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Research article

Induction approach via P-Graph to rank clean technologies

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ABSTRACT

Identification of appropriate clean technologies for industrial implementation requires systematic evaluation based on a set of criteria that normally reflect economic, technical, environmental and other aspects. Such multiple attribute decision-making (MADM) problems involve rating a finite set of alternatives with respect to multiple potentially conflicting criteria. Conventional MADM approaches often involve explicit trade-offs in between criteria based on the expert's or decision maker's priorities. In practice, many experts arrive at decisions based on their tacit knowledge. This paper presents a new induction approach, wherein the implicit preference rules that estimate the expert's thinking pathways can be induced. P-graph framework is applied to the induction approach as it adds the advantage of being able to determine both optimal and near-optimal solutions that best approximate the decision structure of an expert. The method elicits the knowledge of experts from their ranking of a small set of sample alternatives. Then, the information is processed to induce implicit rules which are subsequently used to rank new alternatives. Hence, the expert's preferences are approximated by the new rankings. The proposed induction approach is demonstrated in the case study on the ranking of Negative Emission Technologies (NETs) viability for industry implementation.

1. Introduction

Climate change is a worldwide issue caused mainly by emissions of CO_2. A recent report by the Intergovernmental Panel on Climate Change (IPCC) states that global greenhouse gas (GHG) emissions need to be reduced to zero by mid-century in order to keep temperature rise to a safe level of about 1.5 °C by 2100 [1]. On the other hand, carbon capture and storage and negative emission technologies (NETs) have gained research attention for their potential to address such climate change [2]. Deployment of mature NETs would contribute to the reduction of CO_2 emissions as targeted by the Paris Climate Agreement. According to Le Quéré et al. [3], 82% of the CO_2 emissions from 1959 to 2016 are from the use of fossil fuels and industries. Mitigating CO_2 emissions from the industries with appropriate clean technologies is crucial.

The best technologies can be identified by using multiple attribute decision-making (MADM) methods. These methods are employed for ranking a finite set of alternative technologies based on a set of potentially conflicting criteria which reflect economic, technical, environmental and social aspects [4]. In general, a classical decision-making process relies on the explicit elicitation process. Upon the addition of new alternatives, the elicitation process has to be repeated. Hence, soft computing tools have been developed as decision support systems to encapsulate the expert's knowledge from the problem domains. The soft computing tools have the capability of approximating human thinking pathways by transforming the information that a decision-maker provides into a set of decision rules [5]. As a result, new alternatives can be assessed using the established model which was developed based on previous examples or experiences. For instance, classical MADM approaches such as simple additive weighting (SAW) and the analytic hierarchy process (AHP) rely on explicit prior knowledge of criteria weights based on decision-maker priorities. An enhancement of AHP method with fuzzy set theory (FST) has also been done to capture the vagueness in human decision [6]. Similarly, Rough Set Theory (RST) which was developed by Pawlak (1982) using the concept of discernibility [5] has been utilized for generating rules which can be used for categorizing objects or events according to their attributes. This property enables the use of RST for various machine learning (ML) applications [7].

Using the classical MADM methods, the process of eliciting the preference and knowledge may be burdensome and confusing to the experts when the decision problem becomes more complicated. As a result, a high degree of inconsistency may be introduced into the

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decisions, making the results unreliable [8]. Nevertheless, in practice, many experts arrive at decisions that are based on tacit knowledge that they may be unable to fully articulate [9]. This tacit knowledge contains rich information about the problem domain and can be sampled via appropriate model induction strategies. This inductive approach is conceptually similar to approaches used in ML, where models are generated via training on sample data [9]; in contrast, most MADM techniques rely on a deductive approach where weights are determined by direct elicitation or estimation of the importance of the criteria.

