# ÓMICAS

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Gobierno de Colombia
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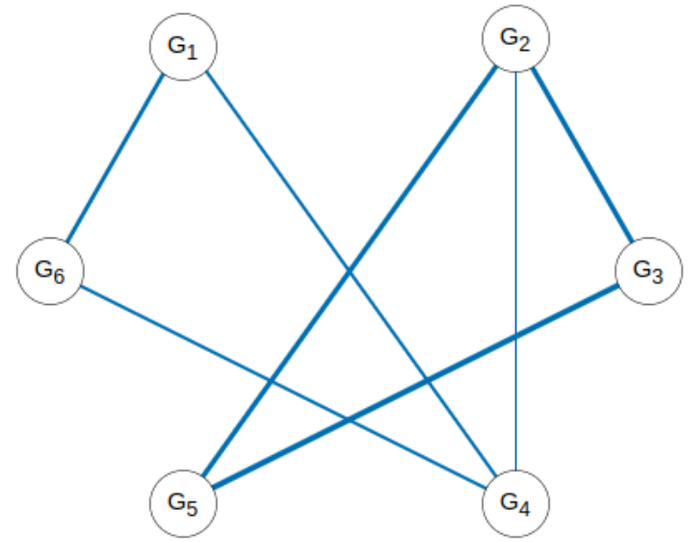
Conocimiento Global para el Desarrollo

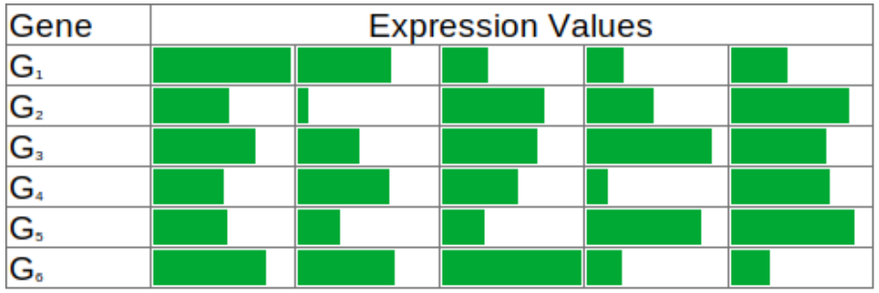
# Characterization of correlation measures with a novel network-based threshold for generating gene co-expression networks. Case study: Rice

