

Gene Ontology Analysis of 3D Microarray Gene Expression Data using Hybrid PSO Optimization

N. Narmadha, R. Rathipriya



Abstract: At present, triclustering is the well known data mining technique for analysis of 3D gene expression data (GST). Triclustering is a simultaneously clustering of subset of Gene (G), subset of Sample (S), and over a subset of Time point (T). Triclustering approach identifies a coherent pattern in the 3D gene expression data using Mean Correlation Value (MCV). In this chapter, Hybrid PSO based algorithm is developed for triclustering of 3D gene expression data. This algorithm can effectively find the coherent pattern with high volume of a tricluster. The experimental study is conducted on yeast cycle dataset to study the biological significance of the coherent tricluster using gene ontology tool.

Ontology, Hybrid Particle Keywords: Gene Optimization (Hybrid PSO), Gene Expression Data, Triclustering, Yeast Cell Cycle data.

I. INTRODUCTION

The 3D time series gene expression data analysis, plays a vital role in identify the most valuable genes along the Gene-Sample-Time (GST) or Gene-Condition-Time (GCT) dimension (Ziv Bar-Joseph, 2002). The analysis of microarray of 3D data represents a computational challenge due to the characteristic of these data. A large number of clustering approaches are proposed for the analysis of gene expression by many literatures. Triclustering techniques are the most recent simultaneous clustering of the 3D microarray data. Tricluster is a subset of genes that have similar patterns over a subset of condition during subset of time points.

Triclustering is treated as one of the optimization problems. Its main objective is to find the quality tricluster with low mean squared residue and high volume. So Partcile Swarm Optimization (PSO) is perfectly suitable for solving this problem.PSO is the optimization approach and it is population based algorithm. The whole populations are maintained throughout the procedure. The potential solution of PSO is said to be particles and every one of the particles is randomized velocity. Each particle is to attain the optimal solution in the solution space. There are two main features there are 1) Convergence Speed and 2) Relative Simplicity these features are suitable for solving the optimization

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problem. The main aim of this work is to find the quality of a tricluster using Hybrid PSO optimization.

This chapter discusses the triclustering of 3D microarray data using Particle Swarm Optimization (Hybrid PSO) to find the maximum optimal tricluster with high MCV value and high volume. Finally, the empricial study is conducted on a Yeast cell cycle dataset to validate the effectiveness of the proposed algorithm. The biological and statistical significance of the result is evaluated using Gene Ontology.

The rest of chapter is organized as follows section II describes the literature review for this research work. Section III discusses the methods and materials. Section IV elaborates the proposed work. Results and discussions need for the studies are shown in section V. Section VI concludes this research work with possible future enhancement.

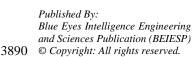
II. LITERATURE REVIEW

This section provides an overview of related works in the field of 3D microarray gene expression data analysis, in particular, the work related to the Particle Swarm Optimization (PSO).

Table- I: List of Existing Evaluation Measure for **Clustering and Biclustering**

C	A (I X7.	T 1	D
S.	Author Name	Techni	Description
No 1	D.W. van der	que	PSO is used to find the centroids
1		Cluster	
	Merwe, A.P.	ing	for user specified number of
	Engelbrecht		clusters
2.	(2004)	C1 4	DGO : 11 C W
2	Rashmi	Cluster	PSO is used before K means to
	Chouhan , Anuradha	ing	find the optimal point. This
			optimal point is taken as a initial cluster for K means to find the
	Purohit (2018)		final cluster
3	Nuria Gómez	Cluster	
3	Blas. Octavio		PSO is to find the user specified
	López Tolic	ing	Cluster.
	(2016)		
4	Jayshree	Cluster	Clustering of multidimensional
· ·	Ghorpade-Aher	ing	data using PSO to reduce the
	and Vishakha	1115	minimum
	A. Metre (2014)		
5	Nadjet Kamel,	Cluster	To cluster web document using
	Imane Ouchen,	ing	PSO and K- means
	and Karim Baali	O	
	(2014)		
6	R.Rathipriya,	Biclust	To find quality of bicluster in
	K.Thangavel,	ering	web usage data
	J.Bagyamani		
	(2011)		
7	R.Rathipriya,	Biclust	to identify the coherent browsing
	K.Thangavel,	ering	pattern using K-Means, Greedy
	J.Bagyamani		Search Procedure and Genetic
	(2011)		Algorithm

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8	Shyama Das, S. M.(2010)	Biclust ering	To find global optimal solution using Particle Swarm Optimization
9	Deepthi P S (2015)	Biclust ering	PSO algorithm gives the good quality of cluster with an accuracy of 70-80 %
`10	Lopamudra Dey (2014)	Biclust ering	The gene expression data clustering K-means, FCM and hierarchical techniques are used for clustering microarray data. But PSO based K-means gives better performance for clustering microarray data
11	(Baiyi Xie, 2007)	Biclust ering	PSO with GA is used to solve the biclustering problem and it provides high accuracy
12	(K.Thangavel, 2011)	Biclust ering	Particle Swarm Optimization (PSO) is used for the best subset generation and for evaluating the subset to uses k-means as wrapper algorithm.

