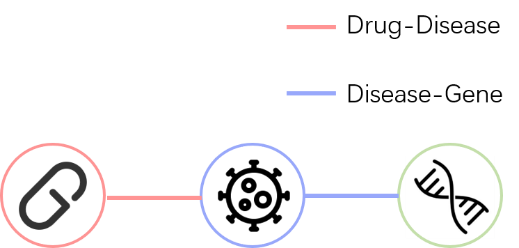
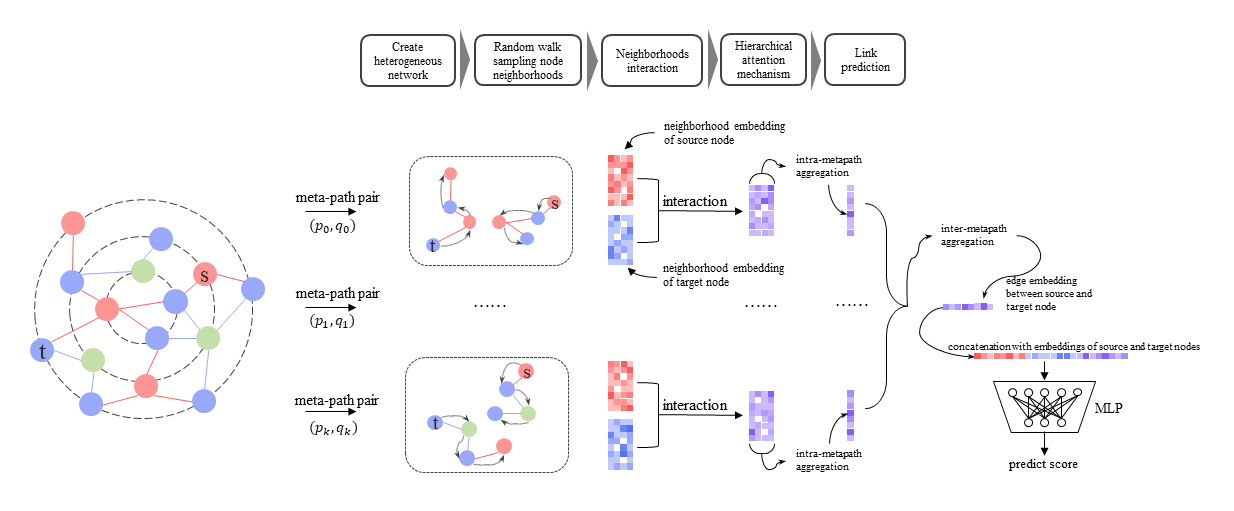
Additional Figures & Table

The following provides a clear version of the figures in the paper and the figures that cannot fit in the original paper due to space limitations. In addition, it also contains a table of 20 drugs predicted for AD in the original paper 4.4 case study part.

