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Application of Gaussian Process Regression (GPR) in Gas Hydrate Mitigation

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ABSTRACT

The production of oil and natural gas contributes to a significant amount of revenue generation in Malaysia thereby strengthening the country's economy. The flow assurance industry is faced with impediments during smooth operation of the transmission pipeline in which gas hydrate formation is the most important. It affects the normal operation of the pipeline by plugging it. Under high pressure and low temperature conditions, gas hydrate is a crystalline structure consisting of a network of hydrogen bonds between host molecules of water and guest molecules of the incoming gases. Industry uses different types of chemical inhibitors in pipeline to suppress hydrate formation. To overcome this problem, machine learning algorithm has been introduced as part of risk management strategies. The objective of this paper is to utilize Machine Learning (ML) model which is Gaussian Process Regression (GPR). GPR is a new approach being applied to mitigate the growth of gas hydrate. The input parameters used are concentration and pressure of Carbon Dioxide (CO_2) and Methane (CH_4) gas hydrates whereas the output parameter is the Average Depression Temperature (ADT). The values for the parameter are taken from available data sets that enable GPR to predict the results accurately in terms of Coefficient of Determination, R^2 and Mean Squared Error, MSE. The outcome from the research showed that GPR model provided with highest R^2 value for training and testing data of 97.25% and 96.71%, respectively. MSE value for GPR was also found to be lowest for training and testing data of 0.019 and 0.023, respectively.

1. Introduction

Gas hydrate was developed in a pipeline where many efforts have been made in the 1930s to understand the clathrate hydrate in terms of structure, compound, balance state and way of managing them due to it poses issues such as plugging of pipelines to produce offshore oil and gas, pressure drop and corrosion plants [1-7]. When sufficient water molecules in the form of oil and hydrocarbon vapour crystallize under intermittent flow conditions, gas hydrate or known as clathrate

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hydrate occurs. It is an ice-like, non-stochiometric crystalline mixture made up of a water cage frame dominated by gas molecules like methane, CH_4, ethane, C_2H_5, and carbon dioxide, CO_2, that forms solid particles that takes place under high pressure and low temperature conditions [3-6]. Gas hydrates are produced in the petroleum and natural gas industries' output, refining and transmission facilities [8-10].

The gas hydrates are formed in 3 structures, which are I, II and H, based on the form and size of guest molecules [7]. Structure I, structure II, and structure H at which smallest and largest formers comprised of mixtures of methane, propane, nitrogen known as type II, CO_2 and CH4 form type I and methyl cyclopentane formers as type H formers are typically formed gas hydrate structures [11-13]. Structure I unit cells contain eight cavities (two smalls and six wide ones) and are formed by 46 water molecules bound to hydrogen. Besides that, there are 136 water molecules for a unit cell of structure II and enclosed 24 cavities, including 16 smalls and 8 wide ones [14]. It is therefore important to resolve the problem of gas hydrate development by introducing appropriate preventive and predictive strategies [3, 16]. There are many risk control techniques that have been used, such as the use of thermodynamic hydrate inhibitor (THI) inhibitors and low-dose hydrate inhibitor (LDHI) inhibitors. Both chemical inhibitors play a key role in preventing gas hydrate development in the pipelines of the oil and gas industry. Two commercially used thermodynamic hydrate inhibition compounds are methanol (MeOH) and monoethylene glycol (MEG), while kinetic hydrate inhibitors (KHI) and anti-agglomerants (AAs) are two types of low-dose hydrate inhibitors [17, 18]. The purpose of THIs, also like water-ice antifreezes, is to disrupt the mechanism in which hydrates develop. In conjunction, the function of KHI is to delay crystallisation of hydrate and the function of AAs is to promote distortion of hydrate molecules [10]. Conversely, because of improvement in deep-sea pipeline placement, the use of THIs is not effective because it creates high operational and capital expense (CAPEX) relative to LDHIs that are more cost-effective [1,13].