Nicolás López-Rozo, Miguel Romero, Jorge Finke, Camilo Rocha

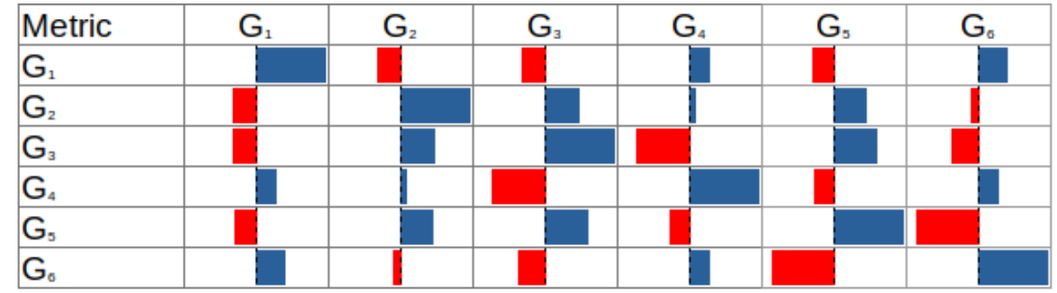



ÓMICAS program – Project P5: In-silico

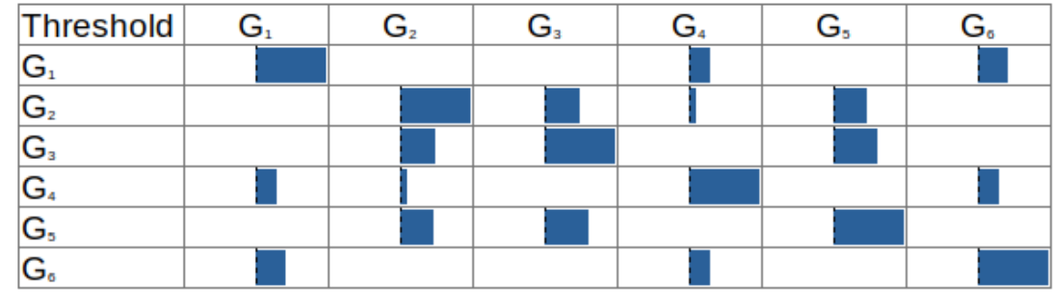
# MOTIVATION: ASSESS CRITICAL STEPS IN GENE ENRICHMENT ANALYSIS



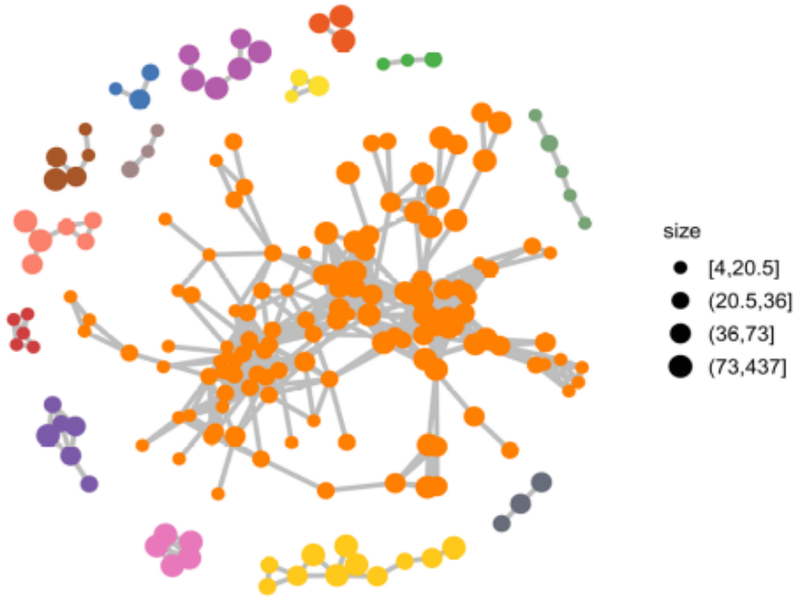

Metric Computation




Threshold Procedure

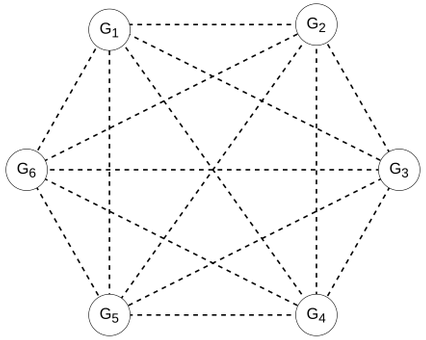


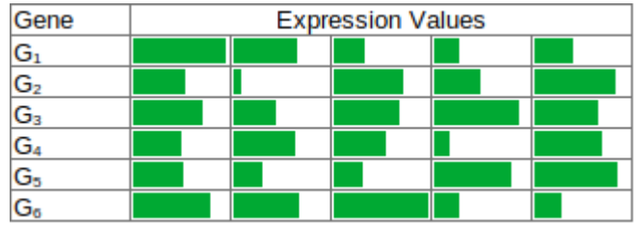

Gene Enrichment



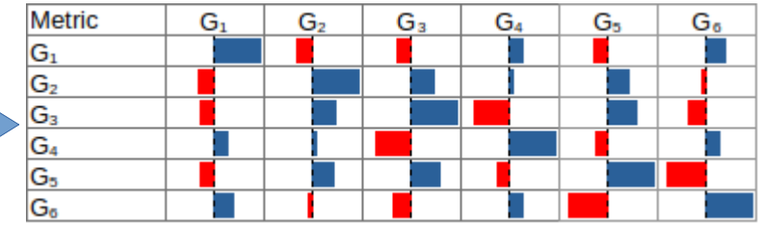

1. Pearson limitations.
2. Threshold is arbitrary.

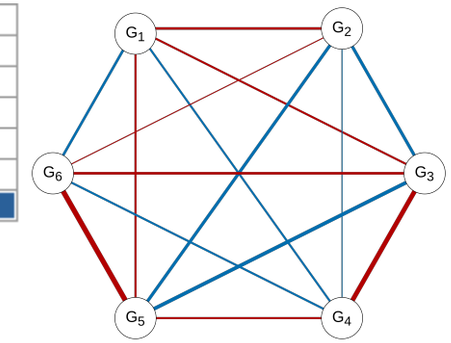
# WORKFLOW: TOWARDS FUNCTION PREDICTION



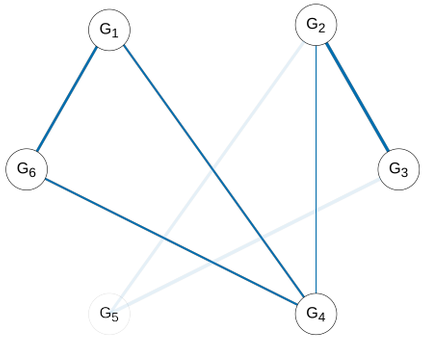



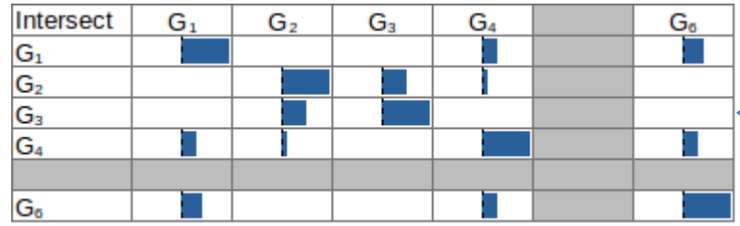

PCC
BICOR
DCORR
MIC
TIC
RIC

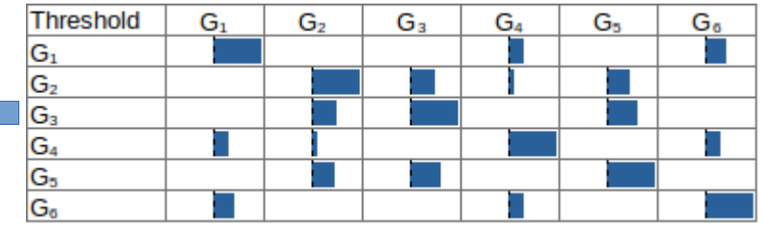


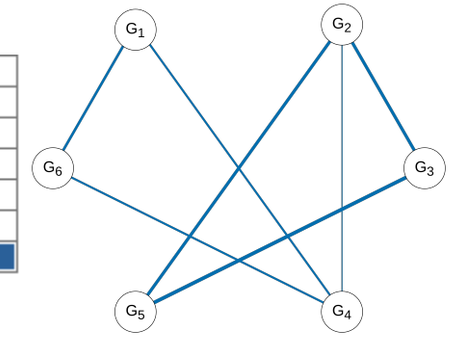



