

Introductory overview

Optimization using evolutionary algorithms and other metaheuristics

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Introductory Overview: Optimization using Evolutionary Algorithms and other Metaheuristics

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Abstract

Environmental models are used extensively to evaluate the effectiveness of a range of design, planning, operational, management and policy options. However, the number of options that can be evaluated manually is generally limited, making it difficult to identify the most suitable options to consider in decision-making processes. By linking environmental models with evolutionary and other metaheuristic optimization algorithms, the decision options that make best use of scarce resources, achieve the best environmental outcomes for a given budget or provide the best trade-offs between competing objectives can be identified. This Introductory Overview presents reasons for embedding formal optimization approaches in environmental decision-making processes, details how environmental problems are formulated as optimization problems and outlines how single- and multi-objective optimization approaches find good solutions to environmental problems. Practical guidance and potential challenges are also provided.

Learning Objectives

As Introductory Overviews are designed to provide a concise topic overview so as to break down barriers to shared understanding and dialogue within multidisciplinary teams, the learning objectives of this paper are:

- To gain an appreciation of the suitability and benefits of using formal optimization approaches, and evolutionary algorithms (EAs) in particular, to support decision-making when using environmental models
- To gain an understanding of how to formulate and solve environmental problems as optimization problems
- To gain an understanding of the way single- and multi-objective EAs work
- To gain an understanding of how to implement EAs in practice
- To gain an understanding of potential challenges associated with the implementation of EAs

Assumed Background Knowledge

- Familiarity with mathematics and environmental modelling
- Familiarity with the use of environmental models to support decision-making
- Familiarity with the calibration of environmental models

1. Introduction and Learning Objectives

Many environmental decision-making problems can be cast as trying to find a preferred option among different alternatives. The use of environmental models can play a central role in this task (Merritt et al., 2017), as they can be used to assess the utility of different decision alternatives (e.g. infrastructure interventions, management strategies, policy options). However, identifying the most suitable option can be difficult, as environmental problems are generally complex and the number of available alternatives is often large. Consequently, significant benefits can be achieved by linking simulation models with a modern family of optimization techniques referred to as “metaheuristics” in order to identify the options that make best use of scarce resources, achieve the best environmental outcomes for a given budget or provide the best trade-offs between competing objectives for further scrutiny. This enables decision-making processes to focus on options that provide the “best bang for buck”, rather than options that are potentially less reliable, more expensive and achieve worse environmental outcomes.

The term “metaheuristic” (coined by Glover, 1986) is composed of two Greek words, the prefix “meta” meaning “beyond” and “heuristic” meaning “to discover”. From an optimization perspective, metaheuristics are high level procedures designed to intelligently utilize heuristics to efficiently find a near-optimal solution to complex optimization problems (for definitions, see Blum and Roli, 2003). From an environmental management perspectives, they provide a means to make use of (existing) environmental models to identify a set of solutions (decision alternatives) that provide (near) optimal trade-offs between desired outcomes. Many metaheuristics are “nature-inspired” (also alternatively called “metaphor-based”), as they involve heuristics that imitate processes in natural systems (Blum et al., 2011; Boussaïd et al., 2013; Dréo et al., 2006; Zavala et al., 2014). Metaheuristics can be divided into two classes, including those that work with populations of solutions and those that do not. Evolutionary algorithms (EAs), which are population based, are a major, and arguably the most popular, class of metaheuristics. Consequently, as was done in Maier et al. (2014), the focus of this paper is on EAs, although many of the concepts discussed also broadly apply to other metaheuristics.

EAs have proven to be highly effective in solving a wide range of environmental problems (Maier et al., 2014), as they can be used in realistic decision-contexts. This is because they (i) can be used as one element in broader, participatory environmental decision-making processes (Di Matteo et al., 2017a; Kaim et al., 2018; Piscopo et al., 2015; Wu et al., 2016), (ii) can be linked with existing simulation models to assist with the exploration of large solution spaces (Maier et al., 2015), (iii) can cater to multiple competing objectives (Newland et al., 2018; Verstegen et al., 2017), (iv) can take into account uncertainties (Beh et al., 2017; Eker and Kwakkel, 2018) and (v) generally provide a number of “good” solutions that can be explored further, rather than being prescriptive (Di Matteo et al., 2017a; Kaim et al., 2018). Their main disadvantages are (i) that they are potentially computationally expensive, although this primarily depends on the computational efficiency of the simulation model with which they are linked, (ii) that they are not guaranteed to identify the globally optimal solution (from a mathematical perspective) and (iii) that they generally need to be tuned to the problem under consideration (Maier et al., 2014; Mala-Jetmarova et al., 2017).

The purpose of this Introductory Overview is to introduce EAs to the environmental modelling community, where environmental models are commonly used to assist with identifying the course of action that should be undertaken (e.g. pollution control, operation of infrastructure system,

implementation of policy option) to produce desired environmental outcomes, but without formal strategies for achieving this. Consequently, before details of EAs are given, a case is made for why formal optimization methods can be useful where environmental models are used to support decisions. In addition, details are given of how to structure environmental decision problems to enable such optimization methods to be used. Then, information is provided on how EAs work, how EAs can be implemented and what some of the challenges are when applying EAs to real-world problems. For ease of understanding, key concepts related to the way decision problems are structured are introduced in the context of five classes of environmental problems, which are illustrated via five specific examples:

- **The mitigation of global climate change impacts:** This problem type is illustrated via the example of designing water distribution systems so as to minimise their impact on greenhouse gas emissions. As climate change is caused by anthropogenic systems, mitigation options typically require modifications to be made to engineered systems. In the specific example presented here, this corresponds to the selection of the components of the systems of pipes, tanks, pumps and valves that deliver water from sources (e.g. rivers, lakes, groundwater) to domestic, industrial and agricultural consumers. Such water distribution systems contribute to greenhouse gas emissions through both the embodied energy of their system components (e.g. pipes, tanks) and the energy required for operating pumps to maintain the required system pressures. By optimizing the design of these systems, the best possible trade-offs between cost and climate change impacts (via greenhouse gas emissions) can be identified, while ensuring such systems perform reliably.
- **Regional resource consumption in urban systems:** This problem type is illustrated via the example of the long-term planning of water resources systems, where optimization can be used to ensure that the best possible balance between the benefits (i.e. water supply security) and impacts (e.g. social and environmental impacts of water extraction) of natural resource consumption can be identified.
- **Natural resource management:** This problem type is illustrated via the example of the operation of reservoir systems, where optimization can be used to determine how to operate an infrastructure system so as to achieve the best possible trade-offs between various economic, social and environmental outcomes in catchments (watersheds).
- **Pollution management in an environmental system:** This problem type is illustrated via the example of the determination of wastewater treatment levels, where optimization can be used to determine the lowest-cost treatment strategies that maintain environmental health in a river system.
- **Environmental model development:** This problem type is illustrated via the example of model calibration, where optimization can be used to identify the model parameters that provide the best match between model outputs and the corresponding measured data.

It should be noted that the above example applications are illustrative only and were selected to ensure that the principles presented are accessible to as wide an audience as possible, which is one of the objectives of Introductory Overviews. This is why examples belonging to five different classes of problems are presented, so that the underlying principles are likely to resonate with as many readers as possible. However, the basic principles on optimization and evolutionary algorithms presented in this paper are applicable to all problems where environmental models are calibrated or

used to support decisions (see Section 2). It should also be noted that as this paper belongs to the Introductory Overview class of papers, it presents fundamental principles in a simple, easy-to-understand fashion. More detailed descriptions can be found elsewhere (e.g. Maier et al., 2014).

2. Why do we need Optimization?

As mentioned in the Introduction, environmental simulation models are used extensively to support decision-making processes in a variety of application areas, such as: the development and evaluation of national and international environmental regulations (Giupponi, 2007; Laniak et al., 2013); land use management (Amato et al., 2018); natural hazard management (Newman et al., 2017); the operation and management of reservoir systems (Razavi et al., 2014); the assessment of environmental and human health (Morley and Gulliver, 2018; Reis et al., 2015); the management of river systems (He, 2003; Humphrey et al., 2016; Hunter et al., 2018; Ravalico et al., 2010); the management of drains (Humphrey et al., 2016); the management of air pollution (Baró et al., 2014; Borge et al., 2014); flood inundation assessment (Teng et al., 2017); groundwater management and remediation (Jakeman et al., 2016; Piscopo et al., 2015; Singh, 2014); the design of water distribution networks so as to minimize global climate impacts (Stokes et al., 2015a; Stokes et al., 2014b; Wu et al., 2010a); the prediction of and adaptation to natural hazards such as floods or droughts (Basher, 2006); crop and livestock management (Moore et al., 2014; van Keulen and Asseng, 2018); the design of green infrastructure for stormwater management and urban renewal (Liu et al., 2014; Yigitcanlar and Teriman, 2015); and evaluating the effects of resource extraction by the petroleum (Fiori and Zalba, 2003), natural gas (McJeon et al., 2014), mining (Côte et al., 2010) and timber (Alavalapati and Adamowicz, 2000) industries. Environmental models are in such widespread use because they can be designed to effectively reproduce the dynamics of real-world systems under traditional management situations as well as *alternative* virtual realities, including different environmental conditions and management alternatives, enabling optimal designs, strategies and policies to be developed under a range of scenarios (Maier et al., 2016).

In order to use environmental simulation models to support decisions, the model inputs have to correspond to the proposed decision alternatives (e.g. infrastructure interventions, management strategies, policy options) and the model outputs have to correspond to the environmental (and other) outcomes of interest. In a decision-support context, the outcomes of interest are generally referred to as *objectives*, but can also correspond to system *constraints* (e.g. allowable pollution levels), and the available decision alternatives are referred to as *decision variables*. The environmental model is then used to find the values of the *decision variables* (i.e. model inputs) that optimize (maximize or minimize) the environmental (and other) *objectives* (i.e. corresponding values of model outputs) and ensure that any *constraints* are satisfied. The selected values for all *decision variable* are referred to as a *solution* to the problem under consideration. These terms are illustrated below for the five example environmental problems introduced in Section 1 (see also Figure 1):

- **The design of water distribution systems to mitigate global climate change impacts:** For this problem, the *objectives* (i.e. outcomes of interest) are to minimize greenhouse gas emissions and system cost by selecting appropriate sizes of pipes, valves, pumps, tanks etc., which are the *decision variables* (i.e. interventions). The *constraints* are that water of sufficient pressure and

quality has to be delivered to consumers. A *solution* consists of the selected sizes for the pipes, valves, pumps, tanks etc.

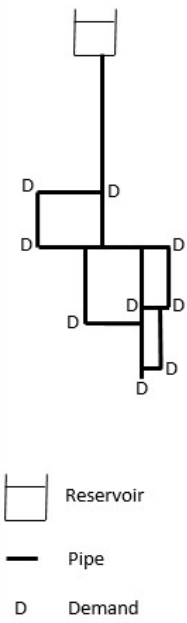
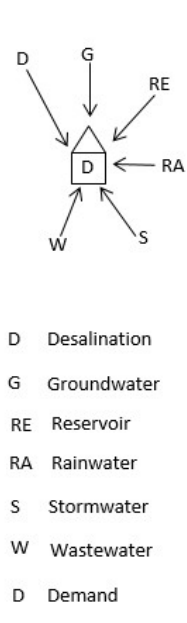
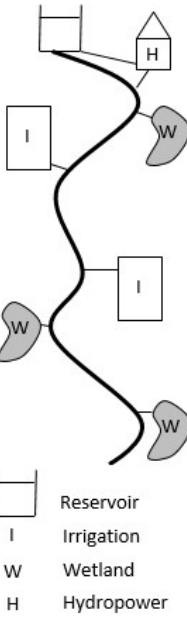
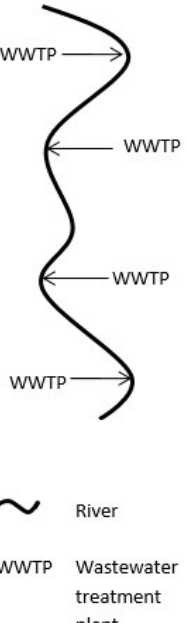
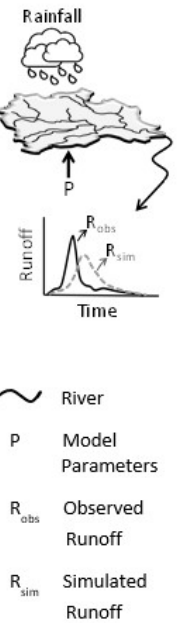
Problem	Design of Water Distribution Systems	Planning of Urban Water Supply Systems	Operation of Reservoir Systems	Wasteload allocation	Model Calibration
	 <p>Reservoir Pipe D Demand</p>	 <p>D Desalination G Groundwater RE Reservoir RA Rainwater S Stormwater W Wastewater D Demand</p>	 <p>Reservoir I Irrigation W Wetland H Hydropower River</p>	 <p>WWTP River WWTP WWTP WWTP</p>	 <p>Rainfall Runoff Time R_{obs} Observed Runoff R_{sim} Simulated Runoff River Model Parameters</p>
Decision Variables	Pipe diameters	Supply source capacities, supply has to be greater than or equal to demand	Reservoir release amounts, duration and timing	Treatment levels	Model Parameters
Constraints	Minimum pressure in pipes	Supply capacity from various sources	Available water	Allowable water quality in river	Physically feasible parameter ranges
Objectives	Minimize: Cost, greenhouse gas emissions	Minimize: Cost of supply, energy usage, greenhouse gas emissions, impact on available water resources	Maximize: hydropower production, environmental health, crop production Minimize: Downstream flooding	Minimize: Total treatment costs	Minimize the model errors, e.g., difference between simulated and observed runoff
Examples	Basupi et al. (2013); Herstein et al. (2010); Stokes et al. (2014a); Stokes et al. (2015b)	Kasprzyk et al. (2013); Paton et al. (2014); Wu et al. (2017); Wu et al. (2016)	Razavi et al. (2013); Reddy and Kumar (2006); Szemis et al. (2014); Teegavarapu and Simonovic (2002)	Burn and Yulianti (2001); Cho et al. (2004); Vasquez et al. (2000); Yandamuri et al. (2006)	Gupta et al. (1999); Razavi and Tolson (2013); Vrugt et al. (2003); Yapo et al. (1998)

Figure 1. Details of formulation of five example environmental problems, including problem representation as well as example decision variables, constraints and objectives.

