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Optimization Examples for Water Allocation, Energy, Carbon Emissions, and Costs

Angelos Alamanos [1] and Jorge Andres Garcia [2,*]

[1] Independent Researcher, 10243 Berlin, Germany
[2] The Water Institute, University of Waterloo, Waterloo, ON N2L 3G1, Canada
* Correspondence: ja4garciahernandez@uwaterloo.ca

Definition: The field of Water Resources Management (WRM) is becoming increasingly interdisciplinary, realizing its direct connections with energy, food, and social and economic sciences, among others. Computationally, this leads to more complex models, wherein the achievement of multiple goals is sought. Optimization processes have found various applications in such complex WRM problems. This entry considers the main factors involved in modern WRM, and puts them in a single optimization problem, including water allocation from different sources to different uses and non-renewable and renewable energy supplies, with their associated carbon emissions and costs. The entry explores the problem mathematically by presenting different optimization approaches, such as linear, fuzzy, dynamic, goal, and non-linear programming models. Furthermore, codes for each model are provided in Python, an open-source language. This entry has an educational character, and the examples presented are easily reproducible, so this is expected to be a useful resource for students, modelers, researchers, and water managers.

Keywords: optimization; water-energy; carbon emissions; economics; linear programming; fuzzy optimization; dynamic optimization; non-linear programming; goal programming; Python

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1. Introduction and Background Concepts

The main themes of this encyclopaedia entry are an integrated resources management problem considering environmental and economic parameters, and its representation through different optimization types.

1.1. Integrated Water Resources Management Optimization Applications

Water Resources Management (WRM) involves all measures and actions that we apply to water resources (surface, groundwater, freshwater, and seawater), to convert or improve their status and cover the multiple needs of societies and ecosystems [1,2]. As one can imagine, WRM is subject to multiple factors (e.g., meteorological, natural, ecological, and socio-economic), and should take into account various water sources and different users, with different characteristics [3]. There are also multiple direct and indirect implications of WRM in the short and long term, applicable to multiple sectors (such as ecology, biodiversity, hydrology, economy, energy, industry, urban planning, policy, etc.) [4]. Integrated Water Resources Management (IWRM) acknowledges the intricate nature of WRM, encompassing various factors, stakeholders, and short- and long-term implications across multiple sectors. Thus, WRM is often meant to be a holistic and integrated process, by nature [5,6]. Since water resources utilization is connected with multiple other uses and activities, WRM deals with complex problems that must take into account many different variables reflecting this complexity (different sources, different users, and gains from using water, as mentioned). These complex problems have theoretically infinite management solutions. The achievement of WRM objectives under the various restrictions posed by their natural, social, economic, and regulatory aspects can be closely related to an optimization process approach that aims to find the optimum solution(s) under specific constraints [7]. This logic has been a useful approach for several aspects of WRM research and practice, with various applications [8,9], including water resources allocation [10–12], water infrastructure, irrigation networks, dams and reservoirs, hydropower works, etc. [13–15], hydrology and hydraulics [16–18], disaster analysis and management [19–21], water quality management [22–25], transboundary water management [26–29], policy/governance/development [30–35], Water-Energy-Food Nexus [36–38], and other cross-disciplinary fields such as hydro-economics, socio-hydrology, ecohydrology, etc. [39–46].

1.2. Optimization Logic

Optimization is a mathematical representation of a problem that we want to solve in the best possible way, satisfying many (often conflicting) objectives. The solutions of such problems are not evident or clearly standing out, so optimization formulates the problems in a structured way (mathematically), helping us solve them while quantifying the impacts of these solutions, or their trade-offs with the constraints of the problem [13].

An objective (goal) is selected for our problem and the optimal solution to the problem will result from its minimization or maximization (e.g., maximum water supply, minimum costs, etc.). This is described mathematically by an objective function.

The objective function is subject to the constraints of the problem, which, as mentioned, express the physical, technical, economic, environmental, or regulatory restrictions of the problem. Each one of these constraints is expressed by a function, and all should be met. The variables in all these functions represent the decision parameters (decision variables) under our control to define them (i.e., the solutions of the optimization problem). The optimal solution values will provide the minimum or maximum result of the objective function, having met all the constraints of the problem [37].

For example, an objective function (Z) is set as a goal to maximize (or minimize), under constraints, which are all functions (h) of the decision variables $x_1,\ x_2, x_3, \ldots, x_n$ (1):

$$Z_{\max\ (\text{or min})} = h(x_1,\ x_2, x_3, \ldots, x_n) \tag{1}$$

The objective function must satisfy a set (i) of constraints (functions y). These are subject to thresholds (e.g., a_i, which are known values), expressing the acceptable range of values (2):

$$y_i(x_1,\ x_2, x_3, \ldots, x_n) \leq a_i \tag{2}$$

The system's optimum solution must meet all the constraints and the objective function. This practically provides a useful set-up for several problems, because an objective set, as in Z, can be maximized or minimized, while securing the optimum levels of the other parameters of the system (controlled as $y_i -$ constraints), all depending on the decision variables [47].

This describes the idea of the general (in this case linear) optimization logic. The different techniques are building on this logic, by following necessary modifications. Depending on the relations of the variables and constraints involved and the mathematical form of the functions used, there are many different optimization techniques, such as non-linear, fuzzy, dynamic, quadratic, or goal programming.