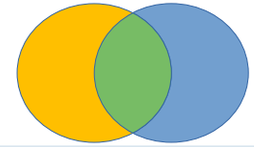

Compute
Topological
Threshold



# DATA

Expression data for *Oryza sativa Japonica:*

- Number of genes: 23374
- Number of samples: 2678
- Data source: NCBI GEO
- Expression value range: 0.009 – 280954

For the classification models:

- 5-fold cross-validation
- 50 repetitions for each model

Selected correlation metrics:

- Pearson's Correlation Coeficient (PCC)
- Biweight Midcorrelation (BICOR)
- Distance Correlation (DCORR)
- Maximal Information Coefficient (MIC)
- Total Information Coefficient (TIC)
- Randomized Information Coefficient (RIC)

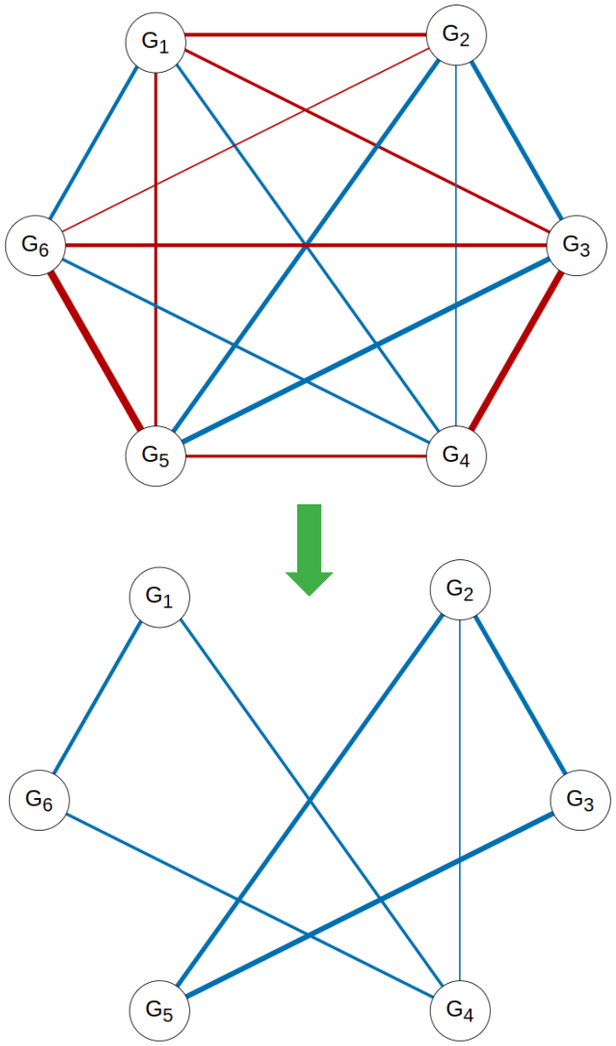
$$\mathrm{PCC}(X,Y) = \frac{\sum_{i=1}^{n}(x_i-\bar{x})(y_i-\bar{y})}{\sqrt{\sum_{i=1}^{n}(x_i-\bar{x})^2}\sqrt{\sum_{i=1}^{n}(y_i-\bar{y})^2}}$$