- **The long-term planning of water resources systems for managing regional resource consumption:** For this problem, the *objectives* (i.e. outcomes of interest) are to minimize the impact on available water resources, energy usage and system cost while maximizing water supply security by selecting an appropriate portfolio of supply and demand interventions, which are the *decision variables*. The *constraints* are the available water supply and demand management options. A *solution* consists of the selected portfolio of supply and demand interventions.
- **The operation of reservoir systems for natural resources management:** For this problem, the *objectives* (i.e. outcomes of interest) are to maximize environmental, social and economic benefits

and to minimize environmental, social and economic costs by selecting appropriate reservoir release magnitudes and durations over time, which are the decision *variables* (i.e. interventions). The *constraints* are the available water resources and limits on reservoir outflows. A *solution* consists of the selected reservoir release schedule.

- **The determination of wastewater treatment levels for pollution control in environmental systems:** For this problem, the outcomes of interest correspond to both *constraints* (i.e. the maintenance of acceptable water quality levels in the river system under consideration) and *objectives* (i.e. minimizing the cost of the interventions required to achieve the desired water quality outcomes). The *decision variables* (i.e. interventions) are the required wastewater treatment levels and a *solution* consists of the selected treatment levels at each wastewater treatment plant.
- **The calibration of simulation models:** For this problem, the *objectives* (i.e. outcomes of interest) are to minimize an error measure between simulated flux/state variables and corresponding measured flux/state variables by selecting appropriate values of the parameters of a simulation model, which are the *decision variables*. The *constraints* are the allowable ranges of the parameters. A *solution* consists of a selected value for each of the model parameters to be obtained by calibration.

Once an environmental problem has been formulated in terms of *objectives* (i.e. the values to be maximized or minimized), *decision variables* (i.e. the values that can be changed to maximize or minimize the objective(s)) and *constraints* (i.e. the allowable values of decision variables and/or objectives/constraints), the best *solutions* are generally identified using an informal “optimization” process, where the “best” solutions are identified via trial-and-error (Simon, 1996), as illustrated in Figure 2. The first step of this process involves the selection of a plausible solution to the problem under consideration from the available alternatives. This selection is generally based on domain knowledge, experience and intuition. For example:

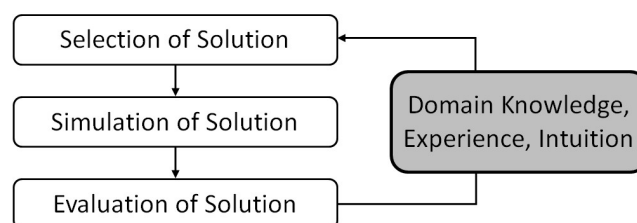


Figure 2. Steps in a traditional informal “optimization” process for finding optimal solutions to environmental problems with the aid of environmental simulation models via trial-and-error.

- For the water distribution system design problem, this would involve the selection of the diameters of all of the pipes in the network, the sizes and locations of all of the tanks and the types, locations and sizes of the valves and pumps.

- For the long-term water resources planning problem, this would involve the selection of the capacities of the various potential supply sources, as well as the various demand management strategies.
- For the reservoir operation problem, this would involve the selection of when to release water, how much to release and how long for.
- For the wastewater treatment problem, this would involve the selection of the treatment level at each wastewater treatment plant.
- For the model calibration problem, this would involve the selection of values for each model parameter to be obtained by calibration.

The performance of the selected solution in terms of objective function values and constraint violation (i.e. the outcomes of interest) is then evaluated, typically with the aid of one or more environmental simulation models. For example:

- For the water distribution system design problem, a hydraulic simulation model (e.g. Rossman, 2000) would typically be used to check whether minimum pressure constraints are violated for the selected pipe diameters, in addition to the calculation of the values of the cost and greenhouse gas emission objectives.
- For the long-term water resources planning problem, a river basin planning model would generally be used to simulate the interactions between various sources and demands throughout the year in order to enable the impact on water resources, supply cost, energy and greenhouse gas emissions, as well as reliability of supply, to be calculated for different combinations of water sources and extraction amounts/capacities and demand management strategies.
- For the reservoir operation problem, an integrated model would be required, linking reservoir releases to the hydropower, environmental health, crop production and flood protection objectives.
- For the wastewater treatment problem, a water quality model (e.g. Ambrose et al., 2017) would generally be used to check whether the water quality constraints in the river are violated for the selected treatment levels, in addition to the calculation of the corresponding treatment costs.
- For the model calibration problem, the simulation model to be calibrated (e.g. Arnold et al., 1998) would be run with the selected parameter values, and the error metric (see Bennett et al., 2013) for a comprehensive range of metrics) would be calculated between the simulated model outputs for a set of inputs and the corresponding measured outputs.

The next step in the informal “optimization” process involves selection of an alternative, hopefully improved, solution. This selection takes into account the performance of the solution that was selected initially, as well as experience, domain knowledge, and intuition. For example:

- For the water distribution system design problem, if the previously selected solution resulted in a violation of the pressure constraint in a particular part of the system, some of the pipe diameters in this region of the network might be increased, reducing pressure losses, but increasing cost and greenhouse gas emissions. Conversely, if the previously selected solution resulted in a large pressure excess in a particular part of the system, some of the pipe diameters in this region of the

network might be decreased, increasing pressure losses, but decreasing cost and greenhouse gas emissions.

- For the long-term water resources planning problem, if the previously selected solution resulted in a demand shortfall, the capacities of one or more of the sources might be increased, resulting in increased cost and water resources impact. In contrast, if the previously selected solution resulted in a large supply excess, the capacities of one or more of the sources might be decreased, reducing cost and water resources impact.
- For the reservoir operation problem, if the previously selected solution resulted in unacceptably high levels of spillage (water flowing over the spillway and not generating power), less water might be held back in the reservoir prior to the spillage event, increasing the storage capacity at the cost of reducing the amount of water available for irrigation and environmental flows. Conversely, if the previously selected solution resulted in very low levels of flood risk, more water might be stored in the reservoir for hydropower, environmental and irrigation usage.
- For the wastewater treatment problem, if the previously selected solution resulted in a violation of the water quality standard in the river, some of the upstream treatment levels might be increased, improving water quality, but increasing cost. Conversely, if the previously selected solution resulted in water quality that is above the required level, some of the treatment levels might be decreased, reducing water quality, but decreasing cost.
- For the model calibration problem, in the case of a rainfall-runoff model, if the previously selected solution resulted in an underestimation of peak flows, the value of the runoff curve number parameter might be increased to intensify the runoff response to rainfall, and vice versa. Conversely, if that solution resulted in a longer time-to-peak than reality, the value of the roughness coefficient might be decreased to allow faster movement of water through channels.

The steps of selecting a trial solution, evaluating its performance with the aid of one or more environmental models and selecting a new (hopefully improved) solution based on experience and domain knowledge, as well as the performance of the previously selected solution(s), are repeated until no further improvement in objective function values can be achieved or the analyst is satisfied with the selected solution.

While the informal optimization approach described above works reasonably well when the problem under consideration and simulation model used are well understood by the analyst, and the number of decision variables and their feasible ranges (i.e., number of alternative solutions) are relatively small, it is unlikely to yield the best possible outcome for the majority of environmental problems. This is because the size of the solution space of typical environmental problems is extremely large, as illustrated in Table 1 for particular instances of the five example problems considered previously. While a vast majority of these solutions might not be considered reasonable from a practical perspective, and would thus be excluded from consideration as part of the informal optimization process outlined above, the resulting search spaces would still be extremely large, as shown in the last column of Table 1, which shows the size of the solution spaces after 99.99% of possible solutions have been discarded. As a result, it is extremely unlikely that optimal, or even near-optimal, solutions can be identified by using the informal optimization process outlined above, as only a very small fraction of the search space is explored. This problem is exacerbated by the fact that many environmental

problems are complex and poorly understood, making it more difficult to bring domain knowledge to bear, especially for inexperienced analysts.

At the other end of the spectrum of possible solution approaches, every possible value in the solution space could be evaluated (i.e. complete enumeration of the search space), such that the best possible solution is guaranteed to be identified. However, this is generally not possible from a practical perspective, as the simulation times associated with the search space sizes in Table 1 are likely to be prohibitively long. Assuming each run of the simulation model(s) used to evaluate the utility of the solutions takes only one second, the total simulation times for the examples in Table 1 will range from ~35,000 to ~2x10⁷⁰ years (for example, in the water distribution system problem, the total simulation time is calculated as (6.5x10⁷⁷x 1second) / (60second x60minute x24hour x365day) ~ 2x10⁷⁰ years). In real-world problems, simulation models can be computationally expensive, taking minutes or longer for a single run, making the full enumeration of all possible solutions even less feasible.

The fact that informal optimization approaches are unlikely to enable near-optimal solutions to be identified and that the evaluation of every possible solution is computationally intractable provides a compelling case for the use of *formal* optimization methods in order to identify optimal or near-optimal solutions to complex environmental problems in a reasonably computationally efficient manner. Thus, formal optimization approaches enable innovative solutions to complex problems to be identified and result in the most efficient use of increasingly constrained economic and natural resources. In fact, the use of formal optimization methods can result in improvements on the order of 10% to 50% compared with the use of the informal trial-and-error process outlined in Figure 2 (Liner and Maier, 2015). In addition, the use of formal optimization methods provides a more consistent approach to solving environmental problems with conflicting objectives (Liebman, 1976), especially for complex problems that are poorly understood (Di Matteo et al., 2017b).

Table 1: Example search space sizes for the five environmental problems considered for illustration purposes in Figure 1. It should be noted that for problems for which potential decision variable values are continuous, as is generally the case for model calibration, the size of the search space is theoretically infinite.

Problem	Number of decision variables	Number of decision variable options (levels)	Number of potential solutions (i.e. size of search space)	0.01% of number of potential solutions
Water distribution system design	100 pipes	6 diameters	$6^{100} = 6.5 \times 10^{77}$	6.5×10^{73}
Long-term water resources planning	25 potential sources	10 potential capacities	$10^{25} = 1.0 \times 10^{25}$	1.0×10^{21}
Reservoir operation	52 weeks	5 different releases	$5^{52} = 2.2 \times 10^{36}$	2.2×10^{32}
Wastewater treatment	20 WWTPs	4 treatment levels	$4^{20} = 1.1 \times 10^{12}$	1.1×10^8
Model Calibration	15 parameters	100 values	$100^{15} = 1.0 \times 10^{30}$	1.0×10^{34}

3. How do we Formulate and Solve Optimization Problems?

3.1 Problem formulation

The formulation of formal optimization problems is very similar to that of problems that are solved using the informal optimization process outlined in Section 2, requiring the specification of the following three components:

- Objective functions, which represent the values that should be maximized (e.g. system performance) or minimized (e.g. environmental impact) (see Figure 1).
- Decision variables, which are the values that can be manipulated in order to maximize or minimize the objective functions (see Figure 1). These can take on discrete (e.g. integer) or continuous (real) values, depending on the problem under consideration.
- Constraints, which can generally be placed on the values that decision variables can take, or used to avoid undesirable/infeasible system responses (see Figure 1).

