Review

Artificial Intelligence techniques applied as estimator in chemical process systems – A literature survey

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ABSTRACT

The versatility of Artificial Intelligence (AI) in process systems is not restricted to modelling and control only, but also as estimators to estimate the unmeasured parameters as an alternative to the conventional observers and hardware sensors. These estimators, also known as software sensors have been successfully applied in many chemical process systems such as reactors, distillation columns, and heat exchanger due to their robustness, simple formulation, adaptation capabilities and minimum modelling requirements for the design. However, the various types of AI methods available make it difficult to decide on the most suitable algorithm to be applied for any particular system. Hence, in this paper, we provide a broad literature survey of several AI algorithms implemented as estimators in chemical systems together with their advantages, limitations, practical implications and comparisons between one another to guide researchers in selecting and designing the AI-based estimators. Future research suggestions and directions in improvising and extending the usage of these estimators in various chemical operating units are also presented.

1. Introduction

Artificial Intelligence (AI), by definition is the ability of computers or other machines in performing activities that require human intelligence. It has attracted researchers on its theories and principles since the 1956 Dartmouth conference (Negnevitsky, 2005). Today, this method has been widely used in various applications including games, automation, medical and process control. In process control, its application has recently expanded not only being used in modelling and control but also as tools to estimate difficult-to-measure parameters, known as estimators. Those AI-based estimators are computational algorithms designed to predict the unmeasured parameters that are significant in developing the state feedback control law of a system. They are also addressed as software or virtual sensors and encompass several algorithms including artificial neural network (ANN), fuzzy logic, genetic algorithm (GA) and expert system (ES). They can be developed using software such as MATLAB and LabView and implemented on the specific process unit to predict unmeasured states such as concentration, temperature, heat flux, molecular weight and impurities. Other practical simulation software used for estimating states are PROCESS (Simulation Sciences code) (Himmelblau, 2008), SIAMOD (Siemens adaptive modelling of dynamic system) (Horn, 2001), NeuralWorks Professional II/(PLUS) (Yeh, Huang, & Huang, 2003) and dynamic simulator (Dynafrag) (Du, del Villar, & Thibault, 1997).

Before AI-based estimators were introduced, researchers have been using the conventional observers in chemical process systems, for example the Luenberger observer, Extended Kalman Filter (EKF), sliding mode observer and observers. These observers also offer good estimation performances and have their relative advantages when applied in chemical unit operations, as quoted in several literatures (Aguilar-López, 2003; Damour, Benne, Boillereaux, Grondin-Perez, & Chabriat, 2010; Dochain, 2000; Dochain, Couenne, & Jallut, 2009; Gonzalez, Fernandez, Aguilar, Barron, & Alvarez-Ramirez, 2001; Kam & Tadé, 1999; Mesbah, Huesman, Kramer, & Van den Hof, 2011; Tronci, Bezzo, Barolo, & Baratti, 2005; Velardi, Hammouri, & Barresi, 2009; Wang, Peng, & Huang, 1997; Zarei & Poshtan, 2010). However, AI-based estimators are generally easier to retune whenever there are changes in the parameters and are able to avoid time delays compared to the conventional observers. Besides that, these AI-based soft-sensors are able to work in parallel with hardware sensors for

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Nomenclature

T_r	reactor temperature	ρ_j	density of jacket
T_j	jacket temperature	F_t	feed rate at time t
Q_r	heat released by reaction	Q_c	specific CO_2 evolution rate
Q_j	heat input	Q_o	specific O_2 uptake rate
ΔH_i	heat of reaction i	e	process error
R_i	rate of reaction i	Δe	change of process error
k	reaction rate constant	C_m	monomer concentration
U	heat transfer coefficient	T	reactor temperature
A	heat transfer area	k_r	reaction rate constants
M_i	number of moles of component i	Q	heat transfer rate
V	volume	R_m	product rate of monomer
τ_j	response time	ε	volume expansion factor

providing information especially to detect faults in the systems (Fortuna, Graziani, & Xibilia, 2005). However in certain applications, AI elements have been combined with conventional observers known as hybrid estimators, which include fuzzy Kalman filter (FKF) (Prakash & Senthil, 2008; Senthil, Janarthanan, & Prakash, 2006) and differential neural network observer (DNNO) (Chairez, Poznyak, & Poznyak, 2007; Porru, Aragonese, Baratti, & Alberto, 2000) mainly to increase their performances.

Based on the increasing popularity of applying AI as estimators in chemical process systems, several review papers are available in literature but they are not comprehensive and involve only certain AI algorithms. For example, de Assis and Filho (2000) have provided a short review of ANN only and compared it with EKF and adaptive observers. Himmelblau (2008) has explained several applications of ANN in chemical engineering including its usage as estimators while Kamimura and co-workers have (Kamimura, Konstantinov, & Stephanopoulos, 1996) provided a review on ANN and knowledge-based systems in biotechnology. Katare and coworkers also compared various parameter estimation using hybrid GA in several kinetic models (Katare, Bhan, Caruthers, Delgass, & Venkatasubramanian, 2004) and several applications of intelligence systems in process engineering have also been reviewed by Stephanopoulos and Han (Stephanopoulos & Han, 1996). Another review has been done by Kadlec and coworkers whereby they explained several soft sensors in process industries (Kadlec, Gabrys, & Strandt, 2009) and the adaptation mechanisms of the techniques (Kadlec, Grbić, & Gabrys, 2011). Besides that, Kalogirou (2003) and Shioya, Shimizu, and Yoshida (1999) have compiled all AI applications in the combustion and bioprocess respectively. In addition, Porter and co-workers have discussed on GA as estimators in general linear and nonlinear systems (Porter li & Passino, 1995).

Therefore, in this paper, we have reviewed and provided a comprehensive list of AI algorithms that have been applied as estimators in chemical process systems by highlighting their advantages, limitations and practical implications since it is not available in any literature at present. Guidelines in selecting the possible algorithm for a specific system are also given, to help researchers in choosing the most appropriate algorithm that suits their system if they are to apply AI algorithms as estimators. Examples are also given to show how to develop these AI-based estimators, all of which are novel and important contributions of this paper. After the introduction section, AI applied as estimators in chemical process systems are discussed in Section 2. Section 3 discusses the guideline and examples of the applications while the advantages, limitations and future directions are given in Sections 4. Section 5 concludes the review.