In this work, a new inductive approach based on the P-graph framework is developed to identify feasible sets of criteria as well as their weights, based on an expert's ranking of a small set of alternatives. A SAW model is then calibrated to approximate the expert's opinion, and subsequently used to rank a larger set of alternatives. A similar approach is used in the classical LINMAP technique [10] where weight induction is done using linear programming (LP). In this work, the Process Graph or P-graph, which was initially utilized for process network synthesis (PNS) [11]. However, no prior use of P-graph for MADM has been reported in the literature. Furthermore, the inherent capabilities of P-graph and its network structure, allows for the superior elucidation of decision structure.

In the next section, a formal problem statement is described, Section 3 then focuses on the development of the induction model framework based on P-graph. A case study on Negative Emissions Technologies (NETs) is used to demonstrate the proposed induction model. Finally, conclusions and directions for future work are discussed.

2. Problem statement

The formal problem statement is as follows. Two sets of technology alternatives: I and I' are given, in which Set I is the extended set with P number of alternatives whereas Set I' is a subset of Set I referred to as the training set with M number of alternatives. There are N number of criteria to be considered in Set J. Alternatives in Set I' are ranked by an expert according to their professional tacit knowledge based on the performance data of the alternatives with respect to the given criteria. In the SAW approach, the final score of any alternative can be calculated using Eq. (1)

$$\vec{D} \times \vec{w} = \vec{s} \tag{1}$$

where $\vec{D}$ = decision matrix, $\vec{w}$ = column vector of criteria weights, and $\vec{s}$ = total score vector of the alternatives. Note that this backward induction approach can make use of the partial information from the given alternatives' ranking without necessitating the scoring (global vector) of alternatives, $\vec{s}$, when determining $\vec{w}$. The objective is to determine optimal and near-optimal weight vectors that result in SAW rankings that are consistent with the rankings given by the expert based on tacit knowledge. The implicit mental process used by the expert is approximated by the proposed induction approach.

3. Model induction framework

This section discusses the development of an optimization model for inducing the decision structure, the general principles of P-graph, and how the optimization model is translated into the proposed P-graph Induction model.

3.1. Optimization model

In this work, the weight vector needs to be determined based on a small training data set consisting of ranked alternatives. It is necessary to limit the sample size to a small number (e.g. 4–7 alternatives) so that the human mind can easily process the information [12]. The objective function as defined by Eq. (2), is to determine a set of consistent criteria weights with minimum deviation from a default assumption of equal weights:

$$\min = \sum_{j\in J}^{n} abs\left(w_j - \frac{1}{N}\right) \tag{2}$$

However, to linearize Eq. (2) and translate it into Eq. (3), it was necessary to introduce two parameters which correspond to the positive deviation (DUW_j) and negative deviation (DLW_j) of the parameter weights from a scenario where all criteria are considered to be of equal importance.

$$\min = \sum_{j}\left(DUW_j + DLW_j\right) \quad \forall j \in J \tag{3}$$

Subject to:

$$w_j - \frac{1}{N} \leq DUW_j \ \forall j \in J \tag{4}$$

$$\frac{1}{N} - w_j \leq DLW_j \ \forall j \in J \tag{5}$$

$$DUW_j, DLW_j \geq 0 \ \forall j \in J \tag{6}$$

$$\sum_{j\in J} w_j = 1 \tag{7}$$

$$\sum_{j\in J}\left[\Delta_{ii',j} w_j\right] \geq d \ \forall i, \ \forall i' \in I' \tag{8}$$

The optimization model is subject to Eq. (4) and Eq. (5), which calculate the difference between the optimal criterion weight and the weight for equal preference. The two constraints are mutually exclusive of each other. Furthermore, DUW_j and DLW_j should be non-negative as indicated in Eq. (6), to ensure that only either Eq. (4) or Eq. (5) is activated. Eq. (7) ensures that the weights of criteria sum up to unity. Eq. (8) extracts partial information by conducting pairwise comparisons between alternatives based on the *a priori* ranks given by the expert. Note that alternative i always outranks alternative i' in Eq. (8). By utilizing Eqs. (3), (4), (5), (6), (7), and (8), the decision structure can be extracted and converted into a matrix-based model which can be implemented using the P-graph framework. This is described in more detail in the succeeding section. The criteria weights induced from the P-graph are used to rank a larger number of alternatives using the SAW approach.