$$\mathrm{BICOR}(X,Y) = \sum_{i=1}^{n} \tilde{x}_i \tilde{y}_i,$$

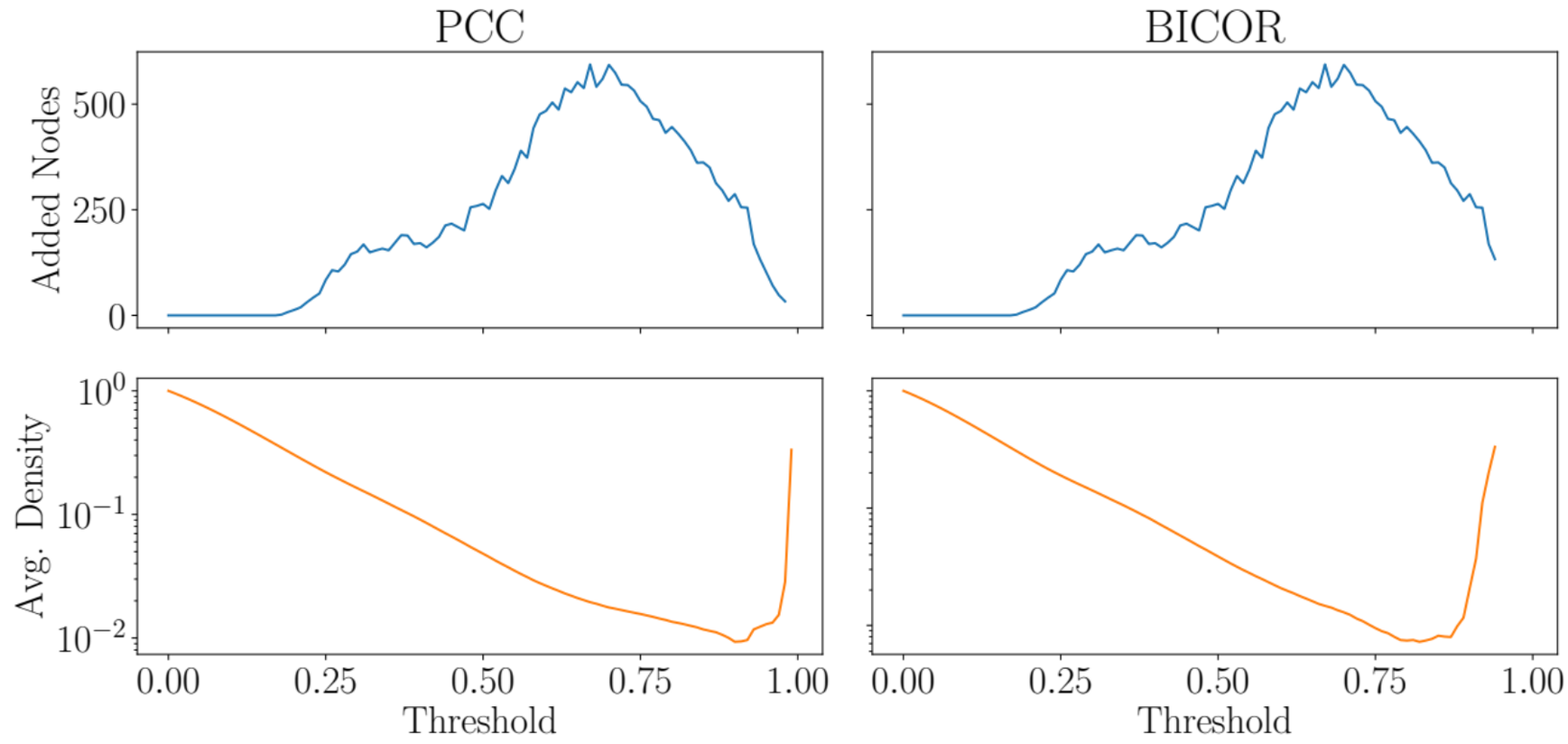
$$\tilde{x}_i = \frac{(x_i - \mathrm{med}(x))w_i^{(x)}}{\sqrt{\sum_{j=1}^{n}[(x_j - \mathrm{med}(x))w_j^{(x)}]^2}}$$

$$\mathrm{DCORR}(X,Y) = \frac{\mathrm{DCov}^2(X,Y)}{\sqrt{\mathrm{DCov}^2(X,X)\,\mathrm{DCov}^2(Y,Y)}}$$

# PROPOSED THRESHOLD COMPUTATION, BASED ON THE TOPOLOGY




$$t_{\mathbf{C}} = \min\left(\text{argmax}(|\Delta V_{I,\mathbf{C}}|), \text{argmin}(\bar{\rho}_{\mathbf{C}})\right)$$