Advance management approach is the implementation of expertise focused on predictive study of multiphase flow, fluid chemistry, hydrate kinetics and plugging processes that do not require power calculation [10]. The use of Machine Learning (ML) is an innovative risk control technique that is currently being applied. ML is basically a numerical representation of a phenomenon, given with a certain significance and based on a certain environment, aimed at performing a job [8]. Deployment of ML models would allow us to do predictive analysis of gas hydrate growth because the value of determining hydrate formation is also that the solid crystalline structure which forms like ice will plug the oil and gas pipes as hydrate forms, either during gas production or transmission. This presents a potentially expensive situation for the organisation as it often takes additional time and cost to conduct a corrective intervention. Laboratory experiments are required to determine at which conditions for hydrate to perform. The best practise, therefore, is to predict the formation of hydrates by using the ML model to minimise gas hydrate growth.

2. Methods and Theory

A universal workspace is called Machine Learning, ML, ready to be used for classification problems, identifying a fitting category for a new set of outcomes, and regression tasks that estimate the relationship between data groups given. ML is essentially a numerical description of a phenomenon aimed at completing a job, assigned a certain value and based on a certain environment. The ML system can be referred to as knowledge discovery in the database (KDD) which focuses on the creation of algorithms and the test cycle. Initially, ML models are built in a training step where data is collected from historical datasets and pre-processed to delete or normalise outliers, manage incomplete data, search, and aggregate parameters. The next step is data migration,

collection of suitable data attributes, minimization of redundancies, adaptation of data format to the specified task, which is a critical step in the ML workflow [14]. The algorithms can be further divided into three distinct families of learning that are supervised learning, unsupervised learning, and reinforcement learning. Molecular modelling and statistical algorithms such as quantitative structure-activity relationship (QSAR) models have previously been used in drug industry [15].

Throughout this study, supervised learning will be based on the most widely used machine learning algorithm, wherein the input data is referred to as training data and has a predetermined mark for predicting predetermined output. Based on whether discrete or continuous output features are used, supervised learning can be further divided into classification and regression activities [14]. Several existing ML models, such as Artificial Neural Network (ANN), Gaussian Process Regression (GPR) and other existing ML models, are present in the mitigation of gas hydrate formation [16-27].

2.1 Least Square Version of Support Vector Machine (LSSVM)

LSSVM development aims to reduce the complexity of the Support Vector Machine (SVM) and eradicate ambiguity in the optimization phase by deciphering linear formulas using linear coding rather than solving quadratic encoding equations. LSSVM algorithm's output can be overcome by fixed linear equality rather than inequality constraints [13,28]. General formulation that being used in approximating a given data set $\{(x_{1,}y_1),(x_{2,}y_2),\ldots,(x_{N,}y_N)\}$ into consideration by employing following nonlinear function [29]:

$$f(x) = \langle w, \Phi(\mathrm{x})\rangle + b \tag{1}$$

where $\langle .,. \rangle$ represent dot product; $\Phi(\mathrm{x})$ denotes the nonlinear function that performs regression; b and w are bias terms and weight vector, respectively. The LSSVM model structure can be seen in Figure 1 where the $K(x_i, x_j)$ is defined as kernel function [23].

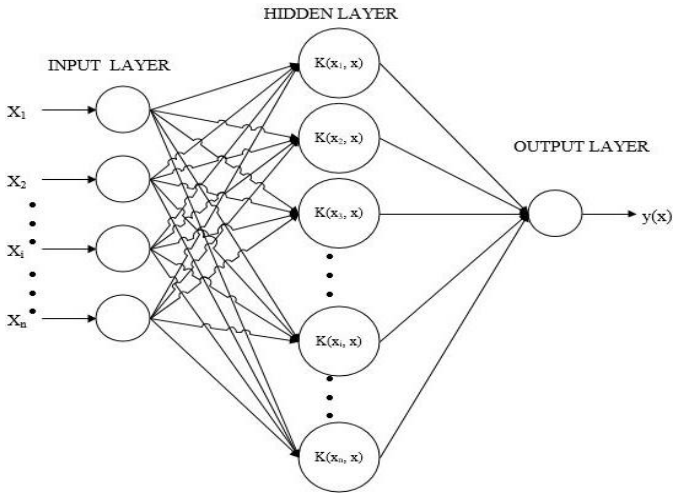


Fig. 1. LSSVM model architecture

2.2 Artificial Neural Network (ANN)

ANN is a measurement tool based on how measurements are carried out by the brain [19,23]. It has been developed for a wide range of topics, such as classification, approximation of functions and prediction [25-27]. Inside and between the layers, there are several similarities showing the strength and weights between neurons that can be seen in Figure 2.