3.2. P-graph methodology

P-graph is a graph theoretic framework developed by Friedler et al. [13] to solve process network synthesis (PNS) problems. It makes use of bipartite graphs consisting of nodes representing operating units and material streams which can be linked by arcs. The three component algorithms of P-graph methodology are Maximal Structure Generation (MSG) [14], Solution Structure Generation (SSG) [15], and Accelerated Branch and Bound (ABB) [16]. MSG enables rigorous and automated generation of superstructures in PNS, and eliminates the risk of human error in problem specification. SSG generates all combinations of feasible network structures (subsets of the maximal structure), each of which contains a potential local optimum. ABB enables computationally efficient optimization by taking advantage of embedded information that is implicit in all PNS problems. Compared to conventional branch-and-bound, redundant structures are excluded, thus achieving accelerated search that is particularly advantageous for large-scale problems.

P-graph has been successfully applied to solving problems which exhibit a similar structure to PNS like chemical reaction pathways [17], carbon management networks [18], economic systems [19], workforce allocation [20] and human resource planning [21] to a name a few. A comprehensive review regarding such applications are discussed in the work of Tan et. al [22]. This similarity in problem structure is exploited in this work to develop the P-graph induction model as described in Figure 1.

Step 1 involves the identification of the training set matrix from the extended set matrix. This simply means that a subset of alternatives together with their performance in the criteria considered will be used to train the induction model.

Step 2 is the construction of the Delta Matrix from the information in the training matrix. The rows of the training matrix correspond to the constraints of the optimization model (Eqs. (4), (5), (6), (7), and (8)) and the columns correspond to the model variables.

Step 3 then calculates for the criteria weights using the optimization model.

The optimization model is then translated into P-graph as shown in Figure 2. Figure 2a shows a simple decision structure with 2 criteria and 2 alternatives. The alternatives will be rated with respect to different criteria in which each criterion has individual weights according to the decision maker's preference. Figure 2b is a P-graph representation translated from the Delta Matrix and illustrates the decision structure in Figure 2a. Figure 2b on the other hand is the P-graph representation of the induction model where the process units correspond to the variables (columns) while the nodes correspond to the constraints (rows) of the induction framework's Delta Matrix. It should be noted that a positive entry in the Delta Matrix refers to an output from the "process unit" while a negative entry refers to an input into the "process unit". The nodes in the P-graph are also defined by parameters in net output, y, or the last column of the Delta Matrix. The blue nodes (RDU1, RDL1, RDU2 and RDL2) are treated as fictitious raw materials which are meant to represent the deviation of the optimal weights from equal preference (i.e. 1/N). RDU1 and RDU2 are activated if the optimal weight is greater than 1/N while RDL1 and RDL2 are activated if the optimal weight is less than 1/N. These are used to model the objective function described in Eq. (3). These nodes are linked to the optimal criteria weights (W1 and W2) via nodes EUW1, ELW2, EUW2 and ELW2. These nodes regulate the activation of the fictitious units by ensuring that ELW1 and ELW2 should have a minimum of 1/N units and a maximum of 1.0 units while EUW1 and EUW2 should have a minimum of 0.0 units and a maximum of 1/N units. The green nodes (material_1 and material_2) are meant to fulfil the axioms of P-graph (i.e. every vertex of the O-type has at least one path leading to a vertex of the M-type representing a final product). In addition, a minimum difference in performance between Alternative 1 and Alternative 2 (D12) has to be indicated to establish that one alternative is preferred to another. The arcs flowing into the node D12 from process unit W1 represents the difference in performance of Alternative 1 with respect to Alternative 2 in criterion 1. Similarly, the arc flowing into node D12 from process unit W2 represents the difference in performance of Alternative 1 with respect to Alternative 2 in criterion 2. The capabilities of the model are demonstrated using a case study on Negative Emission Technologies as discussed in the succeeding section.

