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Optimization Models in Water Resources Management and Security: A Critical Review

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Abstract
This paper reviews optimization models in the context of water resources management and security. The article is instituted on four fundamental pillars: (a) an understanding of the quantum of key optimization techniques adopted by the researchers over the past few decades in managing water resources, (b) an enumeration of these techniques, both in terms of their brief mathematical structures and with reference to their representative applications in managing water resources so as to conform to one of the four perspectives of water security, viz. welfare, equity, sustainability, and risk, (c) an evaluation of major challenges associated with these conventional equation-based optimization techniques, including the perceptive account of the distinction between the gradient-based local optimization and non-gradient global optimization, and finally, (d) an assessment of context-sensitive appropriateness of simulation-based bottom-up modeling schemes, with special reference to evolutionary algorithms. The review emphasizes that the ontology of conventional equation-based models lies in an aggregate manifestation of social behavior and, as a result, it fails to capture individuals' behaviors juxtaposed with ecological and hydrological systems while modeling complex water resources. On the contrary, the expediency of the domain of operational research in responding to societal problems ensuing from a scarce natural resource like water lies in bottom-up optimization schemes, which are more obliging in the sense that they can incarcerate such social explanations in the modeling frame based on local values.

Keywords- Water resources optimization, Water resources management, Water security, Simulation-optimization model, Social explanation, ObR-E, Agent-based model.

1. Introduction

The continuous rise in population, followed by increasing per capita consumption of water resources, has raised concern about water scarcity in the near future globally for human survival. An additional two billion people will be in need of food and energy across the world. They will have to feed and provide energy for an additional 2–2.5 billion people as well as meet the current unmet power needs of a billion (Cosgrove and Loucks, 2015). The availability of adequate, clean drinking water plays a very significant role in economic development as well as healthy ecosystems. Optimization for decision-making, especially in cases of limited resources, is one of the most accepted ones among decision-makers. Growing focus on sustainable development coupled with better utilization of water resources has compelled agencies or organizations to use of optimization methods and techniques. As far as wealth management is concerned, the notion of optimization is embedded in Aristotle's (1106–1119) philosophy of the "mean state," positioned in between two extremes, viz., deficiency and excess (Crisp, 2014). To achieve this optimum state, the philosopher's idea is often deciphered as the process of averting from these two extremes, which are more contrasting to the mean, and at the same time, gathering perceptions of the degree of errors while moving away in opposite directions. Thus, Schwefel (1981), quoted by Katsifarakis (2012), perceives optimization as the process of arriving at "a better or best alternative from among a number of possible states of affairs". In water resources management, while modeling the demand side of the water balance equation is a subject of prediction and estimation under uncertainty, the corresponding narrative due to its limited availability pertains to the optimal management of scarce resources to establish a water-secure world. It is necessary to formulate adaptive water resource management policies. In order to achieve social, economic, and environmental sustainability, the formulation of policies for adaptive water management is required (Naghdi et al., 2021). The present discourse attempts to investigate various optimization models adopted in diverse domains of water resources, along with the various procedural challenges associated with each technique. Although a wide range of such techniques are found in the literature, the review focuses on some key techniques deployed in selective contexts of water resource management. First, in order to gather a sense of the quantum of research efforts that have been undergone to deploy such techniques in this context, the review uses the Scopus database generated by PoP software (https://harzing.com/resources/publish-or-perish) (Harzing, 2007) for the period 1970–2019, using appropriate "keywords" and "titles". The decadal pattern demonstrated in Table 1 indicates that although there has been a steady increase in the number of studies involving various optimization techniques in the domain of water resources, a sharp rise in literature has been observed during the last two decades. Again, among various techniques found in the literature, simulation-based optimizations have been observed to dominate over others during the last decade.

Table 1. The decadal trend in the application of optimization techniques in water resources.

Optimization Technique	**1970's**	**1980's**	**1990's**	**2000's**	**2010's**
Cost-Benefit Analysis	9	22	5	22	57
Linear Programming	19	10	10	22	62
Non-Linear Programming	7	4	2	8	35
Dynamic Programming	29	27	12	28	38
Fuzzy Optimization	0	3	5	37	116
Simulation-based Optimization Scheme	5	6	9	42	138

Source: *Scopus database obtained using PoP software: https://harzing.com/resources/publish-or-perish. Decadal definitions: 1970's (1970-'79); 1980's (1980-'89); 1990's (1990-'99); 2000's (2000-'09); 2010's (2010-'19).*

The present research work is organized into eight sections with subsections. The first section introduces the importance of a welfare-centric modeling approach in managing scarce water resource systems. The second section describes the scope of literature reviewing the optimization models for managing water resources. The third section explains the cost-benefit analysis with an equation-based model structure and applications for water resources systems. The fourth section describes the linear, nonlinear, and dynamic programming-based models for water allocation and reservoir systems. The fifth section reviews the fuzzy optimization model and structure for managing water quality. The sixth section summarizes and compares various conventional optimization schemes discussed in the previous sections. The seventh section conceptualizes the socio-hydrological space and social explanation phenomena involving a bottom-up modeling process, feedback mechanism, and evolutionary algorithm. And, finally, the last section proposes the exploration of an agent-based modeling approach for managing water resources as a scope for further research.

The review article first enumerates a set of conventional optimization techniques, both in terms of their brief mathematical structures and with reference to a specific representative application area under each technique, so as to conform to one of the four broad perspectives of water security, viz. welfare, equity, sustainability, and risk (Hoekstra et al., 2018). Next, the major procedural challenges associated with each technique are evaluated. The review also offers a critical perceptive account of the distinction between gradient-based local optimization and non-gradient global optimization as part of the choice for superior solutions. Finally, as it is widely recognized that the dynamics of water resources systems pertain to the science of "complexity" (Wilensky and Rand, 2015), the real motivation of the present discourse is ingrained in the contention of choice between conventional equation-based top-down approaches and simulation-based bottom-up modeling frameworks like evolutionary algorithms (Koziel and Michalewicz, 1999). The fact remains that humans, as the basic ingredients of society, behave based on their individual value systems, which are echoed in their actions and behaviors against various policy interventions. The question remains whether the equation-based optimization techniques are appropriate in the said direction.