This entry presents a typical problem of integrated WRM, by providing its general formulation, and then its approach from different optimization types offering different representations and answers. The entry is expected to contribute as an educational resource, providing tangible and easily reproducible examples, along with the respective codes.

2. Problem Definition

One WRM problem that is increasingly being studied by water modelers and managers is the optimal and cost-efficient water-energy resource allocation and production, under natural (hydrological) restrictions and sustainability-related goals, such as decarbonization [48,49].

Here, we develop a simple optimization problem considering these factors, and synthesize them in a single model. In particular, we consider water supply from different sources that can be allocated to different users, along with energy considerations. Let us assume we want to optimize the water and energy use, to achieve the minimum costs in an environmentally friendly way.

First, we define our decision variables (we want to find their optimum values, which are not obvious or known from the beginning):

- SW: amount of surface water to use [m^3 for a specific time, *t*] (>0);
- GW: amount of groundwater to use [m^3 for a specific time, *t*] (>0);
- E: amount of non-renewable energy to produce [kWh for a specific time, *t*] (>0);
- ER: amount of renewable energy to produce [kWh for a specific time, *t*] (>0).

The units are m^3 for SW and GW, and kWh for E and ER, respectively, for a specific time-step *t*, which is defined by the analyst, depending on the problem's need (e.g., annual, monthly, etc.).

Next, we define the problem's parameters, i.e., the factors that play a role in the broader context of our problem. The parameters' values are known, and we will use them to estimate the decision variables. So, in a way, these are the data we have (or need to find), in order to solve the problem:

- SWA: Surface water use allowance (Surface water availability) [m^3]. Surface water is considered to be a renewable supply source, in general (depending on the hydrological cycle). The amount of surface water we can exploit depends also on the infrastructure (dams and reservoirs, rainwater storage structures, etc.).
- GWA: Groundwater use allowance (Groundwater availability) [m^3]. Groundwater is replenishing through infiltration, at a much lower rate than surface water, so it is considered to be a non-renewable supply source. Its availability for usage is determined by hydrological models that show what part of the groundwater stocks are renewable (groundwater recharge).
- TWA: Total Water Availability [m^3]. This will be the sum of GWA and SWA.
- EA: Energy production capacity from non-renewable sources (Energy Availability) [kWh]. This will include power generation from sources that are finite and not naturally replenished within a human timescale, such as coal, natural gas, oil, or nuclear power.
- ERA: Energy production capacity from renewable sources (Energy Renewable Availability) [kWh]. This refers to the power generation from environmentally sustainable sources such as wind, solar, hydroelectric, or geothermal power.
- TEA: Total Energy Availability. This will be the sum of EA and ERA [kWh].
- WD: Water Demand (total) to cover the various uses (urban, agricultural, industrial) [m^3].
- ED: Energy Demand (total) to cover the various uses (urban, agricultural, industrial) [kWh].
- GWC: Cost for using groundwater (e.g., pumping, treatment, works) [USD/m^3].
- SWC: Cost for using surface water (e.g., storage and distribution works, treatment) [USD/m^3].
- EC: Cost for using non-renewable energy (e.g., works, production, distribution) [USD/kWh].
- ERC: Cost for using renewable energy [USD/kWh].
- GWE: Groundwater-associated emissions (CO_2 emissions resulting from water treatment and distribution) [kg CO_2/m^3].
- SWE: Surface water-associated emissions (CO_2 emissions resulting from water treatment and distribution) [kg CO_2/m^3].
- EE: Non-renewable energy-associated emissions (CO_2 emissions resulting from energy production and distribution) [kg CO_2/kWh].
- ERE: Renewable energy-associated emissions (CO_2 emissions resulting from energy production and distribution) [kg CO_2/kWh].
- GHG: Emissions (maximum allowable CO_2 emissions—Green-House-Gases) [kg CO_2].

- B: Budget (maximum amount of money available to provide water and energy to serve the users) [USD].

Again, all units refer to a specific time-step t, predefined by the analyst.

Some potential (and common) concerns when optimizing such a system, which are expressed as constraints:

- Not exceed the water availability;
- Not exceed the energy availability;
- Meet the water demand;
- Meet the energy demand;
- Not exceed the CO_2 emissions based on the predefined level of allowable emissions (GHG);
- Not exceed the costs based on the available budget (B);
- Not exceed the groundwater available resources (avoid over-exploitation of non-renewable water stocks);
- Not exceed the surface water available to use (avoid over-pumping);
- Not exceed the energy production capacity from non-renewable sources;
- Not exceed the energy production capacity from renewable sources.

In the following sections, we will formulate the described problem using different optimization techniques. In the Supplementary Material, we provide a set of indicative input data for the problem, along with publicly available Python scripts for solving each example.

3. Linear Problem Formulation

In linear programming, the Objective Function (OF) and the constraints are connected with the decision variables with linear functions (as described in Section 1.2). In particular:

OF: Minimize total costs of using water and energy (3). Often, this is the decision-maker's preference, so cost minimization is a common and practical objective for many real-world optimization problems:

$$Z_{\min} = GWC{\cdot}GW + SWC{\cdot}SW + EC{\cdot}E + ERC{\cdot}ER \tag{3}$$

Subject to the following constraints, according to the ones described in the last paragraph of Section 2:

Water availability constraint (4):

$$GW + SW \leq TWA, \quad [\mathrm{m}^3] \tag{4}$$

Energy availability constraint (5):

$$E + ER \leq TEA, \quad [\mathrm{kWh}] \tag{5}$$

Water demand constraint (6):

$$GW + SW = WD, \quad [\mathrm{m}^3] \tag{6}$$

Energy demand constraint (7):

$$E + ER = ED, \quad [\mathrm{kWh}] \tag{7}$$

We observe here that the left-hand sides of constraints (4) and (6), and of constraints (5) and (7), are the same. This is fine because both sets of constraints represent different conditions on the same variables.

