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Non-linear Programming via P-graph Framework

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P-graph is a graph-theoretic method which is designed to solve process network synthesis (PNS) problem using combinatorial and optimisation algorithms. Due to its visual interface for data encoding and results display; and its capability of generating multiple solutions (optimal and sub-optimal) simultaneously, the utility of P-graph has expanded into a broad range of studies recently. However, this powerful graph-theoretic method still falls short of dealing with non-linear problems. The problem can be found from the cost estimation provided by P-graph software. Despite it allows users to input the sizing cost (noted as “proportional cost” in P-graph software), the capacity and the cost are assumed to be linearly correlated. This inaccurate and unreliable cost estimation has increased the difficulty of making optimal decisions and therefore lead to undesirable profit loss. This paper proposes to solve the fundamental linearity problem by implementing trained artificial neural networks (ANN) into P-graph. To achieve this, an ANN model which utilised thresholded rectified linear unit (ReLU) activation function is developed in a segregated computational tool. The identified neurons are then modelled in P-graph in order to convert the input into the nonlinear output. To demonstrate the effectiveness of the proposed method, an illustrative case study of biomass transportation is used. With the use of the trained neurons, the non-linear estimation of transportation cost which considered fuel consumption cost, vehicle maintenance cost and labour cost are successfully modelled in P-graph. This work is expected to pave ways for P-graph users to expand the utility of P-graph in solving other more complex non-linear problems.

1. Introduction

P-graph framework has gained increasing attention in the fields of process system engineering (PSE) nowadays. It is a graph-theoretic approach which was developed by Friedler et al. (1992) in the early 1990s. Due to its visual appealing nature, the framework has been granted as one of the most “attractive and user-friendly optimisation tool” by researchers and students (Lam et al., 2016). A more recent work conducted by Promentilla et al. (2017) further highlighted the pedagogical advantages of the framework in Problem-Based Learning (PBL). Over the past two decades, P-graph-based methodologies had been applied to solve a wide range of PNS problems, including conventional chemical process design synthesis (e.g., reaction pathway identification (Fan et al., 2001), azeotropic distillation system (Feng et al., 2003)); biological process synthesis (Fan et al., 2019); biomass network optimisation (How et al., 2018); optimisation of Total Site utility system (Walmsley et al., 2018); and carbon management networks (Aviso et al., 2019). Aside from journal articles, P-graph has also been successfully penetrated to the current chemical engineering community. Evidently, P-graph framework has been introduced in undergraduate textbooks (Peters et al., 2003), reference books (Klemeš et al., 2011) and chemical engineering magazine (Cabezas et al., 2015). However, the main drawback of the graph-theoretic method is its incapability in solving non-linear problems. Nevertheless, few researchers have

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attempted to address this critical limitation. For instance, Aviso and Tan (2018) had implemented the fuzzy P-graph approach in synthesising a poly-generation system. Despite the implementation being fuzzy linear programming, the work showed the possibility of extending P-graph toward non-linear programming. Süle et al. (2018) on the other hand, had successfully modelled the safety-critical optimisation of a process system using P-graph with the help of a black-box algorithm. Earlier, Ong et al. (2016) had modelled the non-linear cost function using a piece-wise linear approach. The concept of using virtual operating units to represent the segmented sub-cost-functions is admirable, but its key limitations include i) the non-linear functions must be known; and ii) ineffective for problems with more than two dimensions.

To further extend the capability of P-graph in solving non-linear problems, this work proposes a hybrid approach which utilise P-graph framework in conjunction with the use of artificial neural networks (ANN). The proposition is to utilise the trained neural network to convert linear-input-neurons into nonlinear P-graph model.

