of Optimization Methods

After conducting a sensitivity analysis for each of the three optimization approaches independently, the performance of the three methods was compared. For this comparison, the best set of parameters for each method was implemented. Figs. 5-a, b, and c show the convergence profile of each of the three approaches. The results showed that all three approaches displayed somewhat comparable performance in terms of the final value of the objective function. However, it is crucial to note that the x-axis represents different metrics for each method. For GA (Fig. 5-a), the x-axis represents the number of generations, where each generation is comprised of 100 individuals (i.e., the population size). Each individual requires evaluating the objective function, which involves conducting a full water quality simulation of the WDS. Similarly, for PSO (Fig. 5-b), the x-axis represents the number of swarms, where each swarm consists of 150 particles. On the other hand, for BO (Fig. 5-c), the x-axis represents the number of sequential iterations. Each BO iteration requires only one evaluation of the objective function. Therefore, BO appears to achieve convergence using significantly fewer evaluations of the objective function, i.e., fewer WQ simulations, compared to both GA and PSO. Figure 5-d shows a comparison of the objective function achieved by each of the three methods after 500 evaluations of the objective function. For BO, this corresponds to the final value of the objective function of 11.9 achieved after 500 sequential iterations. On the other hand, the corresponding objective function value achieved after 5 generations of GA (i.e., 500 individuals) is 41.7, while that achieved after 3 swarms of PSO (i.e., 450 particles) is 42.4. Taken together, these results indicate that BO is significantly more computationally efficient than EAs, especially for the optimization of expensive black-box models.

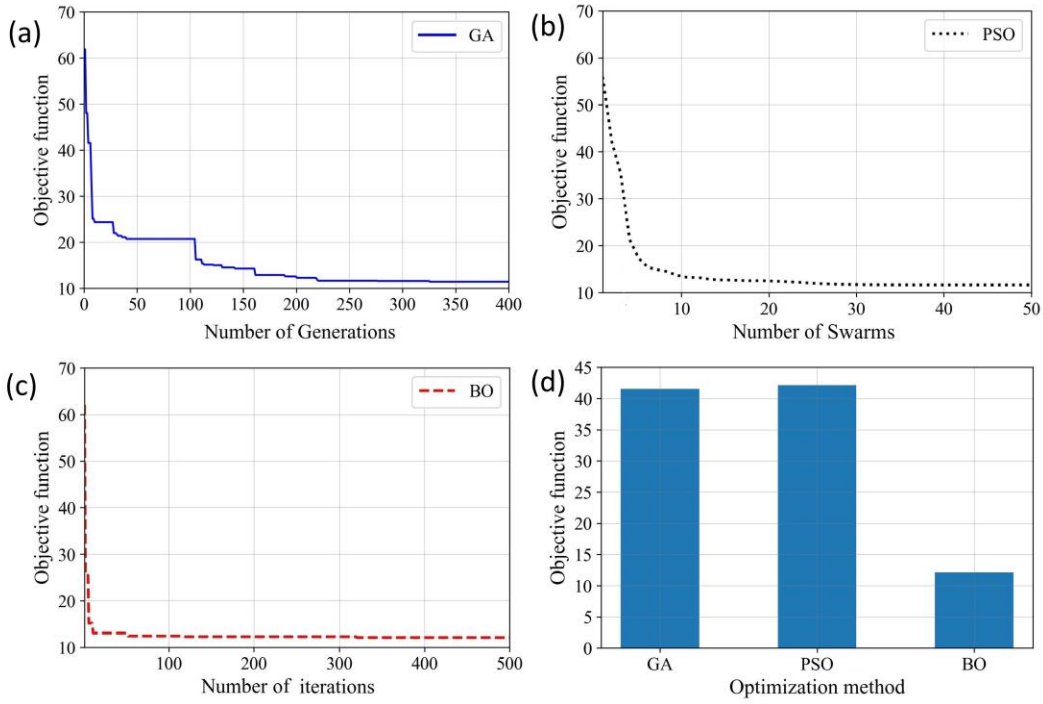

Figure 5. Comparison between the performance of Bayesian Optimization (BO), Genetic Algorithm (GA), and Particle Swarm Optimization (PSO).

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CONCLUSIONS

In this study, we performed a comparative analysis of the performance of three different optimization techniques, namely, Bayesian optimization (BO), genetic algorithm (GA), and particle swarm optimization (PSO), for optimizing the scheduling of chlorine injection sources in drinking water distribution systems. A comprehensive sensitivity analysis was conducted to understand the role of different optimization parameters in controlling the performance of the three optimization techniques and to identify the best set of parameters for each technique. The performance of BO was significantly dependent on the choice of the acquisition function, where the upper confidence bound (UCB) acquisition function showed considerably better performance than expected improvement (EI) and probability of improvement (PI). GA showed the least sensitivity towards different optimization parameters (population size, mutation, and crossover probability), while PSO showed significant dependence on the choice of the inertia parameter. Overall, the results revealed that the convergence of BO requires significantly fewer evaluations of the objective function than both GA and PSO. Yet, BO was found to be more sensitive to the choice of the optimization parameters than both evolutionary optimization methods.

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