Output of the ANN assuming a linear output neuron *j*, a single hidden layer with h sigmoid hidden nodes and the output variable (x_t) is given by [23]:

$$x_t = g\left(\sum_{j=1}^{h} w_j f\left(s_j\right) + b_k\right) \quad (2)$$

where g(.) is the linear transfer function of the output neuron k and b_k is its bias, w_j is the connection weights between hidden layers and output units, f(.) is the transfer function of the hidden layer.

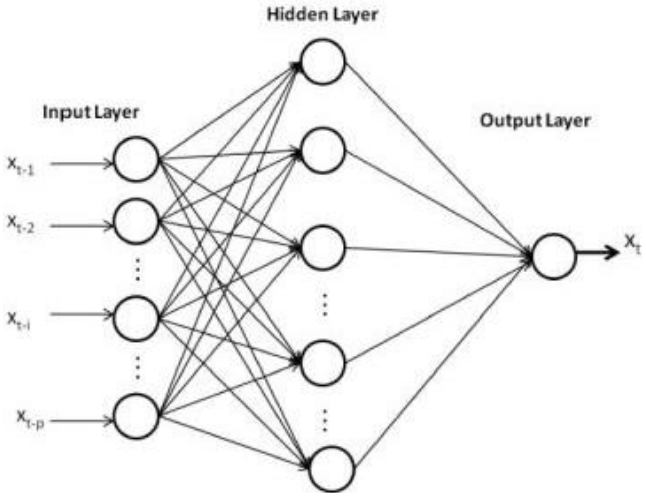


Fig. 2. Framework of ANN

2.3 Gaussian Process Regression (GPR)

GPR can be a valuable method to dynamically perform inference where it defines the maximum possible output based on given data sets and performs precise function approximation in high-dimensional space [30-35]. GPR is a non-parametric Bayesian approach to the issue of regression by using Bayesian inference to capture a wide spectrum of relations between input and output [36-48]. The general formulation for GPR, based on Bayesian analysis, can be seen from Eq. (3) [32]:

$$\mathcal{y} = f(x) + \epsilon \quad (3)$$

Where f is the function value, $\mathcal{y}$ is the observed target value, ϵ is the additive noise which is independent and adhere to normal distribution with zero mean, and variance, σ_n^2 as seen from the Eq. (4).

$$\epsilon \sim \mathcal{N}(0, \sigma_n^2) \quad (4)$$

This will be written in matrix algebra as [31]:

$$\mathcal{y} = x^T w + \epsilon \quad (5)$$

where x^T is the input vector and w is the vector of weights (parameters) of the linear model. The formula to find w is stated in Eq. (6):

$$w \sim \mathcal{N}(0, \sum p) \quad (6)$$

which it adheres to Gaussian prior with covariance matrix, $\sum p$. The Bayesian linear model's inferences are based on the posterior distribution over the weights, determined by the Bayes law, as can be seen in Eq. (7) and Eq. (8) [31].

$$posterior = \frac{likelihood\ x\ prior}{marginal\ likelihood} \tag{7}$$

$$p(w|y,X) = \frac{p(y|X,w)p(w)}{p(y|X)} \tag{8}$$

In addition to that, the newest solution is found to be the GPR application in mitigating the growth of the gas hydrate. The concentration and pressure of the CH_4 and CO_2 in the hydrated gas are the inputs to be used. Whereas average depression temperature (ADT) will be the output of the GPR. The results obtained will be evaluated in terms of Determination Coefficient, R^2, and Mean Squared Error, MSE. Then the R^2 and MSE values will be compared with other ML models. The following equation can be used as the formulation for R^2 and MSE:

$$R^2\% = 100\left(1 - \frac{\sum_i^n (o_i - t_i)^2}{\sum_i^n (o_i - average(t_i))^2}\right) \tag{9}$$

$$MSE\ \% = 100\left(\frac{\sum_i^n (o_i - t_i)^2}{N}\right) \tag{10}$$

where n denotes the number of samples; o_i and t_i are the predictions of the model and corresponding targets, respectively.