2. AI applied as estimators in chemical process systems

The usage of AI algorithms as estimators in chemical process systems is becoming popular due to their robustness, simple formulation, easy-to-design and flexible adaptation capabilities. They also do not require full knowledge of process kinetics, which are at times difficult to be obtained from the highly nonlinear behaviour of chemical processes themselves. The AI algorithms that have been applied include the artificial neural network (ANN), fuzzy logic, genetic algorithm (GA), expert systems (ES) and hybrid systems. However, the variety and unique features of these algorithms make it difficult to decide on the suitable method to be used in any particular system. Therefore a survey of each algorithm applied as estimators in chemical process systems, as presented in this paper, is important to highlight the significance of each algorithm and guide researchers towards the design of the AI-based estimators for any particular chemical process system.

ANN is the most popular algorithms applied since its capability is promising and can be trained to learn the process based on historical data (Devogelaere, Rijckaert, Leon, & Lemus, 2002). Besides that, it provides high accuracy and consistent estimations even when changes occur in the process (Sharma, Singh, Singhal, & Ghosh, 2004). In general, ANN relates to the function of the human brain, consists of a number of simple processors or neurons, which are arranged into layers as illustrated in Fig. 2.1. In the figure, part A represents the neuron in human while part B shows neuron in the ANN (Maltarollo, Honório, & Silva, 2013). Neurons in adjacent layers of ANN are connected by weighted links passing signals from one layer to the next adjacent layer. Those links have numerical weights that are applied to the inputs of a neuron. ANN learns through the repeated adjustment of the weights to obtain the desired output signal. The feed forward structure of ANN consists of a multilayer structure whereby there are hidden nodes in

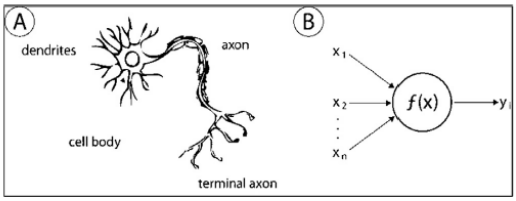

Fig. 2.1. Human and ANN neuron concept. Picture taken from Maltarollo et al. (2013): Applications of artificial neural networks in chemical problems.

between the input and output layers. However, there is no specific method to obtain the number of the hidden nodes and it is commonly based on trial and error basis to find the appropriate number of nodes that will provide the best results (Lashkarbolooki, Vaferi, & Mowla, 2012).

Details and issues regarding the implementation of ANN such as the improvement of neural network generalisation, regularisation, cross validation, learning methods, local minima problem and curse of dimensionality can be found in various references (Buntine & Weigend, 1991; Caruana, Lawrence, & Giles, 2001; Crucianu, Boné, & Asselin de Beauville, 2001; Guyon & Yao, 1999; Hagiwara & Kuno, 2000; Himmelblau, 2008; Lampinen & Vehtari, 2001; MacKay, 1992; Mc Loone & Irwin, 2001; Morgan & Bourlard, 1989; Neal, 1995; Priddy & Keller, 2005; Touretzky, 1990; Wang, Zhang, & Okazaki, 2007; Ytlcetiirk, Herdagdelenz, Uyanikzet, & Lisesi, 1999; Zhang & Friedrich, 2003; Zhang & Morris, 1998; Zhang, 2001; (Zhang, 1999a, 1999b); Zhang, Martin, Morris, & Kiparissides, 1997). We have also highlighted some of these details in Appendix A. Furthermore, the computational cost and time for implementing the neural networks can be minimized if proper steps of training as highlighted in the appendix can be followed closely.

For estimating parameters in chemical process systems, several types of ANN can be used such as the feed forward neural networks (FFN), internally recurrent net (IRN), externally recurrent net (ERN), radial basis function networks (RBFN), and the shape-tuneable neural network (MNN) (Chen & Chang, 1996). Each structure has their own features and the comparisons are listed out in Table 2.1. In addition, Table 2.2(a) provides the details of the applications of ANN in chemical process systems, which include the objective of the estimations, their positive highlights, unit operations involved and relevant references related to each of the applications.

Another AI-based algorithm that has been applied as estimators in chemical processes is the fuzzy logic approach. Fuzzy logic works on fuzzy sets that indicate the maximum limits of an element. By definition, it is a type of logic or multi-valued logic that distinguishes more than just TRUE and FALSE values. It can be represented with degrees of truthfulness and falseness in the range of [0,1] where 0 is absolute FALSE and 1 is absolute TRUE. It was introduced by Zadeh in 1964 through his paper on fuzzy sets and the application has become very popular since 1987 (Negnevitsky, 2005). Fuzzy logic consists of several elements such as the linguistic variable and values, fuzzy rules, membership function, fuzzy inference and defuzzification. These details may be found in several references (Leondes, 1998; Yetilmezsoy, Fingas, & Fieldhouse, 2011). Fuzzy Takagi Sugeno, Fuzzy Mamdani inferences and Fuzzy-C-means are among the fuzzy logic structures that have been used to develop estimators in chemical process units.

Fuzzy logic has been applied as estimators due to their simple formulation and ability to accurately describe imprecise values of parameters, for example temperature, speed and height. Nevertheless, one disadvantages of fuzzy logic is that the results sometimes depend on the number of rules, inference systems and the type of membership function applied. Furthermore, there is no guideline to obtain them but with trial and error or based on past experiences similar to ANN (Delrot, Guerra, Dambrine, & Delmotte, 2012; Frank & Köppen-Seliger, 1997; Liu, 2007). Table 2.2(b) lists out all the application of fuzzy logic as estimators in chemical process systems.