In Figure 2(b), the P-graph contains fictitious units of DUW1, DUW2, RDU1, and RDU2 that activate when criterion weight is >1/N. Other fictitious units (DLW1, DLW2, RDL1, RDL2) activate when the criterion weight is <1/N. On the other hand, W1 and W2 are the optimal weights for criteria 1 and 2 and they make the TOTAL equals to 1.

4. Case study

A set of Negative Emission Technology (NET) alternatives is used here for illustration based on data reported by McLaren [23]. Seven NETs are considered here, with additional data for the different systems obtained from several resources including the techno-economic assessment results of McGlashan et al. [24], process description of electrochemical splitting of $CaCO_3$ described in Rau [25] and the definitions of technology readiness [26]. The selected NETs can be categorized into three, namely mineral, pressurized, and oceanic. Table 1 summarizes the description of each NET alternative. Table 2 describes the four criteria which are considered relevant for evaluating NETs. This includes technical status (C1), potential capture capacity (C2), cost (C3), and energy requirement (C4). The Extended Decision Matrix is formed by normalizing the raw data into dimensionless form using Min-Max approach as shown in Table 3. Note that the relative magnitudes of the scores reflect the preference among the NETs with respect to each criterion, with the value of 1.0 indicating the best performing alternative for a given criterion. For the Training Set Matrix, 3 NET alternatives are chosen and ranked in descending order by an expert based on industry implementation viability. The ranking order of preference is biochar > BECCS > artificial tree.

The maximal structure for the training set is illustrated in Figure 3. This structure provides all the possible solutions that approximate the decision structure of the expert.

Optimizing the system such that the deviation from the default equal weights is minimized results in the network shown in Figure 4, which

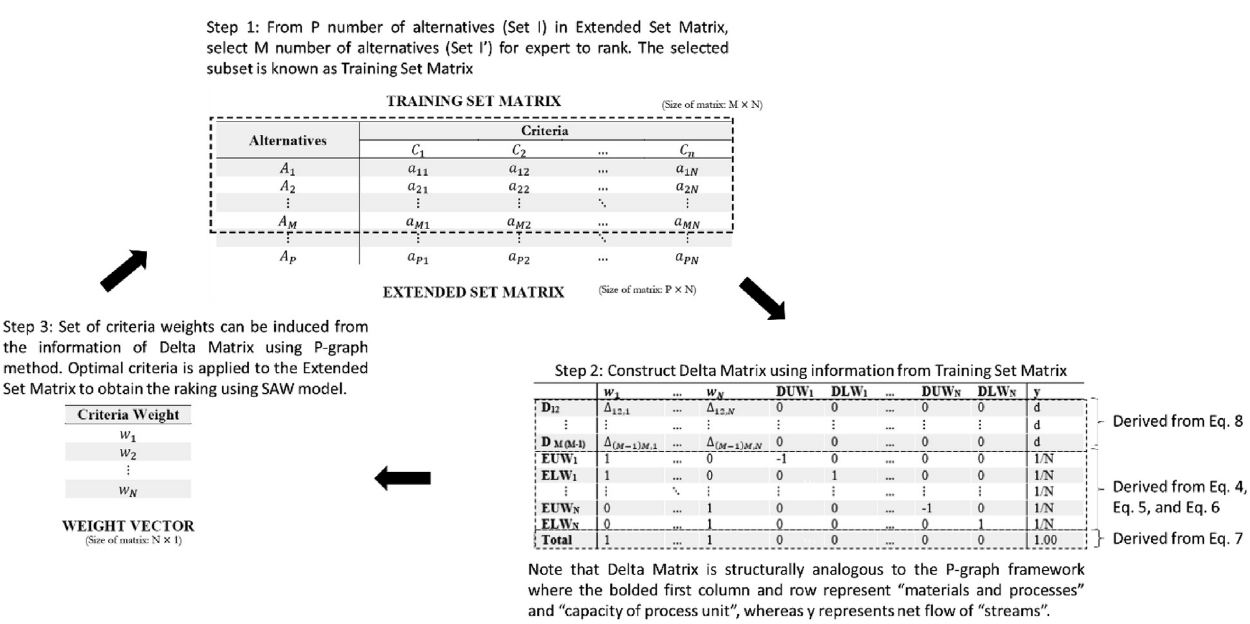

Figure 1. The flow of proposed induction network.