This literature study clearly depicts that PSO or Hybrid PSO based approaches mainly used for one and two dimensional clustering of GST i.e. 3D microarray data. Moreover, there are many studies which highlights the benefits of Hybrid PSO over the evolutionary algorithm such as GA for gene based clustering/ biclustering is shown in table 1. Hence therefore, Hybrid PSO based triclustering approach is proposed in this work for 3D gene expression data to extract large volume tricluster with high coherent quality.

III. METHODS AND MATERIALS

This section provides the methods and materials needed for this research work

A. Tricluster

Three dimensional (3D) dataset A with r (genes) is denoted as G, c (columns) is denoted as S and t (time point) is denoted as T; that is Tricluster B = (G,S,T) is the subset of original dataset, where I is the subset of G ($I \subseteq G$), J is subset of S ($J \subseteq G$) S) and K is subset of T ($K\subseteq T$)

B. GST Microarray data /Triclustering Definition

In GST Microarray data / Tricluster is represented by $T(g \subseteq$ $G, s \subseteq S, t \subseteq T$

Where

- $G = \{g1, g2, g3...gn\}$ be a set of 'n' genes
- $S = \{s1, s2, s3, ..., sm\}$ be a set of 'm' biological samples
- $T = \{t1,t2,t3....tl\}$ be a set of '1' time points
- A three dimensional (3D) microarray dataset is a real-valued n*m*l matrix
- D = G*S*T whose three dimensions correspond to genes, samples and time points whereas simultaneously clustering of GST is said to be GST Microarray data or Triclustering

C. Encoding of Tricluster

First, two way K-means clustering algorithm is applied along the two dimensions of A(G, S, T) to generate kg and ks cluster and combined these clusters to get kg*ks initial bicluster for every time point 't' in T.

The biclusters generated from the seed generation phase are used to create an initial tricluster population (npop) for Hybrid PSO. First, to select the top 'npop' bicluster based on their Average Correlation Value from the entire set of biclusters. Secondly, to create initial tricluster population, generate random time point of size nb*nT and add these points with the 'nb' biclusters. Figure 2 shows single binary-encoded tricluster A(nG+nS+nT) as binary string of length nG+nS+nT.

- 1	,,,,,,		Subset					~				
gl	g 2		gnG-1	gn	sl	s2		snS	tl	t2		tn'T'
	8832			9			24					

D. Mean Correlation Value for Tricluster

Mean Correlation Value of a Tricluster (MCV) is defined as:

$$\sum_{m}\sum_{n}(A_{mn}-\bar{A})(B_{mn}-\bar{B}) / \left(\sum_{m}\sum_{n}(A_{mn}-\bar{A})^{2}\right)\left(\sum_{m}\sum_{n}(B_{mn}-\bar{B})^{2}\right)$$

$$\text{Where } \bar{A} = \frac{\sum_{m}\sum_{n}(A_{mn})}{m*n}, \bar{B} = \frac{\sum_{m}\sum_{n}(B_{mn})}{m*n}$$

Equation 1 shows the Mean Correlation Value (MCV) of a tricluster. The range of MCV is [0,1]. Value close to '1' signifies high correlated tricluster otherwise low or null correlated tricluster. Therefore, MCV based fitness is designed to extract the optimal tricluster from GST gene expression data.

E. Fitness Function

The main objective of this work is to discover high volume triclusters with high MCV from GST dataset. The following fitness function F (I, J, K) is used to extract optimal tricluster is shown in equation 2.

Fig 2. Encoded tricluster of length nG+nS+nT icluster
$$F(I, J, K) = \begin{cases} |I| * |J| * |K|, \text{if MCV}(\text{Tricluster}) \ge \delta \\ 0, & \text{Otherwise} \end{cases}$$
or (MCV) is defined as:

where |I|, |J|, |K| are number of rows, columns and the time points of Tricluster and MCV threshold '5' which range from 0 to 1. In this study, δ is set as 0.91 to 0.95.

