

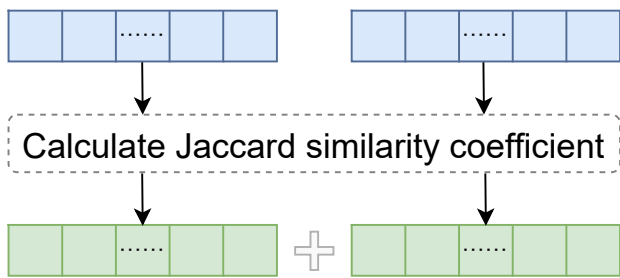
drugA 

drugB 

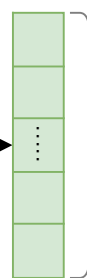
multimodal deep neural network

decision fusion module

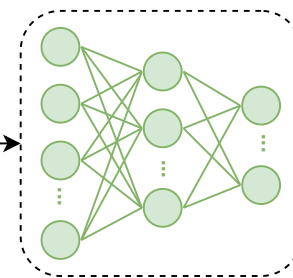
substructure



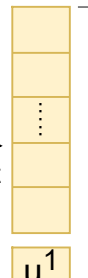
PCA



1258\*2



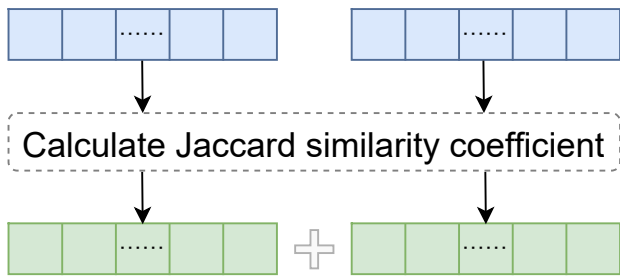
Dirichlet



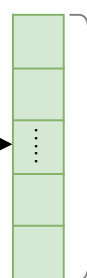
$E^1$

$u^1$

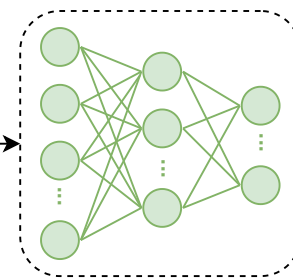
target



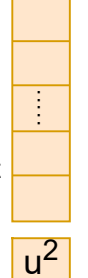
PCA



1258\*2



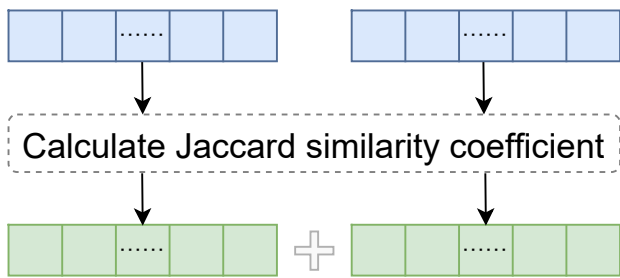
Dirichlet



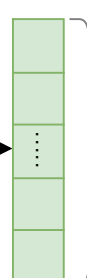
$E^2$

$u^2$

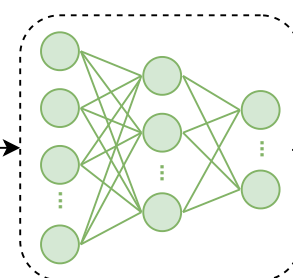
enzyme



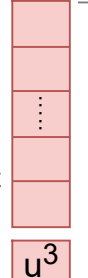
PCA



1258\*2



Dirichlet



$E^3$

$u^3$

DST

$p$



$u$