CO_2 emissions constraint (8):

$$GWE \cdot GW + SWE \cdot SW + EE \cdot E + ERE \cdot ER \leq GHG, \quad [\mathrm{kg\ CO_2}] \tag{8}$$

Budget constraint (ensures feasibility of the OF's solution and consistency with real-life budget constraints) (9):

$$GWC \cdot GW + SWC \cdot SW + EC \cdot E + ERC \cdot ER \ \leq \ B, \quad [\mathrm{USD}] \tag{9}$$

Groundwater capacity limits (10):

$$GW \ \leq GWA, \quad [\mathrm{m}^3] \tag{10}$$

Surface water capacity limits (11):

$$SW = SWA, \quad [\mathrm{m}^3] \tag{11}$$

Non-renewable energy production capacity limits (12):

$$E \ \leq EA, \quad [\mathrm{kWh}] \tag{12}$$

Renewable energy production capacity limits (13):

$$ER \ \leq ERA, \quad [\mathrm{kWh}] \tag{13}$$

The problem solution will be practically the set of values for *GW*, *SW*, *E*, and *ER*, which will satisfy all other equations, giving them also a value. This example problem, as currently formulated, provides a solution for a specific time period (e.g., a year—considering annual averages); hence, the units are not time-dependent. The script for the linear problem algorithm allows the user to input their own values for the desired time period.

Linear programming models are widely used, as they are simple and straightforward, and less computationally demanding compared to other optimization types [50,51].

4. Fuzzy Problem Formulation

Some parameters of the problem described above can be considered fuzzy (i.e., uncertain, with only some indication about the range of values they can potentially take). Fuzzy optimization allows to deal with imprecise, vague, or uncertain parameters, which is a common situation in real-world WRM problems [52,53].

So, let us assume that the GWA and SWA parameters are fuzzy, which is a quite realistic consideration, since the groundwater and surface water availability depend on natural phenomena and the water cycle [54,55]. Sometimes, more parameters can be fuzzy. For example, WD and ED can also be uncertain, but usually engineers use upper-end values for safe design, so here we consider them as not fuzzy in this example [52,56].

Practically, the fuzzy parameters can vary within a range of values (fuzzy sets), which can be defined by the user. For example: GWA, Groundwater use allowance [m^3]: low = 1000, medium = 2000, high = 4000. SWA: Surface water use allowance [m^3]: low = 500, medium = 1000, high = 3000. The values of the fuzzy sets do not necessarily have to increase or decrease around the same number, nor do they have to be equal in size. The choice of the values and the sizes of the fuzzy sets depend on the problem and the available data. In cases of uncertain problems or limited data, the fuzzy sets can be even chosen arbitrarily, as long as they capture the degree of membership of the input variables in each set, and represent the uncertainty and vagueness associated with the input variables [57]. For a more "accurate" choice of the fuzzy sets, the user should consider the available data, expert knowledge, and the context of the problem. For example, in our model, we could study the time-series of hydrological data and capture a possible range for GWA and SWA [58]. Mathematically, the fuzzy optimization problem can be the same as the linear one developed in the previous section, with the difference now that GWA and SWA input parameters are fuzzy sets of values.

In particular, that would be: OF—Minimize total costs of using water and energy (14):

$$Z_{min} = GWC \cdot GW + SWC \cdot SW + EC \cdot E + ERC \cdot ER \tag{14}$$

Subject to the following constraints, as in the previous problem set-up:
Water availability constraint (15):

$$GW + SW \leq TWA, \quad [\mathrm{m}^3] \tag{15}$$

where TWA is now the total water availability, defined as the minimum of the fuzzy sets GWA and SWA. (In fuzzy optimization, the minimum operator is commonly used to define the intersection between fuzzy sets [57]. In this case, the TWA is defined as the minimum of the fuzzy sets GWA and SWA because it represents the lower bound of water availability between the two sources (to make a realistic constraint among the three values of each fuzzy set of values, for each GWA and SWA).) So, TWA is the minimum value of the alpha-cuts of GWA and SWA at the alpha-cut level of 0.5 (a usual parameter expressing a medium contribution of the variables—more details below).

Energy availability constraint (16):

$$E + ER \leq TEA, \quad [\mathrm{kWh}] \tag{16}$$

Water demand constraint (17):

$$GW + SW = WD, \quad \left[\mathrm{m}^3\right] \tag{17}$$

Energy demand constraint (18):

$$E + ER = ED, \quad [\mathrm{kWh}] \tag{18}$$

CO_2 emissions constraint (19):

$$GWE \cdot GW + SWE \cdot SW + EE \cdot E + ERE \cdot ER \leq GHG, \quad [\mathrm{kg\ CO_2}] \tag{19}$$

Budget constraint (20):

$$GWC \cdot GW + SWC \cdot SW + EC \cdot E + ERC \cdot ER \leq B, \quad [\mathrm{USD}] \tag{20}$$

Groundwater capacity limits (21):

$$GW \leq GWA, \quad [\mathrm{m}^3] \tag{21}$$

where GWA, in this case, is the fuzzy set representing the groundwater availability: namely, the upper (high) value of the GWA fuzzy set, which cannot be exceeded.

