

HyPnOBrain

your homology based HPO neural network predictor

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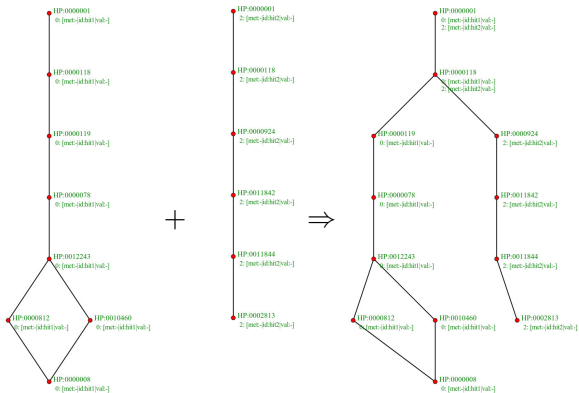
Homology based function prediction

General approach:

- ▶ Search for annotated similar sequences with blast and hhblits (hits)
- ▶ Build subgraph of HPO containing the found annotations
- ▶ Calculate confidence for every annotation from some distance measure to the hits

Preparations

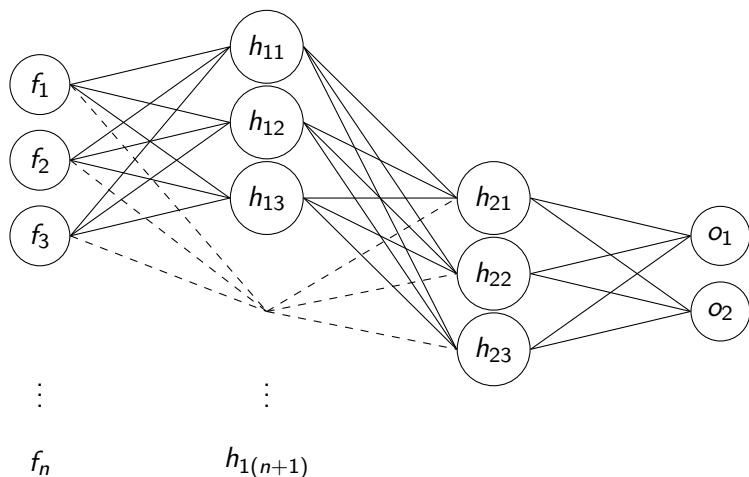
- ▶ Prepare databases for annotated sequences
- ▶ Represent HPO Graph in predictor
- ▶ Merge trees corresponding to hits



Features

- ▶ use neural network to calculate confidence per node
 - ▶ each node is assigned 12 features derived from the merged tree
 - ▶ number of hits
 - ▶ min. E-value
 - ▶ avg. E-value
 - ▶ product of E-values
 - ▶ longest hit
 - ▶ ...
- } [3, 0.0074, 0.45, 4.2e-7, 84, ...]

Network architecture

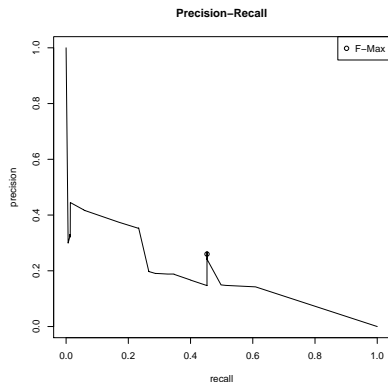


- ▶ fully connected net with two hidden layers
- ▶ two output nodes trained for the two possible predictions
- ▶ difference of predictions as confidence

Validation

- ▶ Inspection of the dataset shows: Most sequences have pairwise similarity $< 80\%$
 \Rightarrow reduce set at 80%-level to remove highly similar clusters
- ▶ Crossvalidate over reduced set but allow non-reduced trainingset for similarity search during testing
- ▶ Calculate precision and recall per test sequence and average over all sequences

Results



- ▶ F-measure 0.33 ± 0.03 (at confidence level 0.25)
- ▶ Precision 0.26 ± 0.04 (at same confidence level)
- ▶ Recall 0.45 ± 0.10 (at same confidence level)