A solution is defined as a set of selected values of the decision variables, and a feasible solution is one that satisfies all problem constraints. The quality of different solutions is evaluated using the objective function. As mentioned previously, the (environmental) outcomes of interest are represented by the objectives and constraints, which generally correspond to the outputs of environmental models, and the potential interventions/choices are represented by the decision variables, which generally correspond to the inputs of environmental models. Generally, decision variables correspond to anthropogenic changes to natural systems, either directly (e.g. revegetation) or via an engineered system (e.g. pollution control).

Formally, optimization problems are represented (Cohon and Marks, 1975) as a maximization problem of an objective function, subject to inequality (and sometimes equality) constraints, as follows:

$$\text{maximize } f(\mathbf{x}) \tag{1}$$

subject to

$$g_i(\mathbf{x}) \leq 0, \quad i = 1, 2, \dots, m \tag{2}$$

$$x_{jl} \leq x_j \leq x_{ju} \quad j = 1, 2, \dots, n \tag{3}$$

where \mathbf{x} is the vector of decision variables, x_j indicates the j^{th} value in this vector, and x_{jl} and x_{ju} are lower and upper bounds on the decision variables, respectively; f is the objective function and g_i is the i^{th} constraint function of vector \mathbf{x} . These functions can be highly non-linear and complex, and their collective evaluation for any given \mathbf{x} requires the running of environmental simulation models.

For minimization problems, the maximization formulation above can be easily transformed into a minimization formulation by multiplying the objective function by minus one (i.e., maximize $-f(\mathbf{x})$ is equivalent to minimize $f(\mathbf{x})$). Also, the “single-objective” optimization formulation above can be extended to a “multi-objective” optimization formulation by introducing more objective functions to be maximized simultaneously in Eq. (1) above; that is, to maximize $(f_1(\mathbf{x}), \dots, f_k(\mathbf{x}))$, where k is the number of objective functions.

It should be noted that the translation of environmental and water resources management problems into the somewhat rigid formulation outlined above can be challenging, especially for real-world problems, which are often complex, high-dimensional, ill-defined and not well structured. Consequently, where possible, stakeholders should be directly involved in the formulation of optimization problems, informing the objectives, decisions and constraints as part of an interactive process (Di Matteo et al., 2017a; Smith et al., 2017; Wu et al., 2016).

3.2 Problem representation

Optimization problems can be represented geometrically by considering a “fitness landscape”. A fitness landscape, or synonymously called a “response surface”, depicts the shape of the fitness (objective) function for a particular objective with respect to the decision variables (e.g. model error as a function of different values of model parameters for model calibration problems). For an optimization problem with only one decision variable, the resulting fitness landscape is a (typically nonlinear) line, and for a problem with two decision variables, the fitness landscape is a plane (see Figure 3). For higher-dimensional problems with three or more decision variables, the fitness landscape becomes a hyperplane that cannot be visualised easily.

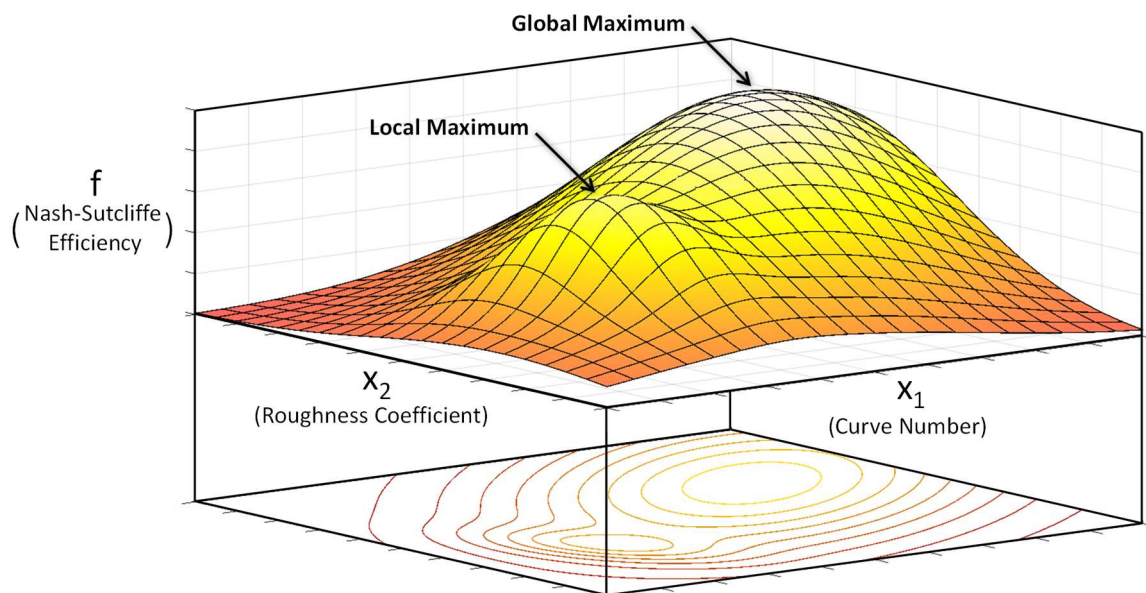


Figure 3. A typical fitness landscape (response surface) and its contour plot for a model calibration problem, where the objective function f is a goodness-of-fit metric to be maximized and the decision variables x_1 and x_2 are model parameters. This optimization problem has two regions of attraction (one local maximum in addition to the global maximum).

When there is a single objective to be maximized, there is a single fitness landscape and the purpose of optimization is to identify the highest peak (or the lowest trough for minimization problems) in the fitness landscape for the problem under consideration. In other words, the purpose of optimization is to identify the feasible combination of decision variable values that results in the largest value of the objective function (fitness). Consequently, the optimization process is akin to identifying the “highest hill” in the fitness landscape, which is referred to as the “global optimum”, as it is the best performing

among all possible solutions. It should be noted that there may exist one or multiple other hills in the fitness landscape with lower peaks, which are referred to as “local optima”, as their respective solutions are optimal only within their *neighbourhood* in the decision variable space.

When there is more than one objective, each objective has its own fitness landscape, as variations in objective values with changes in decision variable values are likely to be different for different objectives. For many problems, objectives compete with each other, so that solutions that improve values of one objective might degrade values in another. For example, a reservoir release schedule that increases ecological health in the river is unlikely to also increase agricultural production. Consequently, when considering competing objectives, it is less clear which solutions are better than others, as the solution that results in the highest peak in the fitness landscape for one objective might result in the lowest peak in the fitness landscape for the other objective and vice versa. In such cases, the optimality of a solution is determined using the concept of dominance.

If a solution (\mathbf{x}_i) performs better than another (\mathbf{x}_j) in at least one objective and does not perform worse in any of the other objectives (e.g. $f_1(\mathbf{x}_i) < f_1(\mathbf{x}_j)$ and $f_l(\mathbf{x}_i) \leq f_l(\mathbf{x}_j)$ for $l = 2 \dots k$), then the first solution (\mathbf{x}_i) is said to dominate the other solution (\mathbf{x}_j), as it is clearly better with respect to all objectives. However, given a pair of solutions ($\mathbf{x}_p, \mathbf{x}_q$) where each solution performs better than the other in at least one objective (e.g. $f_1(\mathbf{x}_p) < f_1(\mathbf{x}_q)$ and $f_2(\mathbf{x}_p) > f_2(\mathbf{x}_q)$), it is not possible to determine which solution is best without some value judgement about the relative importance of different objectives. Consequently, for problems with more than one competing objective, it is not possible to determine a single best solution, as there are a number of solutions (e.g. \mathbf{x}_p and \mathbf{x}_q above) that are not dominated by any others. This set of non-dominated solutions forms the Pareto front (Pareto, 1896), which is unique and provides the optimal trade-off between objectives.

The above concepts are illustrated in Figures 4 and 5 for a hypothetical problem with two decision variables (2-dimensional decision space) and two objective functions (2-dimensional objective space), both of which are to be minimized. Figure 4 illustrates the mapping from the solution to the objective space, which is generally done with the aid of one or more simulation models. As can be seen, the solutions that are non-dominated in the objective space lie on the Pareto front, whereas dominated solutions do not. The relationship between the different fitness landscapes for the two objectives and the Pareto front is illustrated in Figure 5.

3.3 Problem solution

As mentioned previously, the solution of single objective optimization problems corresponds to the process of searching the fitness landscape for the highest peak or lowest trough, depending on whether the objective is to maximize or minimize the objective function. For problems with more than one objective, the optimization process corresponds to searching the fitness landscapes for each of the objectives so as to identify non-dominated solutions. As the globally optimal objective function value(s), and the corresponding decision variable values (i.e. the solution), are unknown for real-life optimization problems (i.e. the whole purpose of the optimization process is to identify these), it is not possible to assess how well an optimization algorithm has performed. The exception to this is model calibration, where the “best” value that can possibly be achieved (i.e. a calibration error of zero) is known. Consequently, split sample testing (i.e. using a subset of the available data for calibration and a subset for validation) can be used for these types of optimization problems to obtain a measure of the “robustness” of the calibration process. This, however, is generally affected by a

number of factors in addition to the optimization method used, including the statistical properties of the available data and how they are divided in calibration and validation subsets (Wu et al., 2013; Zheng et al., 2018).

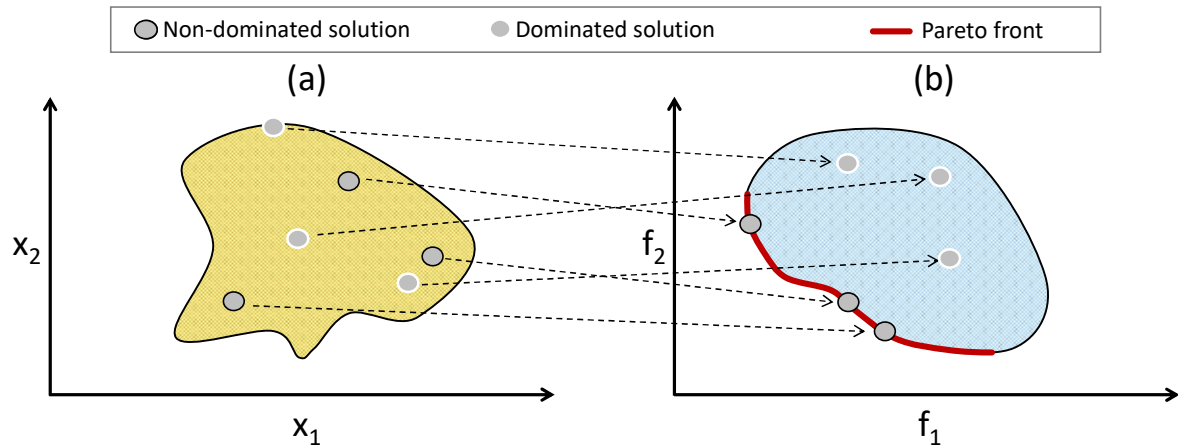


Figure 4. Mapping of (a) a decision space onto (b) an objective space, where both objectives are to be minimized.

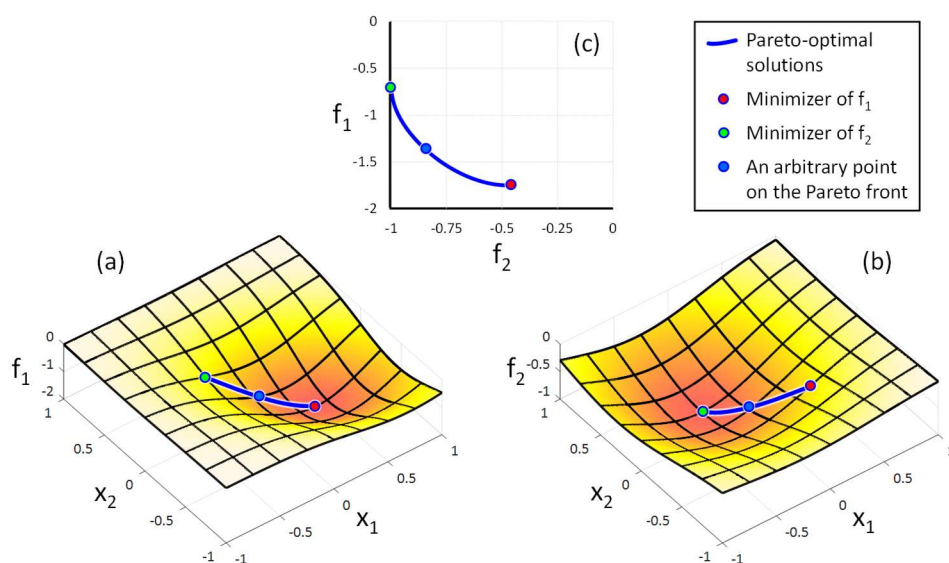


Figure 5. Illustration of the relationship between (a) the fitness landscape of objective 1, (b) the fitness landscape of objective 2 and (c) the Pareto-front of the two-objective optimization problem.