2. Literature Scope

Applications of optimization models in the context of managing water resources boil down to serving one of the four impending concerns before society, viz. welfare, equity, sustainability, and risk (Hoekstra et al., 2018). Using the Scopus database generated by PoP software (https://harzing.com/resources/publish-or-perish) (Harzing, 2007) for the period 1980-2019, the trend of adoption of various conventional optimization techniques in different domains of water resources management reveals the fact that some of the techniques are widely deployed in certain domains over others (Figure 1). In the present review, the criterion of selecting literature on conventional optimization techniques in a particular domain of water resources management, denoted by "s" in circles, is primarily governed by the major contributory share of that technique towards that specific domain of water resources management. In addition, literature on optimization techniques like bi-level programming, fuzzy optimization, Jalingo equation model, and multi-criteria optimization has been critically reviewed and published between the years 2019 and 2023.

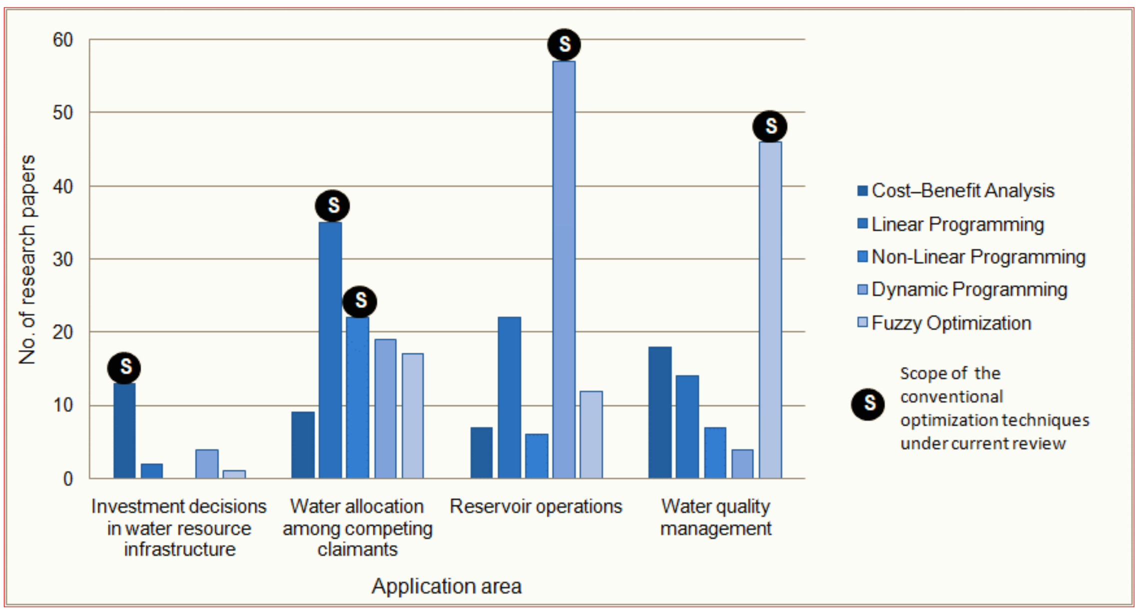

Figure 1. Conventional optimization techniques used in different domains of water resources management. Time period: 1980-2019. Source: Scopus database obtained using PoP software: https://harzing.com/resources/publish-or-perish. "s": Scope of the literature review.

In line with the above scoping of conventional optimization techniques, policy interventions translating into various water-security measures often call for (i) a welfare-theoretic approach in taking the economic decision of investments among alternative choices of water resources systems, (ii) allocating scarcely available water in a logical and fair way to all its competing claimants, enabling the notion of equity to conform to the fundamental right to the natural resource, (iii) designing the capacity of water infrastructures to reduce water-related risks, and finally, (iv) edging off the quality-induced scarcity of water, and thus, striking the chord of sustainability on a temporal scale. These four perspectives on water security, each deployed under a specific conventional optimization technique, form the context-sensitive literature review in the next six sections (sections 3 to 8) of the present discourse.

3. Cost-Benefit Analysis for Water Resource Systems

Cost-benefit analysis (CBA) is one of the basic optimization techniques that attempts to estimate the future benefits vis-à-vis the present costs incurred or benefits foregone. The CBA, as an analytical tool, is grounded in the principles of economics for measuring economic efficiency by comparing alternative investment choices among different public water projects in the face of constrained resources (Freeman III and Haveman, 1970). Although CBA's origin can be traced back to the commencement of the 19th century in France, its extensive applications can first be noted in the US around "the politics of financing water projects in the early 1900s" (Ward, 2012).

3.1 Mathematical Structure of Cost-Benefit Analysis (CBA)

In order to estimate the cost and benefits associated with a project, it is important to understand the model structure that influences the decision alternatives. The essential philosophy of CBA lies in its ability to compare multiple water resource projects engaging various time series of costs and benefits (Loucks and Beek, 2017). Following the authors' work, the technique entails the use of the "present value" criterion, wherein the total present value $B_0{}^p$ of the water resources project *p* is denoted by the summation of the values of the net benefits $B_t{}^p$ accrued at the end of each time period t of the economic planning horizon *T*, multiplied by the discount factor pertaining to that period with the interest or discount rate *i*:

$$B_0P = \sum_t^T B_t^P/(1+i)^t \qquad (1)$$

The equivalent present value criterion represented above forms the economic basis of project selection from the multiple projects possessing the same economic planning horizon *T*.