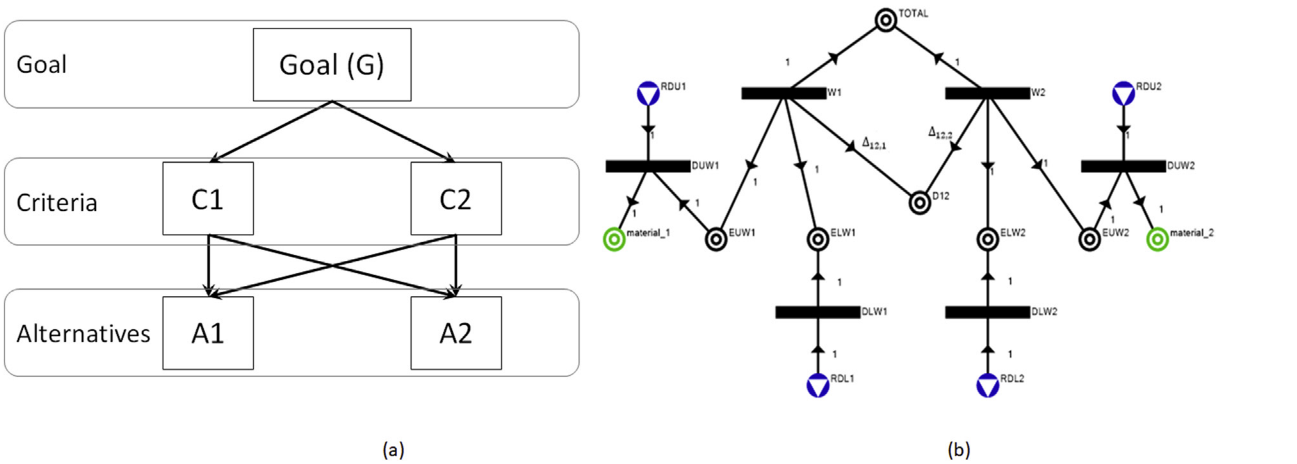

Figure 2. (a) Hierarchical decision structure for 2 criteria and 2 alternatives and (b) P-graph representation translated from Delta Matrix which illustrates the decision structure in part (a).

corresponds to a total deviation of 0.456. Additional 6 sub-optimal solutions are generated due to the unique feature of P-graph. For the optimal structure, the highest weight of 0.460 is allocated to technical status (C1) followed by the energy requirement (C4) and cost (C3) with allocated weights of 0.268 and 0.250 respectively, resulting in the criteria order of preference C1 > C4 > C3 > C2. The influence of potential capture capacity criteria, C2, on selecting NETs can be seen to be almost negligible based on its allocated weight of 0.022. Subsequently, the deviation from equal preference is 0.210 for C1 (0.460–0.250 = 0.210), 0.228 for C2, 0.00 for C3 and 0.018 for C4 such that the total deviation is 0.456 (0.210 + 0.228 + 0.00 + 0.018 = 0.456). An example of a sub-optimal solution has 7.8% increase in the total deviation of criteria weights compared to the optimal solution. The order of criteria importance of the solution according to weight is C1 > C3 > C4 > C2 with corresponding weights of 0.429 > 0.318 > 0.250 > 0.003. Note that there is a rank reversal in the criteria preference when comparing the optimal and the sub-optimal solution. It is notable that the weight of technical status is quite steady and comparably robust. We can deduce that this criterion is prioritized for the NETs deployment in industry. The induced criteria are then used to evaluate the final rankings of the extended set of alternatives using SAW approach and is shown in Table 3.

