Re-engineering of a tool for drug repositioning with NMTF

Application note on bioinformatics

Elena Danchenko

Politecnico di Milano Master, expected graduation time April 2020

February 2020



Objective and applied modifications

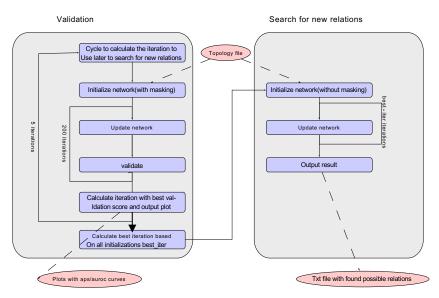
Objective

The generalization of already existing functionality

Applied modifications

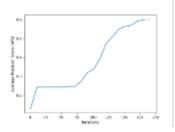
- Testing of existing functionality
- Adding validation
- Adding intra-data relations influence
- Adding output
- Implementing rank calculation
- Adjusting application flow

Application flow



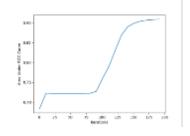
Output

APS/AUROC validation results



APS plot example

Newly found connections file



AUROC plot example

```
DB00005
DB00005
         Immunoalobulins
                          0.5510323395313135
DB00008
         Carbohydrates
DB00041
DB00042
                         0.6860733637208515
DB00054
         Antibodies, Monoclonal
                                 0.6259975668233332
DB00056
         Enzyme Inhibitors
                            0.5346958632240236
DB00056
         Nucleic Acids, Nucleotides, and Nucleosides
                                                       0.5034638372435417
         Antibodies Monoclonal 0.627168743063233
```