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Cancer Detection based on Microarray Data Classification Using Principal Component Analysis and Functional Link Neural Network

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Abstract

Cancer is a deadly disease caused by abnormal growth of tissue cells that are not controlled in the body. In 2018, according to Globocan data, the number of cancer sufferers has increased from the previous years which was 18.1 million people, with a mortality rate of 9.6 million. In recent years, cancer prediction using DNA microarrays data can help medical experts in analyzing whether a person has cancer or not. DNA microarray data have very large and complex gene expression, therefore a dimensional reduction method is needed. Then, the dimension reduction results will be used for classification into types of cancer or not. In this paper, Principal Component Analysis (PCA) is used as a feature extraction to reduce dimension and Functional Link Neural Network as a classifier. Based on the simulation, the average of accuracy using the FLNN and PCA about 76.08%. The purpose of this study is to analyze the effect of PCA dimension reduction and the effect of the Polynomial Order on the classification of microarray data.

***Keywords**:* cancer detection, Microarray data, Functional Link Neural Network, Principal Component Analysis.
Kata Kunci: deteksi kanker, data Microarray, Functional Link Neural Network, Principal Component Analysis.

I. INTRODUCTION

Cancer is a disease caused by the abnormal growth of tissue cells that are not controlled in the body. This abnormal cell growth can damage the normal cells around and in other parts of the body. In 2018, according to Globocan data, the number of cancer sufferers has increased from the previous years which was 18.1 million people, with a mortality rate of 9.6 million people [1]. In general, people with cancer do not feel the initial symptoms of the development of abnormal cells in the body, but only when they have experienced an advanced stage [2].

Along with the times, the use of technology, especially in the field of biotechnology is increasingly high. One example is DNA microarrays, a technology used for medical diagnosis and simultaneous analysis of

gene expression at the same time. Analysis of gene expression is more effective to help medical experts in detecting cancer, rather than using traditional methods to see a symptom or signs [3].

DNA microarrays have very large gene expression and very high complexity [4]. This can affect the accuracy of classification results [5]. Therefore, the solution to overcome this is to use dimensional reduction, which is a process of identifying informative genes that can be used to predict. In a paper entitled "Dimensionality reduction using Principal Component Analysis for cancer detection based on microarray data classification" [3] researched with Leukemia, Ovarian, Central Nervous System, Colon, Lung, Prostate datasets using the PCA method as a feature extraction with SVM and LMBP for classification resulted in an accuracy of 94.98% and 96.07%, respectively. In the Principal Component Analysis method, there is a proportion of variance (PPV) parameter, which is an eigen value taken from the total eigenvalue, the greater the PPV, the greater the eigenvalue and features obtained, and vice versa. In a paper entitled "Deteksi Kanker Berdasarkan Klasifikasi Microarray Data Menggunakan Principal Component Analysis dan Backpropagation Termodifikasi dengan Conjugate Gradient Fletcher Reeves" [6] the resulting PCA+MBP accuracy of 82.15%.

In the classification process, there is a Functional Link Neural Network (FLNN) method, which is a classification of a part of an artificial neural network that has a flat or single layer architecture, so that it is faster in computing (calculation) [7]. In classification, Functional Link Neural Network has several basic functions, one of which is the Legendre Polynomial base function which produces the highest accuracy among others in the study in a paper entitled "Classification of Microarray Data using Functional Link Neural Network" [8]. Legendre Polynomial is a function of differential equations that can change the value of the original input.

Principal Component Analysis is one of the dimension reduction methods that is often used with an average accuracy result above 80%, while the Legendre Polynomial base function is one of the best methods to obtain accuracy than others, but the Functional Link Neural Network base function has a gap with Principal Component Analysis because research has not been too much, so updates with this method are carried out in the classification of cancer detection.

Thus, this research was conducted using the Principal Component Analysis (PCA) method as dimension reduction and Functional Link Neural Network (FLNN) on the basis of Legendre Polynomial for classification, in order to contribute to find out how much influence the reduction of Principal Component Analysis dimensions and the influence of the Polynomial Order parameters on classification. The data that be used for research are Colon Tumors, Ovarian Cancer, and Lung Cancer taken from Kent Ridge Bio-medical dataset [9].

In this introductory chapter, the author explains the background, problem formulation, boundaries, and goals. Then in the related study chapter, the author will discuss related research to the method used. Furthermore, in the system built chapter, the author will discuss the flow classification by the PCA and FLNN methods, and the last in the evaluation chapter, the author will discuss the results of the research that has been done.