A similar P-graph approach has been conducted using 5 NET alternatives with respect to the same set of criteria such that the ranking is given by the same expert (i.e. Biochar > BECCS > Artificial Tree > Calcination Ocean Liming > Lime-Soda Process). The performance of all alternatives using the optimal criteria weights obtained can be calculated using Eq. (1) are shown in Table 4. The comparison in the performance between the training and validation sets are summarized in Table 5. Both training set and validation set yield biochar as the most feasible NET for deployment due to its comparably higher technology status and lower energy requirement. From Table 5, the results are in close agreement, except that rank reversal happens with the Artificial Tree and Ocean Liming Calcination NET. This implies that final ranking of the training sets is not consistent with the initial ranking given by the expert. Apart from the possible ambiguity and uncertainty incorporated during the human decision-making process, the reason could also be that these two alternatives work almost using the same principle as well as in the same technical status (Table 3). Artificial tree uses amine-based resins to capture CO_2 in the atmosphere, while ocean liming captures CO_2 in the ocean. Both are capturing CO_2 directly in a passive manner, by just simply adding artificial trees on the surface of the earth and adding lime

Table 1. Descriptions of NET alternatives in Set I (adapted from [23] to [26]).

Category	NET alternatives	Descriptions
Mineralization	Biochar	Sequestration of thermochemically stabilized biomass carbon in soil.
	Enhanced weathering	Acceleration of mineral carbonation process in soil.
Pressurized	Bioenergy and Carbon Capture Storage (BECCS)	Combination of biomass and Carbon Capture and Storage (CCS) technology.
	Direct Air Capture (Artificial Tree)	Adsorption and sequestration of CO_2 using amine-based sorbent and CCS technology.
	Direct Air Capture (Lime-soda Process)	Adsorption and sequestration of CO_2 using sodium hydroxide in scrubbing tower and CCS.
Oceanic	Ocean Liming (Calcination)	Addition of lime into ocean for carbonation process.
	Ocean Liming (Electrochemical Splitting)	Sequestration of $Ca(HCO_3)_{2\ aq.}$ produced from the electrolysis process into the ocean.

Table 2. Descriptions of the criteria involved in the decision-making problem.

Criteria	Descriptions
Technology Status (C1)	To approximate the technology status of NETs by considering a technology's scalability and maturity for industry deployment [26].
Potential Capture Capacity (C2)	To estimate the capability of the NETs to remove anthropogenic CO_2.
Cost (C3)	To estimate the financial feasibility of the NETs by considering the costs of material inputs, equipment, utility and implementation.
Energy Requirement (C4)	To approximate the energy feasibility of the NETs.

Table 3. Extended Decision Matrix of 7 alternatives with respect to the 4 criteria (adapted from [23] to [26]).

NET alternatives	Criteria			
	Technical status (TRL)	Potential Capacity	Cost	Energy Requirement
Biochar	1.00	0.11	0.65	1.00
BECCS (Combustion)	1.00	0.58	0.63	0.42
DAC (Artificial Tree)	0.67	1.00	0.60	0.42
DAC (lime-soda process)	1.00	1.00	0.00	0.00
Ocean Liming (Calcination)	0.67	0.00	0.92	0.24
Ocean Liming (Electrochemical splitting)	0.33	0.00	0.69	0.19
Enhanced weathering	0.00	0.00	1.00	0.16

