Process-Monitoring-for-Quality — A Model Selection Criterion for Shallow Neural Networks

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ABSTRACT

Since most manufacturing systems generate only a few defects per million of opportunities, rare quality event detection is one of the main applications of the Process Monitoring for Quality philosophy. Single-hidden-layer feed-forward neural networks have been successfully applied to perform this task. However, since the best network structure is not known in advance, many models need to be learned and tested to select a *final model* with the right number of hidden neurons. A new three-dimensional model selection criterion ($3D-NN$) is introduced for the application of shallow neural networks to highly/ultra unbalanced binary data structures. Proposed criterion combines three of the most important attributes – prediction, fit, complexity – of a network structure and map them into a three dimensional space to select the *best* one. It is simple, intuitive and more stable than widely used criteria – Akaike information criterion, Bayesian information criterion and validation cross-entropy error – when dealing with these data structures.

1. INTRODUCTION

Process Monitoring for Quality (PMQ) is a *big data*-driven quality philosophy aimed at defect detection through binary classification (Abell et al., 2017). It is founded on *Big Models (BM)*, a modeling paradigm based on optimization, machine learning and statistics, Fig. 1. It includes a learning component that requires many models to be created to find the *final model* (classifier) (Escobar, Abell, Hernández-de Menéndez, & Morales-Menendez, 2018). Since many *Candidates Models (CM)* are created, *Model Selection (MS)* is one of the main challenges. The concept of using three attributes to evaluate the fitness of a *CM* was initially introduced in (Escobar, Wegner, Gaur, & Morales-Menendez, 2019) for genetic programming, extended to the support vector machine (Escobar & Morales-Menendez, 2019b) and logistic regression (Escobar & Morales-Menendez, 2019a). However, these criteria cannot be directly applied to the *Artificial Neural Network (ANN)* algorithm.

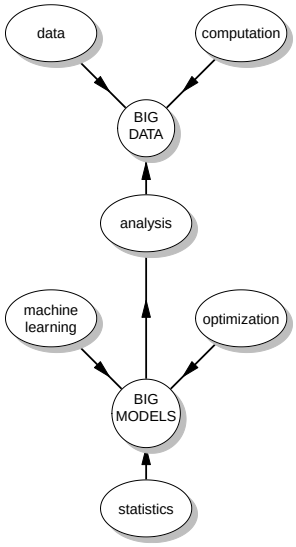

Figure 1. Big Data – Big Models

Feed-Forward Neural Network(s) (FFNN) are universal approximators (Hornik, Stinchcombe, & White, 1989). Their widespread popularity in many domains is mainly due to their ability to approximate complex nonlinear patterns directly from the input samples, without assuming any parametric form for distinguishing between classes. In manufacturing, shallow *ANN* have been successfully applied for rare quality event detection (Escobar et al., 2018), as depicted in Fig 3.

In designing a functional *ANN* structure, determining the number of *hidden neurons (H_n)* is one of the most important challenges because there is no analytical method to define the optimal structure in advance. In the context of generalization (prediction on unseen data), if the *ANN* is too large (too small), it could potentially overfit (underfit) the data. In either of these cases, the network would not generalize well. Existing methods (Sheela & Deepa, 2013) to determine H_n are heuristic in nature and/or trial-and-error dependent – training and estimating the generalization capacity. Since many *ANN* structures – different numbers of H_n – need to be learned and tested to find the best one (*final model*), *MS* is one of the most important steps in the development of a functional structure.

In today's high conformance manufacturing environment, data sets for binary classification of quality (*good*,*bad*) tend to be highly/ultra (*bad* class count $< 1\%$) unbalanced. Therefore, detecting these few *Defects Per Million of Opportunities (DPMO)* is one of the main challenges addressed by *PMQ*. Therefore, in manufacturing modeling, functional refers to a parsimonious (Burnham & Anderson, 2003) classifier with high detection ability.

A new *Three Dimensional (3D) MS* criterion ($3D - NN$) for single-hidden-layer *FFNN* is presented. It is based on three of the most relevant attributes of an *ANN* structure: (1) prediction (generalization), (2) fit (robustness of predictions), and (3) complexity (H_n). Criterion enables the development of a structure with high defect detection ability while avoiding overcomplexity; extra neurons with negligible contribution to the first two attributes.