How difficult it is to search the fitness landscape(s) and find the globally optimal solution(s) is dependent on the following factors:

1. The size of the area to be searched. The size of the search space is a function of the number of decision variables (e.g. how many pipes have to be sized in a water distribution system), the ranges of

the decision variables (e.g. what is the smallest and what is the largest diameter to be considered), and the level of discretization (resolution) in cases where discrete variables are considered (e.g. how many commercially available diameters are considered within the selected range of diameters). The larger the number of decision variables, the larger the ranges of the decision variables and the finer the resolution, the larger the search space and the more difficult it is likely to be to identify the optimal solution(s).

However, it is not only the size of the total search space that matters, but also the size of the feasible portion of this space (i.e. the size of the space for which all constraints are met). For some problems, many of the decision variable combinations result in solutions that violate constraints related to target system performance (i.e. infeasible solutions). For example, for the wastewater treatment problem (Figure 1), various combinations of treatment levels at the WWTPs might result in better objective function values (i.e. lower treatment costs), but might result in water quality levels in the receiving waters that do not satisfy minimum water quality constraints. If the size of the feasible portion of the decision variable space is small, it might be difficult to find a combination of decision variables that results in feasible solutions. Consequently, the ability to find optimal solutions can not only be made more difficult if the size of the search space is very large, but also if the feasible region of the total search space is very small.

2. The properties of the fitness landscape. If the fitness landscape is very smooth, like the “big bowl” in Figure 6a, the search is relatively easy, as there is a single optimum (for a minimization problem). However, if the fitness landscape is very rugged, as shown in Figure 6b, finding the lowest point in the landscape is very difficult. This is because there are many troughs, making it difficult to navigate the landscape and to know if a trough that has been found is the lowest trough (i.e. the global optimum), or just a local optimum. For real-world problems, fitness landscapes tend to be complex (e.g. Gibbs et al., 2011, 2015; Kingston et al., 2005), characterized by a range of features from small-scale features, such as roughness or noise, to large-scale features, such as multimodality (Razavi and Gupta, 2015). Consequently, the fitness landscapes for many environmental problems are likely to be rugged and characterized by many local optima, a large degree of non-linearity and possibly discontinuities, especially if objective function values are calculated with the aid of complex simulation or integrated assessment models (Hamilton et al., 2015).

Although increasing the difficulty of the optimization problem, the presence of multiple local optima with similar objective function values in the fitness landscape can be either advantageous or disadvantageous from a practical perspective. A potential advantage is the provision of choice (diversity) to decision-makers in relation to which option to implement based on factors not formally considered during the optimization. For example, if there are a number of equally “good” management options, these can be fed into a participatory decision-making process to determine which should be implemented. However, the existence of multiple local optima with similar objective function values in the fitness landscape creates problems with model identifiability during model calibration (Shin et al., 2015), as it is difficult to determine which set of model parameters is the “correct” one. Another potential complicating factor related to model calibration is that the global optimum in the fitness landscape might not necessarily correspond to the model parameterization that results in the model that best represents the underlying physical processes. This is because for model calibration problems, the fitness landscape is a function of which error measure is used, how much data are available for calibration and which subset of the available data are used for model

calibration and which subset for model validation (e.g. see Zheng et al., 2018), all of which can have a significant impact on the properties of the fitness landscape.

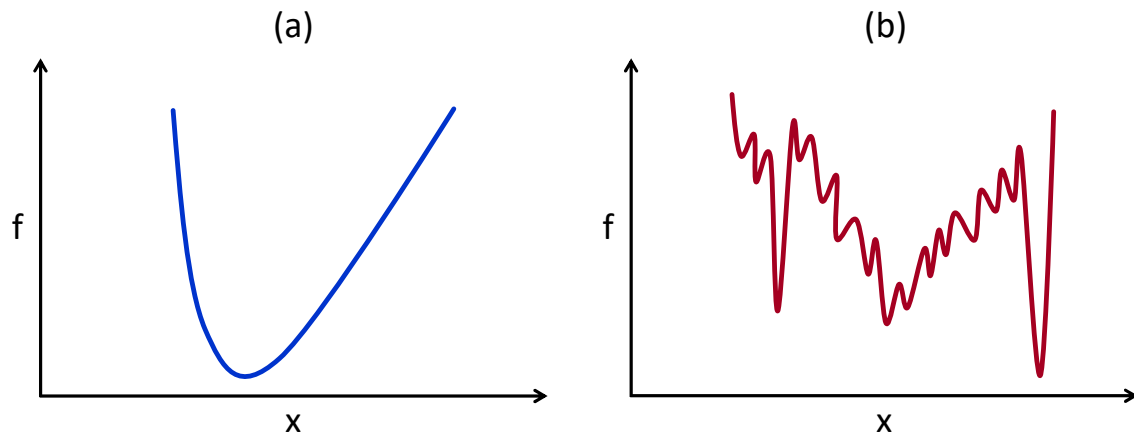


Figure 6. Illustrations of smooth (a) and rugged (b) fitness landscapes for minimization problems, where f represents an objective function and x represents a decision variable.

3. The behaviour of the search method. How well a search space of a particular size and ruggedness can be explored, both in terms of the ability to find globally optimal or near-globally optimal solutions and the computational efficiency with which this is achieved, is a function of the way a particular optimization algorithm navigates the fitness landscape(s). All optimization algorithms generally search the fitness landscape(s) in a stepwise fashion, starting from a random point and making incremental improvements over a number of iterations, as formalized in Equation 4 below, with the only difference between optimization algorithms being the mechanism that is used to decide how to make adjustments to the decision variables from one iteration to the next (i.e. $\Delta \mathbf{x}_{t-1}$). If we write

$$\mathbf{x}_t = \mathbf{x}_{t-1} + \Delta \mathbf{x}_{t-1} \quad (4)$$

where t denotes the iteration number, then \mathbf{x}_{t-1} is the vector of decision variables (solutions) in the previous iteration, \mathbf{x}_t is the updated vector of decision variables, and $\Delta \mathbf{x}_{t-1}$ denotes the change in the vector of decision variables from one iteration to the next.

The adjustment mechanisms used by different optimization algorithms are generally characterised by two competing processes: diversification (exploration) and intensification (exploitation). The goal of diversification is to explore the search space as widely as possible. This is an advantage if the search space is rugged and characterised by a large number of local optima, as illustrated in Figure 6b, so that the region containing the global optimum can be found. This is particularly important for large search spaces. However, an algorithm that explores more than is needed is less computationally efficient and, while it might be able to find the region of the search space that contains the global optimum, it might not be able to converge on this solution.

The goal of intensification is to exploit any information about the fitness landscape in order to converge to good solutions as quickly as possible. This works well for relatively smooth fitness landscapes, such as the one illustrated in Figure 6a, as globally optimal solutions can be identified in a computationally efficient manner. However, for rugged fitness landscapes (Figure 6b), exploitative searching behaviour generally results in convergence to local optima that are in the vicinity of the starting position of the search, as there is insufficient exploration of other regions of the search space. Consequently, for rugged fitness landscapes, the performance of algorithms that exhibit exploitative behaviour can be highly variable, depending on the starting position in the search space.

4. Why should we use Evolutionary Algorithms?

There are a number of reasons why EAs are a good choice for finding optimal solutions to environmental problems, as discussed below.

EAs are able to find (near-) globally optimal solutions: A major advantage of EAs is that they are population-based. This is analogous to having an entire search party exploring the fitness landscape(s) on the lookout for the globally optimal solution(s), rather than a single person. As a result, large and rugged search spaces can be explored more effectively and efficiently because the use of a search party, rather than a single person, enables a greater area of the search space to be covered. In addition, the members of the search party often exchange and share information with each other using a range of mechanisms (see Sections 5 and 6), enabling promising regions of the search space to be identified more effectively and subsequently enabling the search to be concentrated in these regions.

The searching behaviour of EAs can be customised to the problem under consideration: EAs have the ability to be tuned to determine $\Delta\mathbf{x}_{t-1}$ values (Equation 4) that represent an appropriate balance between exploration (diversification) and exploitation (intensification), depending on the properties of the fitness landscape (i.e. the problem under consideration). This enables EAs to escape local optima in the fitness landscape, while still being able to converge relatively quickly (to global, or near-global, optima). In contrast, most conventional optimization algorithms do not have this ability.

For example, gradient methods, which are a classical optimization strategy, calculate $\Delta\mathbf{x}_{t-1}$ as a function of the local gradient of the current solution (\mathbf{x}_{t-1}) in the fitness landscape and a step size (Figure 7a). Consequently, gradient-based methods exhibit a high degree of exploitation (intensification) and therefore only search locally in certain regions of the fitness landscape, but they do not have the ability to escape local optima. In contrast, as part of traditionally used random search strategies, $\Delta\mathbf{x}_{t-1}$ is chosen randomly by sampling the feasible space, as shown in Figure 7b. Consequently, this strategy exhibits a high degree of exploration (diversification), enabling larger areas of the fitness landscape to be searched, but does not have the ability to converge to good solutions.

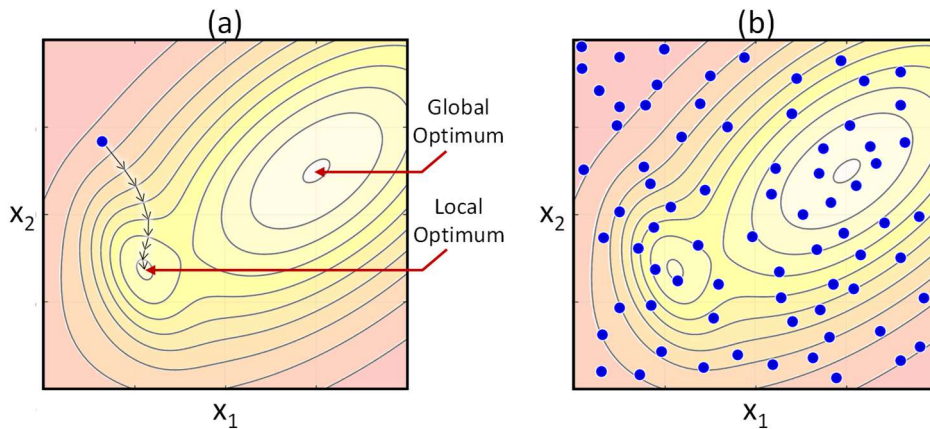


Figure 7. Examples of (a) search using a gradient-based approach, and (b) random (exhaustive) search that “blindly” samples the search space. Here, the response surface of Figure 1 is shown as contour plots.

The fact that these more traditional optimization algorithms exhibit fixed searching behaviours that cannot be tailored to match the characteristics of the fitness landscape limits their range of applicability, as they are generally only suited to certain types of problems. For example, gradient-based methods are generally only suited to problems with relatively smooth fitness landscapes with a single basin of attraction (see Figure 6a), whereas random search methods are generally only suited to problems with very rough and unstructured search spaces (see Figure 6b). However, as mentioned previously, the searching behaviour of EAs can be adjusted to achieve the most appropriate balance between diversification and intensification for the problem under consideration.

EAs are easily linked with (existing) simulation models: One of the greatest advantages of using EAs is that they can be easily linked with existing simulation and integrated assessment models (see Section 8). This can be achieved in a straightforward manner, only requiring a two-way coupling between the optimization algorithm and an (existing) simulation model (Figure 8). In the coupling, (i) the optimization algorithm determines decision variable values that are passed to the simulation model, (ii) the simulation model evaluates the corresponding objective function and constraint values and (iii) the objective function and constraint values are passed back to the optimization algorithm. Consequently, if the performance of a system can be simulated using an existing model, it can also be optimized using EAs. This facilitates the comparison of solutions created via informal optimization (using the simulation model as an engine) with the solutions coming from the EA optimization process, which can aid in users’ trust of the optimization results (Smith et al., 2015).