II. RELATED WORK

In a paper entitled "Deteksi Kanker Berdasarkan Klasifikasi Microarray Data" [10], The dimensions of DNA microarrays to find informative genes in DNA data can affect the level of accuracy. For this reason, a dimension reduction method is needed, one of which is Principal Component Analysis which is one technique that can improve classification accuracy. Many classification techniques are also applied in DNA microarrays, one of them is Back Propagation Neural Network (BPNN) chosen as a classification method and PCA as a dimension reduction method because both of them have been tested in several previous studies. The results of research conducted on colon, leukemia, ovarian, central nervous, lung cancer and prostate tumors obtained an accuracy of more than 80%. Strengthened in a paper entitled "Cancer detection based on microarray data classification using PCA and modified back propagation" [11], the author implements Principal Component Analysis (PCA) as a dimension reduction and Modified Back Propagation (MBP) as a classifier by comparing

Principal Component Analysis (PCA) and Back Propagation (BP). From the results of research conducted by the author, it is said that the proposed MBP + PCA system is better than BP + PCA. From the results done with colon, ovarian and leukemia data, MBP + PCA accuracy of 96%, 76.92% and 97.14% were obtained respectively.

In a paper entitled "Classification of Microarray Data using Functional Link Neural Network" [8] Functional Link Neural Network has four basic functions, namely; Power Series Polynomial, Trigonometric, Chebyshev Polynomial, and Legendre Polynomial. From the four basic functions, the Legendre Polynomial is the base function that is most suitable to use in classification compared to other base functions. The parameter for evaluating is F1-Measure. In a paper "Deteksi Kanker berdasarkan Klasifikasi Data Microarray menggunakan Functional Link Neural Network dengan Seleksi Fitur Genetic Algorithm" [12] shows that the Genetic Algorithm (GA) as a feature selection and Functional Link Neural Network with Legendre Polynomial base functions for classification with colon tumor and leukemia data obtained an accuracy of 92.3% and 87.5%. While in a paper entitled "Implementation of mutual information and bayes theorem for classification microarray data" [13] shows that the classification system using Bayesian Network and Naïve Bayes produces F1-Score of 91.06% and 88.85%.

III. RESEARCH METHOD

A. *System Design*

At this stage of the research, the System Design workflows is built to classify cancer data to find out whether a person has cancer or not as follows;

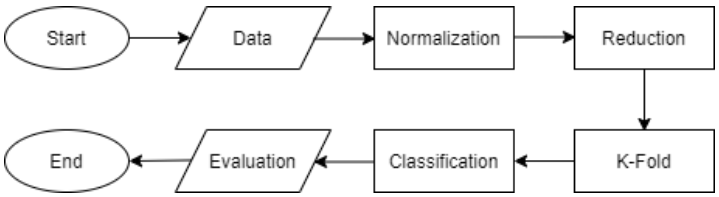

Fig 1. System Design

Cancer data input, then the normalization process is carried out to get the range 0-1. After that, the process of dimension reduction is carried out to retrieve attributes that are considered more important. After that, the K-Fold Cross Validation process for training and testing data is carried out alternately, then the classification process is performed using Functional Link Neural Network, after which the Evaluation process is carried out to find out how well the system has been built.

B. *Dataset*

The data used for this study were obtained from Kent Ridge Biomedical that are Colon Tumor, Ovarian Cancer and Lung Cancer data. The data has often been used for research into DNA microarrays classification. The data details are written as follows:

TABLE 1.
DATA CANCER [9]

Data	Number of Features	Number of Data	Number of Class	Sample
Colon Tumor	2000	62	2	62(22 Positive, 40 Negative)
Ovarian Cancer	15154	253	2	253(91 Normal, 162 Cancer)
Lung Cancer	12533	181	2	I81(31 Mesothelioma, 150 ADCA)

C. *Preprocessing Data*

In the data preprocessing stage, there are 2 processes, namely the normalization process and data splitting. The normalization process is used so that the value of each feature is in the range of 0 to 1. Normalization techniques are used with the following equation;

$$Normalization(N) = \frac{N - N_{min}}{N_{max} - N_{min}} \quad (1)$$

Where;
N: microarray data that has not been normalized.
N_max: the largest data in the microarray data that has not been normalized.
N_min: the smallest data in the microarray data that has not been normalized.
Then, the process of splitting the data against the dataset uses the K-fold technique, where the data will be divided into 2 data namely training data and testing data. This stage is carried out after the process of dimension reduction.