3.2 Cost-Benefit Analysis Applications

Academic endeavors in the context of adopting CBA as a welfare-theoretic technique to economically evaluate alternative investment choices in water infrastructure are copious. In the early seventies, the literature by Freeman III and Haveman (1970) was found to critique preceding work done by Major (1969) on the benefit-cost ratio in the context of a multiple objective water resource investment planning framework. A methodology integrated with uncertainty in the CBA of water resources management is found in the work of Goicoechea et al. (1982). As part of the re-allocation of water resources, a cooperative game theory with a hierarchical structure and its temporal variations is modeled by Okada and Sakakibara (1997) in the context of investment choices between basin-wide reservoir re-development and the construction of new reservoirs. Jianbing et al. (2010) show how CBA is adopted for wide-ranging decision-making processes and evaluation of urban water harvesting in the city of Beijing, China. Also, CBA as an instrument to assess the economic feasibility of implementing managed aquifer recharge (MAR) technology is demonstrated in the work of Maliva (2014). The optimization of water resource allocation using the bi-level programming coupling model can help in achieving the balance between economic benefits and environmental pollution discharge (Ge and Wang, 2023).

4. Linear Programming in Managing Water Allocation

The primary goal of CBA, as discussed in the previous section, is to evaluate multiple projects that are competing with each other, considering economic cost and benefit criteria. But mere comparative assessment might not be enough; rather, optimum allocation of water resources plays a dominant role, especially when dealing with water scarcity or a water-stressed scenario. Linear programming is an effective tool for such complexities in decision-making. Although the quest to solve linear equation systems has prevailed over the last two centuries, it is a set of challenges that surfaced before the US Air Force during World War II regarding the allocation of limited military resources. These objectives gave birth to what was popularly called the Simplex Computational Method (Dantzig, 1963). The Ford Foundation sponsored the Harvard Water Programme in the early 1960s, a point of departure for numerous water resource problems to embrace the linear programming (LP) technique in subsequent years (Drobny, 1971).

4.1 Mathematical Structure
A typical LP problem consists of: (i) a linear objective function that is required to be maximized or minimized, (ii) unknown activity levels (variables) that are to be solved to arrive at the solution to the LP problem; (iii) the proportionality of resource consumption by various activities to the activity levels, establishing linearity in their relationships; and (iv) the allowance of only non-negativity in activity levels (Driebeck, 1969; Hadley, 1961). The general formulation structure of the problem is as follows (Loucks and Van Beek, 2017):

$$\left.\begin{array}{l} Max.\text{ or } Min.\ Z = F(\boldsymbol{X}) \\ \text{subject to constraints: } g_i(\boldsymbol{X}) \leq \text{ and/or } = \text{ and/or } \geq b_i,\ i = 1, 2, 3, \ldots, m; \end{array}\right\} \quad (2)$$

where, $\mathbf{X}$ is the vector of all x_j; $j = 1, 2, 3, \ldots, n$; and $F(\boldsymbol{X})$ and $g_i(\boldsymbol{X})$ are all linear.

The non-negativity requirements state $x_j \geq 0\ \forall\ j$.

4.2 Linear Programming Applications
In the context of water resources management, the fundamental motivation behind an LP problem (and mathematical programming in general) is ingrained in the philosophy of how to allocate the scarce natural resource on spatial and temporal scales to all its competing claimants so that some quantifiable objectives like benefits or costs are maximized or minimized, respectively. This essentially translates into an equity-based approach embedded in the broad notion of water security. Jacovkis et al. (1989) formulate an LP model to optimize a multi-purpose water resource system subject to technical, economic, financial, social, and political constraints. Also, a "separable" LP model is found in the literature, which talks about the maximization of the net income of the farm obtained from various crops under varied water availabilities and cropping areas (Frizzone et al., 1997). Iancheva and Kelevedzhiev (2001) illustrate a model based on the LP approach, termed multi-stage network flows, aiming to simultaneously optimize large-scale water distribution networks on a temporal scale. The idea of minimization of virtual water and the related concept of water footprints are captured in the LP formulation of Pearson and McRoberts (2010).

5. Revisiting Water Allocation
Water resources management problems ensuing from various complexities often face physical, economic, or operational configurations that are essentially non-linear in nature. In line with this realism, the duality of an LP, transformed into an equivalent saddle value problem by adopting the calculus-based method usually applied to constraining equations, forms the classical Lagrangian expression (Kuhn, 2014). Although the spirit of mathematical programming was found in the late forties, it is the saddle-point problem that is the true point of departure for elucidating Kuhn-Tucker analysis (Kuhn and Tucker, 1951). Three components are engaged under this calculus-based non-linear programming (NLP) technique, often called generalized deterministic mathematical programming: a continuous objective function, concave or convex, is maximized or minimized, respectively, subject to a set of constraints to arrive at the optimal solution for the decision variables involved in the phenomenon of interest.