F. Particle Swarm Optimization (PSO)

Particle swarm optimization (PSO) is an optimization technique. It's a population-based stochastic algorithm inspired by social behaviour of fish schooling and bird flocking developed by Dr Eberhart and Dr Kennedy in 1995. PSO shares various similarities with an evolutionary computation technique such as Genetic Algorithm (GA). PSO is initialized with random population solutions and updating generations to search for optima. In GA evolution operators like crossover and mutation are used. But in PSO there are no evolution operators. In PSO by following current optimum particles it flies through the problem space to attain the potential solutions is called as particles.





For each particle to track its coordinates in the problem space and it checks whether they are associated with the best solution (fitness). The steps in PSO each time changing the velocity for accelerating then each particle moves toward its pbest and lbest. Random numbers are generated for acceleration toward pbest and lbest locations. In PSO the fitness is also be stored this value is said to be pbest. Then to find the other best value to track the particle swarm optimizer and check whether any particle is the neighbour of the particle, this location of the particle is said to lbest. In that, the entire particle takes all the population as its topological neighbours and the best value is said to be global best then it is called gbest. When compared to GA, PSO is easy to implement and to adjust the few parameters by researchers. PSO is applied successfully in many areas such as Function Optimization (FO), Artificial Neural Network (ANN), Fuzzy System Control (FSC) and others area like Genetic Algorithm (GA) can be applied.

G. Hybrid PSO (K -Means + PSO)

There are two phases in Hybrid PSO. They are:

1. Seed Generation

Algorithm 1 mentions the step by step procedure for the seed generation phase using greedy approach. The output of this algorithm is treated as initial population or particle for Hybrid PSO.

2. Optimal Coherent Tricluster

Algorithm 2 depicts the optimal coherent triclustering approach using Hybrid PSO. Its aim is to extract the high volume coherent tricluster.

H. Parameters of Hybrid PSO Algorithm

The parameter settings needed for this research work is in table 2. It tabulates the number of population, fitness value, number of gene id in optimal tricluster, threshold value, mean correlation of the population, inertia weight, mean volume of the population, learning factors and range of velocity etc.

Table II: The parameter setup of Hybrid PSO algorithm

Parameters	Values
No. of Population	24
Fitness Values	1
No. of Gene Id in Optimal Tricluster	7744
Threshold	0.910.95
Mean Correlation of the population	1
Inertia Weight	0.7-0.9
Mean volume of the population	46331
Learning Factor (c1 & c2)	2
Range of Velocity[min to max]	-20 to 20

IV. PROPOSED WORK

This section elaborates the proposed work and discusses the application of hybrid Hybrid PSO algorithm for triclustering of gene expression data.

1	Algorithm 1: Seed Formation using Greedy Approach	
Input : In	nitialization of (nG+nS)	

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Output: Gene Enlargement and Refined tricluster

Step 1: Compute k_g gene cluster and k_s sample cluster from (nG+nS)

Step 2: Compute k_g and k_s clusters to form $k_g * k_s$ biclusters called genes.

Step 3: For each gene

i) Call gene Enlargement (gene (G', S', T'))

ii) Call gene Refinement (gene (G', S', T'))

Step 4: Return the Gene Enlargement and Refined tricluster Step 5:

// Sub functions of Gene Enlargement and Refined tricluster

Call gene Enlargement (gene (G', S', T'))

Step 1: Set of genes 'g' not in G'

Step 2: Set of samples 's' not in S'

Step 3: Set of time point 't' not in T'

Step 4: For each node g/s/t

If MCV (union (gene, (g/s/t)))> MCV (gene (G,S,T)) then

1. Add g/s/t to gene (G,S,T)

2. End (if)

End (for)

Step 5: Return Enlarged gene set

Call gene Refinement (gene (G',S', T'))

Step 1: For each node g/s/t in Enlarged gene

Remove node g/s/t in Enlarged gene

G"/S"/T' be set of rows /columns/timepoint in G'/S'/T' but not contained g/s/t

If MCV Enlarged gene (G",S", T")> MCV (Enlarged gene (G'/S'/T'))

Update G'/S'/T'

End (if)

End (for)

Step 2: Return refined gene set G", and A(G",S',T') as refined tricluster.