The rest of the paper is organized as follows. Acronyms in Table 1, a brief theoretical background is in section 2. Section 3 describes the *MS* criterion. To evaluate the performance of the criterion, a comparative analysis using many public data sets is presented in section 4. Section 5 shows the conclusions and future research.

2. ARTIFICIAL NEURAL NETWORKS

Although *ANN* approach can be applied for different purposes: function approximation, probability estimation, pattern recognition, clustering, and prediction (Demuth, Beale, De Jess, & Hagan, 2014), the type of *Neural Network (NN)* for which the $3D - NN$ *MS* is developed is very specific, and widely used in manufacturing. In this section, a brief overview of the *ANN* architecture of interest is provided.

2.1. Single Hidden Layer Feed-Forward

The *FFNN* was the first and simplest type of *ANN* developed. It has been successfully applied to solve a wide range of complex-classification problems across domains (Escobar et al., 2018; Boland & Murphy, 2001; Saxena & Saad, 2007). In this network, the information moves in just one direction, forward. There are no cycles or loops from the outputs of the neurons towards the inputs throughout the network (Sazli, 2006; Auer, Burgsteiner, & Maass, 2008). To explain in brief, the information enters the network through the input neurons of the first layer, which then develop a mathematical process (F. Amato nd A. López, na Méndez, Vaďhara, Hampl, & Havel, 2013) by using activation functions (Valente Klaine, Ali Imran, Onireti, & Demo Souza, 2017) and finally is transferred to the neurons of the following layer. Each neuron is connected to each neuron of the forward layer by a weighted relation, which indicates the strength of the link. Finally, the neurons of the last layer provide the outcome.

Figure 2 shows the *ANN* structure of interest, which is suitable for binary classification problems. A single hidden layer *FFNN* with sigmoid transfer and activation functions, the classification threshold, γ, is tuned with respect to the *Maximum Probability of Correct Decision (MPCD)* following the *OCTM* algorithm (Escobar & Morales-Menendez, 2017). For the purposes of this paper, a network with only a single hidden layer is called *shallow*.

The process of assigning the predicted label ($\hat{y}$) to a manufactured item is defined as follows:

$$\hat{y}_i = \begin{cases} 1 & \text{if } O(y=1|x;\theta) \geq \gamma \Rightarrow i^{th} \text{ predicted bad (+)} \\ 0 & \text{if } O(y=1|x;\theta) < \gamma \Rightarrow i^{th} \text{ predicted good (–).} \end{cases} \quad (1)$$

Since the number of hidden layers is constant and the transfer/activation functions are the same, complexity (Kon & Plaskota, 2006) can be efficiently defined in function of *number of parameters (N_p)*.

$$Np = (m \times n) + (n \times 1) \quad (2)$$

2.2. Maximum Probability of Correct Decision

In the field of machine learning, specifically applied to classification problems, a confusion matrix (Fawcett, 2006) is a technique for summarizing the performance of a classifier. It is a table with two rows and two columns that contrasts predictions with real-world values Table 2.

Table 2. Confusion matrix.

	Predicted good	Predicted bad
Real-world good	True Negative (TN)	False Positive (FP)
Real-world bad	False Negative (FN)	True Positive (TP)

A type-I error (α) may be compared with a *FP* prediction; a type-II (β) error may be compared with a false *FN* (Devore, 2015):

$$\alpha = \frac{\text{FP}}{\text{FP} + \text{TN}}, \quad \beta = \frac{\text{FN}}{\text{FN} + \text{TP}} \quad (3)$$

Table 1. Acronyms Definition

Acronyms	Definition
ANN	Artificial Neural Network
AIC	Akaike Information Criterion
BIC	Bayesian Information Criterion
BM	Big Models
CEE	Cross-Entropy Error
CM	Candidate Model
DPMO	Defect Per Million of Opportunities
FFNN	Feed-Forward Neural Network(s)
LSW	Laser Spot Welding
MPCD	Maximum Probability of Correct Decision
MS	Model Selection
NN	Neural Network(s)
OCTM	Optimal Classification Threshold with respect to MPCD
3D	Three Dimension
UMW	Ultrasonic Metal Welding