Apart from ANN and fuzzy logic, expert systems (ES) and genetic algorithms (GA) have also been applied to build estimators in several chemical process systems. ES is an intelligent system that can provide information and expert advice and is also known as Knowledge-Based-Expert-System as it depends on large amount of knowledge to solve problems. There are basically five types of Expert System namely Rule-Based ES, Frame-Based ES, Case-Based ES, Fuzzy ES and Neuro-Fuzzy ES. Rule-Based ES is an expression of knowledge in the form of rules to solve problems. It is divided into two parts which are IF: Antecedent (premise/condition) and THEN: Consequent (conclusion/action). If there are many antecedents, the operator AND as well as OR is used to combined them all. These rules are the most popular type of knowledge representation. ES has been applied as estimators due to its ability in expressing relations, recommendations, directives, strategies and heuristics. It has five basic components namely knowledge base, database, inference engine, explanation facilities and user interface (Rich & Knight, 1991) as depicted in Fig. 2.2 (Kishan, Chadha, & Maini, 2012). However, it is seldom applied as estimators since it is limited in its capability to narrow down the problems domain (Krishnamoorthy & Rajeev, 1996) and it also only

Table 2.1
Comparison of several ANN structures.

No.	Types of ANN	Key features	Advantages	Limitations
1	Feed forward neural networks (FFN)	• Fixed function and require large amount of training data	• Accurately approximate continuous functions • Easy to implement	• Slow convergence • Lack dynamics • Mainly used for static function approximation
2	Internally recurrent net (IRN)	• Characterised by time-delayed feedback connections from output of hidden nodes back to inputs of hidden nodes	• Capable of estimating process with changing variable dynamics • No limit for the number of states	• Difficult to initialize • Training can be time consuming
3	Externally recurrent net (ERN)	• Contain time-delayed feedback connections from output layer to a hidden layer	• Easy to initialize • Simple design and can use current values to initialize states	• Number of states must be the same as model outputs • Training can be time consuming
4	Radial basis function neural networks (RBFNN)	• Basis function used can be Gaussian or wavelets • Do not apply back-propagation for training	• Less sensitive to sensor noise • Faster training	• Most suitable for classification problem • Large number of hidden nodes needed
5	Recurrent trainable neural network (RTNN)	• Hidden layer is the recurrent layer and the other two layer is based on back propagation	• Faster convergence • Less complexity in the design	• Not versatile • Slow training due to sequential structure
6	Shape-tuneable neural network (MNN)	• Allow tuning of weight between neurons and saturation function of each neurons simultaneously	• Sensitive to plant changes but still provide good estimation even with varied parameters	• Greatly depends on sampling time and initial parameters

Table 2.2
Various applications of AI-based estimators in chemical process systems.

Types	Objective/estimate(s)	Systems applied	Positive highlights	References
(a) *ANN as estimators in chemical process systems*				
FFN	Conductivity	Evaporator	Small validation error (7%)	(Devogelaere et al., 2002)
ANN	Gasoline and butane concentration	Debutanizer	Able to overcome delay	(Fortuna et al., 2005)
ANN	Distillate composition	Distillation column	Good for binary distillation without multi-component	(Singh, Gupta, & Gupta, 2005)
ANN	Distillate composition	Distillation column	Handle many inputs with accurate results	(Singh, Gupta, & Gupta, 2007)
Adaptive neural network	Product composition	Binary distillation column	High accuracy with faster response	(de Canete et al., 2012)
ANN	Mole fraction of distillate product	Binary distillation column	Satisfactory estimation performance, help to enhance overall control	(González, Aguilar, Alvarez-Ramírez, Fernández, & Barrón, 1999)
ANN	Product composition	Reactive distillation column	Allow error refinement	(Bahar & Özgen, 2010)
ANN	Top, bottom composition, reflux ratio	Batch distillation	Able to speed up training for better prediction	(Frattini Fileti, Cruz, & Pereira, 2000)
RANN	Product compositions	Batch distillation	Good agreement with actual value	(Zamprogna, Barolo, & Seborg, 2001)
ANN	Faults	Packed distillation column	Consistent results even with disturbances	(Sharma et al., 2004)
IRN	Polymer product quality	Polymerization reactor	Excellent prediction especially in grade transition region	(Himmelblau, 2008)
IRN	Outlet reactor concentration	CSTR	Good prediction compare with Extended Kalman Filter (EKF)	(Himmelblau, 2008)
MNN	Heat of reaction, heat coefficient	CSTR	Handle system with noise	(Chen & Peng, 1999)
ANN	Kinetic parameters	Bioreactor	Good estimation for on-line application	(de Assis & Filho, 2000)
RANN	Biomass concentration	Bioreactor	Stable estimation based on corrective action during training	(Acuña, Latrille, Béal, & Corrieu, 1998)
MLPFF	Cellular concentration	Bioreactor	Accurate estimation at all three phases (lag, exponential, stationary)	(Silva et al., 2008)
FFN	Oxygen uptake rate, carbon dioxide evolution rate	Bioreactor	High accuracy even the training data is reduced and save cost due to the reduction	(Komives & Parker, 2003)
ANN	Oxygen mass transfer coefficient	STR	Good prediction even with noise	(García-Ochoa & Castro, 2001)
ANN	Overall reaction rates of anhydrite	Stirred cell reactor	Good estimation even without initial assumption	(Molga & Cherbański, 2003)
ANN	Substrate, ethanol concentration	Fed-batch reactor (Experimental)	Estimation can be done outside domain	(Gadkar, Mehra, & Gomes, 2005)
ANN	Heat-released	Batch reactor	Accurate and fast estimation	(Aziz, Hussain, & Mujtaba, 2000)
FFN	Reactive impurities, polymer product quality	Polymerization reactor	Effective estimation if based only on the initial batch condition of reactive impurities	(Zhang, Morris, Martin, & Kiparissides, 1998)
Stacked NN	Reactive impurities, fouling	Polymerization reactor	Good prediction with impurities	(Zhang, Morris, Martin, & Kiparissides, 1999)
ANN	Initiator concentration, heat of reaction	Polymerization reactor	Only need measurement of one variable for training	(Horn, 2001)
ANN	Monomer, Initiator concentration	Polymerization reactor	Satisfactory estimation performance	(Yang, Chung, & Brooks, 1999)
MLRN	Chain length	Polymerization reactor	Good estimation that allow variety of measured variables during training	(Meert & Rijckaert, 1998)
ANN	Reactor temperature	Polymerization reactor	Small estimation error	(Kuroda & Kim, 2002)
Bootstrap NN	Weight and number of average MW	Polymerization reactor	Reduce estimation error	(Zhang, 1999a, 1999b)
IRN	Polymer product quality	Polymerization reactor (Experimental)	Accurate prediction over wide range of transition period	(Barton & Himmelblau, 1997)
ANN	Ethanol concentration	Flash fermentor	Optimum performances	(Rivera, Atala, Filho, Carvalho da Costa, & Filho, 2010)
ANN	Sugar concentration,	Fermentation process	Good agreement with the	(Dai, Wang, Ding, & Sun, 2006)