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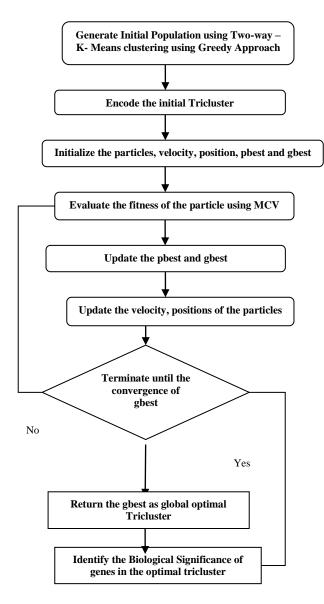


Fig 3. An overview of Hybrid PSO based Triclustering

Table III: Effect of inertia weight on global volume of tricluster (Gbest) in Hybrid PSO

Particle Size	Inertia Weight	Gbest volume	Gbest MCV
24	0.2	45808	0.9503
	0.3	45808	0.9503
	0.4	45808	0.9503

The table 3 shows the experimental results of Hybrid PSO Triclustering method with the different inertia weight from 0.2 to 0.4. It has revealed that there is no change in the global volume of optimal tricluster when inertia weight falls between 0.2 and 0.4. The Volume and MCV of this optimal tricluster is 45808 and 0.9503 respectively.

Table IV: Effect of inertia weight on global volume of tricluster (Gbest) in Hybrid PSO

Particle Size	Inertia Weight	Gbest volume	Gbest MCV
24	0.7	46928	0.9515
	0.8	46928	0.9515
	0.9	46928	0.9515

Similarly, the table 4 shows the experimental results of Hybrid PSO Triclustering method with the different inertia weight from 0.7 to 0.9. It has observed that there is no change in the global volume of optimal tricluster when inertia weight falls between 0.7 and 0.9. The Volume and MCV of this optimal tricluster is 46928 and 0.9515 respectively. But the volume and MCV of the optimal tricluster are increased significantly. It means that upper range of inertia weight extracts the higher volume of tricluster.

From the above tables 3 and 4, it has evidented that lower range inertia weight favors local search whereas upper range inertia weight favors global search. Hence for this reason, higher inertia weight identifies the large volume tricluster with high coherent pattern.

Table V: Characteristics of Optimal Coherent **Tricluster**

Characteristics	gpopulation	rpopulation
MCV	0.9515	0.900
Volume	46928	21
No.of Gene	8828	50
No.of Sample	7	16
No.of Time point	21	6
Gene Coverage %	99.95 %	74 %
Sample Coverage %	77.78%	93.75%
Time point Coverage %	87.5%	67%

The number of genes, samples and time point in the optimal tricluster are shown in table 5. Similarly gene coverage, sample coverage and time point coverage for the same is calculated using equations 3, 4, 5 is given below and their values are given in this table. Thus, the optimal tricluster for gpopulation covers the 99.95 % of genes from gene set G, 74 % of samples from sample set S and 77.78% of time points from time set T. But, the optimal tricluster for rpopulation covers 74% of genes from gene set G, 93.75 % of samples from sample set S and 67 % of time points from time set T respectively. The study of the biological significance of these genes will be shown in the following sections

$$Gene\ coverge = \frac{No.\ of\ genes\ extracted}{Total\ no.\ genes} * 100$$

$$Sample\ coverge = \frac{\frac{No.of\ samples\ extracted}{Total\ no.Sample}}{Total\ no.Sample} * 100$$

$$Time\ point\ coverge = \frac{\frac{No.of\ time\ points\ extracted}{Total\ no.\ time\ points}}{Total\ no.\ time\ points} * 100$$

Algorithm 2: Optimal Coherent Triclustering (OCT) using **Hybrid PSO** Input: 3D Matrix Output: Highly Correlated tricluster // Initial Tricluster Formation Step 1: Perform Two-way K-means clustering on Microarray data to create initial tricluster Step 2: Initialize the velocity and position 'x' of each particle Step 3: Set initial position as pbest and maximum of pbest is set as gbest Step 4: Repeat For each particle in the population current fitness = fitness (particle) if current fitness > fitness (pbest (particle)) Update pbest with position of current particle end (if) end(if) Update gbest Update velocity equation using this $v_n^{t+1} = Iw * v_n^t + l_1 * ran_1 * (Pbest_n)$ Update position using this equation $s(v_{ij}) = \frac{1}{1+e^{-v_{ij}}}$ If(rand < s(vi,j)) then xi,j = 1; else xi,j =0 Until stopping criteria is met Step 5: Return gbest as global best optimal tricluster

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V. RESULTS AND DISCUSSION

This section shows the graphical representation for the Biological Significant of CDC15 Experiment for Yeast Cell Cycle data. Thus the dataset downloaded using the link (http://genome-www.stanford.edu/cellcycle/) it is the yeast cell cycle analysis projects are publicly available for the researchers. An experimental study is conducted with the CDC15 Data with 8832 number of genes, 9 number of samples and the 24 number of time point. There are three gene ontology annotation is processed the gene expression data are shown in figure 4.