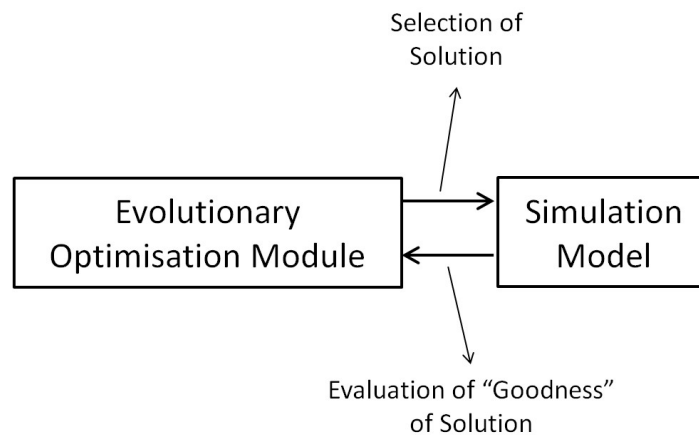


Figure 8. Illustration of coupling between the evolutionary optimization module and the simulation model, where the optimization module can be “bolted onto” any simulation model. The optimization module identifies which solutions to try and passes these to the simulation model, which evaluates the utility of these solutions (i.e., objective function and constraints). This information is passed back to the optimization module, where it is used to determine which solutions to try next.

An implication of this is that EAs have a wider range of applicability compared with many more traditional optimization approaches, such as linear programming (Md. Azamathulla et al., 2008) and gradient-based methods (Kessler and Shamir, 1989). For example:

- Linear programming works when the objective function and constraints are linear, while many environmental processes are highly non-linear. Therefore, when linear programming is used, the outputs from simulation models can generally not be used directly, and instead, a simplified (linear approximation) version of the problem has to be solved. In this way, although linear programming is very computationally efficient and guaranteed to find the globally optimal solution, the solution that is found is generally not to the actual problem (unless the problem is linear), but a simplified version of the problem.
- When gradient methods are used, information about the gradient of the fitness function is used to decide in which direction the search should proceed (i.e., how $\Delta \mathbf{x}_{t+1}$ is determined), as mentioned previously. However, the gradient (derivative) information of environmental models is not typically available, requiring the derivative of the objective function to be approximated numerically. This increases the computational demand, as many more objective function values (i.e., model runs) need to be evaluated. In addition, in fitness landscapes with significant roughness/noise (small-scale features that might be due to simulation model errors), the resulting derivative information might be deceptive and misguide the search. Related to this, the objective function might be non-differentiable (e.g. due to discontinuity) in some areas of the feasible space. The derivative-free nature of EAs, however, makes them insensitive to possible discontinuity and ruggedness in fitness landscapes.

The way EAs are used is intuitive: The application of EAs is intuitive, as the optimization process that is used mirrors the informal optimization process adopted when using simulation models to assist with the identification of solutions to environmental problems (Figure 2). The major difference between the informal optimization process in Figure 2 and the formal EA-based optimization process is in how solutions are altered (i.e., how $\Delta\mathbf{x}_{t-1}$ is obtained). As part of informal optimization processes, values of $\Delta\mathbf{x}_{t-1}$ are obtained using personal domain knowledge, experience and intuition, but in the EA-based process, these changes in decision variable values from one iteration to the next are obtained automatically with the aid of evolutionary operators (Figure 9). The operators are generally based on optimization strategies found in nature, such as survival of the fittest, although this is not always the case (see Sections 5 and 6 for details).

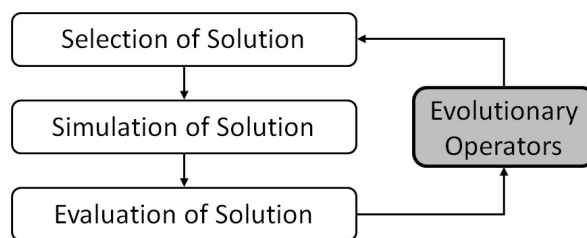


Figure 9. Process of identifying optimal solutions when evolutionary algorithms are used.

EAs are applicable to discrete and continuous decision variables: Another advantage of EAs is that they can generally work with both discrete and continuous decision variables, as opposed to most traditional optimization methods, which require continuous decision variables (exceptions include integer programming (Samani and Mottaghi, 2006) and combinatorial optimization methods (Da Conceição Cunha and Sousa, 1999)). This is of benefit for a large number of real-world applications where decision variables are either categorical (e.g. distinct crop choices, distinct infrastructure options) or where continuous variables are constrained by practical considerations (e.g. pipes are only manufactured in discrete diameters, wasteload reduction levels are aligned with particular treatment processes). However, while EAs can cater to both discrete and continuous variables, the mechanisms that aim to improve solution quality from one iteration to the next are different for discrete and continuous variables, requiring these mechanisms to be implemented in a single algorithm, as is done for example in the Exploratory Modeling Workbench (Kwakkel, 2017), the Water System Multi Objective Genetic Algorithm (WSMGA) (<https://github.com/jeffrey-newman/WSMGA-with-Wrapper-and-Analytics>; Wu et al., 2010b) and the mixed integer implementation of the Pareto Archived Dynamically Dimensioned Search algorithm applied in Tolson et al. (2012).

EAs can handle constraints in a straightforward manner: Constraint handling in EAs is easy and straightforward. The most common approach to handling constraints is to use penalty functions. The idea is to transform a constrained optimization problem into an unconstrained problem by adding a penalty value to the objective function based on the amount of constraint violation of a candidate solution (see Section 5.3). As reviewed by (Coello, 2002), there are other constraint handling techniques that work well, such as restricted tournament selection for multi-objective optimization,

in which the feasibility of solutions is integrated into the selection procedure (see Section 5.3 for details, especially Figure 13).

EAs have the ability to deal with multiple objectives simultaneously: Many traditional approaches to solving multi-objective optimization problems merge the different fitness landscapes into one, typically through their weighted summation based on their perceived importance, thereby turning a multi-objective optimization problem into a single objective problem. Such approaches, however, limit any insights that can be gained into the problem and its solutions, as trade-offs between objectives are not able to be explored. EAs, however, are able to overcome this limitation, as they typically have multi-objective analogues. Such analogues navigate multiple fitness landscapes simultaneously during the optimization process and are able to approximate Pareto fronts in a single algorithm run, as explained in Section 3.2.

EAs are easily parallelizable: EAs are naturally suited to being implemented in parallel computing environments. At each generation, individual solutions in the population can be evaluated in parallel on multiple processors to accelerate the search. This can result in a significant saving in (computational) time, compared with most traditional optimization methods, where candidate solutions would have to be evaluated serially during the search.

EAs are not prescriptive: As EAs work with populations of solutions, they produce a number of near-optimal solutions, which might be similar in objective function space, but quite different in decision variable space (either for single- or multi-objective problems). This enables consideration of factors other than those captured in the mathematical formulation of the optimization problem when selecting the final “optimal” solution. As a result, decision-makers have greater control in terms of using their judgement and intuition to select the final solution based on a number of good solutions “suggested” by the optimization algorithm (Di Matteo et al., 2017b). In this way, EAs are used to assist with “sifting through” the very large solution spaces that are a feature of environmental problems (see Table 1) in order to identify a set of near-optimal candidate solutions that can then be scrutinized by decision-makers to identify those that make most sense, either informally or with the aid of multi-criteria decision analysis methods (e.g. Hyde and Maier, 2006).

EAs result in increased trust in optimization results: The fact that the evaluation of objectives and constraints when EAs are used is based on the outputs of (existing) environmental simulation models, and that the iterative process of identifying improved solutions mimics that used by experienced environmental modellers, reduces the black-box nature of the optimization process and increases trust in the optimal solutions identified. This is in contrast to the use of more traditional optimization methods, such as linear programming, where simplified versions of existing models are likely to be used, the application of which is unlikely to evoke the same level of trust. The fact that solutions are not “prescriptive”, as outlined above, is also likely to increase trust in the overall optimization process. However, the degree to which the solutions developed with the aid of simulation-optimization approaches are trusted is likely to be a function of the degree to which decision-makers are familiar with and trust the simulation model, especially if the optimal solutions do not correspond with expectations (Di Matteo et al., 2018).

5. How do Single Objective EAs and other Metaheuristics work?

As mentioned previously, EAs are similar to many conventional optimization algorithms in that they update decision variable values in an iterative fashion (Equation 4) in order to identify solutions that optimize the objective function. However, as shown in the high-level pseudo-code for single-objective EAs below, they work with populations of solutions, rather than a single solution, as discussed in Section 4, and update decision variable values using heuristic operators. These operators can vary significantly between different types of EAs, but are usually inspired by examples from nature. In general, there are two major philosophies for determining $\Delta\mathbf{x}_{t-1}$, “evolutionary computation” and “swarm intelligence”. The former, such as Genetic Algorithms (GAs) (Goldberg, 1989), was inspired by biological evolution, such as selection, recombination (crossover), and mutation, while the latter, such as Particle Swarm Optimization (PSO) (Kennedy and Eberhart, 1995) and Ant Colony Optimization (ACO) (Dorigo et al., 1996), was inspired by the collective social behaviour of natural organisms such as birds, ants, and fish.

A range of “operators” has been developed over the past decades to mimic the functioning of these natural systems for optimization purposes. An EA utilizes a collection of such operators that work together to determine $\Delta\mathbf{x}_{t-1}$ intelligently based on feedback from the performance of the solutions generated in the previous iteration (Figure 9), while keeping “some” balance between diversification and intensification. The relative degree of exploration and exploitation of the search is adjusted by changing the values of a number of parameters that control the function of these operators, which can be done in a variety of ways (see e.g. Zheng et al., 2017).

A high-level pseudo-code for single-objective EAs

- Generate an initial population of solutions, \mathbf{x}_0 , and evaluate their fitness
- REPEAT
 - Generate a new population, \mathbf{x}_t , by updating \mathbf{x}_{t-1} using heuristic operators (e.g. evolution operators including selection, recombination, and mutation that focus on the best solutions in the set so far)
 - Evaluate the fitness of solutions in the new population by using the simulation model to evaluate the fitness function
- UNTIL stopping criteria are met

In general, as shown in Figure 10 for an example with a 2-dimensional fitness landscape, EAs begin with a randomly distributed initial population (Figure 10a) and an exploration-oriented search in the first iterations to locate the main regions of attraction (Figure 10b). As the search continues, it becomes more exploitation-oriented in the regions of attraction, and identifies the best solution in the final iteration (Figure 10c). Examples of how this is achieved using evolutionary computation- and swarm intelligence-based algorithms are given in Sections 5.1 and 5.2, respectively.

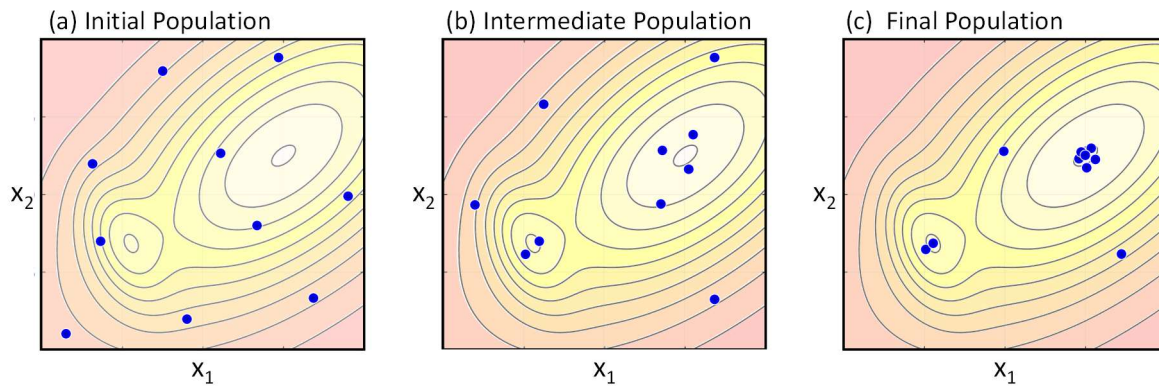


Figure 10. An example performance of an evolutionary algorithm. Plot (a) shown an initial population of solutions randomly distributed in the decision variable space (population size=10). Plot (b) shows the “evolving” population after a limited number of generations where both regions of attraction have been identified. Plot (c) shows the final population that has converged to the global optimum.

5.1 Genetic algorithms

Figure 11 shows how a set of operators works consecutively to determine $\Delta \mathbf{x}_{t-1}$ in Genetic Algorithms (GAs). Individual solutions (sets of decision variables) of a population and their individual decision variables are analogous to chromosomes (or genotypes) and genes, respectively. To update the current population, the algorithm utilizes some “selection” operator to repeatedly select parent chromosomes (a pair of individual solutions) from the current population, typically based on their fitness function. The selected parent chromosomes are then used for breeding via some “crossover” and “mutation” operators, and the resulting pair of offspring are used to form the next-generation population.