5.1 Lagrangian Expression

The present discourse refers to the standard form of a non-linear maximization using Lagrange multipliers, where the differentiable concave net benefit objective functions $B_j(x_j)$ of a typical water allocation project are maximized subject to a set of differentiable techno-commercial and environmental constraints $g_i(x_i)$. The problem, involving n decision variables x_j (water allocations) and m constraints i, translates into maximizing the net benefit function (Loucks and Beek, 2017):

$$\left.\begin{array}{l} Max.\ B(\boldsymbol{X}) \\ \text{Subject to constraints: } g_i(\boldsymbol{X}) = b_i;\ i = 1, 2, 3, \ldots, m; \\ \text{where } \boldsymbol{X} \text{ is the vector of all } x_j;\ j = 1, 2, 3, \ldots, n. \end{array}\right\} \tag{3}$$

The corresponding Lagrange function is represented by the following equation:

$$L(\boldsymbol{X}, \boldsymbol{\lambda}) = B(\boldsymbol{X}) - \sum \lambda_i \left(g_i(\boldsymbol{X}) - b_i\right).$$

A particular vector $\boldsymbol{X}^*$ maximizes $B(\boldsymbol{X})$ subject to the constraints if, and only if, there is some vector $\boldsymbol{\lambda}^*$ with non-negative components such that $L(\boldsymbol{X}, \boldsymbol{\lambda}^*) \le L(\boldsymbol{X}^*, \boldsymbol{\lambda}^*) \le L(\boldsymbol{X}^*, \boldsymbol{\lambda})\ \forall\ x_j$ and $\lambda_i \ge 0$. While the saddle point $(\boldsymbol{X}^*, \boldsymbol{\lambda}^*)$ offers a solution for the corresponding two-person zero-sum game, the bi-linear symmetry of $L(\boldsymbol{X}, \boldsymbol{\lambda})$ in $\boldsymbol{X}$ and $\boldsymbol{\lambda}$ characterizes the duality of linear programming (Von Neumann and Morgenstern, 1947). The unit of weight or multiplier λ_i, connected to each constraint is interpreted as the marginal benefit with respect to a change in the constant b_i pertaining to the constraint i.

As most of the local optimization techniques are gradient-based, and with gradient information available, the solutions for possible local optima are obtained through the Karush-Kuhn-Tucker (KKT) necessary conditions slated in the following simultaneous equation system:

$$\left.\begin{array}{l} \partial L/\partial x_j = 0\ \forall\ j; \text{ and} \\ \partial L/\partial \lambda_i = 0\ \forall\ i. \end{array}\right\} \tag{4}$$

With m constraints ($m < n$), the sufficient (second-order) conditions to ensure a maximum is reached are omitted here in this sector-specific discussion.

5.2 Nonlinear Programming in Water Allocation

Many attempts have been made in the domain of water research to study the optimal allocation of water using various nonlinear programming (NLP) techniques. In their interdisciplinary work on the optimum allocation of scarcely available surface and groundwater to the irrigational areas in the Jordan Valley, Rydzewski and Rashid (1981) follow NLP optimization to maximize the net benefit of agricultural productivity. Cullinane et al. (1992) use the NLP algorithm to establish a novel concept of reliability-based least-cost design of water-distribution networks. An application of NLP to model intra-seasonal water allocation among the stipulated crops from a reservoir dam in Iran is found in the work of Ghahraman and Sepaskhah (2002). In an intricate work in recent times, Aljanabi et al. (2018) uses a mixed-integer NLP model to find out the optimum allocation of reclaimed water for agriculture in Baghdad, subject to constraints of reclaimed water availability, the area of cultivation, farm-crop, and farm-reclaimed-water connectivity, and a minimum permissible net benefit.

6. Dynamic Programming in Water Reservoir Operations

Optimal allocation of water resources using either linear programming or a non-linear programming approach might not be enough to address water stress or water scarcity. Decisions are to be taken in various stages over a period of time and are sequential in nature. Optimization problems, in reality, often deal with functional forms that may not necessarily be strictly continuous, perfectly concave for maximization, or perfectly convex for minimization. The riposte to such challenges lies in the path-breaking technique, comprising deterministic "multi-stage decision processes", also termed "optimal control problems" (OCP). It splits the original optimization problem into a smaller set of problems, each of which is required to be deciphered to arrive at an approximately optimum solution for the original problem (Bellman, 1957). Thus, dynamic programming (DP) problems fundamentally engage "state" and "control" variables.

6.1 Mathematical Structure

Dynamic optimization models include (i) a feasible set of policies from which a particular policy is decided; (ii) an objective function that measures benefits or costs associated with the policy; and (iii) a mathematical model that demonstrates system responses to the policy selected, subject to the initial conditions and exogenous factors (Williams, 1989). The present review paper refers to the mathematical structure pertaining to a typical scenario involving the minimization of the cost of future capacity expansion of water resources infrastructure, wherein the optimization question hovers around "how much capacity" and "when" (Loucks and Beek, 2017) in order to institute the notion of "risk neutrality with respect to uncertainty" (Al-Adhadh, 1978). With an initial capacity K_t and a planned capacity expansion Δ_t, the objective is to minimize the present value of the cost of total capacity expansion C_t pertaining to the time period t. The constraints in the optimization problem comprise conditions: (i) the following period's initial capacity K_{t+1} equals the current period's initial capacity K_t plus each expansion Δ_t all over the time horizon, (ii) the current period's closing capacity, i.e. the following period's initial capacity K_{t+1} must not fall short of K_t^*, the capacity required at the end of the current period, and (iii) the planned capacity expansion Δ_t of each period t belongs to a set of feasible capacity expansions Ω_t pertaining to the period t.

$$\left.\begin{array}{l} Min. \sum C_t\,(K_t, \Delta_t)i. \\ \text{subject to constraints: } K_{t+1} = K_t + \sum\limits_{i=1} \Delta_i \ \text{ for } t = 1, 2, 3, \dots, T; \\ K_{t+1} \geq K_t^* \ \text{ for } t = 1, 2, 3, \dots, T; \\ \Delta_t \ \varepsilon\ \Omega_t . \end{array}\right\} \tag{5}$$

6.2 Dynamic Programming Applications

With the notion of "risk" inherent, Al-Adhadh (1978) shows a DP application incorporated with chance-constrained programming in the context of water reservoir operations by introducing a penalty function, which brings economic interpretations to the technical obligations of a maximization problem. The study done by Chandramouli et al. (2002), applying a neural network based on DP in the context of a multi-reservoir system for supplying irrigational water, is worth mentioning. The adoption of a folded DP (FDP) with superior computational performance and flexibility under transitory hydrological scenarios and varied risk regimes is noted in the case study on Hirakund Reservoir in the Mahanadi basin of India (Nagesh Kumar et al., 2009). Lai et al. (2022) reviewed the various approaches (including the dynamic programming model) to reservoir operations optimization.