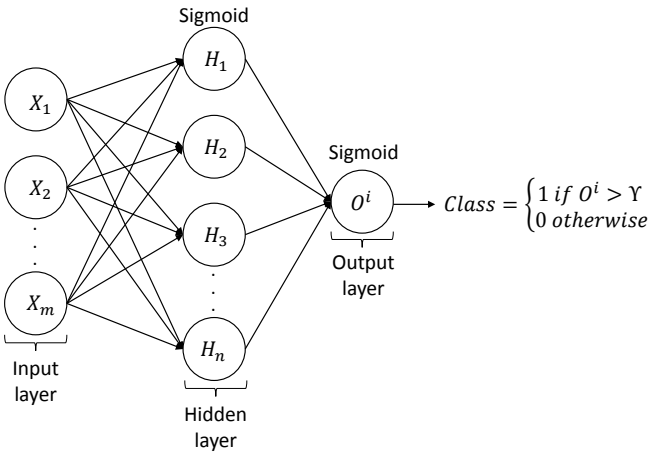

Figure 2. Single-hidden-layer *FFNN* (fully connected) structure with sigmoid transfer function and sigmoid activation function.

The *MPCD* is a probabilistic-based measure of classification performance – driven by detection – that is highly sensitive to *FN* in highly/ultra unbalanced classes. The α, and beta β errors are combined to estimate its score:

$$\text{MPCD} = (1-\alpha)(1-\beta) \tag{4}$$

where higher score ($0 \leq MPCD \leq 1$) indicates better classification performance.

Figure 3 shows how *BM* is applied to process data to monitor and detect those very few *DPMO* that are generated by the manufacturing process. Where the predominant goal for a classifier is detection ($\beta = 0$) with a small as possible false alarm rate – *FP* (α).

2.3. Cross-Entropy Error

The probability distribution of the class label y, given a feature vector x is modeled by (S. Lee, Lee, Abbeel, & Ng, 2006):

$$O(y=1|x;\theta) = \sigma(\theta^T x) = \frac{1}{1+\exp(-\theta^T x)} \tag{5}$$

where $\theta \in \mathbb{R}^N$ are the parameters of the model and $\sigma(\cdot)$ is the sigmoid function that maps values from $(-\infty, \infty)$ to $[0, 1]$. The *Cross-Entropy Error (CEE)* of the *NN* is defined by (Murphy, 2012):

$$\sum_{i=1}^{M} [y^{(i)} log O^{(i)} + (1-y^{(i)}) log(1-O^{(i)})] \tag{6}$$

3. THE CRITERION

A $3D$ *MS* criterion ($3D-NN$) is presented which is aimed at analyzing highly/ultra unbalanced data structures. Due to the importance of detecting rare quality events generated by manufacturing systems, proposed criterion is mainly driven by detection ability. It uses three of the most important attributes of an *ANN* structure – prediction (rewarding attribute), fit (re-

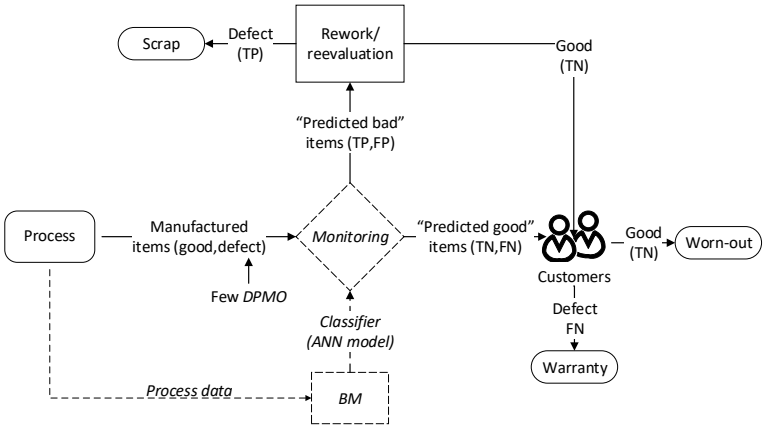

Figure 3. *PMQ*-based quality control.

warding attribute), complexity (penalizing attribute) – of each *CM* to map them into a three dimensional space to select the *best* one. Criterion avoids overcomplexity; extra neurons with negligible contribution to the rewarding attributes.

Once a set of *Candidate Models*, (CM_j^m), $j = 1, ..., m$, – where m is the number of models – are trained by exploring different numbers of H_n, the three attribute values are computed. To match the *MPCD* scale, fit and complexity attributes are rescaled to $[0, 1]$ using the $Min - Max$ (Mohamad & Usman, 2013) normalization method.