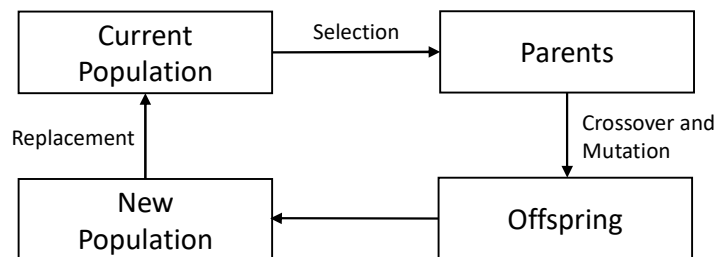


Figure 11. Genetic heuristic operators for population updating in EAs

A selection operator is generally based on the “survival of the fittest” concept from Darwinian evolution theory and picks probabilistically the fittest candidate solutions (best in terms of objective function) in the current population for breeding. An example selection operator is called “Roulette wheel”, named after a casino game for gambling, where the fitness level is used to associate a probability of selection to each candidate solution of the population. Alternatively, fitter candidate solutions can be identified by comparing the fitness of a subset of solutions (usually pairs) in

“tournaments”, with the winner of the tournament selected for reproduction. Selection can also directly carry over the best solution(s) in a population to the next. This mechanism is called “elitism” and is to guarantee that solution quality will not degrade during optimization. Overall, selection promotes intensification during search.

When two parent solutions are selected, the crossover operator is applied to reproduce two offspring solutions. Figure 12a shows two parent solutions (chromosomes) i and j of a 5-decision variable problem (5 genes) where a “single-point crossover” is applied. In this crossover, a single point on the chromosomes is selected randomly, and all genes (decision variable values) beyond that point are swapped between the two parents to reproduce the two offspring. Figure 12c illustrates how a single-point crossover operator functions with 2 decision variables on the fitness landscape of Figure 10. Crossover operators may work for both intensification and diversification during the search, depending on the type of the crossover operator and the locations of parents with respect to each other.

A mutation operator may be applied to mutate a small number of offspring that resulted from the crossover. Figure 12b shows an example mutation where one of the decision variables (genes) is randomly selected and replaced by a uniformly distributed random number in its feasible range. Figure 12d illustrates how this mutation works in the 2-decision variable space where x_1 is mutated. Mutation works to preserve and introduce diversity during the search. It enables the EA to escape local optima.

The heuristic operators above can be easily applied to both continuous and discrete problems. In case of continuous problems, such as model calibration, the procedure explained above directly applies to model parameters that can be varied within their feasible ranges. In case of discrete problems, such as water distribution system design where the optimal size of pipes is of interest, the feasible range of each decision variable is reduced to a set of possible values (e.g. commercially available pipe sizes) that can be directly incorporated into the procedure. For example, for mutation of Figure 12b, the pipe size can be directly replaced by another pipe size chosen randomly from the available set of pipe sizes. Further details on GAs can be found in Holland (1975), Goldberg (1989), Michalewicz (1992) Coley (1999), Nicklow et al. (2009) and Maier et al. (2014).

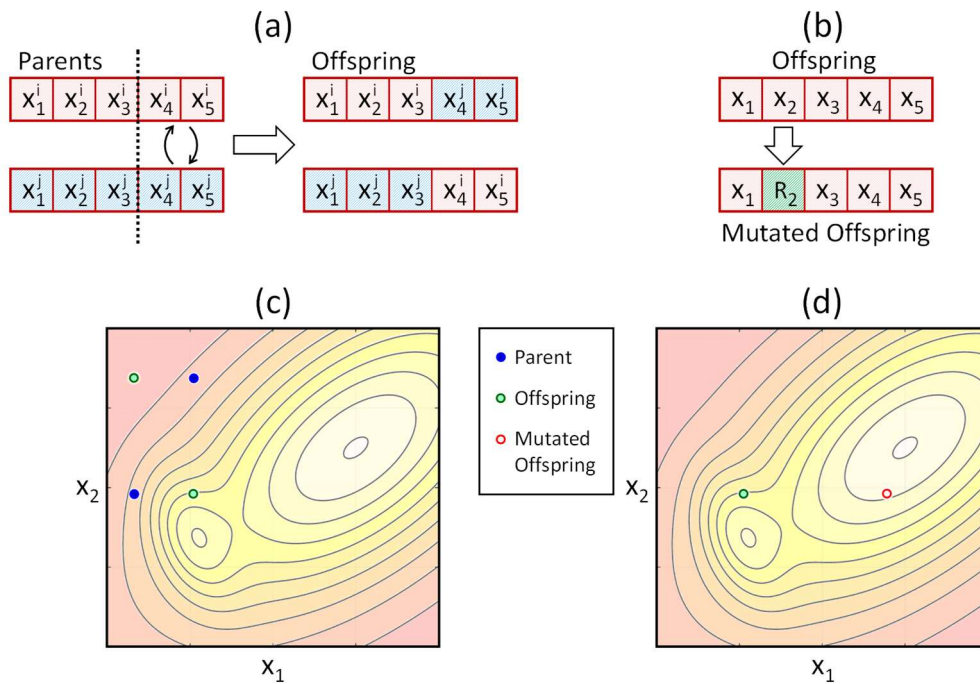


Figure 12. Example crossover and mutation operators and their performance on a fitness landscape. (a) Single-point crossover that reproduces two offspring from two parents in a 5D decision variable space. (b) Uniform mutation that replaces the value of a decision variable by a uniformly distributed random number between the variable lower and upper bounds ($R_2 = \text{random number in } [x_{2l}, x_{2u}]$). Example outcome of (c) single-point crossover and (d) uniform mutation in a 2D decision variable space.

5.2 Ant colony optimization algorithms

In contrast to GAs, in ACO algorithms (ACOs), the evolutionary operators are not applied to solutions directly. Instead, the solution space is modified to encourage the selection of decision variable values that have resulted in good solutions in previous iterations. As a result, completely new solutions are generated in each iteration, rather than modifying solutions from previous iterations.

This searching behaviour is inspired by the way colonies of ants look for food in nature. As part of this process, ants deposit pheromone, leaving trails, and other ants are more likely to follow trails with higher concentrations of pheromone. As shorter paths between a colony's nest and a food source can be traversed more quickly, shorter paths receive more pheromone per unit time, encouraging more ants to follow this path, further increasing its pheromone concentration. In this way, a positive feedback loop is created, reinforcing shorter paths (i.e. better solutions) from one iteration to the next. At the same time, the attractiveness of longer paths diminishes over time due to pheromone evaporation.

When using ACO to identify optimal solutions to environmental problems, the values particular decision variables can take correspond to the different paths ants can traverse (e.g. Golding et al., 2017; Nguyen et al., 2016; Szemis et al., 2012). As these paths are discrete, the decision variable options also have to be discrete, which requires continuous decision variables to be discretized using

an appropriate resolution. In the example in Figure 13, there are two decision variables, X_1 and X_2 , each of which can take on nine discrete values (i.e. $X_{1,1}, X_{1,2}, \dots, X_{1,9}; X_{2,1}, X_{2,2}, \dots, X_{2,9}$). At the beginning of the optimization process, the same pheromone concentrations are assigned to all decision variable options, as indicated by the same thickness of blue shading for each of the nine paths for both decision variables in Figure 13a. As the optimization process progresses, decision variable options (i.e. paths) that result in better solutions (i.e. better objective function values) receive more pheromone, increasing their chances of being selected in subsequent iterations, creating the positive reinforcement loop observed in nature. Consequently, at the end of the optimization process, the paths that result in the globally optimal solution have significantly larger pheromone concentrations than the other paths, as shown in Figure 13b (i.e. the paths corresponding to decision variable options ($X_{1,7}$ and $X_{2,6}$)).

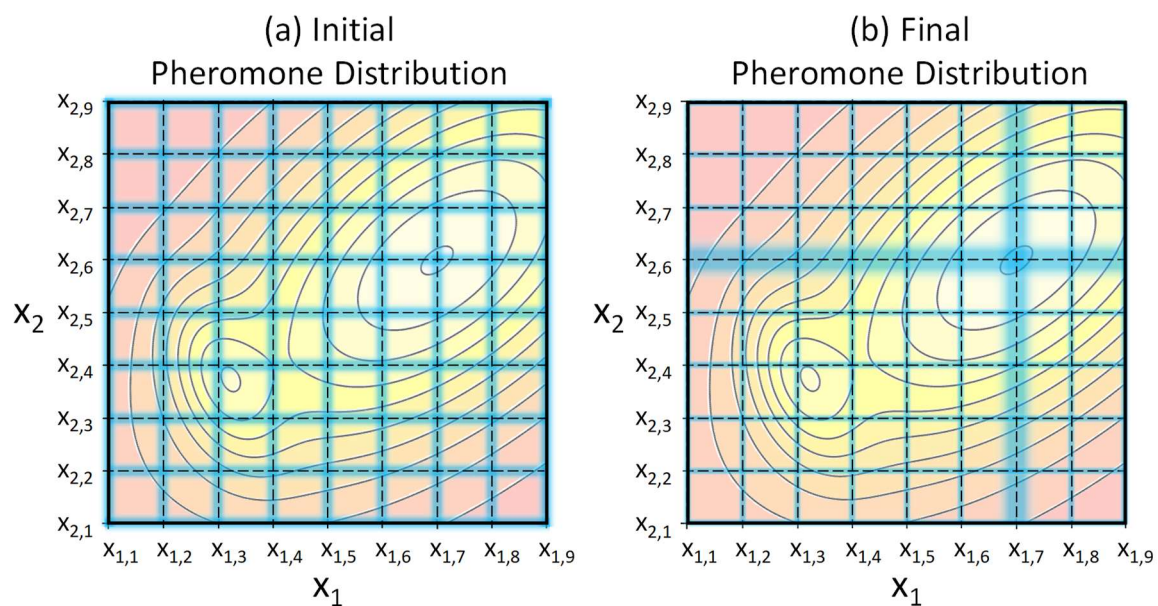


Figure 13. Illustration of the evolution of pheromone concentrations over a large number of iterations, where the thickness of the blue shading of the paths corresponding to discrete decision variable choices corresponds to pheromone concentration. As can be seen, the discrete values of X_1 and X_2 that correspond to the globally optimal solution (i.e. $X_{1,7}$ and $X_{2,6}$) have higher pheromone concentrations during the final iteration, thereby increasing the probability that these decision variable values will be selected.

At each iteration of the optimization process, decision variable options (i.e. paths) are selected as a function of the relative pheromone concentrations on different paths. A common way of achieving this is by using a biased roulette wheel, although the way the probabilities of selecting a particular path are calculated generally varies between algorithms (Dorigo and Gambardella, 1997; Dorigo et al., 1996). For example, in many algorithms, these probabilities are often also a function of a preference for locally optimal solutions (i.e. decision variable values that are known to increase objective function values (for a maximization problem)), in addition to pheromone levels, with the relative contribution

of these two mechanisms based on user-selected weightings. Once paths have been selected for each decision variable, a trial solution to the problem under consideration has been obtained. In general, a number of solutions is obtained in each iteration, which is akin to the size of the ant colony in natural systems and is equivalent to the population size in GAs.

The way pheromone levels on each of the paths are updated from one iteration to the next is generally a function of the quality of the solutions obtained, where paths that contribute to solutions with better objective function values receive a greater amount of pheromone than paths that contribute to poorer quality solutions. The specific way in which this is achieved varies between algorithms, where some algorithms use information from all ants in the colony, while others only use information from ants that select high-performing solutions (Bullnheimer et al., 1999; Dorigo et al., 1996; Stützle and Hoos, 2000). Further details on ACO algorithms and their applications can be found in Dorigo et al. (1996), Stützle and Hoos (2000), Dorigo et al. (2006), García-Martínez et al. (2007), Zecchin et al. (2007) and Afshar et al. (2015).

5.3 Constraint handling

The design of EAs and other metaheuristics is typically such that they can search for optimal solutions in a hypercube decision space, where there are only bound constraints (see Equation 3). In some cases, the design of an algorithm functions naturally to respect bound constraints (e.g. binary decision variable problem solved with a GA). However, in many algorithms, some special constraint handling procedures, often invisible to users, are required to respect bound constraints. If during the search a generated solution goes beyond a bound, it may be rejected (and a new solution would be generated), absorbed to the bound, or reflected back into the hypercube. Figure 14 shows an example with these three simple “constraint handling” mechanisms for bound constraints.