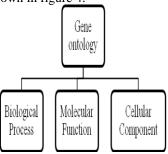


Fig 4. Gene Ontology Annotation

The experimental study is conducted to CDC15 dataset is a microarray gene expression data with https://www.yeastgenome.org/goTermFinder. Using this link biological process, molecular function and the cellular component are evaluated. The experimental study is tested and conducted on CDC15 experiment using Hybrid PSO algorithm. Table 5 shows the Hybrid PSO Algorithm and the characteristics of optimal tricluster such as threshold value, number of genes, number of samples, number of time points, volume and optimal correlated tricluster value are given in table 6 for different threshold value. Eventhough, threshold value varies from 0.91 to 0.95 the proposed algorithm identifies the same tricluster. This is because, the optimal tricluster of the CDC15 dataset is the only one tricluster with larger volume which satisfies the given tricluster function. The threshold values beyond 0.96 the Hybrid PSO algorithm not able to identify any tricluster.

Table VI: Hybrid PSO algorithm and its parameter for **CDC15 Experiment**

CDC13 Experiment							
Optimal Tricluster	Threshold value	No. of Genes	No. of Samples	No. of Time Points	Volume	Optimal Correlated Tricluster Value	
Optimal Tricluster	0.91	419	7	16	46928	0.9515	
Optimal Tricluster 2	0.92	419	7	16	46928	0.9515	
Optimal Tricluster 3	0.93	419	7	16	46928	0.9515	
Optimal Tricluster 4	0.94	419	7	16	46928	0.9515	
Optimal Tricluster 5	0.95	419	7	16	46928	0.9515	

A. Biological Process

The biological process is evaluated using gene ontology tool. This tool helps to discover the number of similar genes in the list. From the input list, 6126 genes are either identified or unidentified but not clear. Unidentified shows the annotation providers are still included in the statistics. Also, 1026 duplicates were removed from the input list. The total

number of genes used to calculate the background distribution of Gene Ontology (GO) terms is 7166. Displaying 341 terms out of a total of 4268 found. Thus the Biological Process networks for CDC15 dataset is shown in figure 5.

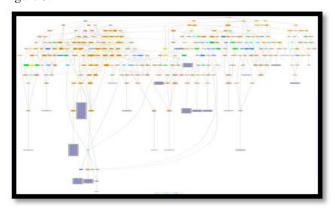


Figure 5: Biological Process networks for CDC15 dataset using Gene Ontology

The gene ontology tool not only displays the network and similar gene in the list. It also helps to identify the standard name, systematic name, SGD ID, description of the name with the physical interaction and genetic interaction for biological process. Here all this kind of details is shown in

Table VII: Technical Names and terms for Biological process with their interaction

Standard Name	Systematic Name	SGD ID	Name Descripti on	Physical Interaction	Genetic Interaction				
				Affinity Capture-MS: 377	Dosage Growth Defect: 2				
				 Affinity Capture -RNA: 6 	 Dosage Lethality: 6 				
				Affinity Capture-Western: 87	• Dosage Rescue: 15				
				 Biochemical Activity: 48 	 Negative Genetic: 265 				
	CN5 ¹ YGR252W SGD5000003484	General Control	Co-crystal Structure: 2	• Phenotypi c Enhancement : 30					
GCN5 ¹			Nonderepr	• Co-Fractionati on: 3	• Phenotypi c Suppression: 21				
				1	Co-Localizati on: 5	 Positive Genetic: 61 			
				Co-Purificatio n: 16	Synthetic Growth Defect: 158				
									Protein-Peptid e: 1
				 Reconstituted Complex: 19 	Synthetic Rescue: 40				
The		:42.1£ .:		• Two-hybrid: 5					

The gene ontology itself gives the graphical representation of the biological process for CDC15 dataset and it shows the number of conditions and their log ratio is shown in figure 6.



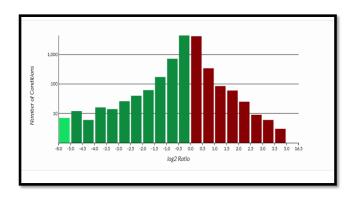


Fig 6. Graphical Representation for Biological Process

The biological significance of an overall experiment for the biological process is in table 8 with the help of gene ontology tool.