Table 2.2 (*continued*)

Types	Objective/estimate(s)	Systems applied	Positive highlights	References
	chemical potency		value from production process	
ANN	Glucose and Galactose concentration, residual carbon concentration	Fermentor (Experimental)	Error of estimation is almost zero (0.06%)	(Jin, Ye, Shimizu, & Nikawa, 1996)
ANN	Consumed sugar concentration, optical cell density	Fermentor (Experimental)	Satisfactory despite variation in substrate	(Yet-Pole, Wen-Tengu, & Yung-Chuan, 1996)
FFN, RBFNN	Biomass concentration	Fermentor	Good estimation even with variation in yield coefficient	(James, Legge, & Budman, 2002)
ANN	Fluid and particle temperature, Biot number (B_i)	Fluid-particle system	Able to reduce the error of estimation	(Sablani, 2001)
RNNM	Process kinetics	Fermentor (Experimental)	Reliable estimates and able to avoid over-fitting of NN during learning	(Valdez-Castro, Baruch, & Barrera-Cortes, 2003)
ANN	Density, viscosity, refractive index	Binary system (water–methanol–acetonitrile–tetrahydrofuran mixtures)	Small estimation error	(Mehlman, Wentzell, & McGuffin, 1998)
ANN	Heat transfer rate	Heat exchanger	Consistent prediction value compared with actual value	(Islamoglu, 2003)
ANN	Heat flux	Heat exchanger	Prediction is based on known experimental data	(Su et al., 2002)
ANN	Pressure drop	Rotating fed bed	Accurate estimation compare with actual values in wet bed	(Lashkarbolooki et al., 2012)
ANN	Activated carbon	Absorber	Satisfactory prediction performance	(Faur-Brasquet & Le Cloirec, 2003)
ANN	Iron oxide conversion rate	Iron oxide reduction process	High convergence	(Wiltowski et al., 2005)
ANN	Thermal conductivity response factor	Gas chromatography	Good agreement with actual value	(Jalali-Heravi & Fatemi, 2000)
ANN	Particle size	Cyclone (grinding process)	Simple formulation	(Du et al., 1997)
FFN	Coal combustion rate	Coal combustion process	High accuracy and robust compared with actual value	(Zhu, Jones, Williams, & Thomas, 1999)
BPNN	Hydrogen content of coal	Coal combustion process	Prediction is based on proximate analysis	(Yao, Vuthaluru, Tadé, & Djukanovic, 2005)
ANN	Slurry velocity, solid concentration	Pipeline for conveying bulk material	Suitable for difficult model development process	(Lahiri & Ghanta, 2008)
FFN	Dynamic compositions	Tennessee Eastman plant	Reliable estimates upon calibration of the estimator	(Yeh et al., 2003)
ANN	Lipase, biomass concentration	Enzyme process (Experimental)	Good estimation based only one online measured parameters	(Linko, Zhu, & Linko, 1999)
RBFNN	Permeate and residue hydrogen concentration, permeate gas flux	Gas membrane separator	Predict by omitting many boundary values	(Wang et al., 2006)
FFN	Moisture content of bananas	Fruit dehydration process	Superior ability in predicting moisture content	(Mohebbi et al., 2011)
ANN	Critical odour release	Waste water treatment plant (refinery)	Good prediction even when number of nodes are reduced	(Kordon et al., 1996)
(b) *Fuzzy Logic as estimators in chemical process systems*				
Fuzzy Takagi–Sugeno (FTS)	Fouling parameters	Heat exchanger	Accurate estimate without any additional sensors	(Delrot et al., 2012)
Fuzzy Takagi–Sugeno (FTS)	Specific CO_2 evolution rate, specific O_2 uptake rate	Fermentor	Eliminate defuzzification part since output can be directly obtained from rule part	(Hisbullah et al., 2003)
Fuzzy	Energy efficiencies of ethylene	Furnace	High efficiencies, able to reduce more than 50% of the cost	(Geng, Han, Gu, & Zhu, 2012)
Fuzzy	Size of Algae population	Wastewater treatment plant	High accuracy that able to improve the runtime	(Shen & Chouchoulas, 2001)
Intelligent Fuzzy Weighted	Heat flux	Thermal fluid hollow cylinder pipeline	Fast convergence	(Chen & Lee, 2008)
Fuzzy	Product concentration	Fed-batch reactor	Easy design	(Patnaik, 1997)

(*continued on next page*)

Table 2.2 (*continued*)