1. Prediction (p)
   A rewarding attribute based on validation *MPCD*. In highly unbalanced data structures, this measure of classification performance tends to reflect the model's capacity in detecting the minority class.

$$p_j = 1 - MPCD_j \tag{7}$$

2. Fit (f)
   A rewarding attribute based on the validation *CEE*. It is a relative measure that describes how well a candidate model fits the validation data, where smaller values describe more robust predictions.

$$f_j = CEE_j \tag{8}$$

$$\text{MM}(f_j) = \frac{f_j - \min(f)}{\max(f) - \min(f)} \tag{9}$$

3. Complexity (c)
   A penalizing attribute based on N_p.

$$c_j = N_{pj} \tag{10}$$

$$\text{MM}(c_j) = \frac{c_j - \min(c)}{\max(c) - \min(c)}. \tag{11}$$

For each CM_j the tree associated attribute values are mapped into a three-dimensional space and the weighted *Euclidean* (E_{wj}) distance (Deza & Deza, 2009) to the *utopian point* $(0, 0, 0)$ is computed, eqn 12. Then, the closest model ($3D - NN^*$) to the utopian point is selected, Eq. 13. The utopian point, is an ideal model that optimizes the three attribute-functions simultaneously; however, most of the times, a model cannot be improved in any of the attributes without degrading at least one of the others. An overview of the *MS* process is illustrated in Fig. 4.

$$E_{wj} = \sqrt{w_p(p_j - 0)^2 + w_f(f_j - 0)^2 + w_c(c_j - 0)^2} \tag{12}$$

where $w_p = 1$, $w_f = 1$ and $w_c = 0.01$

$$3D - NN^* = \min(E_{wj})_j^m. \tag{13}$$

3.1. Discussion

The fundamental principle of *BM* learning paradigm, is that none of the models developed using process (empirical) data is the *true model* that generates the observed data. Based on this premise, proposed criterion's objective is not to search for the *true model*, but to efficiently solve the posed tradeoff between these three competing attributes.

There is no universal *best Euclidean* weight-combination, instead they are hyper-parameters that can be adjusted based on the goals of a particular project. Since complexity increases very rapidly, its influence is kept low, otherwise it would become a dominating attribute. Proposed weights maintain prediction ($w_p = 1$) and fit ($w_f = 1$) as the main drivers. However, the light penalization for complexity ($w_c = 0.01$) prevents the selection of over-complex structures.

3.2. The *MS* Process

To illustrate the *MS* process, a case study is derived from *Ultrasonic Metal Welding (UMW)* (Shao et al., 2013) of bat-

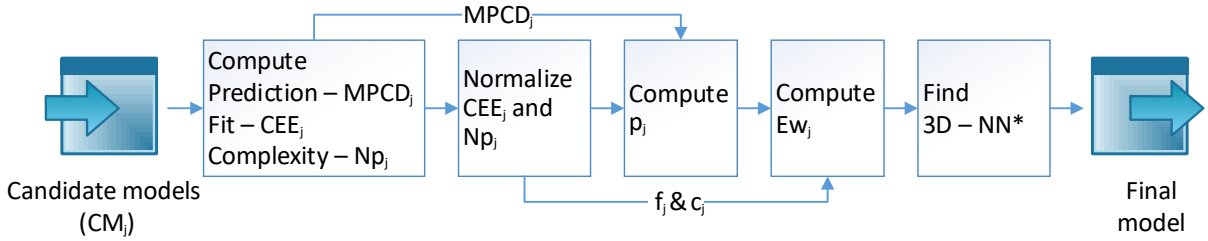

Figure 4. Model selection process.

tery tabs for the Chevrolet Volt (Abell et al., 2017), an extended range electric vehicle. A very stable process, that only generates a few defective welds per million of opportunities. The data set has 54 features and a binary outcome (*good*/*bad*). It is highly unbalanced, since it contains only 29 bad batteries out of 30,731 examples (0.0944%). Because manufacturing systems tend to be time-dependent, the data set is partitioned following the time-ordered hold-out validation scheme (Escobar et al., 2018): training set (18,495 - including 20 *bads*), validation set (12,236 - 9 *bads*). Following a widely used rule-of-thumb "the number of hidden neurons should be less than twice the size of the input layer" (Heaton, 2008), 108 candidate models, CM_j, are generated using early stopping (Demuth et al., 2014) with the scaled conjugate gradient algorithm (Møller, 1993).