7. Managing Water Quality Under a Fuzzy Environment

Traditional optimization procedures, addressing the so-called "hard system" with definitive configurations, often confront objective functions, constraints, and decision variables that are not crisp and specific; rather, reality is often overwhelmed by "ambiguity" and "vagueness". While ambiguity may ensue from either a preference-based or possibility-based source, depending on whether the origins of ambiguity are subjectivity in knowledge or lack of knowledge, respectively, the basis of vagueness lies in the obscurity of deciphering information in a precise manner (Tang et al., 2004). Fuzzy set theory was developed by Zadeh in the 1960s (Zadeh, 1965). Subsequently, the adoption of fuzzy modeling based on information analyzed and the associated fuzzy optimization (FO) technique seeking "optimality" are seen as responses to the inability of mathematical programming-based or probability-based stochastic optimization techniques to tackle such "soft systems" in fuzzy environments (Bellman and Zadeh, 1970). While FO problems pertaining to vagueness and preference-based ambiguity entail the use of subjectively determined membership functions, scenarios under possibility-based ambiguity, often called "imprecision", are handled with a subjectively or objectively expressed possibility distribution function, a possible measure of the occurrence of an event or an object.

7.1 Mathematical Structure

The present discourse refers to a schematic form of constrained FO, otherwise called fuzzy mathematical programming (Tang et al., 2004):

$$f(x, r)\ max, \tag{6}$$

subject to $x\ \varepsilon\ C = \{x\ \boldsymbol{\varepsilon}\ X \mid g_i\,(\mathrm{x, s}) \leq\ \tilde{}\ 0, i = 1, 2, \cdots, m\}$;

where, universe $X = \{x\}$ is a set of alternatives, the domain C may be configured as a crisp system of constraints or fuzzy system of constraints involving fuzzy equations, fuzzy inequalities, inequalities/equations with fuzzy coefficients, r is either a crisp constant or a fuzzy coefficient, $f(x, r)$ is either a crisp objective function or an objective function with fuzzy coefficients. The formulation above is interpreted as how to find out an x "belonging" to the domain C such that $f(x, r)$ can reach a possibly "maximum"; various construal of the terms "belonging" and "maximum" in a fuzzy sense contribute to the varieties of FO problem as conceived by different academicians. (Tang et al., 2004), for example, opine that "the formulation and classification of the fuzzy mathematical programming problems depend on what and where the fuzziness is involved", e.g., fuzzy emergence based out of fuzzy goal, fuzzy constraints, or fuzzy coefficients in the objective function and/or constraints. Addressing water quality issues in the long term is one of the key considerations while tackling water resources management. The next section reviews the key literature on the application of fuzzy optimization in this direction.

7.2 Applications of Fuzzy Optimization

In the literature, applications of FO drifting around water quality issues and challenges are quite prominent, with the focus being on long-term sustainability. Esogbue (1984) uses fuzzy sets and hierarchal models in nonpoint source (NPS) water quality management in urban contexts. In order to evaluate the drinking water quality grade supplied by various water plants in the city of Wuhan, China. Jin et al. (1996) establish that the fuzzy mathematical synthetic method is a superior choice compared to the prevailing pollution index method, as the latter tends to overstate water quality accuracy. The study done by Mpimpas et al. (1999) on the distribution of pollutants in the Gulf of Thermaikos, Greece, is one of the many attempts to apply fuzzy set theoryton characterizing the imprecise parameters used in a water pollution model. In more recent work, Aminravan et al. (2013) propose an enhanced fuzzy evidential reasoning (EFER) approach as an instrument to monitor the quality of water in water distribution networks engulfed with uncertainty and subjectivity. Cho and Lee (2020) developed a waste load allocation problem that minimizes the cost related to water quality management. Hao et al. (2022) applied the interval fuzzy two-stage (IFTS) optimization method to identify the impact of the maximum availability of water in the river basin on the economic benefits.