B. Molecular Function

From the input list, 6126 genes are either identified or unidentified but not clear. Unidentified genes shows the annotation providers are still included in the statistics. Also, 1026 duplicates were removed from the input list. The total number of genes used to calculate the background distribution of Gene Ontology (GO) terms is 7166. Displaying 80 terms out of a total of 1573 found. When compared to biological process the molecular function identifies more similarity gene. Thus the graphical representation of molecular function networks for CDC15 dataset using gene ontology is depicted in figure 7.

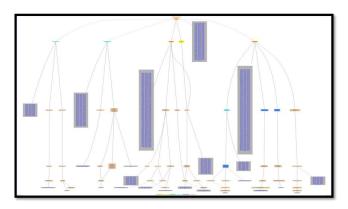


Fig 7. Molecular Function networks for CDC15 dataset using Gene Ontology

The technical names and the terms used for the molecular function with their interactions are described in table 9.

Table IX: Technical Names and terms for Molecular Function with their interaction

Standard Name	Systematic Name	SGD ID	Name Description	Physical Interaction	Genetic Interaction
UBP14	YBR058C	\$GD\$00000262	UBiquitin-specific Protease	Affinity Capture-MS: 17 Affinity Capture RNA: 2 Biochemical Activity. 2 Co-Purification: 1 Reconstituted Complex: 2	Doage Growth Defect 6 Doage Resour. 2 Negative Genetic: 28 Phenotypic Enhancement: 2 Phenotypic Enhancement: 1 Positive Genetic: 24 Synthetic Growth Defect 26 Synthetic Growth Defect 26 Synthetic Lethality: 7

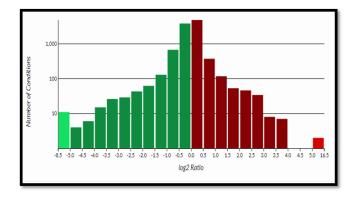


Fig 8. Graphical Representation for Molecular Function

The graphical representations of the molecular function are represented in figure 8. The overall experiment for biological significance for the molecular function is given in table 10. Thus the table shows the gene ontology term with their cluster frequency, their genome frequency with the corrected P-value.

C. Cellular Component

From the input list, 6126 genes are either identified or unidentified but not clear. Unidentified genes shows the annotation providers are still included in the statistics. Also, 1026 duplicates were removed from the input list. The total number of genes used to calculate the background distribution of Gene Ontology (GO) terms is 7166. Displaying 101 terms out of a total of 958 found.

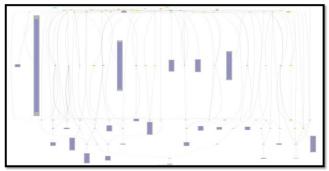


Fig 9. Cellular Component networks for CDC15 dataset using Gene Ontology

The cellular component networks for CDC15 dataset using gene ontology are shown in figure 9. The technical names and the terms for this cellular component with their interaction are also tabulated in table 11.





Table XI: Technical Names and terms for Cellular Component with their Interaction

Stan dard Nam e	Syste matic Name	SG D ID	Name Descripti on	Physical Interaction	Genetic Interaction
UTP 11	YKL 099C	SGD S00 0001 582	U Three Protein	Affinity Capture-MS: 20 Affinity Capture -RNA: 5 Biochem ical Activity: 1 Co-Purif ication: 1 Two-hyb rid: 3	Dosage Growth Defect: 1 Negative Genetic: 5 Positive Genetic: 4 Synthetic Lethality: 3

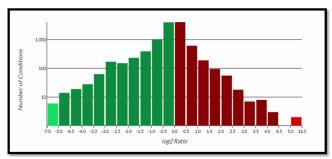


Fig 10. Graphical Representation for Biological Process

The graphical representations for the biological process are shown in figure 10. Thus the biological significance of the overall experiment for the cellular component is described in table 12.

VI. CONCLUSION

In this paper, a novel triclustering algorithm based using Hybrid PSO has proposed to extract the high quality of tricluster. The study has carried out with different inertia weight of the particles in Hybrid PSO for identification of optimal tricluster. It has observed that higher inertia weight converges to global optima of the particle. The result has shown in the work clearly pin point the performance of the proposed work in extracting the high volume tricluster with high MCV. The optimal tricluster holds the higher level of coherent pattern among the genes.

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