Candidate model information is summarized in Fig. 5, and the *MS* process is illustrated in Fig. 6. First, the three attributes of each CM_j are mapped into a three dimensional space, Fig. 6(a), then, the *weighted Euclidean* distance of each CM_j is computed, and the one closest to the utopian point is selected, Fig. 6(b). According to the *MS* criterion, CM_7 should be selected ($E_{w7} = 0.0258$) – $H_n = 7$, $MPCD = 0.97677$ and $CEE = 64.4580$. This model has the highest prediction, relatively low *CEE* (good fit) and low complexity.

4. COMPARATIVE ANALYSIS

To verify the performance of proposed criterion, the *final model* selected by $3D - NN$ is compared against the *final model* selected by three criteria/method, which have been widely used to search for the most efficient *NN* structure: (1) *Akaike information criterion (AIC)* (Panchal, Ganatra, Kosta, & Panchal, 2010), (2) *Bayesian information criterion (BIC)* (H. K. Lee, 2001), (3) validation *CEE* (Demuth et al., 2014), and (4) validation *MPCD* (Escobar & Morales-Menendez, 2017). To perform this analysis, 10 highly/ultra unbalanced data sets (8 publicly available) are used, Table 3. The associated attribute values of each *final model* by data set are summarized in Table 4.

$3D - NN$ vs:

- *AIC*, the *final models* selected by the $3D - NN$ criterion show significantly better generalization ability and fitting properties. This gain is obtained at the expense of a slightly higher complexity than the structures selected by *AIC*.
- *BIC*, the $3D - NN$ criterion show significantly better generalization ability and fitting properties. This gain is obtained at the expense of a slightly higher complexity.
- Validation *CEE* and *MPCD*, the $3D-NN$ criterion show competitive generalization ability. However, both approaches show competitive generalization at the expense of overcomplexity.

Proposed criterion shows competitive performance at solving the posed tradeoff between the three competing attributes. The *AIC*, *BIC* and validation *CEE* raise a red flag when dealing with highly/ultra unbalanced data structures, as they selected *myope* structures – a solution that fails to capture the pattern (e.g., $MPCD = 0.3078$, $MPCD = 0.3338$, $MPCD = 0.4000$ respectively).

Whereas measures of classification performance (e.g., *MPCD*) can be used as a *MS* criterion, there is a risk associated – as shown in by data set 8 – since the *final model* may be an overcomplex *NN* structure with virtually the same prediction ability of a simpler one – e.g., $MPCD = 0.8621$ with $N_p = 30$ Vs $MPCD = 0.8678$ with $N_p = 1650$.

5. CONCLUSIONS

A new model selection criterion for a single-hidden-layer *FFNN* structures was developed. It maps three of the most important attributes of an *ANN* structure – prediction, fit, complexity – into a three dimensional space and uses the *weighted Euclidean* distance to the utopian point – where the three attributes are optimized simultaneously.

Based on empirical results, proposed criterion shows better performance and stability at solving the posed tradeoff between these three competing attribute than conventional model selection criteria when dealing with highly/ultra unbalanced data structures. As it selected structures with high detection ability, avoided overcomplexity and never selected a *myope* solution.

Table 3. Data sets information (preprocessing details are provided in Appendix A).

Data set	Description	Features	Instances (T/V)	Negative class (T/V)	Overall %
1	UMW	54	18,495/12,236	20/9	0.09††
2	LSW	240	1,502/760	32/15	2.07†
3	AID373*	155	47,831/11,957	50/12	0.10††
4	AID604AID644*	154	47,826/11,956	54/13	0.11††
5	AID746AID1284*	154	47,828/11,956	46/11	0.09††
6	Statlog (class 1)	36	4,435/2,000	1,072/461	23.82†
7	Statlog (class 2)	36	4,435/2,000	479/224	10.92†
8	Credit Card Fraud	29	200,000/84,807	385/107	0.17††
9	Occupancy Detection	5	6,587/1,791	173/98	3.23†
10	HTRU2	8	12,000/5,898	1,484/155	9.15†

T=Training set V=Validation set *Subsets of PubChem Bioassay Data
†highly unbalanced ††ultra unbalanced

Table 4. Characteristics of the selected model based on $3D-NN$, *AIC*, *BIC* and validation *CEE*