8. Optimization Techniques for Achieving Water Security

8.1 Motivations and Challenges

The challenges in managing scarce water resources encompass the entire biophysical and socio-economic processes. In this way, it can be said that optimizing the allocation of water resources is multi-dimensional. Thus, the dynamics of water resource systems are "complex systems" (Wilensky and Rand, 2015). Depleting the level of urban groundwater due to increased demand from both industrial and domestic users is one of the biggest challenges being faced globally (Hoekstra et al., 2018). As per the definition of the Global Water Partnership (GWP, 2000), the concept of water security comprises an "overarching goal" for the management of water resources on spatial and temporal scales (Hoekstra et al., 2018), while reviewing urban water security, construes the philosophy from four different perspectives, viz. welfare, equity, sustainability, and risk. Sustainable water resources management involves water resources planning and decision-making by using feedback views and models. Integrating all aspects of the water system, right from water resource planning followed by decision-making using models, is very important to achieve sustainability in water resource management (Behboudian et al., 2021). The entire array of optimization techniques and the motivations behind their applications to scarcely available water resources are ingrained in these four fundamental denominations. Each technique, however, is under the shadow of its own set of challenges. In a conceptual economic framework, Ward (2012) points out certain research challenges while adopting CBA as a tool for decision-making in a water resources system, including (i) a lack of agility to accommodate the onslaught of climate variability, (ii) unimproved sensitivity analyses, (iii) the absence of institutional management control over water pricing, and (iv) a deficiency of meticulous information to compute the opportunity cost. As far as LP is concerned, the majority of the constrained optimization problems pertaining to water resources management find it difficult to fit into reality, which is essentially non-linear in nature. The exponential complexities arising out of multiple iterations of the Simplex method create the urge to adopt a polynomial time algorithm (Klee and Minty, 1972); interior-point methods (IPM) being one such category (Karmakar, 1984). On the NLP front, it is often argued that "an adequate level of adherence to the physical system" is required in order to represent reality better (Liberatore et al., 2006). However, extensive applications of NLP are inhibited as the rigor of the mathematics involved often calls for very high computational resources (Singh, 2012). Moreover, the KKT technique tends to recognize local or relative optima only and doesn't necessarily guarantee a global optimum. The technique is generally considered inept at addressing discrete optimization problems, and it is prone to "numerical noise" (Venter, 2010). Although it is the conceptual simplicity that makes DP widely applicable in water resources systems analyses, the associated computational complexities in terms of computational resource requirements (e.g., computer memory) arise out of the degree of discretization, commonly known as the "curse of dimensionality" (Yakowitz, 1982). In order to avoid this dimensionality problem, various schemes are found in the literature, which entail the use of successive approximation algorithms. Discrete differential dynamic programming (DDDP) (Heidari et al., 1971), incremental dynamic programming (IDP) (Trott and Yeh, 1973; Yurtal et al., 2005), differential dynamic programming (DIFF DP) (Murray and Yakowitz, 1979), and successive improved dynamic programming algorithm (SIDP) (Zhao et al., 2014) are a few of the schemes applied in the optimization of water resources.

8.2 Conventional Optimization Schemes: A Comparison

It is argued that "even the best successive approximation methods can converge to local optima, or may not converge at all, unless the OCP itself satisfies somewhat stringent assumptions" (Yakowitz, 1982). While the transformation of a fuzzy problem into a crisp one is the essence of FO, it is well documented in the literature that the criticality lies with the interpretability of this transformation, which should be appropriate and reasonable. Thus, fuzzy formulation and its interpretation reserve the true perspective to optimize the problem more realistically. Table 2 summarizes the range of conventional optimization schemes reviewed in the present discourse, mapped onto different perspectives of water security along with the principal procedural challenges associated with each technique.

Table 2. Water-security motivations and procedural challenges for conventional optimization schemes.

Optimization scheme	**Water resources management context**	**Water-security perspective**	**Major challenges**	**Relevant literature support**
Cost–benefit analysis (CBA)	Evaluation of optimal investment decisions in alternative water resources projects	*Welfare-centric approach:* enhances benefits from efficient decisions based on the principles of economics	Imprecise information for model construct, lack of sensitivity to changes in parametric values and other factors like climate variability etc., poor control towards equitable water-pricing.	Major (1969), Freeman III and Haveman (1970), Goicoechea et al. (1982), Okada and Sakakibar (1997), Jianbing et al. (2010), Molinos-Senante et al. (2010), Ward (2012), Maliva (2014),, Kind et al. (2018).
Linear programming (LP)	Optimal allocation of water resources among its competing claimants subject to techno-economic, socio-political constraints etc.	*Embedded in the notion of equity:* brings distributional justice to water resources	Unrealistic; multiple iterations of Simplex method add exponential complexities to modeling	Hadley (1961), Dantzig (1963), Driebeck (1969), Drobny (1971), Klee and Minty (1972), Andrews and Weyric (1973), Karmakar (1984); Jacovkis et al. (1989), Frizzone et al. (1997), Iancheva and Kelevedzhiev (2001), Pearson and McRoberts (2010).
Non-linear programming (NLP) using Lagrange multipliers			High computational costs are involved, and various linearization schemes are adopted; local instead of global optimum; numerical noise	Von Neumann and Morgenstern (1947), Kuhn and Tucker (1951), Kuhn (2014), Rydzewski and Rashid (1981),, Cullinane et al. (1992), Berghoue and Kuczeraz (1997), Ghahraman and Sepaskhah (2002), Liberatore et al. (2006),, Ahlfeld and Baro-Montes (2008), Venter (2010), Singh (2012), Aljanabi et al. (2018).
Dynamic programming (DP)	Constrained cost optimization of future capacity expansion for reservoir operations in terms of decisions involving expansion volume and expansion-timing	*Risk reduction*: conservation measures through the capacity creation of water infrastructures, reducing scarcity and various water-related risks	"Curse of dimensionality": computational memory requirements arise out of the degree of discretization; local optima	Bellman (1957), Bellman and Dreyfus (1962), Heidari et al. (1971), Trott and Yeh (1973), Al-Adhadh (1978), Murray and Yakowitz (1979), Yakowitz (1982); Williams (1989), Ozelkan et al. (1997), Chandramouli et al. (2002), Yurtal et al. (2005), Nagesh Kumar et al. (2009), Zhao et al. (2014).
Fuzzy optimization (FO)	Optimization of water quality parameters and cost of treatment of polluted water	*Long-term sustainability on the temporal scale*: through stakeholders' aspirations on water quality improvement	Interpretability of the transformation of the fuzzy problem into a crisp one should be appropriate and reasonable	Zadeh (1965), Esogbue (1984), Jin et al. (1996), Mpimpas et al. (1999), Tang et al. (2004), Aminravan et al. (2013).

8.3 Local vs. Global Solutions

Conventional optimization methods are usually dependent on gradient information to search for the local optimum. The differences among various gradient-based algorithms that we come across ensue from the different interpretations that go behind determining the search directions to find out the local optimum. According to Venter (2010), scenarios involving: (i) a large number of design variables; (ii) the affordability of expensive computational costs; (iii) inconsequential numerical noise; (iv) the availability of gradient information; and (v) the permissibility of solutions based on local optimization, usually motivate the researchers to undertake local optimization techniques.