Surface water capacity limits (22):

$$SW = SWA, \quad [\mathrm{m}^3] \tag{22}$$

Similarly, here the SWA is the fuzzy set representing the surface water availability, namely, the upper (high) value of the SWA fuzzy set, which we cannot exceed.

Non-renewable energy production capacity limits (23):

$$E \leq EA, \quad [\mathrm{kWh}] \tag{23}$$

Renewable energy production capacity limits (24):

$$ER \leq ERA, \quad [\mathrm{kWh}] \tag{24}$$

This example problem, as currently formulated, provides a solution (optimum) for a specific snapshot in time, or a predefined time-period, hence the units are not time-dependent. The script for the fuzzy problem algorithm allows the user to input his own values for the desired time-period.

This fuzzy optimization problem can be solved using fuzzy linear programming techniques, such as fuzzy simplex or fuzzy goal programming [59,60]. In a fuzzy optimization problem, it is also important to interpret the fuzzy results, as the solutions are also fuzzy sets (or fuzzy numbers), which indicate the degree of membership of each value in the solution space to the optimal solution. The degree of membership is determined by the degree of satisfaction of the constraints and OF. The alpha-cut level in fuzzy set theory represents a threshold value that defines the degree of membership of elements in a fuzzy set (membership of SWA and GWA values satisfying the OF and constraints) [61]. It is used to "cut" or "truncate" the fuzzy set to obtain a crisp (non-fuzzy) set of elements that have a membership degree equal to or greater than the alpha-cut level. So, this alpha-cut level is used to calculate the TWA by taking the minimum membership values of GWA and SWA at the specified alpha-cut level. We used an alpha-cut level of 0.5 in this example, which is commonly used to obtain a "midpoint" estimate of the fuzzy set. The user can experiment with different alpha-cut levels to see how they affect the optimization results and the level of uncertainty incorporated into the decision-making process [62]. Below is a short description of what different alpha-cut levels express:

1. Alpha-Cut Level = 0: This corresponds to a crisp set and selects only elements with a membership degree of exactly 0. It effectively eliminates any uncertainty or fuzziness.
2. Alpha-Cut Level = 0.5 (the "default" case): This is a common choice and represents a midpoint between the lowest and highest membership values in the fuzzy set. It provides a balanced estimate between conservative and optimistic scenarios.
3. Alpha-Cut Level = 1: This corresponds to the highest membership degree and selects all elements with a membership degree of 1. It includes all elements in the fuzzy set.
4. Alpha-Cut Level between 0 and 0.5: Lower alpha-cut levels select elements with lower membership values, making the estimate more conservative.
5. Alpha-Cut Level between 0.5 and 1: Higher alpha-cut levels select elements with higher membership values, making the estimate more optimistic.

The choice of the alpha-cut level depends on the specific problem and the degree of conservatism or optimism we want to incorporate into the analysis. A higher alpha-cut level includes more elements in the estimate, while a lower alpha-cut level selects fewer elements, emphasizing higher membership values [61]. For example, in a possible solution situation of the problem described in this section, one might observe that below some alpha-cut levels, there is no feasible solution (where this means simply that there is not enough water availability to satisfy the OF and the constraints), while above some alpha-cut levels there is a feasible solution. Adjusting the alpha-cut level may lead to different feasibility results, so it is essential to consider the level of uncertainty and conservatism in the problem when selecting an appropriate alpha-cut level for decision-making.

5. Dynamic Problem Formulation

Dynamic optimization uses differential and algebraic relations that consider the changing nature of the variables over time, by breaking the problem in smaller and simpler sub-problems, so spanning several points in time. The optimum solutions can involve parameter estimation and be also found based on predictions of future outcomes [25].

Several of the parameters used in our example problem are not constant over time. They change every year, month, week, or even day. Let us see how to describe the problem, if we consider that the following parameters are time-dependent:

- GWA: Groundwater use allowance (Groundwater availability) [m^3/t];
- SWA: Surface water use allowance (Surface water availability) [m^3/t];
- ERA: Energy production capacity from renewable sources (Energy Renewable Availability) [kWh/t];

- WD: the total water demand [m^3/t].

Let us assume that ED: Energy Demand (total) stays stable around the year.

With the above time-dependent parameters, the problem will automatically have also time-dependent decision variables, namely the following:

- GWt: the amount of groundwater used at time *t* [m^3].
- SWt: the amount of surface water used at time *t* [m^3].
- Et: the amount of non-renewable energy produced at time *t* [kWh] (in this example we assume that this is constant, as usually the production of conventional energy sources is more controllable compared to the non-renewable sources).
- ERt: the amount of renewable energy produced at time *t* [kWh].

So, considering the above, the mathematical formulation of the same problem described in the previous sections can be now expressed as a dynamic optimization one.