Data	3D-NN			AIC			BIC			CEE			MPCD		
Set	p	f	c	p	f	c	p	f	c	p	f	c	p	f	c
1	0.9767	64.45	385	0.7659	65.49	55	0.7659	65.49	55	0.7703	50.36	2200	0.9767	64.45	385
2	0.8782	46.05	10485	0.6559	60.41	1687	0.7166	30.74	241	0.4000	20.89	90134	0.8782	46.05	10485
3	0.7667	223.29	27144	0.4784	247.42	47892	0.3338	341.64	156	0.5487	236.91	6240	0.7692	214.68	29328
4	0.7835	336.86	4650	0.3078	420.43	155	0.3078	420.43	155	0.7137	316.57	35650	0.7835	336.86	4650
5	0.8890	213.94	4650	0.6283	329.31	155	0.6283	329.31	155	0.8374	144.88	3100	0.9213	214.68	21700
6	0.9863	48.67	518	0.9694	167.41	37	0.9694	167.41	37	0.9902	36.46	2294	0.9941	67.97	2331
7	0.9755	56.57	185	0.9605	132.13	37	0.9605	132.13	37	0.9821	33.54	777	0.9821	33.54	777
8	0.8621	662.8	30	0.8621	662.8	30	0.8621	662.8	30	0.8621	659.81	1470	0.8678	653.61	1650
9	0.9582	185.03	12	0.9675	190.46	6	0.9675	190.46	6	0.9675	185.33	42	0.9681	196.62	36
10	0.8891	1118.1	18	0.8891	1118.1	18	0.8891	1118.1	18	0.9028	1110	45	0.9028	1110	45

Future research along this path could be the application of the $3D-NN$ criterion to *deep neural network* structures, since the N_p tend to explode, defining its influence on the criterion seems an interesting research challenge.

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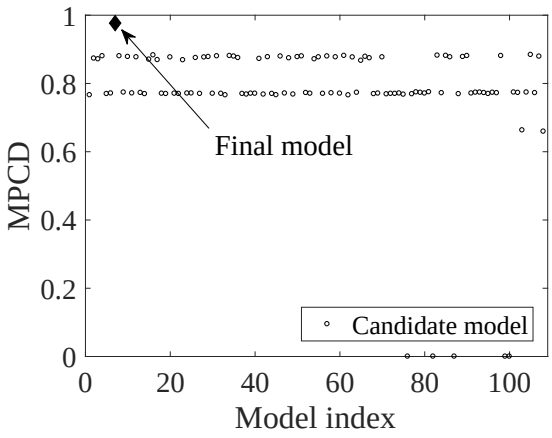
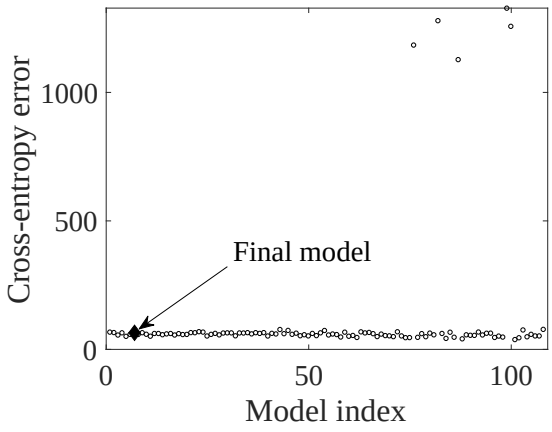
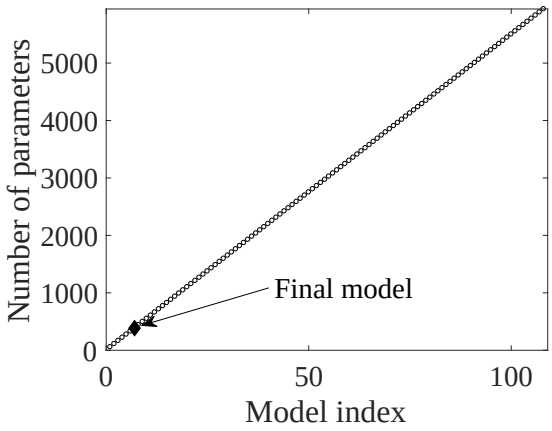


(a) Prediction attribute.