D. *Dimension Reduction (PCA)*

In the Principal Component Analysis (PCA) [14] process, data dimension reduction is done by "combining" or "projecting" the core of each feature by forming a new subset of features so that the feature dimensions become less, therefore PCA is classified into the dimension reduction of extraction features. Thus, using PCA dimension reduction can help the classification process with faster and more efficient computing time. For the steps of the PCA dimension reduction algorithm in a paper entitled "Colorectal Cancer Classification using PCA and Fisherface Feature Extraction Data from Pathology Microscopic Image" [15], as follows;

1) Calculating averages for each dimension using equations;

$$\bar{A} = \frac{1}{n} \sum_{i=1}^{n} A_i \quad (2)$$

Where;
n = the number of samples or the amount of observation data
A_i = observation data

2) Calculating the covariance matrix with equations;

$$k_x = \sum_{i=1}^{n} (A_i - \bar{A})(A_i - \bar{A})^T \quad (3)$$

Where;
n = the number of samples or the amount of observation data
A_i = observation data
$\bar{A}$ = average

3) Calculating eigen vectors and eigen values from a covariance matrix with equation;

$$k_A V_m = \lambda_m V_m \quad (4)$$

Where;

v_m = *eigen* vectors
λ_m = *eigen* values
k_A = covariance matrix
m = number of dimensions

4) Sort the eigen vectors (descending)

5) Take the largest eigen value.

6) Next is data transformation.

$$Y = V^T \text{ x } (A_i - \bar{A}) \quad (5)$$

Where;

V = eigen vectors
A_i = observation data
$\bar{A}$ = average

E. *K-Fold*

K-Fold is a process of sharing training and testing data. The amount of training and testing data depends on the determination of partition K. In this study, the K used is 5, meaning that the data is partitioned by 5 data, 4 for data training and 1 for data testing. In the process of K-Fold training data and testing data are carried out alternately and the classification results taken are the average results, the following is an overview of K-Fold;

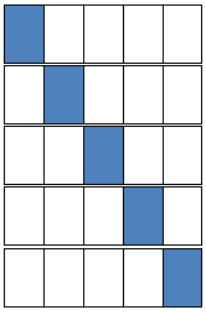

Fig 2. K-Fold

F. *Classification (FLNN)*

Furthermore, the core process of this study is to classify DNA microarray data, whether included in the cancer class or not by using the Functional Link Neural Network (FLNN) algorithm. Functional Link Neural Network (FLNN) is part of an artificial neural network. In the artificial neural network classification model, using FLNN classification is more efficient than using Multi Neural Network (MNN). This is because the Functional Link Neural Network classification uses flat architecture or a single layer, so it is not like a Multi Neural Network that performs computations (calculations) on its hidden layer [7]. On the Functional Link Neural Network (FLNN), there are a number of basic functions that can be used. One of them is the Legendre Polynomial base function which is the best base function compared to the others [8]. FLNN algorithm is basically the same as Artificial Neural Network (ANN) which uses a single layer, only the difference in FLNN is using a base function whose result will be an input vector to ANN. For the steps of the Functional Link Neural Network classification algorithm in a paper entitled "Functional link neural network approach to solve structural system identification problems" [7], as follows;

1) The input value X is expanded by the basic function of the Legendre Polynomial with the following equation;

$$L_{n+1} = \frac{1}{n+1}\,[(2n + 1)\, xL_n - nL_{n-1}(x)] \quad (6)$$

Where;

L_n = Legendre Polynomial
n+1 = order polynomial
x = original data input value

2) After obtaining the value from the polynomial legend, the value becomes a new input value which will be processed to "Linear Amount" with the following equation;

$$S = \sum_{i=1}^{N} w_i L_i(x) + b \quad (7)$$

Where;

S = linear sum value

w_i = weight value

b = bias value

N = amount of data (features) in one object

3) Then the linear sum value is entered into the activation function process using the sigmoid function, with the following equation;

$$f(S) = \frac{1-\exp(S)}{1+\exp(S)} \quad (8)$$

Where;