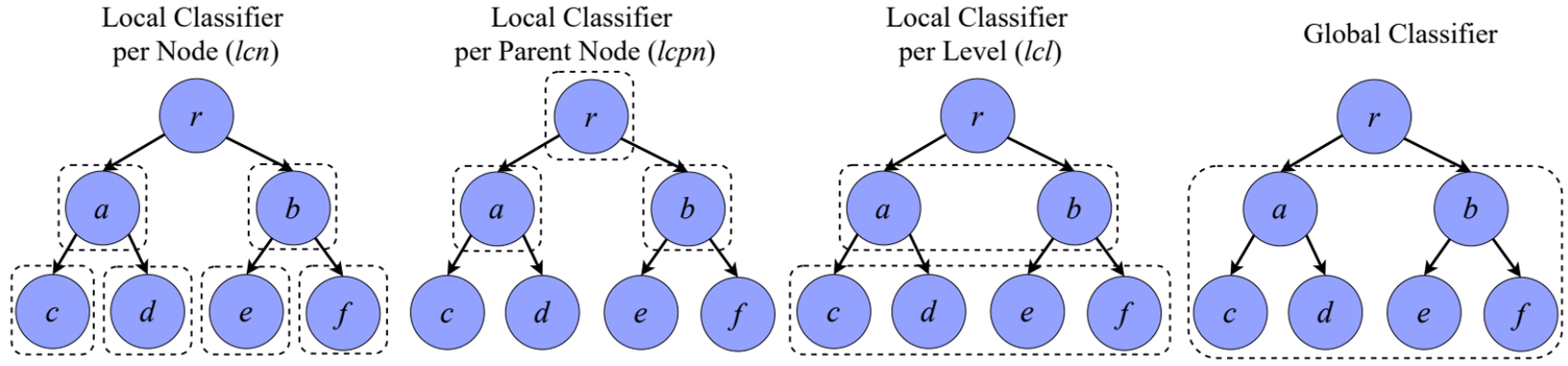


# PERFORMANCE ASSESSMENT: GENE FUNCTION PREDICTION

Four classification models taking advantage of the hierarchical organization of annotations:

- Local Classifier per Node (lcn)
- Local Classifier per Level (lcl)
- Local Classifier per Parent Node (lcpn)
- Global (multi-label) Classifier