9. Socio-Hydrological Space and Social Causal Explanation

9.1 Conceptualizing Bottom-up Modeling Process

Diverse optimization schemes hovering around the philosophy of water security raise one pertinent question: how to incarcerate individuals' social behaviors juxtaposed with ecological and hydrological systems while modeling complex water resources. The complexity of relationships coupled with feedback mechanisms among different systems poses challenges to understanding sustainable water resource management for the purpose of evaluating water policies (Mohamed et al., 2020). Sawyer (2004), while exploring the role of computer simulation in seeking a social causal explanation, emphasizes that the traditional equation-based models entail the use of various social variables purely at the macro level, but the true knowledge of the process of emergence can be effectively unveiled through a dynamic "artificial society". During the process of investigating "the role of ecological expertise in policy-making", Carpenter and Gunderson (2001) observe three key features among all bottom-up models: (i) ecosystem dynamics; (ii) a society consisting of human beings with diverse value systems; and (iii) a capacity engineered to evaluate the ecosystem. The dynamics of water resource systems, too, are characterized by complex interactions of these elements on spatial, temporal, and organizational scales. Saini et al. (2019) analyzed the water-energy nexus in ObR-E's (open but restricted environment) Type I, Type II, and Type III with the help of a difference-differential solution (Jalingo equation). Further, they established the connection of water usage and energy and food usage at high and low occupancy rates in the nexus. In the course of such local interactions, information pertaining to individual social behaviors is propagated from one individual to another and from one community to another, paving the way for establishing a new order in the aggregate social pattern. Any policy intervention in the midst of these locally interacting elements leads to individual behavioral modifications (reactions and/or adaptations), which eventually translate into an "emergent" global pattern in the macro-behavior of the locality as a whole.

9.2 Feedback Mechanism

Tang et al. (2021) came up with an improved model structure for simulating demand as well as supply-side management strategies for water resource management. The "feedback" mechanisms are generated between hydrological and social processes, and further interventions are triggered with necessary modifications in the policy prescriptions until a superior solution is achieved. In order to conceptualize such a bottom-up modeling process, the present review article adopts the framework presented by Parrott et al. (2012), originally transliterated by Ostrom (2009) (Figure 2).

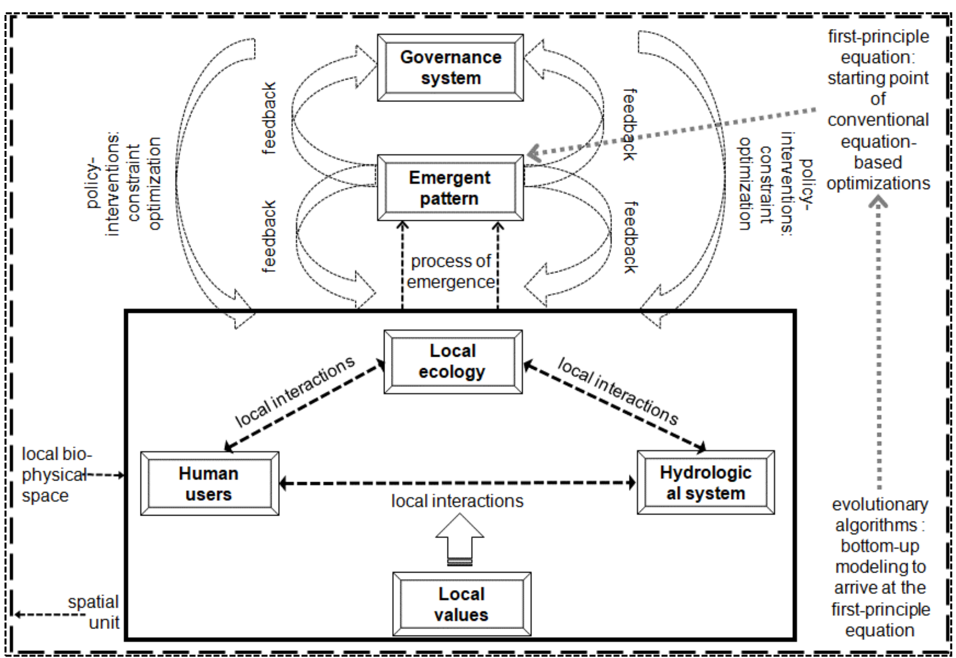

Figure 2. Bottom-up modeling framework in water resources management (Ostrom, 2009; Parrott et al., 2012).

9.3 Evolutionary Algorithms

Entrenching a simulator in an optimization scheme should not be treated as a separate class of optimization technique per se, at least from a purely theoretical perspective, but as a computational strategy that enables even the most expensive optimization programming to achieve superior solutions. Simulation- optimization aims to "minimize the resources spent while maximizing the information" (Carson and Maria, 1997). Among various simulation-optimization techniques, one such method involves heuristic (or meta-heuristic)-based algorithms. These evolutionary algorithms are enormously capable of portraying and addressing complex systems. Genetic algorithms (GA) (Holland, 1992), motivated by biological processes of natural selection (Darwinian principle), and particle swarm optimization (PSO) (Kennedy and Eberhart, 1995), based on a basic social model, are two evolutionary algorithms that are worth mentioning. Other pioneering works belonging to this genre of optimization schemes include tabu search (Glover, 1989; Glover, 1990), ant colony optimization (Colorni et al., 1991), and harmony search (Geem et al., 2001), to name a few. Over the last three decades, a lot of academic efforts have been trending towards these meta-heuristic-based techniques in the context of water resources management, as these algorithms do not necessitate any a priori requisite of concavity, convexity, or differentiability in objective functions and constraints. They entail the use of a population or design points in searching for the global or near-global optimum (Venter, 2010). Figure 3 establishes the increasing trend in the adoption of major evolutionary algorithms in the field of water resources over the last three decades.