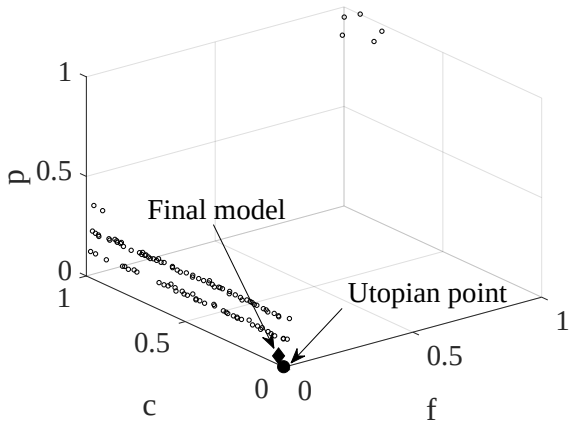


(b) Fit attribute.

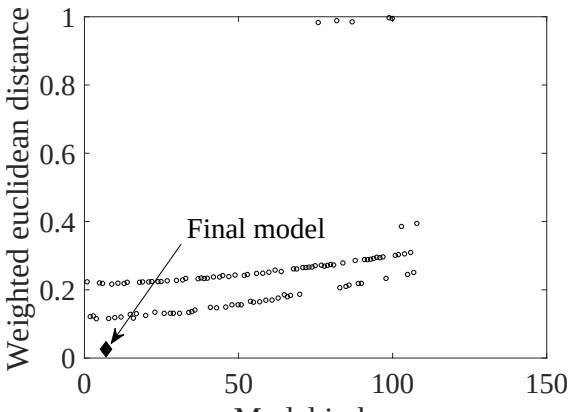


(c) Complexity attribute.

Figure 5. Candidate model information.



(a) 3-Dimensional candidate model location.



(b) *Weighted Euclidean* distance to utopian point.

Figure 6. *MS* process based on the *weighted Euclidean* distance.

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BIOGRAPHIES

Carlos A. Escobar Diaz earned an Industrial Engineering degree with concentration in automated manufacturing from the Instituto Tecnológico de Ciudad Juarez in 2003, a masters degree in engineering with Concentration in Quality and Productivity Systems from the Instituto Tecnológico y de Estudios Superiores de Monterrey, Campus Juarez in 2005, and a master of science in Industrial Engineering from New Mexico State University, Campus Las Cruces, New Mexico in 2015. He was certified six-sigma black belt from Arizona State University in 2008 and design for six-sigma black belt from University of Michigan in 2012. In 2013 he was inducted into the of Alpha Pi Mu Industrial Engineering honor society and into Tau Beta Pi engineering honor society in 2014. In 2017, Carlos was ranked into the top 3 % in TEXATA, the Big Data Analytics World Championships. He received a PhD in Engineering Sciences program from the Instituto Tecnológico y de Estudios Superiores de Monterrey, Campus Monterrey in May 2019.

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APPENDIX

- Data set 1-2
  UMW and *LSW* data sets are privately stored in the Manufacturing Research Lab of General Motors. Because of the active research aimed at understanding and improving these processes, General Motors can not make these data sets publicly available.
- Data set 3-5
  Data sets derived from the PubChem Bioassay data set (Dheeru & Karra Taniskidou, 2017). These highly

imbalanced bioassay data sets are from the differing types of screening that can be performed using HTS technology. These data sets were created from 12 bioassays.

- Data set 6-7
  Data sets derived from the Statlog (Landsat Satellite) data set (Dheeru & Karra Taniskidou, 2017). The original data set contains seven classes (with no instances with class 6). In this study, only classes 1 and 2 are considered – class 1 vs. all, class 2 vs. all.
- Data set 8
  Credit Card Fraud data set (//github.com/ellisvalentiner /credit-card-fraud), it contains credit card transactions over a two day collection period in September 2013 by European cardholders. There are a total of 284,807 transactions, of which 492 (0.172%) are fraudulent. First 200,000 are used for training and the last 84,807 for validation.
- Data set 9

  Occupancy Detection data set (Candanedo & Feldheim, 2016; Dheeru & Karra Taniskidou, 2017). To create an unbalanced data structure, one out of 10 class 1 are included in the data sets (index 1, 10, 20, etc.) and the remaining nine eliminated, all 0 class are included.

- Data set 10

  HTRU2 data set (Lyon, Stappers, Cooper, Brooke, & Knowles, 2016; Dheeru & Karra Taniskidou, 2017). Pulsar candidates collected during the HTRU survey. Pulsars are a type of star, of considerable scientific interest. Candidates must be classified in to pulsar and non-pulsar classes to aid discovery. First 12,000 are used for training and the last 5,898 for validation.