Types	Objective/estimate(s)	Systems applied	Positive highlights	References
Fuzzy matching	Cost	Chemical plant (Chem. Systems Ltd.)	Accurate with minimal estimation effort	(Petley & Edwards, 1995)
Fuzzy (Mamdani inferences)	Biogas, methane production rate	Digester	Satisfactory performance with small deviation	(Turkdogan-Aydınol & Yetilmezsoy, 2010)
Fuzzy c-means (FCM)	Melt index	Fluidized bed reactor	Reduce input variables dimension	(Liu, 2007)
Fuzzy (Mamdani inferences)	Fault on pH sensor and sodium hydroxide frequency	Digestion reactor (Experimental)	Satisfactory even with varied operating condition	(Genovesi et al., 1999)
(c) *ES as estimators in chemical process systems*				
ES	Probability of odour	Waste water treatment plant	Good prediction even when number of nodes are reduced	(Kordon et al., 1996)
ES	Effluent waste colour	Wastewater treatment plant	Provide early warning for further treatment process	(Paraskevas, Pantelakis, & Lekkas, 1999)
ES	Product flow, temperature	Crude oil distillation column	Able to minimise the error	(Motlaghi et al., 2008)
(d) *GA as estimators in chemical process systems*				
GA	Size of Algae population	Wastewater treatment plant	High accuracy that able to reduce the cost	(Shen & Chouchoulas, 2001)
GA	Friction factor	Helically coiled tubes (Experimental)	High accuracy by improving the mean relative error	(Beigzadeh & Rahimi, 2012)
GA	Hydrogen concentration, temperature of coolant and reactant	Catalytic reactor	High conversion	(Rezende et al., 2008)
GA	Temperature	CSTR	Minimize error between the estimated and set point temperature	(Khairi Abdul Wahab et al., 2007)
GA	Moisture content of banana	Fruit dehydration process	Superior ability of on-line estimation	(Mohebbi et al., 2011)
GA	Fuel input parameter	Palm oil mill	Consistent prediction	(Ahmad, Azid, Yusof, & Seetharamu, 2004)
(e) *Hybrid systems as estimators in chemical process systems*				
FuREAP	Size of Algae population	Wastewater treatment plant	High accuracy that able to improve the runtime	(Shen & Chouchoulas, 2001)
ANFIS	Compositions	Multi-component reactive distillation column	Reliable and accurate estimation	(Khazraee & Jahanmiri, 2010)
FNN	Fault signal in valve	Control valve	Good estimation despite model mismatch	(Korbicz & Kowal, 2007)
FNN	Melt index	Polymerization reactor (Experimental)	Able to settle the online training efficiency problem	(Liu & Zhao, 2012)
FNN	MW average	Polymerization reactor	Fast estimation	(Chitanov, Kiparissides, & Petrov, 2004)
FNN	Biomass concentration, viscosity	Bioreactor	Fast convergence	(Araúzo-Bravo et al., 2004)
ANFIS	Emulsion stability	Water-in-oil mixtures	Satisfactory performance with small deviation	(Yetilmezsoy et al., 2011)
ANFIS	Friction factor	Helically coiled tubes	High accuracy by improving the mean relative error	(Beigzadeh & Rahimi, 2012)
HNN	Injection time, injection pressure	Plastic injection moulding process	Small estimation error without the knowledge of injection moulding	(Yarlagadda & Teck Khong, 2001)
HNN	Product yield, gas compositions	Fluidized bed gasifier	Powerful estimator especially for complex process	(Guo, Li, Cheng, Lü, & Shen, 2001)
HNN	Monomer concentration	Polymerization reactor	Accurate estimation without the knowledge of model structure	(Ng & Hussain, 2004)
HNN	Monomer concentration, temperature	Polymerization reactor	Good validation results, fast convergence	(Wei et al., 2007)
HNN	Liquid heads	3-tanks in series	Able to handle noise and variation of the stochastic process	(Wilson & Zorzetto, 1997)
HNN	Food porosity	Food drying process (Experimental)	High accuracy based on increasing number of inputs	(Hussain, Shafiur Rahman, & Ng, 2002)
SAHNN	Reactants rates and concentration	Batch reactor	Fast convergence rate	(Wang et al., 2011)
HMNNRFM	Reaction rate	Fixed bed reactor	Good prediction without use of model equation	(Shiva Kumar & Venkateswarlu, 2012)
ANN-GA (GNN)	Critical heat flux	Heated tubes	Fast convergence,	(Wei, Su, Qiu, Ni, & Yang, 2010)

Table 2.2 (*continued*)

Types	Objective/estimate(s)	Systems applied	Positive highlights	References
			consistent prediction	
FFN-ES	Silicon, sulphur compositions	Furnace	Small estimation error	(Radhakrishnan & Mohamed, 2000)
Fuzzy-ES	Froth density	Flotation column (Experimental)	Satisfactory despite variation in feed rate	(Chuk et al., 2005)
Fuzzy-GA	Kinetic parameters	Sulphuric acid catalyst preparation process	Effective convergence, able to avoid premature convergence	(Yang & Yan, 2011)
Fuzzy-Neural-GA	Injection velocity and cooling water temperature	Plastic injection moulding	Good generalization capabilities	(Li et al., 2002)

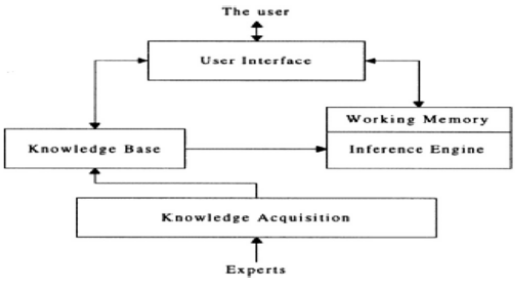

Fig. 2.2. Components of an expert system. Picture taken from Kishan et al. (2012): A review of development and application of expert systems.

generates one solution at a time. This can be seen in Table 2.2(c). An alternative solution is the GA, whereby it is able to generate many feasible solutions and allow researchers to choose from several approaches for obtaining best results (Krishnamoorthy & Rajeev, 1996).

The GA concept was first introduced by Holland in the 1970s with the aim to make computers do what nature does (Fernandez, 1996). In natural computation, chromosomes are blindly selected and are able to manipulate data into binary digits string. Each data is the artificial chromosome that consists of a series of binary elements or genes and is represented by digits known as encoding. Similarly, the evaluation process in GA will select the fittest chromosomes for mating and is expected to produce the fittest offspring within the chromosomes. However, since the selection is stochastic, the population will remain stable until a superior chromosome appears and this is one of its limitations, where the fittest genes will dominate the population for a long time. GA has also been applied widely in several areas including process control, transportation and pattern recognitions. Although GA provides good techniques in assisting decision making such as estimating parameters, it also depends on experience and heuristic method in order to obtain better mutations and generations. It may take several trial and errors steps before reaching the ideal new generations when this concept is applied (Mohebbi, Shahidi, Fathi, Ehtiati, & Noshad, 2011; Porter Ii & Passino, 1995). Table 2.2(d) provides examples of applications of GA as estimators for chemical process systems.

Recently, researchers have developed algorithms that combined two or more AI methods in what is called hybrid systems. These algorithms are applied as estimators to overcome the limitations of the single algorithm and to further increase the estimator's performances. For example, ANN will only allow reasoning from input to outputs and this can be overcome by using the adaptive neuro-fuzzy inference systems (ANFIS) (Yetilmezsoy et al., 2011). Normally, the combination utilised the advantages of each of the algorithms such as the hybrid neural network (HNN), ANFIS, fuzzy neural network (FNN) and expert system neural network (ES-NN) (Sivan, Filo, & Siegelmann, 2007). Details of the applications of hybrid systems as estimators in chemical process systems are given in Table 2.2(e) and the types of hybrid systems are given in Table 2.3 with their advantages and limitations.