The OF will refer to the minimization of the total costs of using water and energy over a time horizon *T* (e.g., *T* = 12 months) (25):

$$\text{Zmin} = \sum_{t=1}^{T=12} (GWC{\cdot}GWt + SWC{\cdot}SWt + EC{\cdot}Et + ERC{\cdot}ERt) \tag{25}$$

Subject to the following constraints, $\forall\, t \in \{1, 2, \ldots, T = 12\}$:

Water availability constraint (26):

$$GWt + SWt \ \leq \ TWAt, \quad [\text{m}^3] \tag{26}$$

Energy availability constraint (27):

$$Et + ERt \ \leq \ TEAt, \quad [\text{kWh}] \tag{27}$$

Water demand constraint (28):

$$GWt + SWt = WDt, \quad [\text{m}^3] \tag{28}$$

Energy demand constraint (29):

$$Et + ERt = EDt, \quad [\text{kWh}] \tag{29}$$

CO_2 emissions constraint (30):

$$GWE \cdot GWt + SWE \cdot SWt + EE \cdot Et + ERE \cdot ERt \ \leq \ GHG, \quad [\text{kg CO}_2] \tag{30}$$

Budget constraint (31):

$$GWC \cdot GWt + SWC \cdot SWt + EC \cdot Et + ERC \cdot ERt \ \leq \ B, \quad [\text{USD}] \tag{31}$$

Groundwater capacity limits (32):

$$GWt \ \leq GWAt, \quad [\text{m}^3] \tag{32}$$

Surface water capacity limits (33):

$$SWt = SWAt, \quad [\text{m}^3] \tag{33}$$

Non-renewable energy production capacity limits (34):

$$Et \ \leq EAt, \quad [\text{kWh}] \tag{34}$$

Renewable energy production capacity limits (35):

$$ERt \ \leq ERAt, \quad [\text{kWh}] \tag{35}$$

For the time horizon $T = 12$ the model will provide a set of 12 solutions, namely one set of decision variables, an OF solution, and constraint values, per month.

6. Multi-Objective Optimization—Goal Programming

Goal Programming (GP) is another technique that can be applied to a variety of decision problems involving multiple objectives [63]. GP formulates an objective function, which gets optimized by reaching as close as possible to the specified goals. It aims, thus, to minimize the set of deviations from multiple pre-specified (desirable) goals that are considered all together. The analyst (or stakeholders) assigns weights to those goals according to their importance [37]. The weights play the role of penalizing the deviations from the desirable goal values (so that lower-order goals are considered only after the higher-order goals are achieved). The general GP model is based on linear programming, wherein the positive (exceedance) and negative (under-performance) deviations from our predefined goals are minimized, following the prioritization imposed by the weights (penalties) [7,11].

The general GP model can be stated as follows, based on the linear programming model:

$$\min Z = \sum_{i=1}^{m} \sum_{k=1}^{K} P_k \left(w_{i,k}^{+} d_i^{+} + w_{i,k}^{-} d_i^{-} \right) \tag{36}$$

where P_k is the priority coefficient for the k-th priority;

$w_{i,k}^{+}$ is the weight for the d_i^{+} variable in the k-th priority level, and

$w_{i,k}^{-}$ is the weight for the d_i^{-} variable in the k-th priority level.

Subject to the following set of constraints (37):

$$\begin{aligned} &\textstyle\sum_{j=1}^{n} a_{ij} x_j + d_i^{-} - d_i^{+} = b_i \quad \text{for } i = 1, 2, \ldots, m \\ &\textstyle\sum_{j=1}^{n} a_{ij} x_j \ (\leq = \geq) \ b_i \quad \text{for } i = m+1, \ldots, m+p \\ &x_j, \ d_i^{-}, d_i^{+} \geq 0 \quad \text{for } j = 1, 2, \ldots, n, \quad i = 1, 2, \ldots, m \end{aligned} \tag{37}$$

where goals are expressed by "m" component column "b_i". The coefficient for the j-th decision variable in the i-th constraint is represented by the a_{ij} variables, and x_j represents the decision variable. As mentioned, w_i are the weights of each goal and d_i^{-}, d_i^{+} are the deviational variables that represent the amount of under-achievement and over-achievement of the i-th goal, respectively.

The goals are classified in k-ranks; the pre-emptive priority factors (P_1, P_2, ...) should be assigned to deviational variables di^- and di^+ according to their order of importance [63]. So, a lower-priority goal can never be achieved at the expense of higher-priority level.

The problem we demonstrated in our example will have the same decision variables and parameters as the linear model. The constraints (Goal Programming Targets) are Equations (38)–(47):

$$\text{Min Costs}: \ GWC \cdot GW + SWC \cdot SW + EC \cdot E + ERC \cdot ER - d_c^{+} \ \leq \ B, \quad [USD] \tag{38}$$

$$\text{Min } CO_2 \text{ emissions}: GWE \cdot GW + SWE \cdot SW + EE \cdot E + ERE \cdot ER - d_{CO2}^{+} \ \leq \ GHG, \ [\text{kg } CO_2] \tag{39}$$

$$\text{Min Groundwater use}: \ GW - d_{gw}^{+} \leq GWA, \quad [\text{m}^3] \tag{40}$$

$$\text{Reach Surface water availability}: \ SW - d_{sw}^{+} + d_{sw}^{-} <=> SWA, \ [\text{m}^3] \tag{41}$$

$$\text{Minimize non} - \text{renewable energy production}: E - d_e^{+} \ \leq EA, \quad [\text{kWh}] \tag{42}$$

$$\text{Maximize renewable energy production} : ER + d_{er}^{-} \geq ERA, \quad [\text{kWh}] \tag{43}$$