2. Methods

2.1 Embedding of trained neural network in the P-graph structure

ANN was first introduced by McCulloch and Pitts (1943) to model nervous activity in the human brain. It can now be served as a universal black box model which can be applied in a wide range of researches (Hornik et al., 1989). In Lek et al. (1996), its capability of modelling non-linear problem had been further demonstrated in their ecology study. As an illustrative example, a multi-layer perceptron type artificial network is implemented in this study. All neurons in the former layer are directly linked to the neurons in the next layer. They receive the signals from the neurons located in the previous layer directly before it and transmit signals to all the neurons located in the subsequent layer directly after it. The signal propagation can be formulated as:

$$A_j = f_{ac} \left(\sum_{i=1}^{n} A_i w_i + B_j \right) \tag{1}$$

where A_j denotes the activation of the j^{th} neuron in one layer; while the activation of i^{th} neuron in the layer directly before the layer of j^{th} neuron is referred to as A_i. The assigned weight for each connection between the connecting neurons is indicated as w_i; while B_j refers to the "bias" which improves the modelling capabilities of the neural network. Note that the thresholded rectified linear units (ReLU) is used as the activation function (Konda et al., 2014), f_{ac} in this work (see Eq(3), where a refers to the threshold limits; $z \in \mathbb{R}$) since it is found more efficient compared to the conventional sigmoid units (Rynkiewicz, 2019). These parameters can be determined by minimising the mean square error (MSE) between the actual values (X^{ACT}) and estimated values (X^{EST}), where N indicates the total number of sample sizes. Note that the optimal number of neurons (i.e., lead to least MSE) can be determined by iterating through different number of neurons. After the neurons were trained, they can be represented by P-graph. Figure 1 shows how a multi-layer perceptron type of neural network can be represented in P-graph model. M-type vertices are used to represent the input and bias; while the assigned weight can be input as the "rate" on the arcs. Note that the construction of hidden layers might be different due to the neuron condition. This is to ensure the activation function in Eq(3) is fully satisfied.

$$\min \quad MSE = \frac{\sum (X^{EST} - X^{ACT})}{N} \tag{2}$$

$$f_{ac}(z) = \begin{cases} z\,, & z > a \\ 0\,, & otherwise \end{cases} \tag{3}$$

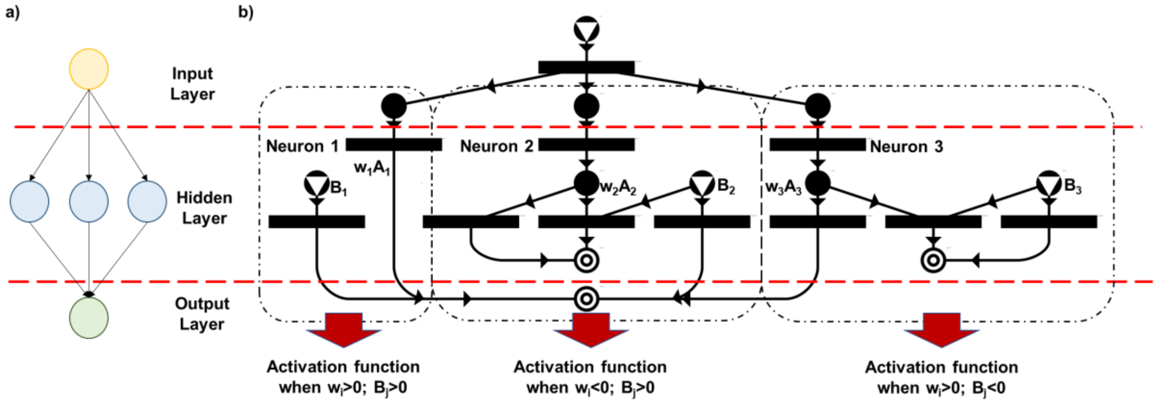

Figure 1: Illustration of a) typical multi-layer perceptron type neural network; b) neural network in P-graph model

2.2 Transportation cost estimation

A biomass transportation example is used to demonstrate the proposed method. The non-linear transportation cost function which was developed by How et al. (2016) is adopted in this work. Note that the total transportation cost, C^{TR} encompasses three components, i.e., fuel consumption cost, C^{FUEL}, vehicle maintenance cost C^{MAINT} and labour cost C^{LAB}. These components are expressed in Eq(5) to Eq(7):

$$\min \; C^{TR} = C^{FUEL} + C^{MAINT} + C^{LAB} \tag{4}$$

$$C^{FUEL} = N^{TRIP} \times 2 \times d \times r^{FUEL} \times C^{DIESEL} \tag{5}$$