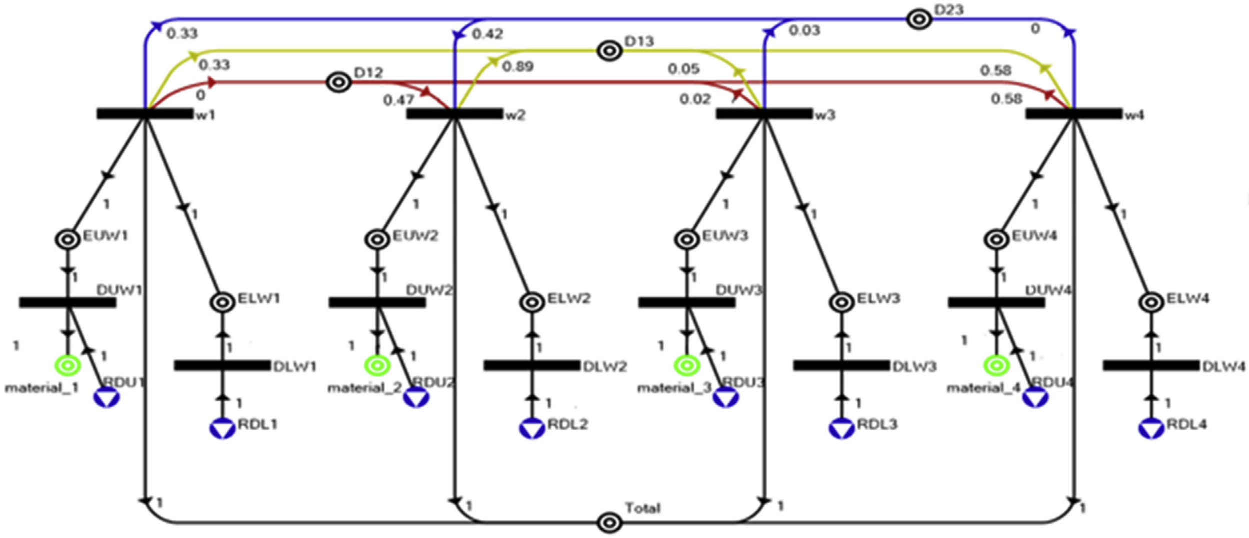

Figure 3. Maximal structure of training set.

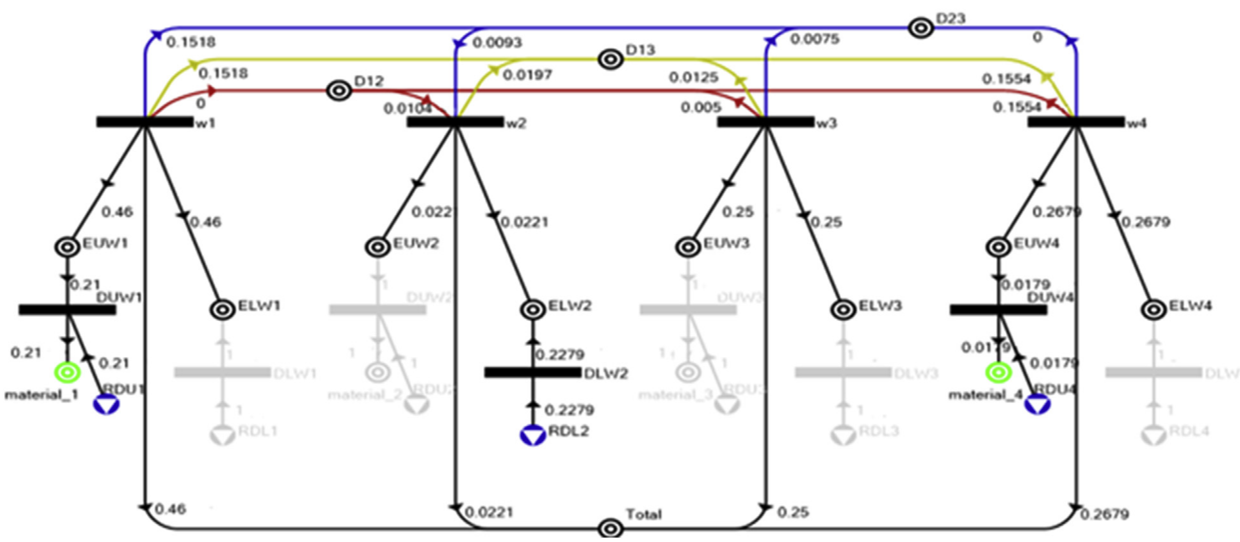

Figure 4. Optimal Network structure.

into the ocean. Hence, one might get these two alternatives as comparable.