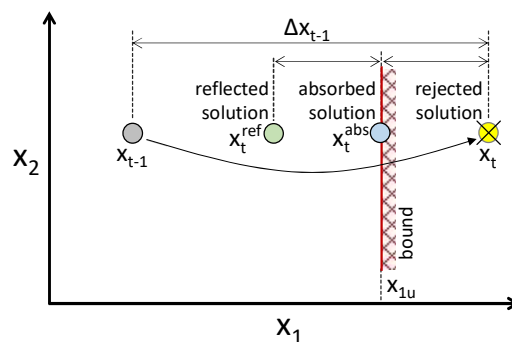


Figure 14. Bound constraint handling in metaheuristic optimization. Three strategies are shown: 1- the new solution violating the constraint is rejected in order to generate another new solution, 2- the new solution is modified and absorbed to the bound, and 3- the new solution is modified and reflected by the bound.

The ability to handle other types of constraints (see Equation 2) may not be as straightforward. In general, the “rejecting” approach is the simplest but most inefficient way of handling any type of constraint. With this approach, any candidate solution that violates a constraint will be rejected and

removed from the search and the degree of constraint violation is not considered. An efficient, and perhaps the most popular, way of handling any type of constraint is the “penalizing” approach. In this general-purpose approach, which is also referred to as the “penalty function” approach, a penalty function is defined to quantify the degree of infeasibility (constraint violation) of an infeasible solution and penalize it proportionally. In this way, the constraint is removed from the optimization formulation, and instead, a corresponding penalty function is integrated into to the objective function. This integration is typically by weighted averaging with a carefully chosen weight for the penalty function. In practice, the user may need to identify the appropriate penalty function and corresponding weights via trial and error.

6. How do Multi-Objective EAs work?

The searching mechanisms of multi-objective EAs (MOEAs) are based on the same basic principles that underpin single objective EAs. However, as shown in the high-level pseudo-code below, a major difference between the two is in the way they evaluate the fitness of a solution. Unlike single-objective optimization, where fitness evaluation is straightforward and is performed simply by evaluating a single objective function, multi-objective optimization requires a more elaborate “fitness assignment” scheme that brings together and unifies the different objective functions. Fitness assignment is a major component of multi-objective EAs and other metaheuristics and basically refers to the process of translating a vector of objective function values into a scalar-valued fitness that can be used for ranking and selecting solutions of higher quality during the course of the search.

A high-level pseudo-code for multi-objective EAs

- Generate an initial population of solutions, \mathbf{x}_0 , and assign their fitness using code a
- REPEAT
 - Generate a new population, \mathbf{x}_t , by updating \mathbf{x}_{t-1} using heuristic operators (e.g. evolution operators including selection, recombination, and mutation)
 - Assign the fitness of solutions in the new population using code A below
- UNTIL stopping criteria are met
- Return the non-dominated solutions in the current population and respective fitness functions

A: Sub-pseudo-code for fitness assignment in multi-objective EAs

- Evaluate the multiple fitness functions for each solution
- Rank the solutions based on their dominance and density

There are different strategies for fitness assignment, but these are generally based on the dominance concept illustrated in Section 3. The idea is to rank candidate solutions based on their dominance strength in objective space and to use the rank numbers of the solutions as their respective fitness values. Figure 15 shows three strategies for ranking the solutions in a population, namely “dominance depth”, “dominance rank” and “dominance count”. In the dominance depth strategy (e.g., used in

NSGA-II developed by Deb et al., 2000), the solutions in a population are grouped into multiple fronts. The non-dominated solutions form the first front and receive rank 1, and the remaining solutions that are non-dominated by all solutions, excluding the solutions on the first front, form the second front and receive rank 2. This will continue to the third and higher fronts. In this strategy, candidate solutions lying on the same front are deemed equally fit. In the dominance rank strategy, the fitness of any given solution is the number of other solutions that dominate that solution (e.g., used in MOGA developed by Fonseca and Fleming, 1993); while in the dominance count strategy, fitness of a given solution is defined as the number of other solutions this solution dominates (e.g., used in SPEA2 developed by Zitzler et al., 2002). Readers may refer Zitzler et al. (2004) for more details on the different fitness assignment strategies for multi-objective optimization.

In multi-objective EAs, diversification is not limited to the decision-variable space. It is also important to introduce diversity in the objective space (see Figure 16) to diversify the optimal solutions and spread them uniformly on the Pareto front. This is because the purpose of the optimization process is not to identify a single, optimal solution, but to identify a set of optimal solutions that are distributed with a uniform “density” over the Pareto front. For this purpose, “crowding distance”, which is a measure to estimate the density of solutions surrounding any given point in the objective space, is often used to encourage solutions to “spread out”. Accurately stated, in a bi-objective space, the crowding distance of a solution is defined as one half of the circumference of the rectangle formed by the two neighbouring solutions of the same front on either side of that solution (Figure 16). In addition, the three ranking strategies in Figure 15 may result in multiple solutions receiving the same rank, while EAs may need to differentiate such solutions in the process of selection. For example, in the dominance depth strategy, all solutions lying on the same front would be seen equally. In this case, *density*, as quantified, for example, by crowding distance, can be used for a second-level fitness assignment of these solutions, indicating that solutions lying on the same front, but with larger crowding distance, would receive a higher fitness value (i.e., a higher chance to be selected).

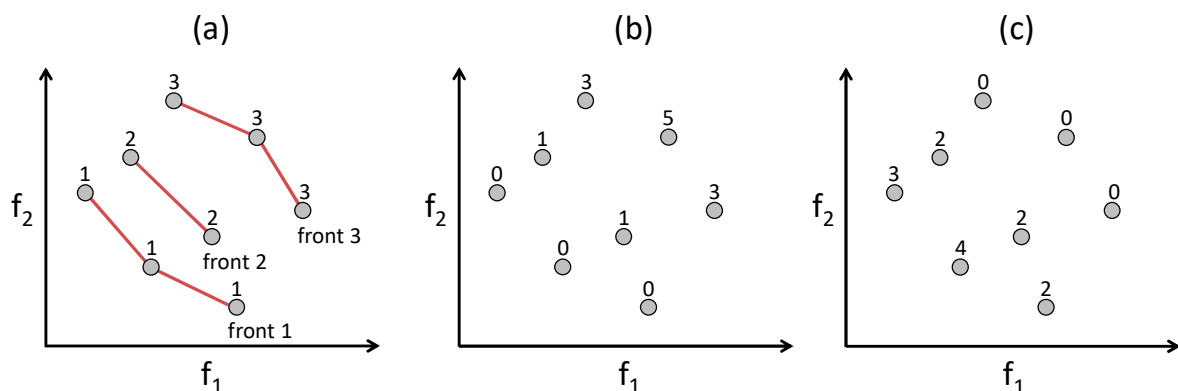


Figure 15. Strategies for dominance-based ranking (fitness assignment) of candidate solutions in the objective space: (a) dominance depth, (b) dominance rank, and (c) dominance count. The number by each candidate solution is the associated rank to that solution; in (a) and (b), a smaller number indicates a better solution, while in (c) a larger number indicates a better solution

Unlike the above strategies for MOEAs, some other algorithms take a more simplified approach and only search from dominance rank 1 (nondominated solutions). That is, the population or set of current solutions maintained during the search only contains those that are currently non-dominated. Two examples would be PAES and PADDs (Asadzadeh and Tolson, 2013; Asadzadeh and Tolson, 2009; Knowles and Corne, 2000). In both of these algorithms, a measure such as crowding distance is utilized to influence algorithm trajectory when preference between two or more non-dominated solutions is required.

It should be noted that the number of Pareto-optimal solutions increases with an increase in the number of objective functions. This is because all of the Pareto-optimal solutions of a k -objective optimization problem would remain Pareto optimal in the same problem with additional objective functions, while any additional objective function would introduce a new dimension in the objective space and extend the Pareto front. So as more objectives are added to a problem, the proportion of feasible solutions being Pareto-optimal also increases. This increase limits the ability of MOEAs (and any multi-objective algorithm) to accurately approximate high dimensional Pareto fronts and as such, the application of MOEAs is often limited to two or three objectives. Further details on MOEAs and their applications can be found in Coello et al. (2007), Deb (2001), Nicklow et al. (2009) and Reed et al. (2013).

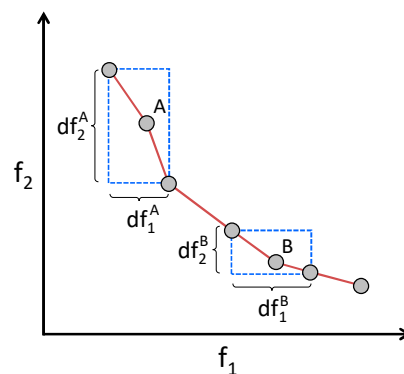


Figure 16. Ranking of solutions lying on the same front by crowding distance. The crowding distances of solutions A and B are $df_1^A + df_2^A$ and $df_1^B + df_2^B$, respectively. As crowding distance of A is larger than that of B, A will receive a better rank for selection.

7. What are the Challenges associated with using EAs?

While EAs have a number of advantages over more conventional optimization methods, as discussed in Section 4, they also present a number of additional challenges, especially related to computational efficiency and the adjustment of their searching behaviour.

Challenges with computational efficiency: As EAs work with populations of solutions and generally evolve better solutions over tens or hundreds of iterations, the number of times objective function and constraint values have to be calculated is the product of the population size and the number of iterations. This can make their use computationally demanding, especially if objective function and/or constraint values are obtained with the aid of environmental models. The application of EAs to complex, real-world problems are of particular concern in this regard, as (i) model run-times can be in

the order of minutes or even hours and (ii) search spaces can be extremely large and rugged, requiring larger population sizes and/or numbers of generations in order to find good solutions. These computational challenges are exacerbated when considering uncertainties, as performance metrics such as risk, resilience, reliability or robustness (Hashimoto et al., 1982; McPhail et al., 2018) generally require simulation models to be run hundreds or even thousands of times during each iteration of the optimization process (Beh et al., 2017).

These computational challenges can be addressed using a number of strategies. A commonly used approach is replace computationally expensive simulation models with more efficient surrogate-, meta- or emulation- models (Razavi et al., 2012), which can increase the computational efficiency of EAs by one to two orders of magnitude (Beh et al., 2017; Broad et al., 2015b; Timani and Peralta, 2017). As EAs are easily parallelizable (see Section 4), the use of parallel computing can also be an effective means of reducing overall runtime (Newland et al., 2018; Tang et al., 2007). Depending on the type of the problem and the EA algorithm used, “pre-emption” strategies can be used to opportunistically evade running computationally expensive models during optimization (Asadzadeh et al., 2014; Razavi et al., 2010). Alternatively, the size and complexity of the optimization problem can be decreased by reducing the size of the search space (Fu et al., 2012) or re-formulating the optimization problem (Garner and Keller, 2018; Quinn et al., 2017).

Challenges with adjustment of searching behaviour: As mentioned in Section 4, one of the advantages of EAs is that their searching behaviour (i.e. their degree of diversification (exploration) and intensification (exploitation)) can be adjusted to match the properties of the fitness landscape for the problem under consideration. However, in practice, this can be a challenge, as the properties of the fitness landscape are unknown. As a result, the parameters that control the searching behaviour of EAs are commonly determined with the aid of extensive sensitivity analysis, although guidelines for the selection of appropriate parameters have been developed for some problem types (e.g. Gibbs et al., 2015; Zecchin et al., 2005). Alternatively, algorithm searching behaviour can be adjusted dynamically throughout the search by automatically adjusting (i) parameter values to achieve pre-determined searching behaviours (Hadka and Reed, 2013; Vrugt et al., 2009; Wang et al., 2017; Zheng et al., 2017) or (ii) the utilisation rate of different operators in response to algorithm performance (Hadka and Reed, 2013; Vrugt et al., 2009; Wang et al., 2017; Zheng et al., 2017).

8. How do we Implement EAs?

A typical implementation strategy for the workflow described by Figure 8 is to view the search algorithm and simulation model as “black box” components that are coupled via an I/O (input/output) interface. This I/O interface manages run-time execution and data transfers of both the algorithm and the simulation model. As discussed in Section 4 (e.g. see Figure 8), data transfer consists of preparing model input and processing model output and can be accomplished by reading and writing files or by in-memory or inter-process communication.

As summarized by Matott et al. (2009), a number of software packages have been built using the black box approach described above, and such packages typically support multiple algorithms and may be written in compiled (i.e., C/C++ or FORTRAN) or interpreted (i.e., R, Python, or MATLAB) languages. Figure 17 illustrates a black-box approach to implementing EAs. As indicated in Figure 16, the primary operators of the optimizer (e.g. elitism, selection, crossover and mutation) are invariant with respect

to the simulation model and linkage between the optimizer and simulation model is only required for evaluation of the fitness of the population of each generation.