S = linear sum value

4) If the sigmoid value does not meet the threshold, then it can be said that the value is an error value. To minimize the error again, the following equation is used;

$$E = \frac{1}{2}\,[d_i - y_i]^2 = \frac{1}{2}\,{e_i}^2 \quad (9)$$

Where;

d_i = prediction value target
y_i = prediction value results
e_i = prediction value

5) After the above process is finished, the last process is to update the weight value with the following equation;

$$w_i(baru) = w_i(lama) + \Delta w_i \quad (10)$$

$$\Delta w_i = [\, -\eta \frac{\partial E}{\partial w_i}\,]$$

$$= [\, -\eta\,(d_i - y_i)(1 - {y_i}^2)\, L_i(x)]$$

Where;

Δw_i = change in weights

η = Learning parameter to reduce *error*

The FLNN picture is as follows;

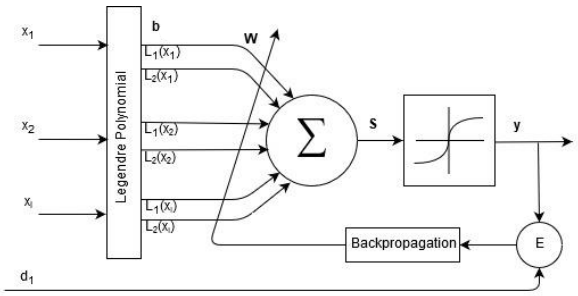

Fig 3. FLNN [7]

G. Testing Scenarios

In this study, two test scenarios were conducted on 3 cancer datasets namely Colon, Ovarian, and Lung. The first scenario, the method of reducing the dimensions of Principal Component Analysis and Order 1 Functional Link Neural Network Classification or can also be said as ANN classification in order to determine the effect of the Proportion of Variance (PPV) parameter on the Accuracy results. The second scenario, PCA and FLNN methods to determine the effect of the Polynomial Order on performance. The results of each scenario used can be seen below. The limits used in this research are PPV 65% - 95% and order 1 – 4.

H. *Performance Evaluation*

In the last stage, the authors conducted an evaluation to see how well the system had been built, a confusion matrix table was used as a basis for determining actual data and predict data. The following is a confusion matrix table;

TABLE 2.
CONFUSION MATRIX

Actual / Predicted	Predicted Positive	Predicted Negative
Actual Positive	True Positive (TP)	False Negative (FN)
Actual Negative	False Positive (FP)	True Negative (TN)

From Table 2, TP (True Positive) is a system that successfully produces cancer output according to actual data, TN (True Negative) is a system that successfully produces non-cancerous output according to actual data, FP (False Positive) is a system that fails to produce non-cancerous output, FN (False Negative) is a system that fails to produce cancer output.

1) Precision: Precision is the ratio of true positive predictions compared to all results predicted positively by the system. The precision equation is as follows;

$$\text{Precision} = \frac{TP}{TP + FP} \quad (11)$$

2) Recall: Recall is the ratio of true positive predictions compared to all results that are true positive. Recall equations as follows;

$$\text{Recall} = \frac{TP}{TP + FN} \quad (12)$$

3) F1-Score: F1-Score is a comparison of average precision and recall. F1-Score equation as follows;

$$\text{F1-Score} = 2 * \frac{(Recall * Precision)}{(Recall + Precision)} \quad (13)$$

4) Accuracy: Accuracy is the ratio of true positive and negative predictions compared to all data. The accuracy equation is as follows.

$$\text{Accuracy} = \frac{(TP + TN)}{(TP + TN + FP + FN)} \quad (14)$$

IV. RESULTS AND DISCUSSION

A. *Effect of PPV on Accuracy*

PPV is a proportion of variance parameter that represents the boundary of the attribute to be chosen, therefore the value of PPV selected is only in the range 65-95. In Figures 4, 5, and 6 show the results of Accuracy using various PPV values for each microarray data as follows;