Evaluation metric for comparison: Area under the average precision-recall curve



# PERFORMANCE RESULTS (1): COMPARISON OF CORRELATION METRICS

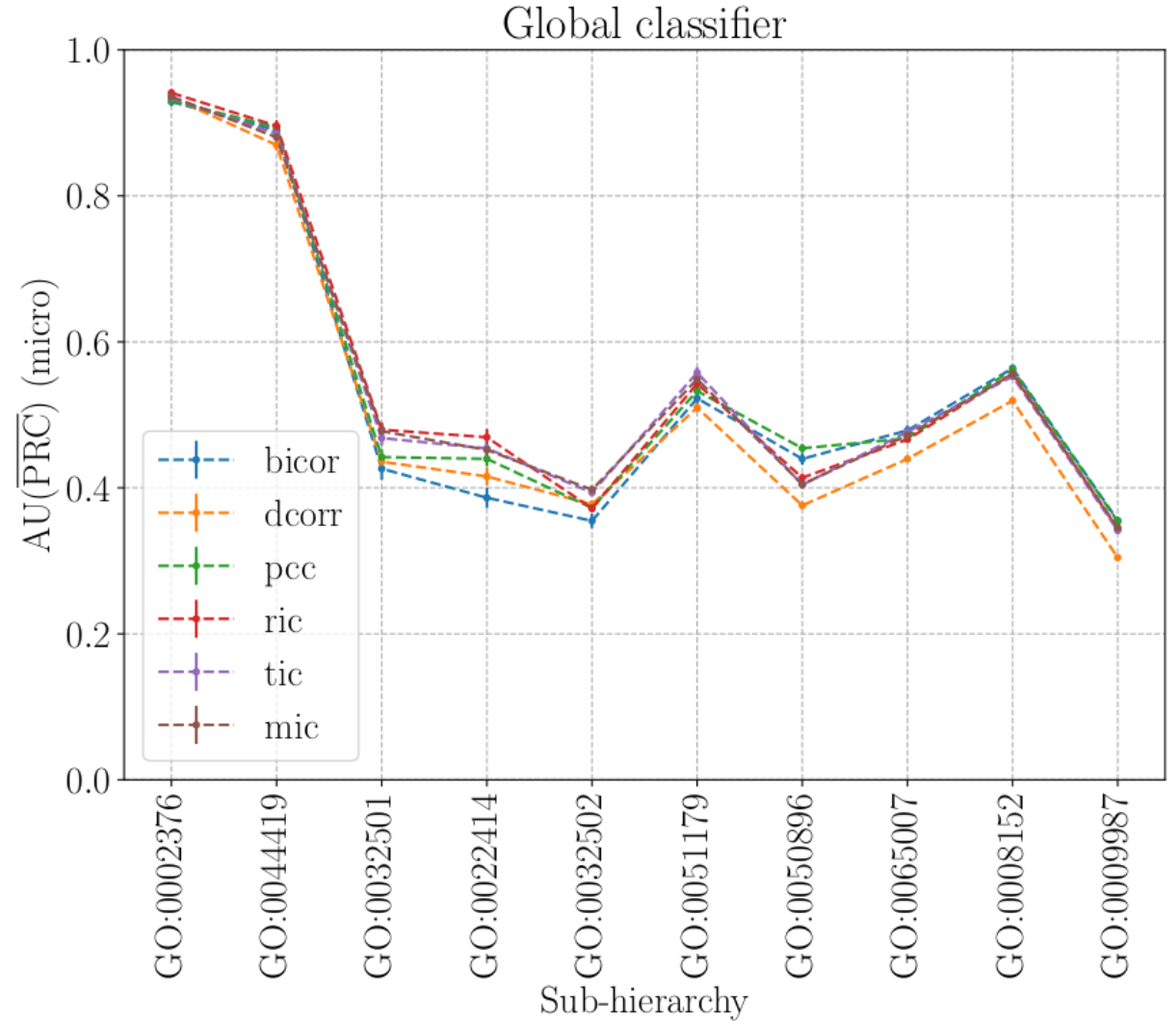
PROPERTIES OF THE RESULTING NETWORKS

| Network | Nodes | Edges | Components | Avg. degree |
|---|---|---|---|---|
| PCC | 11,241 | 1,195,905 | 473 | 212.78 |
| BICOR | 7,344 | 382,202 | 586 | 104.09 |
| DCORR | 13,069 | 2,184,554 | 12 | 334.31 |
| MIC | 14,233 | 5,790,949 | 255 | 813.74 |
| TIC | 13,549 | 5,276,496 | 275 | 778.88 |
| RIC | 13,383 | 3,261,088 | 314 | 487.35 |

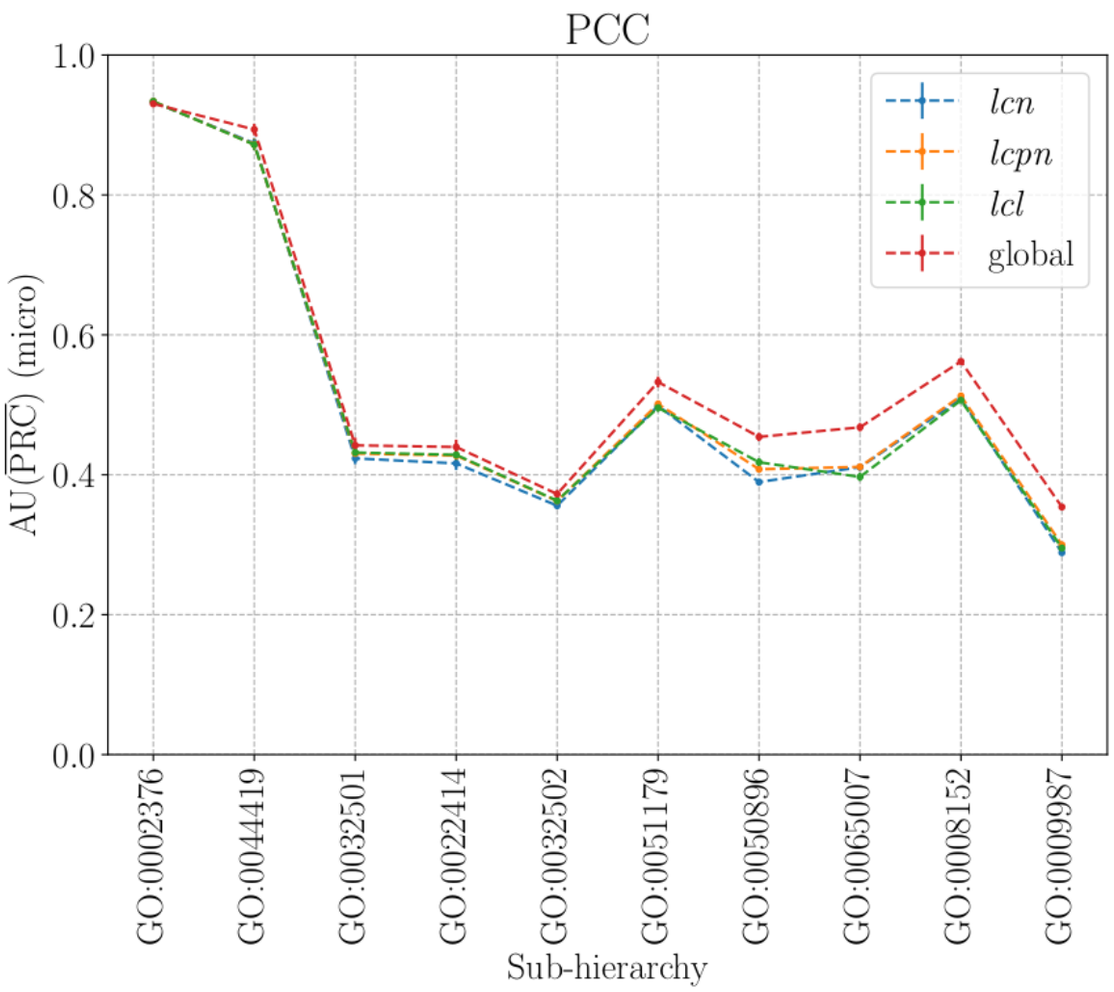
SUB-HIERARCHIES OF BIOLOGICAL PROCESSES[a]