Most applications with AI-based estimators are designed using the MATLAB (Araúzo-Bravo et al., 2004; Bahar & Özgen, 2010; Devogelaere et al., 2002; Ng & Hussain, 2004; Patnaik, 1997; Silva, Pinotti, Cruz, Giordano, & Giordano, 2008; Wang, Shao, Wang, & Wu, 2006; Yarlagadda & Teck Khong, 2001) and LabView software (de Canete, del Saz-Orozco, Gonzalez, &

Table 2.3
Comparisons of several hybrid systems structures.

No.	Types of Hybrid System	Key Features	Advantages	Limitations
1	Adaptive Neuro-Fuzzy Inference System (ANFIS)	• Construct input–output mapping based on human knowledge and simulated input–output data pairs • Consist of two parts: antecedent and conclusion	• Minimize error by applying two learning algorithms (back propagation and hybrid) • Able to handle complex processes • Short learning time • Fast in reaching optimum results	• Optimum structures are based on trial and error
2	Hybrid Neural Network (HNN)	• Hybrid combination of neural network and first principle model	• Fewer nodes • Less training time • Fast convergence	• Bigger mean square error of the estimated parameters
3	Structure Approaching Hybrid Neural Network (SAHNN)	• A hybrid type of neural network • Use approximate mechanistic equation for characterising the unmeasured variables	• Rapid convergence	• Suitable for certain parameters estimation only
4	Fuzzy Neural Network (FNN)	• Contain theory of fuzzy logic and ANN	• Implementation can be either from input to output or output to input	• Accuracy depends on the number of data quality
5	Fuzzy-Rough Set (FuREAP)	• Based on rough set and fuzzy logic theories	• Reduce measurement and data set for reducing cost	• Pre-processor is difficult to be optimised
6	Fuzzy-Expert Systems (Fuzzy-ES)	• Combination of IF-THEN rules with expert systems	• Able to solve problems involving variations in parameters • Reduce quantity of rules	• Expression of fuzzy inference depends on the behaviour of the systems

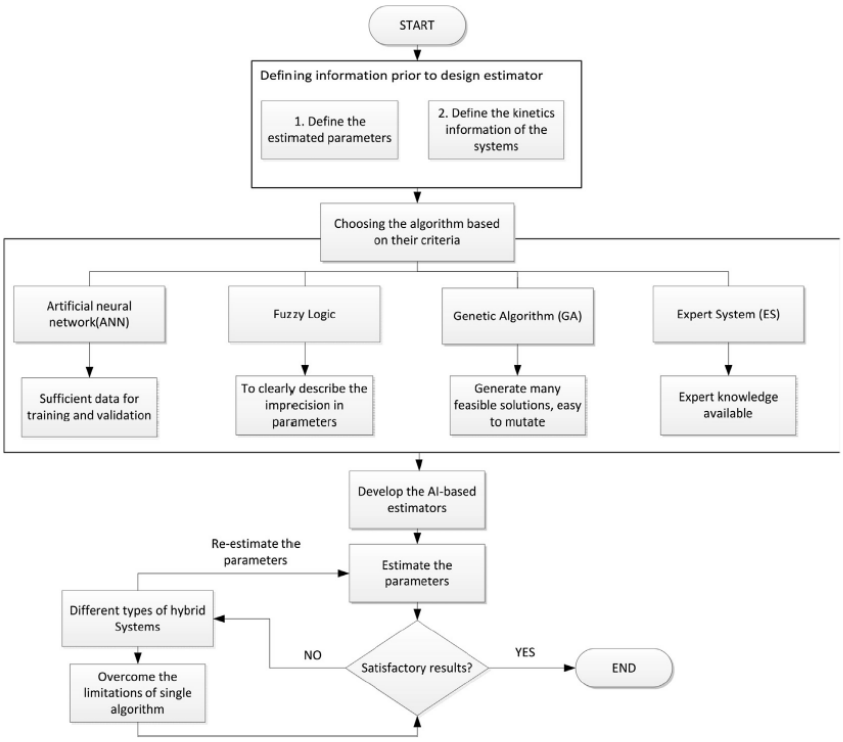

Fig. 3.1. Guideline for choosing AI-based estimators.

Garcia-Moral, 2012) while others utilised their own software such as Simulation Sciences code (PROCESS) (Himmelblau, 2008), Siemens Adaptive Modelling of Dynamic System (SIAMOD) (Horn, 2001), GENSYM G2 (Kordon, Dhurjati, & Bockrath, 1996), DataFit (Turkdogan-Aydınol & Yetilmezsoy, 2010) (Yetilmezsoy et al., 2011), ANSYS Fluent CFD (Delrot et al., 2012) and DAMADICS (Korbicz & Kowal, 2007) to develop the estimators for their systems.

3. Guidelines with examples of application

In this section, we provide the general guidelines on how to select the appropriate AI algorithm to be applied as estimators with example of some typical applications in order to clearly show how to develop AI-based estimators for chemical process systems. Although, the AI-based estimators can be designed without full knowledge of the process kinetics, we will still use the process model to highlight the nonlinearity of the process. Determining the process model and understanding the behaviour of the process is the first step in designing the AI-based estimators. This is followed by defining the estimated parameters for the specific system such as concentration, temperature, melt index and pressure. Once both the behaviour and the estimated parameters have been identified, researcher may proceed to choose the appropriate algorithm to be used.

The variety of those algorithms makes it difficult to decide the most suitable algorithm, thus a guideline as depicted in Fig. 3.1 is helpful in assisting researchers in selecting the algorithm. In this paper, we consider five major algorithms that have been applied as estimators in chemical process systems namely ANN, fuzzy logic, GA, ES and the hybrid systems. Each algorithm differs in terms of formulations and has their own advantages as well as limitations. The comparisons regarding advantages, limitations and practical implications of all the algorithms are given in Table 3.1, which will also help in deciding the combination of the hybrid systems, which is developed based on the advantages of individual algorithms.