$$C^{MAINT} = N^{TRIP} \times 2 \times d \times C^{REPAIR} \tag{6}$$

$$C^{LAB} = N^{TRIP} \times OH^{TRIP} \times C^{WAGES} \tag{7}$$

where N^{TRIP} refers to the total number of trips required (a function of the transferred load and vehicle capacity constraint); d refers to the distance between the two locations; r^{FUEL} denotes the fuel consumption rate; OH^{TRIP} indicates the delivery time required per trip; while C^{DIESEL}, C^{REPAIR} and C^{WAGES} refer to the diesel price, estimated repair cost per unit of distance travelled and the hourly wages for the workers. For more details, please refer to How et al. (2016).

3. Case Study

In this case study, a given amount of biomass is transported to a biorefinery plant via a set of transportation modes (i.e., M1, M2, M3). Table 1 summarises the related vehicle data; while other parameters used in this case study are tabulated in Table 2.

Table 1: Operating specification of transportation modes (How et al., 2016)

Mode	Load Capacity (t)	r^{FUEL} (L/km)	Travel velocity (km/h)	C^{REPAIR} (RM/km)	Loading Delay (h)
M1	15	0.261*	80	0.22	0.50
M2	25	0.278*	75	0.34	0.67
M3	40	0.294*	65	0.45	0.83

*Fuel consumption rate when the vehicle is empty (i.e., r_0^{FUEL}); it is assumed that $r^{FUEL} = 0.001 \times x^2 \times r_0^{FUEL}$, where x refers to the weight of loaded biomass.

Table 2: Other parameters used in the case study

Parameter	Value
C^{DIESEL} (RM/L)	2.18
C^{WAGES} (RM/h)	10.00
Daily transferred biomass load (t/d)	0 to 20
d (km)	20
Annual operating days (d/y)	355
Maximum operating hour per day (h/d)	40

4. Result and discussion

The optimal number of neurons required for each transportation mode can be determined through Table 3. The results show that two neurons are required for the M2 and M3 (having three neurons no longer provide significant improvement); while M1 require three neurons. This is due to the step changes in the outputs for M2-case. In addition, overfitting phenomena (i.e., MSE increases with the number of neurons) had occurred when more than three neurons were used. All the determined parameters for each neuron (i.e., determined using ANN formulation introduced in Section 2.1) are tabulated in Table 4. The formulated neural network is then constructed in the form of P-graph (see Figure 2). The red-coloured section represents the neural network of M1; green-coloured section represents the neural network of M2; while the blue section refers to the neural network for M3. The optimised results are illustrated in Figure 3 and Figure 4. The results show that M1 is the optimal transportation mode when the daily delivered biomass load is less than 15 t/d (illustrated as Figure 3); while M2 is selected when the daily delivered biomass load exceeds 15 t/d (illustrated as Figure 4). This is due to the vehicle capacity constraint of M1, as the biomass loads cannot be fully-transferred in a single trip. The model performance is illustrated in Figure 5. It shows that the proposed P-graph model is now capable to deal with non-linear systems.

Table 3: MSE obtained

Number of neurons	MSE for M1	MSE for M2	MSE for M3
1	0.0174	0.0032	0.0025
2	0.0012	0.0002	0.0002
3	0.0007	0.0002	0.0002
4	0.0070	0.0008	0.0004

Table 4: Parameters for each neuron

Neuron for M1	a	w_i	B_j	Neuron for M2	a	w_i	B_j	Neuron for M3	a	w_i	B_j
1	0.00	0.1111	-0.3312	1	0.50	1.0000	-0.0168	1	0.00	0.5048	-0.5026
2	0.00	0.2979	-0.4652	2	0.00	0.5303	-0.5482	2	0.46	0.9623	-0.0146
3	0.75	0.4503	0.9999								