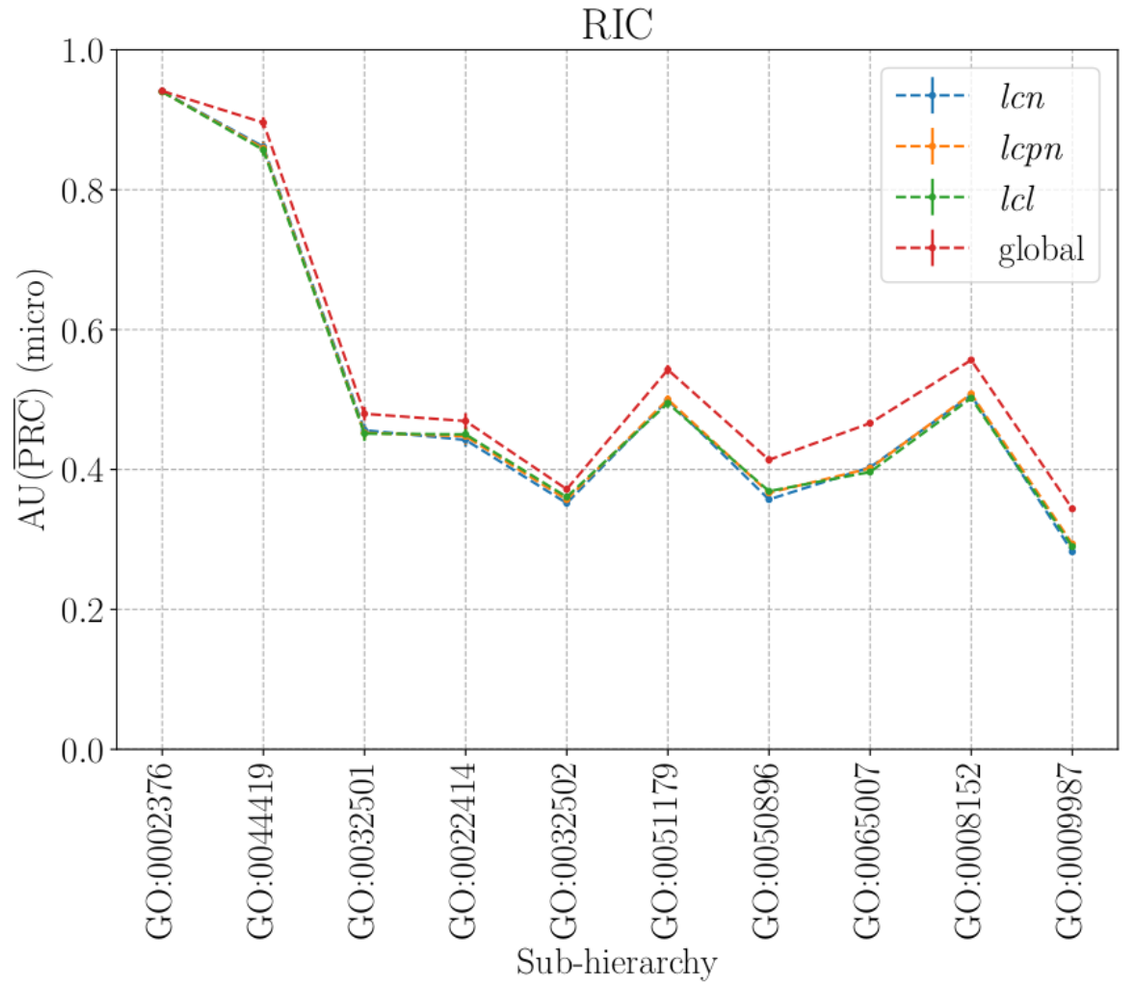
| Hierarchy[b] | Description | Functions |
|---|---|---|
| GO:0002376 | Immune system process | 9 |
| GO:0044419 | Biological process involved in inter-species interaction between organisms | 13 |
| GO:0032501 | Multicellular organismal process | 18 |
| GO:0022414 | Reproductive process | 24 |
| GO:0032502 | Developmental process | 53 |
| GO:0051179 | Localization | 86 |
| GO:0050896 | Response to stimulus | 102 |
| GO:0065007 | Biological regulation | 184 |
| GO:0008152 | Metabolic process | 399 |
| GO:0009987 | Cellular process | 517 |

[a] Each sub-hierarchy is considered an independent dataset.
[b] Each sub-hierarchy is represented by its root.