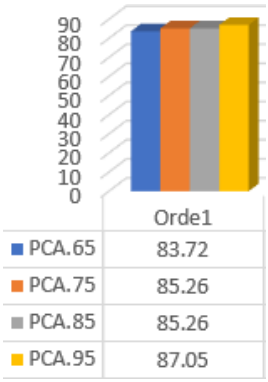

Fig 4. Colon Tumor

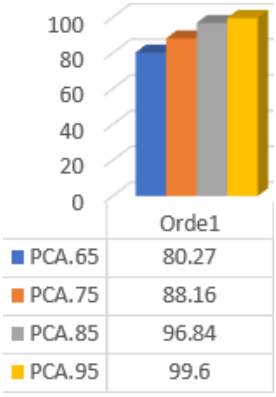

Fig 5. Ovarian

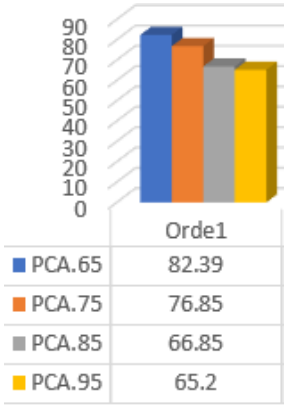

Fig 6. Lung

TABLE 3.
ACCURACY PPV

PPV	Colon Tumor	Ovarian	Lung	Average
65	83.72	80.27	82.39	82.13
75	85.26	88.16	76.85	83.42
85	85.26	96.84	66.85	82.98
95	87.05	99.6	65.2	83.95
Average	85.32	91.22	72.82	83.12

At the dimension reduction stage, feature extraction is performed to reduce very high dimensional features using the Principal Component Analysis (PCA) method. PCA has the proportion of variance (PPV) parameter, which is a feature extraction process carried out by choosing how much PPV to use. PPV itself is an eigenvalue taken from the total overall eigenvalue, the greater the PPV, the greater the eigenvalue and features obtained, and vice versa.

Eigenvalues represent the uniqueness of each feature, the greater the PPV, the smaller the correlation of other features and vice versa. In the PPV parameters experiment in table 3. Accuracy PPV above, the highest Accuracy results were obtained at PPV 95% with an average accuracy of 83.95%, and the highest accuracy results in Ovarian data with an average of 91.22%.

Judging from the average accuracy, the greater the PPV used, the greater the accuracy produced, but this is not a specific guideline that the greater the PPV, the greater the accuracy produced. In Colon Tumor data, there are varying accuracy results and also strengthened in Lung data where the accuracy results always decrease with the amount of PPV used. This makes it possible to still have a correlation between one feature with another feature because the features obtained from PPV (large) are many.

B. *Effect of order polynomial on performance*

In figure 7, 8, 9, 10, 11, and 12 we can see the accuracy and F1-Score by using various order in the FLNN classification for each microarray data;