In order to apply ANN, the data to be used for training and validation must be sufficient to obtain the best results (Lashkarbolooki et al., 2012) while fuzzy logic is normally applied since it can clearly describe the imprecision in the parameters and its ability in avoiding vagueness in the estimation results (Genovesi, Harmand, & Steyer, 1999; Liu, 2007). GA on the other hand, is applicable for process system which is easy to apply the mutation concept and for generating many feasible solutions to choose from while ES is applied for estimation cases in less nonlinear systems where only one solution is sufficient to obtain the best performance (Krishnamoorthy & Rajeev, 1996).

These are the single AI algorithms applied as estimators in chemical process systems and once they have been chosen, the AI-based estimators will be design and validation test will be conducted to observe the performances and upon achieving satisfactory outcomes, the development of AI-based estimators is complete (Chen & Lee, 2008; Motlaghi, Jalali, & Ahmadabadi, 2008; Rezende, Costa, Costa, Maciel, & Filho, 2008; Sharma et al., 2004). However, if the results are unsatisfactory, hybrid approach including the hybrid algorithms should be considered. Hybrid systems are applied to overcome the limitation of any single algorithm including slow rate of estimation and high estimation error but the combination will strongly depend on the behaviour of

Table 3.1
Comparisons of AI algorithms applied as estimators in chemical process systems.

AI algorithm	Advantages	Limitations	Practical implications
ANN	Able to learn based on historical data, high accuracy and consistent estimations when changes occur	No specific numbers of the hidden neurons and it is always based on trial and error	Increase in the accuracy for measurement of parameters in highly nonlinear systems
Fuzzy logic	Simple formulation, easy to design and able to accurately describe imprecise values of parameters	Depends on the number of rules, inference systems and the type of membership function applied	Applicable for imprecise definition of parameters in difficult-to-model systems
GA	Generate many feasible solutions and allow researchers to choose from several approaches for obtaining best results	Several trial and errors before reaching the ideal new generations when this concept is applied	Able to choose best estimation results from several generated solution for complex systems
ES	Ability in expressing relations, recommendations, directives, strategies and heuristics	Generates one solution at a time and expert knowledge must be available	Able to estimate parameters using one accurate solution for nonlinear systems
Hybrid systems	Overcome the limitations of the single algorithms and to increase the estimation performances, faster estimation with more error reduction	The formulation is not simple and require more time to be developed	Improve in the estimation performances, thus allow better estimation especially in dealing with disturbances in processes

Table 3.2
Input–output neural network mapping.

$T_r(k-2)$	$T_r(k-1)$	$T_r(k)$
Input Output	$T_j(k-1)$	$T_j(k)$
	$Q_r(k-1)$	$Q_r(k)$

the system (Li, Jia, & Yu, 2002). Similarly, these hybrid systems will have to be evaluated to observe their performances.

As for the first example, we choose the ANN applied as the estimator since it is the most promising method. We refer the reader to the guideline in Fig. 3.1 and the AI-based estimation research by Aziz, Hussain, and Mujtaba (2000). First of all, the estimated parameter is selected, which is the amount of heat released, Q_r from a jacketed batch reactor, where the reaction is exothermic. Then, the kinetics information will be defined before choosing the appropriate AI algorithm to be used as the estimator. Based on the information, data available is sufficient for applying ANN and it has been proven to be fast and accurate in estimating unknown parameters (Hussain, 1999). The design will proceed with a three layered feed forward neural network with 18 hidden nodes used and the training is based on the Levenberg–Marquardt methodology (Aziz et al., 2000). The process model is also required to relate the reactor temperature, T_r, jacket temperature, T_j and the energy balance with one another as given below.

$$\frac{dT_r}{dt} = \frac{(Q_r + Q_j)}{M_r C_{p_r}} \tag{3.1}$$

$$\frac{dT_j}{dt} = \frac{(T_j^{sp} - T_j)}{\tau_j} - \frac{Q_j}{V_j \rho_j C_{pj}} \tag{3.2}$$

$$Q_r = \Delta H_1 R_1 - \Delta H_2 R_2 \tag{3.3}$$

$$Q_j = UA(T_j - T_r) \tag{3.4}$$

$$R_1 = k_1 M_A M_B \tag{3.5}$$

$$R_2 = k_2 M_A M_C \tag{3.6}$$

$$M_r = M_A + M_B + M_C + M_D \tag{3.7}$$

Here Q_j is the heat input, ΔH_1 and ΔH_2 are the heat of reactions, R_1 and R_2 are the rate of reactions, k_1 and k_2 are the constant reaction rates, M_r is the overall number of moles, M_A, M_B, M_C and M_D are the number of moles for component A, B, C and D respectively.The input layers consist of both present and past values of the reactor and jacket temperature as well as the past heat-release values whereas the output layer will estimate the current heat-release values. Using 6 inputs, the neural network is trained through the forward modelling methodology to obtain the present value of Q_r (the output). A constant bias is added to the hidden (bj) and output layer (bk) node where (wji) and (wkj) are the weights. The data are moved forward at one discrete-time interval until all are fed into the network in a moving window scheme and are continued repeatedly until it achieves the training error criterion.

A cross-validation based early stopping mechanism is implemented and neural network is validated with new set of data, which has not been used during training. The input and output variables are shown in Table 3.2 while the topology of the multi-layered ANN is given in Fig. 3.2. The validation result is seen in Fig. 3.3, and since the validation shows no discrepancies between actual and estimated values the design of the estimator using ANN can be finalized.