The output which is the ADT is the difference between the temperature of the pure water and temperature of the inhibitors mixed with the pure water. Below demonstrates the equation used to calculate ADT [40]:

$$ADT = \frac{1}{n}\sum_{i=1}^{n} \Delta T \tag{11}$$

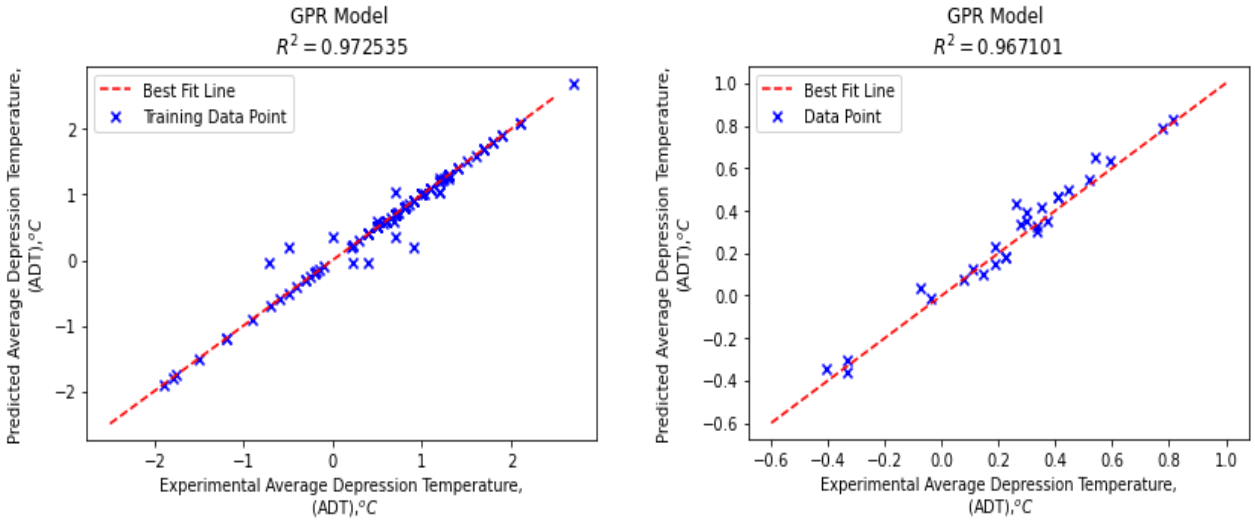
where n is the number of data point, ΔT is the difference between the equilibrium point of temperature in presence of pure water and hydrate inhibitors at a specified pressure, MPa and concentration, wt%.

3. Results and Discussion

Applied different Machine Learning (ML) models such as Least Square Support Vector Machine (LSSVM), Artificial Neural Network (ANN) and Gaussian Process Regression (GPR) to predict the output which is the Average Depression Temperature and inputs are Pressure and Concentration. The data generated from the 140 data points were utilized to plot the Predicted results of ADT versus Experimental results of ADT for each respective ML models. From the 140 data points, 112 data points will be used as training set and remaining 28 data points will be utilized as testing set. The result of training, testing prediction for each ML models in the work are presented.

From the Figure 3, it can be observed that results from the training and testing data to obtain the predicted analysis values of ADT with the experimental values of ADT in terms of °C. This GPR model is constructed with kernel present in it. Kernel is a function that represents feature space and hence, naturally incorporate the similarity measure between data points. Therefore, most used kernel that