While, at the same time, we do not want to exceed the available resources TWA and TEA, and meet the demands WD and ED:

$$\text{Water availability} : GW + SW - d_{w}^{+} \leq TWA, \quad [\text{m}^3] \tag{44}$$

$$\text{Energy availability} : E + ER - d_{en}^{+} \leq TEA, \quad [\text{kWh}] \tag{45}$$

$$\text{Meet Water Demand} : GW + SW - d_{wd}^{+} + d_{wd}^{-} <=> WD, \quad [\text{m}^3] \tag{46}$$

$$\text{Meet Energy Demand} : E + ER - d_{en}^{+} + d_{ed}^{-} <=> ED, \quad [\text{kWh}] \tag{47}$$

This model will provide the optimum mix of m^3 of groundwater and surface water (GW, SW), and kWh of renewable and non-renewable sources (ER, E), to minimize costs, emissions, groundwater use, and non-renewable energy production, while maximizing the surface water use and the renewable energy production. At the same time, the model controls for not exceeding water and energy availability, and meeting the respective water and energy demands.

The OF (48) aims to minimize the deviations from the predefined targets (38)–(47), thus minimizing the positive and negative deviation variables (d_i^+, d_i^-), which will be weighted depending on their importance by weights w_i^+ and w_i^-, respectively. As mentioned, these weights w_i^+ and w_i^- are actually the penalties that the user defines for each deviation. Namely, this is the degree to which we do not want something to happen (e.g., penalty 1 if we exceed the CO_2 emissions threshold, etc.).

$$\begin{gathered}\text{Min } Z = w_c^+ d_c^+ + w_{CO_2}^+ d_{CO_2}^+ + w_{gw}^+ d_{gw}^+ + w_{sw}^+ d_{sw}^+ + w_{sw}^- d_{sw}^- + w_e^+ d_e^+ + w_{er}^- d_{er}^- + w_w^+ d_w^+ \\ + w_{en}^+ d_{en}^+ + w_{wd}^+ d_{wd}^+ + w_{wd}^- d_{wd}^- + w_{ed}^+ d_{ed}^+ + w_{ed}^- d_{ed}^-\end{gathered} \tag{48}$$

Each d_i^+, d_i^- is a deviation we want to minimize, "as much as its importance", which is defined by the respective weight (w). So, each term of the OF corresponds to each goal (as defined in (38)–(47). For this particular example, let us assume three scenarios of weight preferences (which can be represented in custom scales, for this case from 0–1) [7], as Table 1 shows.

Table 1. Indicative weights assigned to the deviation variables of the OF (48) from three scenarios, preferring: the economic-related targets ("Intensive Economy"), the environmental ones ("Environmentalist"), and a more balanced case ("Middle Solution").

Description	Weights w	"Intensive Economy"	"Middle Solution"	"Environmentalist"
Minimize Costs	w_c^+	0.9	0.5	0.2
Minimize Emissions	$w_{CO_2}^+$	0.1	0.4	1
Minimize Groundwater use	w_{gw}^+	0.1	0.4	0.8
Reach surface water use	w_{sw}^+	0.1	0.5	0.7
Reach surface water use	w_{sw}^-	0.1	0.5	0.7
Minimize non-renewable energy use	w_e^+	0.3	0.6	0.8
Maximize renewable energy use	w_{er}^-	0.5	0.7	0.8
Do not exceed water availability	w_w^+	0.2	0.5	0.7
Do not exceed energy availability	w_{en}^+	0.2	0.3	0.5
Meet Water Demand	w_{wd}^+	0.8	0.7	0.5
Meet Water Demand	w_{wd}^-	0.8	0.7	0.5
Meet Energy Demand	w_{ed}^+	0.8	0.6	0.4
Meet Energy Demand	w_{ed}^-	0.8	0.6	0.4

Each scenario will result a set of solutions for each decision variable and set of goals, allowing the user to explore the effects of the weights on the results.

This problem provides a solution (optimum) for a specific snapshot in time, or a predefined time-period; hence, the units are not time-dependent. The provided script for the GP algorithm allows the user to input their own values for the desired time-period.

7. Non-Linear Programming

In the case of non-linear programming (NLP), the general relations of the OF (1) and/or constraints (1) are described by non-linear functions. Although these problems are computationally harder to solve, they are more often closer to reality, and optimality can be guaranteed when certain conditions are met by the problem [7,37]. In particular, the initial linear model example is realistic, but it comes with some unavoidable assumptions: its formulation assumes that the costs and CO_2 emissions for using water and energy sources are linear with respect to the amounts used. It also assumes that the energy production from non-renewable and renewable sources are directly proportional to the amount produced. In real life, these assumptions do not always hold. Thus, to represent such a case, the linear programming formulation must become non-linear, so the problem needs to be adjusted accordingly.

The decision variables and the parameters of the problem remain the same as with the linear case, as well as the general model set-up. The OF (49) will still aim to minimize the total costs of using water and energy:

$$Z\text{min} = GWC \cdot GW \; + \; SWC \cdot SW \; + \; EC \cdot E \; + \; ERC \cdot ER \quad (49)$$

But in the NLP case, the terms are non-linear functions (f) that represent the cost as a function of the amount used. These functions should capture the non-linear relationships between the costs and the decision variables. So, GWC = f(GW), SWC = f(SW), EC = f(E), and ERC = f(ER). For example, one can use polynomial functions, exponential functions, or other non-linear relationships to model these cost functions based on the data (more details on how to estimate these are provided below).

The constraints will be formulated according to the previous cases.