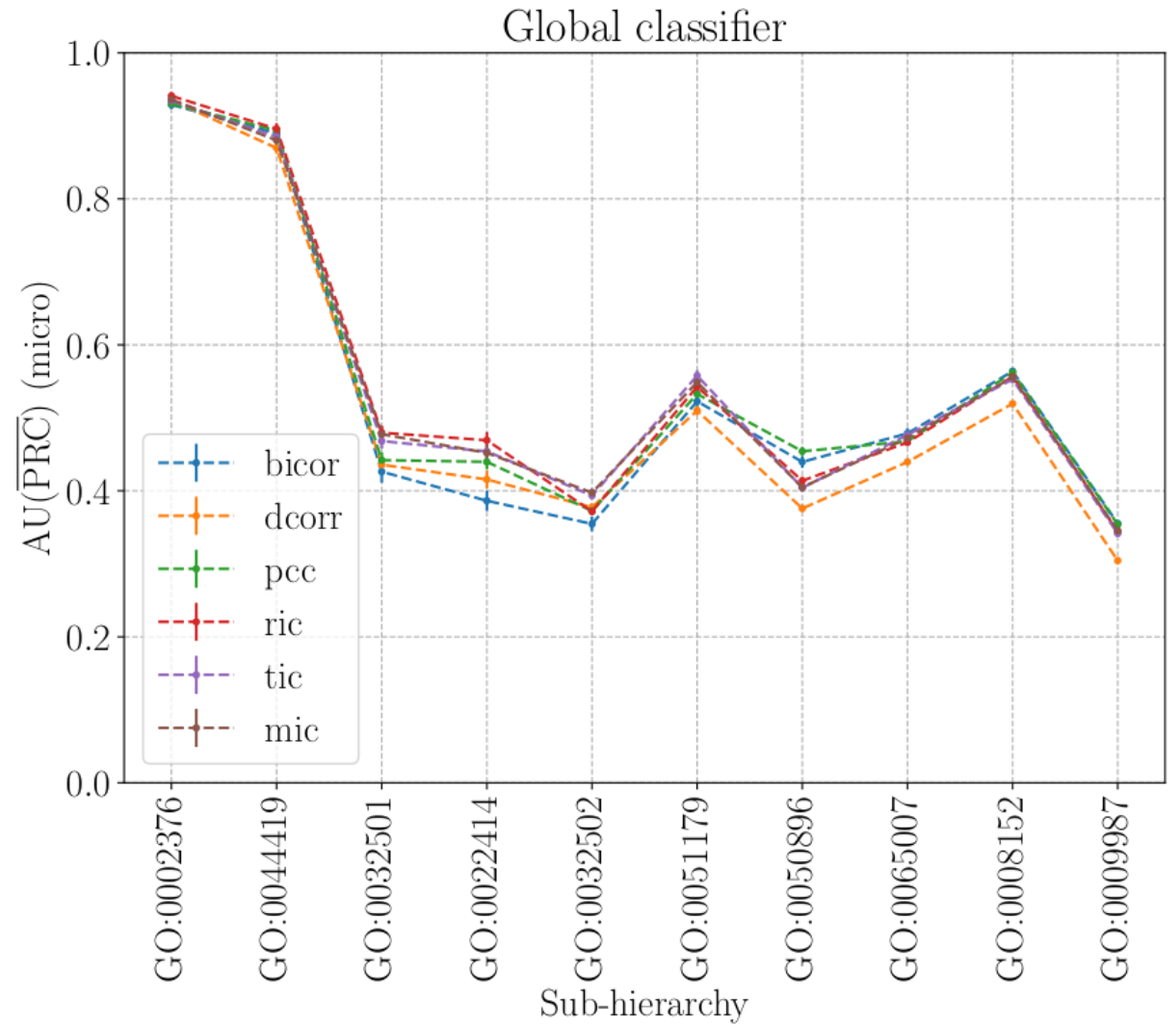
# PERFORMANCE RESULTS (2): COMPARISON OF CLASSIFICATION MODELS



# CONCLUSIONS

- Global multi-label classification model performs better with respect to AU-PRC
- GO hierarchies with less than 25 terms have a better performance with RIC GCN
- Similarly, hierarchies with more than 180 terms get better results with BICOR GCN
- Future work: Explore different threshold approaches and characterize network growth as a function of the cut-off value



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