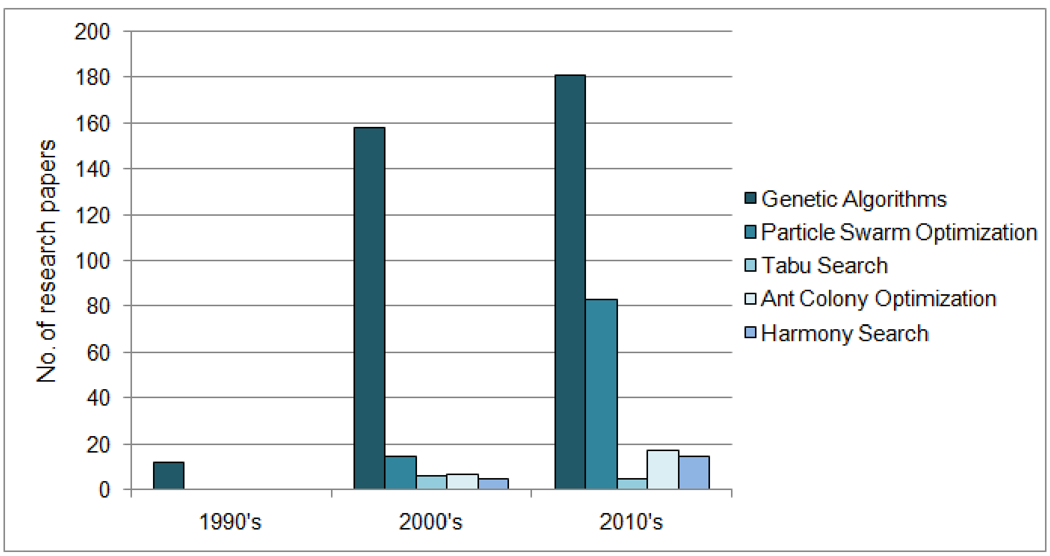

Figure 3. Decadal trends in the adoption of various evolutionary algorithms in the field of water resources. Decadal definition: 1990's (1990-'99); 2000's (2000-'09); 2010's (2010-'19). Source: Scopus database obtained using PoP software (https://harzing.com/resources/publish-or-perish).

9.4 Evolutionary Algorithms Challenges

Although it is intrinsically perceived that most of the evolutionary algorithms fall into the class of unconstrained optimization problems, constraint handling technique is the key challenge while dealing with these algorithms; "penalty function" is the most popular technique frequently adopted by the researchers, as this technique conforms to the conventional gradient-based approach and is easily implementable (Koziel and Michalewicz, 1999). Accurate problem-specific parameter tuning is the essence of model set-up in all evolutionary algorithms, from typically deployed static penalty parameters to the penalty parameters that are dynamically tuned in the course of the optimization process (Poon and Joaquim, 2007). However, the most serious challenge with these algorithms is their high computational cost for a limited problem size (Venter, 2010).

9.5 Agent-Based Modeling: A Future Research Direction
Rooted in the tenet of complex adaptive systems (CAS), bottom-up simulation techniques like Agent-Based Modeling (ABM) (Wilensky and Rand, 2015) have been thriving in academia since the mid-nineties. ABM is a computational methodology that is often considered a "distinct simulation and modeling technique, having characteristics and capabilities in addition to the standard simulation techniques" (Macal, 2016). Deng et al. (2022) used a multi-objective water-resource allocation model in order to interconnect the interaction cognition between hydrology and social systems by all factors (efficiency, equity, and sustainability) simultaneously. Further, Viola et al. (2021) proposed a conceptual socio-hydrological model for studying the mutual interactions between water management systems and society using simulation. Similarly, Sharma (2022) applied multi-criteria optimization and an intelligent water demand forecasting framework to address water resource demand projections using simulation experiments. There are widely used models for water resources management like WEAP, SWAT, WAPOR, and the System Dynamics model (Guemouria et al., 2023). However, in ABM, the system is configured to allow simultaneous agent-agent and agent-environment interactions, and such modeling framework, when integrated with other tools like geographic information systems (GIS), provides the predictive power to achieve global or nearly global optimality in a socio-hydrological space. However, the philosophy of an ABM must be recognized as a subject of its own to understand and explore its appropriateness while modeling with natural resources like water, taking social causal explanation into account.

10. Conclusions
While investigating various optimization techniques in different domains of water resources management, it is observed that there has been a steady increase in the quantum of such research over the past decades. The trend also reveals that some of the conventional techniques are widely deployed in certain domains of water resource management over others. Each of the techniques, with its adoption in managing one of these domains, conforms to one of the four perspectives of water security, viz., welfare, equity, sustainability, and risk. However, every methodology has its own set of inherent challenges. Therefore, the choice is really dependent on what perspective on water security the researcher intends to imbibe and whether the model configuration conforms to a search strategy for local or global optima. Unlike conventional optimizations, simulation-optimization schemes like evolutionary algorithms are not dependent on gradient information and entail the use of a population or design points in searching for the global or near-global optimum. The current study suggests that the choice of conventional equation-based modeling frameworks is insufficient or even inappropriate for incorporating social causal explanations in the socio-hydrological space. The study points out the limitations of conventional optimization techniques or algorithms that must be considered, as they may require technical expertise to be applied more effectively. Further, the availability and accuracy of data through satellite may be affected by unpredictable or adverse climate conditions, posing challenges for modeling groundwater management and interactions between different water users. A bottom-up simulation-based framework like ABM, seeking global or near-global optimality, could be the better alternative that needs to be studied further.

Conflict of Interest
The authors declare that there is no conflict of interest.

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