Water availability constraint (50):

$$GW + SW \; \leq \; TWA, \quad [\text{m}^3] \quad (50)$$

Energy availability constraint (51):

$$E + ER \; \leq \; TEA, \quad [\text{kWh}] \quad (51)$$

Water demand constraint (52):

$$GW + SW = WD, \quad [\text{m}^3] \quad (52)$$

Energy demand constraint (53):

$$E + ER = ED, \quad [\text{kWh}] \quad (53)$$

CO_2 emissions constraint (54):

$$GWE \cdot GW + SWE \cdot SW + EE \cdot E + ERE \cdot ER \; \leq \; GHG, \quad [\text{kg CO}_2] \quad (54)$$

where, again, the emissions coefficients will be non-linear functions of the water or energy used. Namely, GWE = g(GW), SWE = g(SW), EE = g(E), and ERE = g(ER). Similar to functions (f), these non-linear functions (g) represent the emissions according to the amounts used.

Budget constraint (55):

$$GWC \cdot GW + SWC \cdot SW + EC \cdot E + ERC \cdot ER \leq B, \quad [\text{USD}] \tag{55}$$

Groundwater capacity limits (56):

$$GW \leq GWA, \quad [\text{m}^3] \tag{56}$$

Surface water capacity limits (57):

$$SW = SWA, \quad [\text{m}^3] \tag{57}$$

Non-renewable energy production capacity limits (58):

$$E \leq EA, \quad [\text{kWh}] \tag{58}$$

Renewable energy production capacity limits (59):

$$ER \leq ERA, \quad [\text{kWh}] \tag{59}$$

In this formulation, the non-linearity comes from the functions (f) and (g). As mentioned above, these functions can be defined based on the data of the problem, reflecting in this case the actual relationships between the costs and the amounts used [36]. The choice of specific non-linear functions will depend on the nature of the cost data and the relationships, which can be mathematically observed. For example, regression techniques or other data-driven methods have been helpful and widely used for determining the appropriate non-linear functions [64,65]. As soon as these are defined, they can be then incorporated into the NLP problem formulation [66].

Let us assume we have collected some data and performed linear regression to model the cost and the emissions as functions (f and g) of the respective decision variables. The linear regression equations might look like this (60) and (61):

$$\begin{gathered}
\text{Cost for using groundwater, } GWC = \mathrm{f}(GW) = a_1 \cdot GW + b_1 \\
\text{Cost for using surface water, } SWC = \mathrm{f}(SW) = a_2 \cdot SW + b_2 \\
\text{Cost for using non-renewable energy, } EC = \mathrm{f}(\mathrm{E}) = a_3 \cdot \mathrm{E} + b_3 \\
\text{Cost for using renewable energy, } ERC = \mathrm{f}(ER) = a_4 \cdot ER + b_4
\end{gathered} \tag{60}$$

where a_1, a_2, a_3, and a_4 are the coefficients obtained from linear regression, and b_1, b_2, b_3, and b_4 are the intercepts.

$$\begin{gathered}
\text{Emissions from groundwater, } GWE = \mathrm{g}(GW) = c_1 \cdot GW + d_1 \\
\text{Emissions from surface water, } SWE = \mathrm{g}(SW) = c_2 \cdot SW + d_2 \\
\text{Emissions from non-renewable energy, } EC = \mathrm{g}(E) = c_3 \cdot E + d_3 \\
\text{Emissions from renewable energy, } ERE = \mathrm{g}(ER) = c_4 \cdot ER + d_4
\end{gathered} \tag{61}$$

Here, similarly, c_1, c_2, c_3, and c_4 are the coefficients obtained from linear regression, and d_1, d_2, d_3, and d_4 are the intercepts.

These functions (f) and (g) can be inserted in (49) and (54) to solve the NLP problem. It is worth noting that these are simple linear regression-based functions for the sake of providing an example. In practice, the user may need to use more complex functions if the relationships between costs or emissions and usage amounts are non-linear, e.g., considering also the incorporation of higher-order terms.

8. Discussion

The example problems described in this entry (linear, fuzzy, dynamic, GP, NLP) were coded in Python within the Spyder environment of Anaconda. Python's open-source nature, widespread accessibility, and compatibility with various optimization solvers make it a versatile and powerful choice for such models [67]. A link with access to all the scripts is provided in the end matter at the end of this entry. This supplementary material includes a detailed description of the numerical examples provided for the solution of the linear, fuzzy, dynamic, GP, and NLP models. In particular, we assumed some indicative parameter values for a typical year, and provide them as input values to solve each model. All scripts are structured to allow the users to first define the decision variables, then insert manually the values of the parameters, describe the OF and constraints, execute the optimization process (utilizing linear, fuzzy, dynamic, goal, or non-linear programming), solving, thus, the problem, and print the results of the OF and each one of the constraints. The users have the flexibility to modify and, of course, improve the provided examples and tailor them according to their own problems and data. Thus, adaptability and customization are ensured.

The different approaches stand for different problem requirements, offering a spectrum of tools to modelers [68]. For instance, the linear approach is a simpler and more accessible representation of a complex problem, in terms of (linearity) assumptions that one must consider, and computational demand. A simple yet powerful technique such as linear programming is useful when one is first approaching a problem and needs to understand how the variables and parameters interact [69].