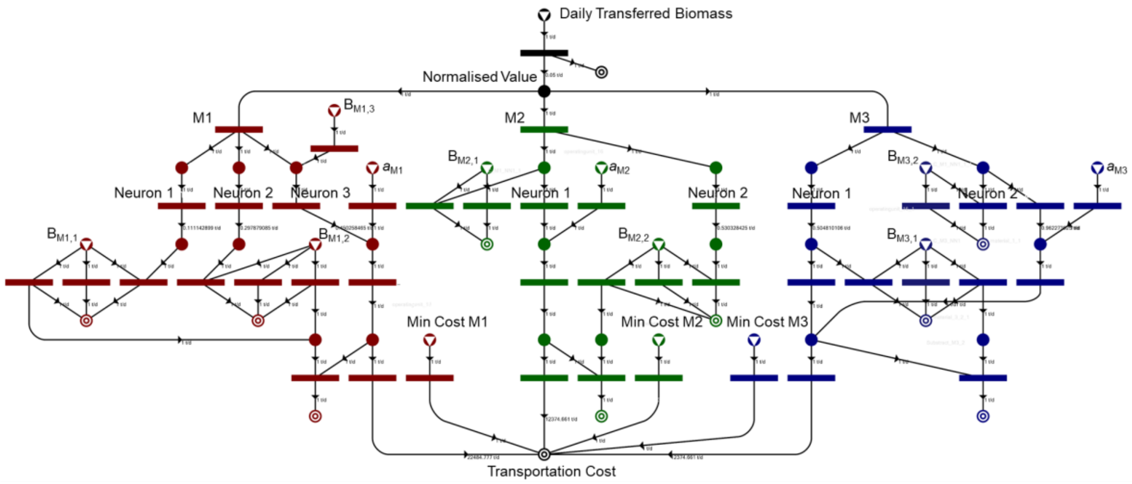

Figure 2: P-graph model with the formulated neural networks

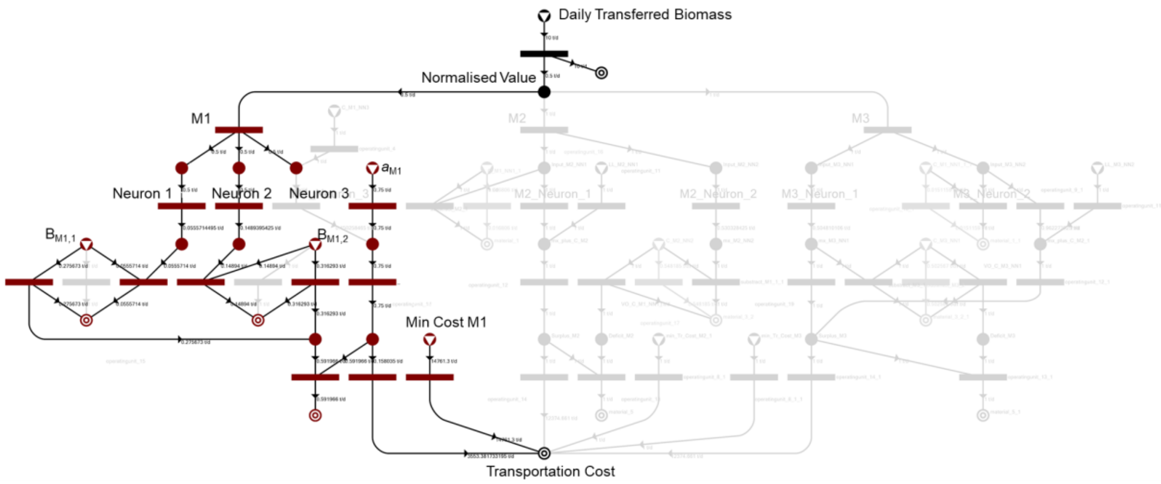

Figure 3: Optimal structure when daily biomass transferred load is less than 15 t/d