Another example is applying fuzzy logic as estimator to predict the specific CO_2 evolution rate, Q_c and specific O_2 uptake rate, Q_o in a fermentor studied by Hisbullah, Hussain, and Ramachandran (2003). Those parameters are estimated to find the differences of both rate $(Q_c - Q_o)$ to be applied in the fermentor as set point for maintaining the glucose level for obtaining the optimum productivity and yield in the process. The estimator is based on the Takagi–Sugeno inference method which consists of fuzzification and IF-THEN rules. The input variables are the process error, e and the change of the error, Δe while output variables are the feed rate, ΔF. Those variables are as follows:

$$e_t = (Q_c - Q_o)_{sp} - (Q_c - Q_o)_t \tag{3.8}$$

$$\Delta e_t = e_t - e_{t-1} \tag{3.9}$$

$$\Delta F_{t+1} = F_{t+1} - F_t \tag{3.10}$$

First, the set point of both rate $(Q_c - Q_o)$ is considered and the present value (initial estimated value of $(Q_c - Q_o)$ is assumed and the error is obtained as e_t. Then, the change of error is calculated based on Eq. (3.9) and the fuzzy estimator is applied to obtained the present value of $(Q_c - Q_o)$ based on the desired output value, ΔF_{t+1}. The rules for the estimation is given below with linguistic term of Z = zero, N = negative and P = positive.

(1) *IF* Δe_t *is P and* e_t *is Z THEN* $\Delta F_{t+1} = GM_Z(-0.002F_t)$
(2) *IF* Δe_t *is P and* e_t *is N THEN* $\Delta F_{t+1} = GM_N(-0.15F_t)$

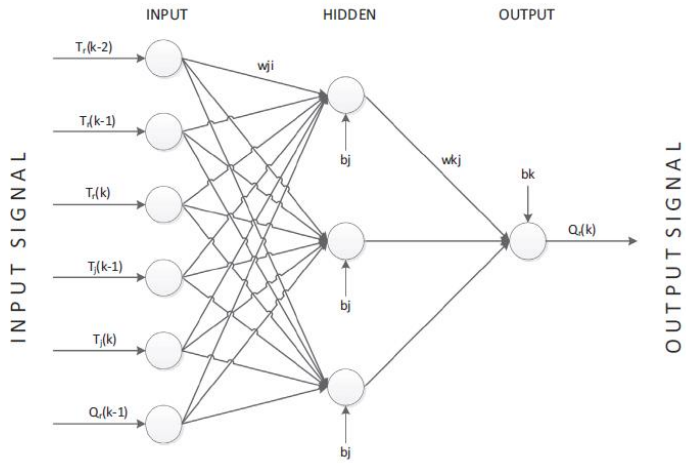

Fig. 3.2. Topology of the ANN.

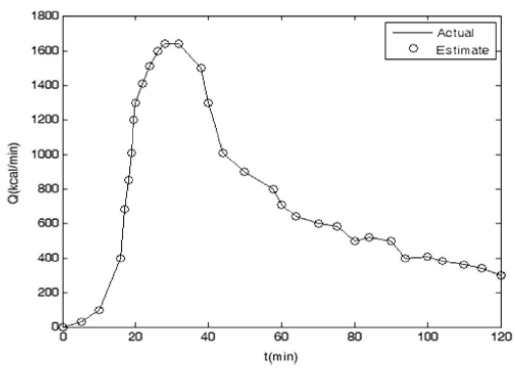

Fig. 3.3. Heat-release estimated using ANN.

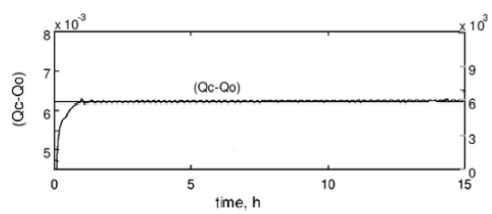

Fig. 3.4. Estimation of $(Q_c - Q_o)$ using fuzzy logic. Picture taken from Hisbullah et al. (2003): Design of a fuzzy logic controller for regulating substrate feed to fed-batch fermentation.

(3) *IF* Δe_t *is P and* e_t *is P THEN* $\Delta F_{t+1} = GM_P(0.1F_t)$
(4) *IF* Δe_t *is N and* e_t *is Z THEN* $\Delta F_{t+1} = GM_z(0.01F_t)$
(5) *IF* Δe_t *is N and* e_t *is N THEN* $\Delta F_{t+1} = GM_N(-0.1F_t)$
(6) *IF* Δe_t *is N and* e_t *is P THEN* $\Delta F_{t+1} = GM_P(0.1F_t)$

The results are shown in Fig. 3.4 where the actual values of $(Q_c - Q_o)$ are in good agreement with the fuzzy estimated values and the advantage of this estimator is being able to achieve good performance, even for a difficult-to-estimate process parameter.

For GA applied as estimator, we consider an example taken from Khairi Abdul Wahab, Azlan Hussain, & Omar, 2007) that used GA to predict the coolant jacket temperature, T_c in a CSTR in order to minimize the error of the reactor temperature, T. The coolant temperature is normally not measured directly. The input used to generate the initial population is the reactor temperature, T where the error between T and T_{sp} is constantly monitored. If this monitored error is over the specified limit, a binary coolant jacket temperature (initial population) will be created and repeated to achieve the minimum error in the reactor temperature. The procedure involving selection of quasi-genetic, crossover and mutation are illustrated in Fig. 3.5.

The selected operators evaluate the population based on the fitness function and emerge with the best individuals. Next, two individuals are randomly chosen and they reproduced new individuals during the crossover step. After that, mutation ability will enhance the method by injecting a random point for a better search in the entire parameters for estimating the temperature. This mutation step contained random value of elements of the chromosomes. The best fitness chromosomes that gave the smallest error will be chosen as the new estimated coolant jacket temperature. The results are illustrated in Fig. 3.6 where the estimated temperature followed the set point or actual temperature.

Finally, HNN will be taken as the example to show how the hybrid systems act as an estimator. It is based on the work done by Hussain et al. (Wei, Hussain, & Wahab, 2007) where HNN is applied for estimating monomer concentration in a polymerization reaction.

Consider the mass balance of the monomer as follows:

$$\frac{dC_m}{dt} = -k_r C_m - \frac{\varepsilon k_r C_m^2}{C_{m_0}} \tag{3.11}$$

Assuming the rate constant, k_r is constant between sampling interval Eq. (3.11) can be integrated to become:

$$C_m^{mod}(k+1) = \frac{e^{-k_r \Delta t} k_r C_m(k)}{k_r - QC_m(k)e^{-k_r \Delta t} + QC_m(k)} \tag{3.12}$$

where $Q = \frac{k_r \varepsilon}{C_{m_0}}$ and $C_m(k+1)$ is the concentration of monomer at sampling $(k+1)$.

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