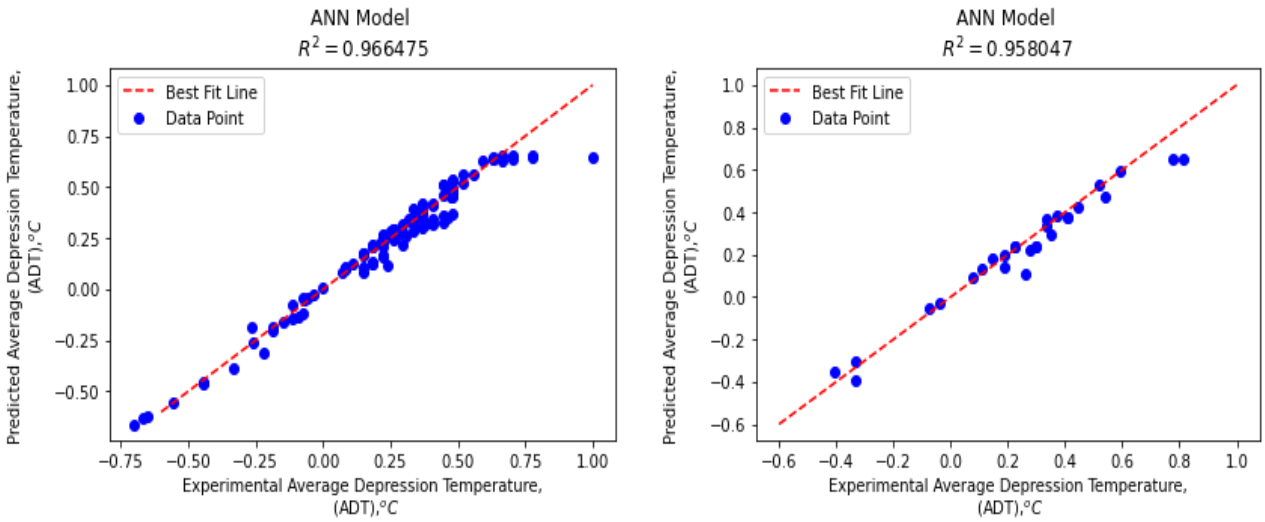
has been implemented in this GPR model is Radial Basis Function (RBF) kernel [31]. The length-scale, λ of the RBF kernel used is 10. This value is embedded to ensure the smoothness of the prediction of the output which is the ADT.



(a) (b)

Fig. 3. GPR model outcomes for (a) training and (b) testing sets

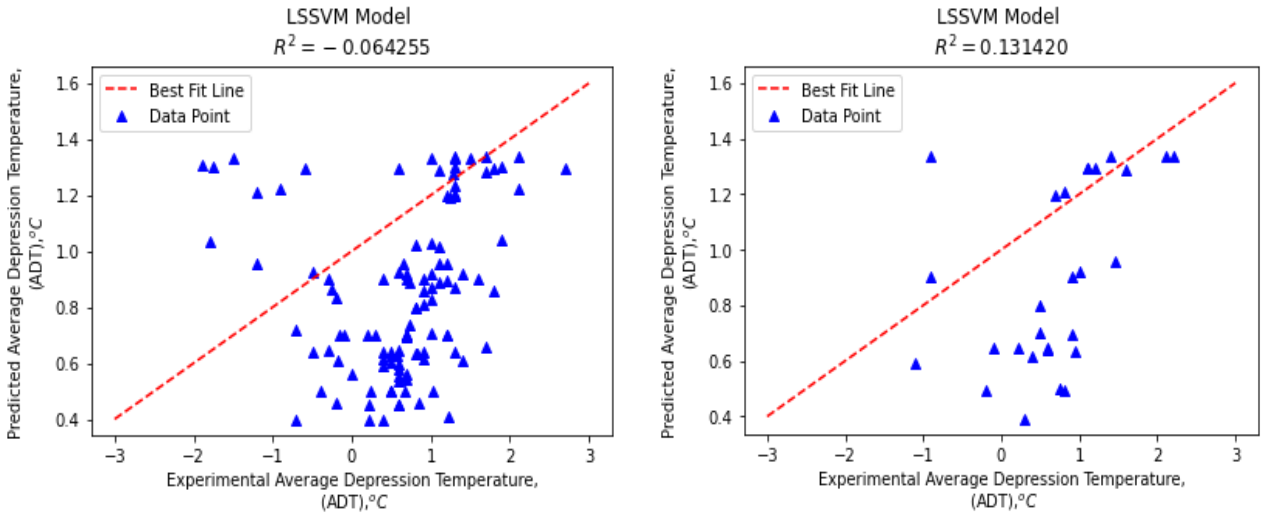
From Figure 4, the results obtained by the predicted ADT versus the experimental ADT gives coefficient of determination for testing and training set approximately 96% and 95% respectively. In the ANN model, the hyperparameter which has been applied is Lbfgs optimizer because due to a smaller number of datasets and gives fast iterations. Lbfgs optimizer employs Quasi-Newton method where the results obtained from this optimizer will converge faster and perform better. The hidden layer size that has been implemented is 6. Nonetheless, this ANN model does gives various local minimum value rather than global minimum value thus more fluctuations of the results tend to occur leading to R^2 and MSE values not to be stable and accurate.