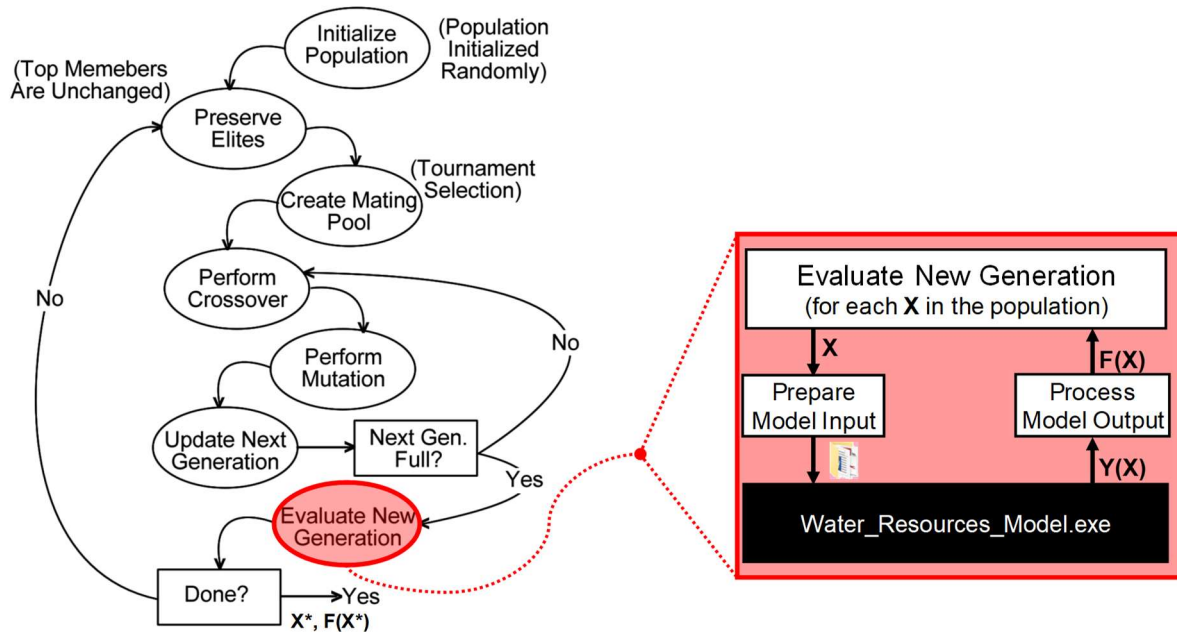


Figure 17. Illustration of the 'black-box' approach to linking an evolutionary algorithm with a water resources model. \mathbf{x} and $f(\mathbf{x})$ are as described in equations 1-3 (see Section 3.1) and $\mathbf{y}(\mathbf{x})$ represents a set of model outputs (response variables) that are computed as a function of the decision variables (i.e. \mathbf{x}) represents a vector of objective functions and/or constraints that are to be optimized and which are computed using the model outputs.

In addition to standalone EA packages, there has been a variety of APIs (application programming interfaces) and libraries developed to support EA implementations (e.g. Hadka, 2016; Wilhelmstötter, 2018). These APIs and libraries generally prescribe a specific I/O interface that will ensure interchangeability and interoperability across algorithms implemented using a given API or library. In this way, libraries and APIs foster a community of practice with respect to EA implementation and their adoption is highly encouraged for advanced users.

The difficulty of comparing alternative algorithm implementations and of assessing incremental changes to a given algorithm is now being increasingly recognized (e.g. Hansen et al., 2016; Sörensen, 2013; Weyland, 2012, 2015). This has led some algorithm developers to formalize “standard” algorithm implementations that can be used to establish the expected baseline reference behaviour and performance of a given algorithm (Bratton and Kennedy, 2007; Swan et al., 2015).

The choice of programming language for implementing an EA algorithm is typically made pragmatically based on the historical preferences and experience of the code developer. In general, compiled languages are capable of delivering significantly better computational performance, relative to interpreted languages. However, these effects are not likely to be significant within a given algorithm implementation since runs of the simulation model usually dominate the overall compute requirements of a given simulation-based optimization exercise.

As mentioned previously, EAs that iteratively operate on a population of candidate solutions sets are readily parallelized using distributed computing, whereby population members are evaluated simultaneously by a team of processors. These processors may reside on the same motherboard (e.g. in a typical desktop system), within the same rack or cluster of a data centre, within multiple data centres that are geographically separated, or, most generally, across multiple interconnected computing devices (e.g. desktops, laptops, tablets, and smartphones). In addition to choosing an appropriate communications interface (e.g. the message passing interface (MPI)(Gibson and Meter, 2000; Gropp et al., 2014), the sockets protocol, network attached storage (NAS), etc.) for relaying information between these processors, implementers must decide whether the processors should operate synchronously or asynchronously. Figure 18 illustrates the difference between the synchronous (left hand side of Figure 18) and asynchronous (right hand side of Figure 18) schemes in the context of evaluating the new generation of an EA using parallel computing.

As illustrated in Figure 18, in the synchronous mode of operation, each processor is assigned a set of a priori compute tasks and these are typically keyed to the processor's unique id. For example, processor 0 might always be responsible for evaluating the first 10 population members, with processor 1 assigned the next 10 members, and so on. While this approach minimizes inter-processor communication overhead, it can result in significant bottlenecks if simulation run times are markedly heterogeneous across the population members. For example, such heterogeneity can occur if model pre-emption is employed (Razavi et al., 2010). Consequently, some processors may take longer than others to complete a given round of evaluations, thereby forcing those that finish early to wait.

As shown in the right hand side of Figure 18, in the asynchronous mode of operation, one or more processors are designated as "managers" or "coordinators". These managers communicate asynchronously and on-demand with the remaining "worker" processors to assign compute tasks. This asynchronous approach entails more inter-processor communication overhead but has the benefit of minimizing the idle time of "worker" processors.

As the use of EAs enters into the state of practice, there has been increased interest in incorporating them into decision support systems and related integrated modelling frameworks (e.g. Babendreier and Castleton, 2005; Laniak et al., 2013). Such "meta-systems" involve complex modelling workflows that can include parameter estimation, uncertainty and sensitivity analysis, and design optimization. Ideally, these systems should be structured to accommodate varied programming languages, libraries and APIs. Furthermore, the execution management used within a given meta-system should be implemented in a manner that can exploit the inherent parallelism of EAs.

Looking to the future, various EA research directions and emerging technologies are already influencing their implementation in computer software. For example, the ubiquity of cloud computing has fostered the emergence of optimization as a service (OaaS) as a practical on-demand tool for decision makers to apply EAs to solve previously intractable problems (Broad et al., 2015a; Kurschl et al., 2014). Rapid and agile OaaS implementation is facilitated by portable and interpreted web-ready languages that support reflection and introspection (e.g. python, php, and javascript). Furthermore, researchers are in the early stages of exploring how EAs can best exploit exascale parallel computing technologies like accelerators and graphics processing units (GPUs) (Alonso, 2015; Cárdenas-Montes et al., 2016; Hadka and Reed, 2015). Finally, the development of hybridized EA algorithms is an

ongoing line of research (e.g. Hadka and Reed, 2013; Lozano and García-Martínez, 2010) that is likely to further motivate the desire for increased interoperability among EA implementations.

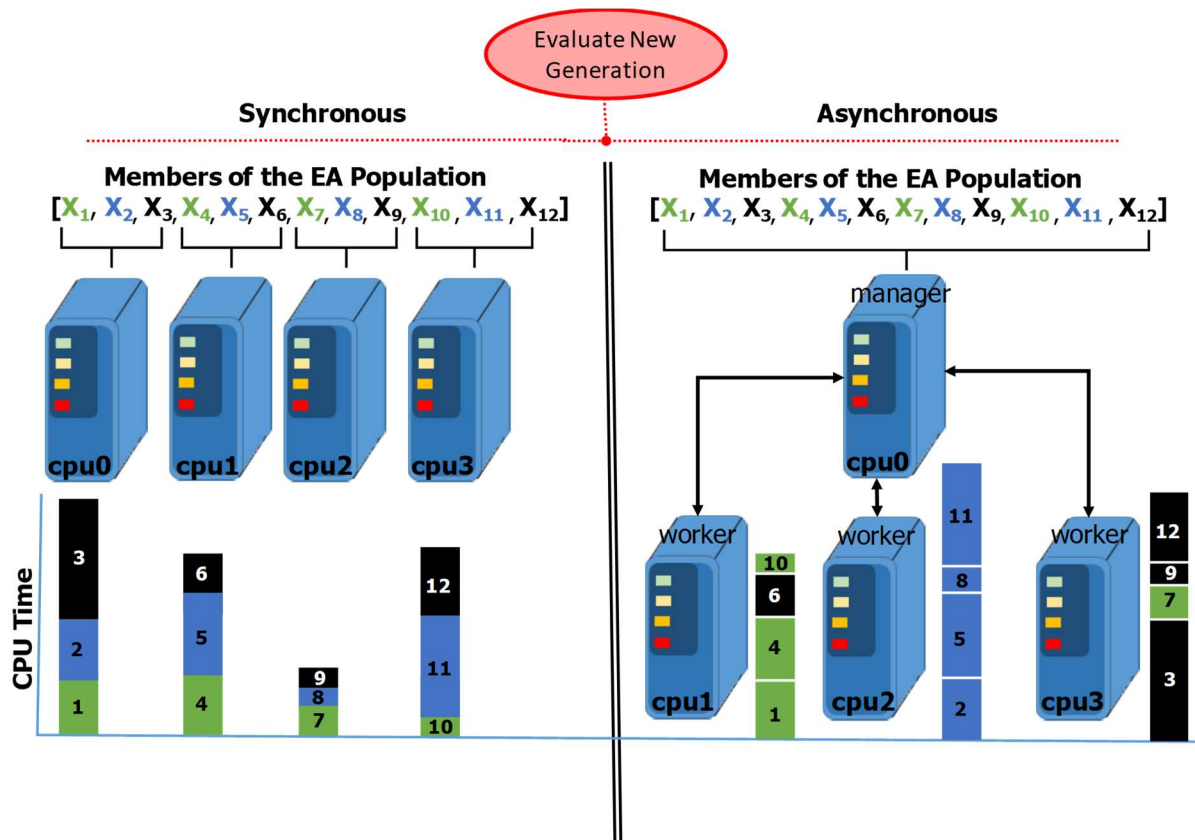


Figure 18. Schematic comparison of synchronous vs. asynchronous approaches to EA parallelization. The hypothetical CPU timings illustrate how different evaluations can get assigned to different processors. Gaps in the asynchronous CPU time graphs represent overhead from interprocess communication.

9. Conclusion

Environmental simulation models are used extensively to support decisions. However, in many instances, the problems being addressed are complex, non-linear, relatively poorly understood and, probably most importantly, characterised by extremely large solution spaces. This makes it almost impossible to identify a set of solutions that provides the best trade-offs between competing objectives, such as minimizing cost and maximizing environmental outcomes, using an informal “optimization” approach, as part of which the best solution is identified with the aid of domain knowledge, experience and intuition, coupled with the outputs from one or more environmental simulation models.

Evolutionary algorithms and other metaheuristics provide a means of addressing the above shortcoming, as they can be linked directly with the environmental simulation models used as part of the commonly used informal optimization approach outlined above, while allowing large search

spaces to be explored in a computationally efficient manner. This is achieved using the same process employed during informal optimization in that a trial solution is proposed, which is then evaluated using a simulation model leading to the selection of a new (hopefully improved) solution and so on. The primary difference is that the decision of which solution to try in the next iteration is not informed by the domain knowledge of the user, but by operators inspired by examples from nature, such as survival of the fittest and the way colonies of ants search for food. This generally enables the identification of solutions that achieve better environmental performance for the same cost or solutions that achieve a particular environmental outcome for reduced financial outlay, rather than solutions that result in inferior environmental outcomes for higher costs. In this way, formal optimization processes can be incorporated into integrated environmental decision-making processes, rather than prescribing a single optimal solution using a black-box process.

However, it is important to note that despite all of the advantages of EAs, they are not necessarily always the best optimization method to use. For example, if in some specific case where the analysed real-life problem could be linearized without losing its key features, and/or a planner needs an answer very quickly (e.g. hydropower scheduling), other optimization methods (such as Linear Programming) may be better suited. This highlights the importance of using any optimization method appropriately. EAs are particularly well suited to solving large, complex, discrete and non-linear real-life problems and are particularly useful for providing decision support in suitably formulated and solved optimization problems accompanied with relevant expert analyses, ideally in some iterative exploratory-type setup. When used in this way, EAs can be very helpful and can reduce the computational burden of the analysed problem, thereby enabling simulation modellers to explore many more options and trade-offs than would otherwise be possible. Thus they allow modellers to focus in general on more important aspects of the analysed problem.

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