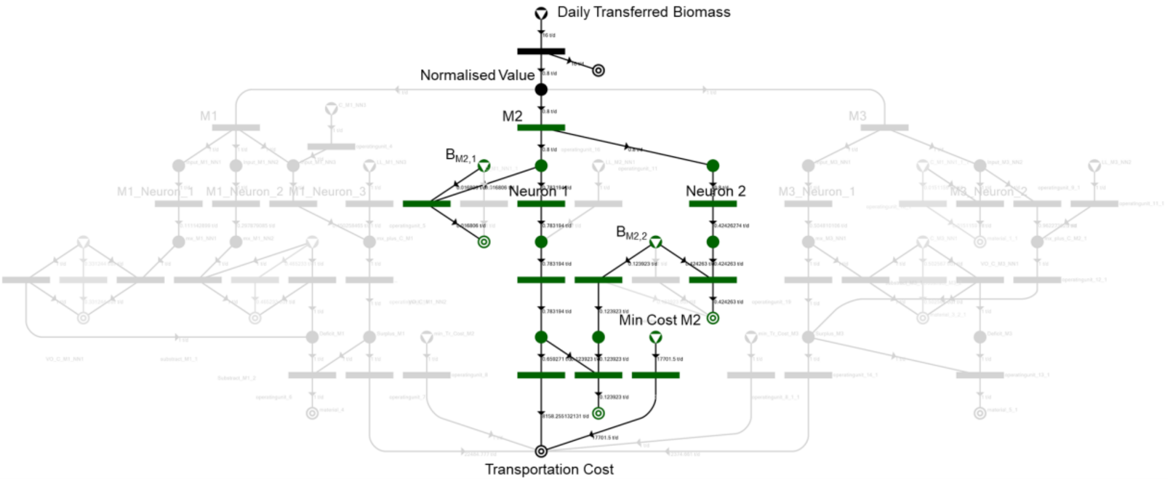

Figure 4: Optimal structure when daily biomass transferred load is more than 15 t/d

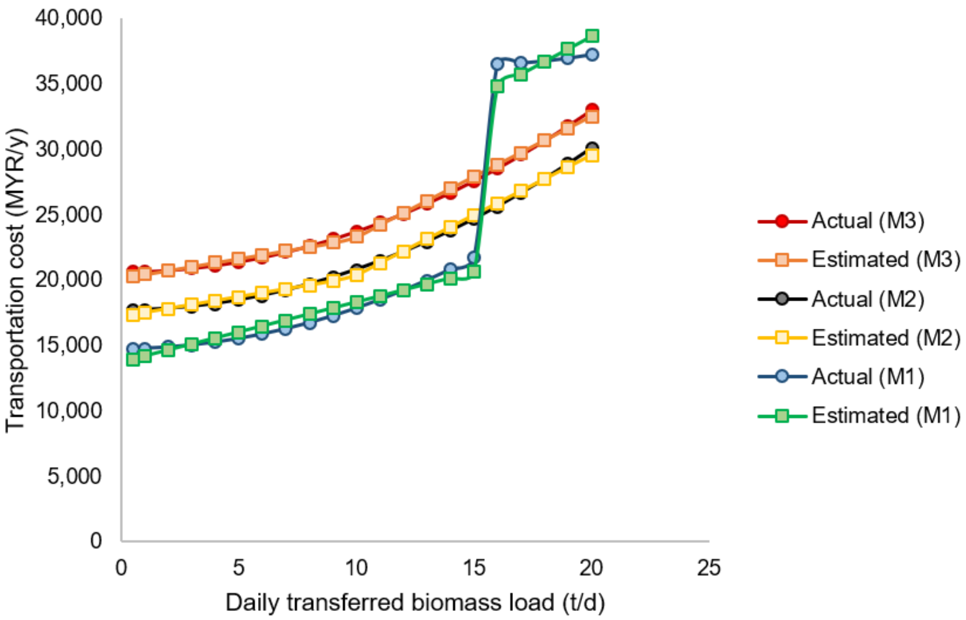

Figure 5: Model performance

5. Conclusions

This work further assures the capability of P-graph framework in non-linear programming by incorporating the use of artificial neural network into the model. The potential of the proposed method can be clearly seen from the model performance chart where the non-linear transportation cost can be determined by using P-graph. With the use of multi-layer perceptron, P-graph is no longer restricted in conventional process system engineering but can also be served as a predictive model without the need to determine the exact non-linear functions. Note that massive amount of data sample is required to ensure the reliability of the attained results. This work can be further extended with the consideration of multiple inputs and outputs in the neural network, in order to solve other complex non-linear problems, including heat exchanger network optimisation, vapour liquid equilibrium, transportation design (with the consideration of both volume and weight constraint), etc. More advanced artificial intelligence method will be described and demonstrated in the future works.

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