Next, the fuzzy model enhances the approach in terms of potentially uncertain values by introducing a range of possible values to some variables. Thus, it makes a first step toward a "not so deterministic" approach. This deviation from the linear model allows users to incorporate a degree of uncertainty into their analysis, acknowledging the variability in input values and, consequently, presenting a spectrum of potential outcomes and associated constraints [59,70]. This extension of the linear model offers a more realistic representation of the inherent uncertainties in many real-world scenarios without introducing a substantial increase in complexity. The fuzzy model's ability to capture and navigate this inherent uncertainty makes it a valuable tool for decision-making in dynamic and unpredictable environments.

The dynamic model demonstrates that the problem is not atemporal in reality, allowing the user to input the values of the variables and parameters per time-step (e.g., per month), and see also sets of results per time-step. Real-world problems are inherently temporal, and this model set-up acknowledges the evolving nature of various factors over time [71]. This is a more computationally demanding process but can offer realistic representations of real problems and show their time-evolving nature. This temporal dimension allows for a deeper understanding of how solutions unfold over time, capturing the dynamic nature of the system under consideration. Thus, such dynamic solutions are recommended in cases where the modelers need to see a specific change in the results over time, or after another change in the input parameters (e.g., exploring seasonal variations in supply and demand) [72].

The GP model follows a different logic, being multi-objective, which is often the case in real situations, and allows the analyst to consider different opinions (e.g., stakeholders' priorities, as in Table 1). Within the corresponding script, users have the flexibility to manually input weights that signify the importance of each goal. This feature empowers analysts to explore a spectrum of scenarios, providing a nuanced understanding of the trade-offs involved in decision-making processes. The ability to consider multiple perspectives makes GP particularly valuable for decision-makers seeking comprehensive and inclusive solutions [73].

Finally, the NLP approach is "free" from the linearity assumption. It allows the user to examine in detail the relations governing the OF and/or the constraints of the problem, describing them with non-linear functions. This flexibility allows for the description of these relationships using non-linear functions, providing a more realistic representation of the intricacies involved. However, it is crucial to note that this increased realism comes at the cost of added complexity, making the computational demands of NLP more substantial.

Despite its computational challenges, the NLP approach remains invaluable for addressing problems wherein non-linearities play a significant role, offering a nuanced and accurate modelling framework.

9. Conclusions and Prospects

This entry described an optimization problem considering the most common concerns of the modern water management processes, including economic (e.g., costs) and sustainability factors (e.g., resources use, GHG emissions). The aim was to provide a useful educational and computational resource, allowing the users to build on the examples provided here, and modify them according to their specific cases.

Depending on the nature of the problem one has to solve, and the mathematical expressions that better describe the relationships among the functions and variables used, there are many more techniques that can be used, e.g., integer programming, quadratic programming, stochastic optimization, unconstraint optimization, etc. [36,74–76]. Genetic Algorithms (GAs) is another widely used technique. GA optimization is a heuristic search algorithm inspired by the process of natural selection—based on Darwin's evolution theory, where the fittest individuals (solutions) are selected for reproduction in order to produce offspring of the next generation of solutions, until a stopping criterion is met [77]. GAs can be applied to solve linear optimization problems, such as the first example we considered, and in such cases, the mathematical formulation remains the same as in linear programming. But GAs provide an alternative approach to finding solutions, and are particularly useful when traditional LP techniques are impractical due to the problem's complexity or constraints. GAs can also handle a wide range of optimization problems beyond linear ones [78].

Choosing the most appropriate optimization model is a critical decision, as there is no specific guideline, but it depends on the specific characteristics and objectives of the problem at hand. Linear optimization models are well suited for problems with linear relationships between variables, providing efficient solutions. Fuzzy optimization models accommodate uncertainties and vagueness in the data, making them valuable for situations wherein precise values are challenging to determine. Dynamic optimization models are apt for problems evolving over time, allowing for the consideration of sequential decision-making processes. Goal Programming is beneficial when dealing with multiple, conflicting objectives, enabling the modelling of trade-offs and finding balanced solutions, while including the opinions/priorities of stakeholders. Non-linear optimization models are essential for addressing complex problems (with non-linear relationships), offering flexibility in capturing less-obvious interactions. The choice among these models hinges on the problem's specific characteristics, and a thoughtful consideration of these aspects will guide modelers toward the most suitable optimization approach for their particular application. This entry provides a solid basis for building on the most common optimization approaches and tailoring any problem based on comprehensive models.

The application of the selected optimization technique is not always easy in all types of problems. Its success depends on the proper problem formulation by the analyst, the data availability and robustness, and the validity of the (often unavoidable) simplifying assumptions considered. The data often play a crucial role, as optimization often needs accurate data from various disciplines and/or models, which usually are not easily available in reality, or they are subject to different units, time or space scales, and other differences.

There are optimization techniques that allow stakeholder input and use it to reach solutions (such as the weights in GP), and others that do not. In any case, optimization will provide an optimal solution, and while everybody may agree that, e.g., maximizing or minimizing the OF is a desirable objective, not everyone, if indeed anyone, will be likely to agree on how best to distribute the necessary actions (including costs, benefits, behavioural changes, etc.) to reach to the optimum results. Of course, for the application of WRM strategies, models alone are not enough. However, they are useful to inform and support decisions [79]. This entry contributes to such efforts, providing usable and practical tools for integrated WRM models and applications.

Supplementary Materials: The Python scripts for all presented models can be downloaded at GitHub: https://github.com/Alamanos11/Water-Energy-Costs-Emissions-Optimizations (accessed on 8 December 2023).

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