Use of the induction approach for determining the expert's implicit weights offer several advantages over conventional MADM approaches. Firstly, this method provides a means of extracting the implicit preference rules from a small set of ranked alternatives instead of relying on the explicit expert's preference elicitation. Secondly, this approach is less time-consuming and eases the burden on expert decision makers despite the seeming computational complexity. The unique feature of the P-

Table 4. Performance of NET alternatives using optimal criteria weights.

NET alternatives	Criteria				Total Score
	Technical status (TRL)	Potential Capacity	Cost	Energy Requirement	
(weights)	(0.460)	(0.022)	(0.250)	(0.268)	
Biochar	1.00	0.11	0.65	1.00	0.893
BECCS (Combustion)	1.00	0.58	0.63	0.42	0.743
DAC (Artificial Tree)	0.67	1.00	0.60	0.42	0.593
DAC (lime-soda process)	1.00	1.00	0.00	0.00	0.482
Ocean Liming (Calcination)	0.67	0.00	0.92	0.24	0.603
Ocean Liming (Electrochemical splitting)	0.33	0.00	0.69	0.19	0.375
Enhanced weathering	0.00	0.00	1.00	0.16	0.293

Table 5. The final NET rankings.

Alternatives	Performance		Ranking	Validation	Ranking from Validation
	Optimal	Sub-optimal			
Biochar	0.893	0.886	1	0.766	1
BECCS (Combustion)	0.743	0.736	2	0.689	2
DAC (Artificial Tree)	0.593	0.586	4	0.639	3
DAC (Lime-soda Process)	0.483	0.432	5	0.477	5
Ocean Liming (Calcination)	0.603	0.641	3	0.528	4
Ocean Liming (Electrochemical Splitting)	0.375	0.408	6	0.342	6
Enhanced Weathering	0.293	0.357	7	0.312	7

graph offers a key advantage to produce optimal and near-optimal solutions and can provide a decision structure which can be consistently used for evaluating future similar alternatives.

5. Conclusion

A novel methodology based on P-graph has been developed and applied for the ranking of NETs. In this approach, criteria weights are determined inductively from training data to generate a SAW model that can then be used to rank additional options. Among the 7 NETs, Biochar is the most feasible clean technology to be implemented in the industry, followed by BECCS and Calcination Ocean Liming. For 4 of the considered criteria, technology status is identified as the determining criterion with the weight of 0.460. In conclusion, the proposed induction approach managed to induce the implicit preference rules of experts by making use of the expert's ranking of a sample set of alternatives. The preferences are reflected as criteria weights that can then be applied to a more complex system with an expanded set of alternatives. The P-graph framework has the additional advantage of identifying alternative near-optimal solutions, which provide alternative sets of preference weights to achieve the ranking given by the expert and might possibly be more realistic for implementation. This approach can be used to solve other similarly structured decision problems in industry. This methodology has critical limitations on the technical issues that usually arise in real problems, such as decision inconsistency and data uncertainty which should be explored in future work. Future works may also integrate this methodology in conjunction with other decision-making tools.

Declarations

Author contribution statement

K. B. Aviso, M. A. B. Promentilla, R. R. Tan: Conceived and designed the experiments; Contributed reagents, materials, analysis tools or data; Wrote the paper.

C. X. Low, W. Y. Ng: Performed the experiments; Analyzed and interpreted the data; Wrote the paper.

Z. A. Putra: Analyzed and interpreted the data; Wrote the paper.

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Competing interest statement

The authors declare no conflict of interest.

Additional information

No additional information is available for this paper.

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