1) F1-Score

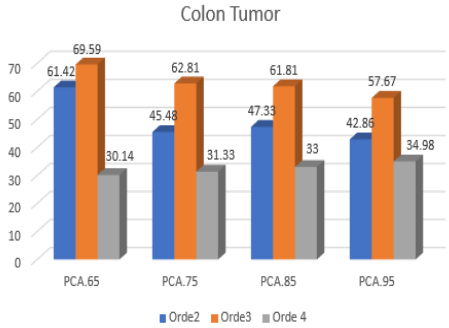

Fig 7. F1-Score for various order

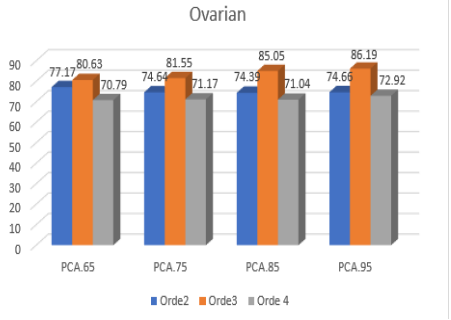

Fig 8. F1-Score for various order

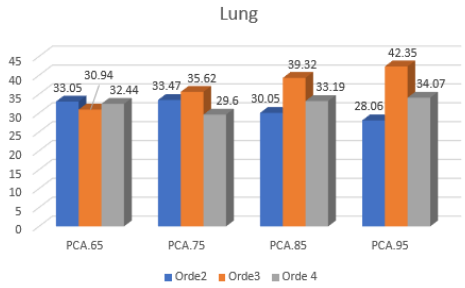

Fig 8. F1-Score for various order

2) Accuracy

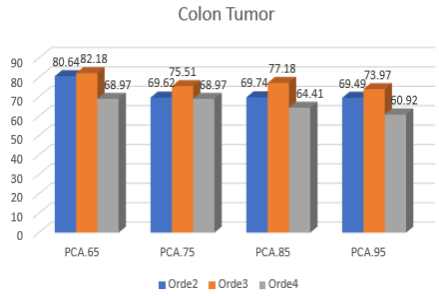

Fig 9. Accuracy for various order

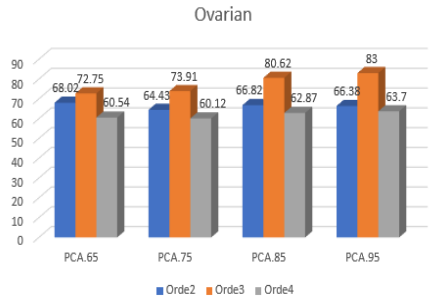

Fig 10. Accuracy for various order

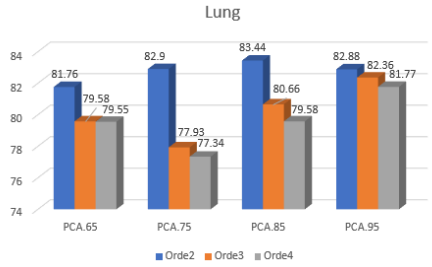

Fig 11. Accuracy for various order

TABLE 4.
EXECUTION TIME

Order	Colon Tumor	Ovarian	Lung
Order 1	77s	144s	112s
Order 2	80s	145s	128s
Order 3	86s	157s	150s
Order 4	99s	196s	230s

TABLE 5.
AVERAGE PERFORMANCE IN EACH DATA

Performance	Order	Colon Tumor	Ovarian	Lung	Average
F1-Score	1	79.88	92.91	37.75	
	2	49.27	75.22	31.16	
	3	62.97	83.36	37.06	
	4	32.36	71.48	32.33	
	Average	56.12	80.74	34.47	57.11
Accuracy	1	85.32	91.22	72.82	
	2	72.37	66.41	82.75	
	3	77.21	77.57	80.13	
	4	65.82	61.81	79.56	
	Average	75.18	74.25	78.82	76.08

TABLE 6.
AVERAGE CONFUSION MATRIX IN EACH DATA

Order 1	Colon	Ovarian	Lung	Order 2	Colon	Ovarian	Lung
Ave. TP	3.75	29.85	3.65	Ave. TP	1.85	26.1	1.7
Ave. TN	6.85	16.3	22.7	Ave. TN	7.1	7.75	28.25
Ave. FP	1.15	1.9	7.3	Ave. FP	1.05	10.45	1.75
Ave. FN	0.65	2.55	2.55	Ave. FN	2.75	6.8	4.5
Class	P:22	P:162	P:31	Class	P:22	P:162	P:31
	N:40	N:91	N:150		N:40	N:91	N:150

The principle of performance in the Polynomial Order is to add features to each data record, the greater the order used, the more features will be added to the data record, so this will add time when the running classification process is seen in Table 4 Execution time. In the experiments that have been carried out above, the results show that the greater polynomial order used can not guarantee an increase in performance results in the classification, because of the dataset used the class difference between Positive and Negative relative in a relatively large range with a ratio of 36:64, so that the False Positive and False Negative obtained are still quite large, but things are different from the Lung data condition which has increased and is relatively convergent in each orders, this is due to more large data differences between classes (positive and negative) by comparison 18:82, therefore the False Positive and False Negative that are obtained every order are relatively small.

The system that has been built can be seen in Table 6 that the system produces predictions of True Negative values that are greater than the results of True Positive, this is due to the dataset used by more classes that are Negative compared to Positive so that the difference in the average results of performance between accuracy and F1-Score show significant differences in results. The average difference between the three classes is 30:70, therefore the performance used in this study is Accuracy. The advantage of the PCA and FLNN methods is that the computation time is quite fast and at each order, the increase does not require a significant increase in optimization time.

V. CONCLUSION

After conducting research on data on Colon Tumors, Ovarian and Lung. It can be concluded that the PPV value used will affect the accuracy obtained, but the greater value of PPV used does not guarantee to improve accuracy results. The best PPV value is at 95% of the three data with an accuracy of 83.95% and from all experiments on some PPV values, Accuracy results reach above 80% with an average of 83.12%. The effect of polynomial order on performance using accuracy performance is better than using F1-Score, the average result obtained is 76.08%. Polynomial order in Colon Tumor and Ovarian data can not improve the accuracy results, but in the Lung data it can improve the accuracy results, so it can be said that using the FLNN method can not improve the accuracy of the ANN method. Therefore, for future research, it can be done with a different dimension reduction, because in research conducted by Ramadhani [12] that by using the Functional Link Neural Network method the average performance is 89.9%.

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