(a) (b)

Fig. 4. Performance of ANN for (a) training and (b) testing sets

From Figure 5, shows the results obtained by the LSSVM model for the training and test set with the value of -0.06% and 0.131%, respectively. Hence, this indicates that the predicted value of ADT does not correspond well to the experimental values of ADT in which variance can be observed as well as number of iterations applied is 6000.This is due to LSSVM model is an embedded with linear programming to solve the regression analysis. With this small dataset, this LSSVM model is prone to overfitting consequently leading to obtaining inaccurate coefficient of determination and higher value of mean squared error.



(a) (b)

Fig. 5. Performance of LSSVM model for (a) training and (b) testing sets

From Table 1, it can be justified that GPR model gives highest R^2 value of 97.25% and 96.71% respectively for training and testing set in comparison to other two models. This shows that GPR model gives higher accuracy in predicting the ADT value depending to the concentration of the inhibitor and the pressure. Mean Square Error (MSE) shows the percentage error of predicted value with the experimental value whereby lower the MSE value, the closer is predicted value to the experimental value. MSE value of GPR for training and testing set gives lowest value of 0.019 and 0.023 respectively compared to ANN and LSSVM model. This signifies that the results of the predicted value of ADT and experimental value of ADT gives low variance with regards to the other ML models leading to lowest prediction error.

Table 1
Error evaluation outcomes for GPR, ANN and LSSVM models

Parameter/Model	GPR		ANN		LSSVM	
	Train	Test	Train	Test	Train	Test
R^2%	97.25	96.71	96.65	95.80	-0.06	0.131
MSE%	0.019	0.023	0.03	0.03	0.733	0.524

4. Conclusion

In this research, the advanced risk management technique in preventing the growth of clathrate hydrate in oil and gas pipelines, known as Machine Learning (ML) models that act as predictive analysis, has been extensively applied. In resolving the growth of gas hydrates, there are several ML models, but Gaussian Process Regression (GPR) is the newest method used in minimizing the growth of hydrates in the natural gas industry. The predictive analysis using GPR will be carried out by

applying the algorithm from the data obtained in terms of pressure, and concentration as the input, while average depression temperature will be the output. To summarize, the ML model that gave the best results in terms of coefficient of determination, R^2 and mean squared error, MSE is Gaussian Procession Regression model in comparison to Artificial Neural Network and Least Square Support Vector Machine models. GPR model gave the best results for test and training data in terms of R^2 which are 97.25% and 96.71% respectively compared to ANN and LSSVM models. MSE value of 0.019 for training set and 0.023 for the testing set obtained is the lowest for GPR model indicating this model gives lowest prediction error of ADT in contrast to other two ML models.

This study is a good example for researchers who want to further understand the correlation between the output which is the ADT and the inputs which are the Pressure and Concentration of the THIs. The researchers will be further understanding the significance of utilizing the ML models to grasp the knowledge of predictive analysis. Nonetheless, it is recommended to obtain more data points before implementing it in this ML model. This is because ML model are data driven analysis where more experimental work needs to be executed to obtain results that will improve and give more accurate predictive analysis for this ML model especially GPR model that needs large data points. Furthermore, to obtain optimized hyperparameter in the GPR model is another recommendation that needs to be addressed. Further study needs to be developed in understanding the hyperparameter where it is configuration that is external to the model and whose value cannot be estimated from data. This hyperparameters presents mostly in all ML models, especially GPR models hyperparameters such as RBF kernel length-scale value needs to be studied and tuned that will lead to obtaining optimized value of the hyperparameter consequently obtaining precise prediction result of the output.

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