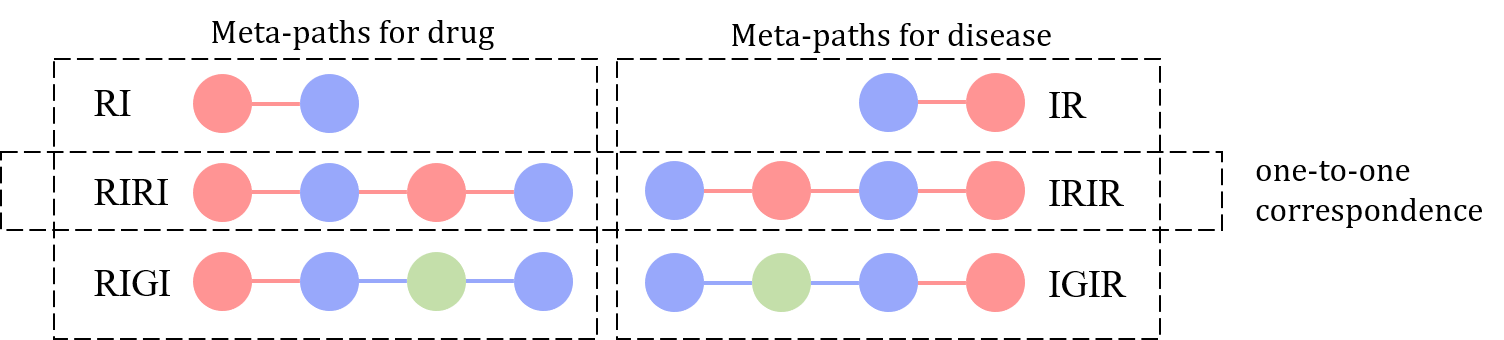


**Fig. 1.** Nodes and Edges used

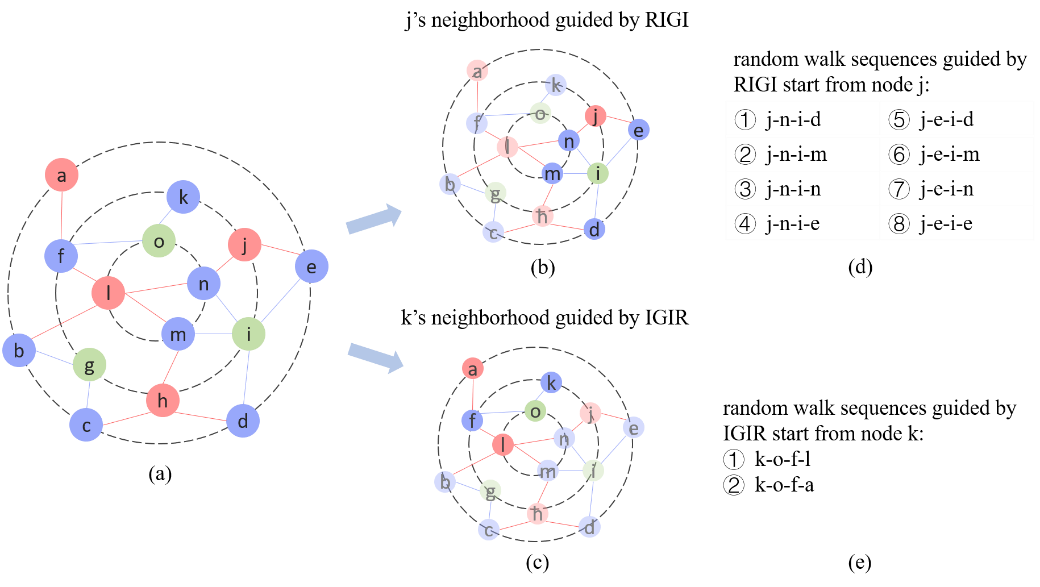
Our dataset bioDDG contains three types of nodes and two types of edges



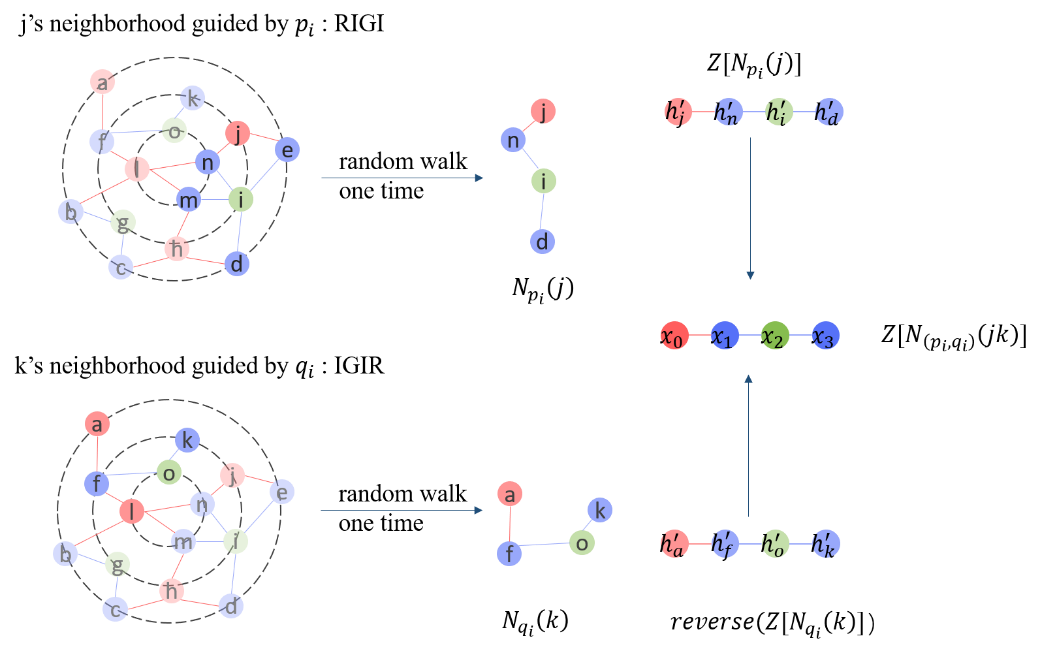
**Fig. 2.** The workflow of the NIEE



**Fig. 3.** Meta-path pairs

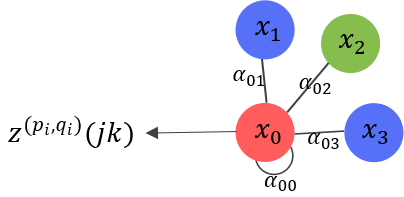


**Fig. 4.** Neighborhoods guided by meta-paths for given nodes (take RIGI & IGIR as example)

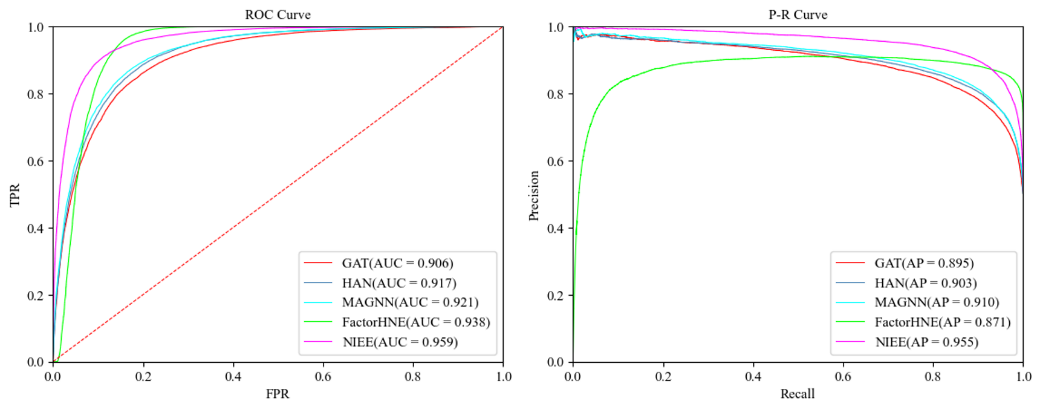


**Fig. 5.** Example of interaction between neighborhoods (take the meta-path pair RIGI & IGIR as an example)

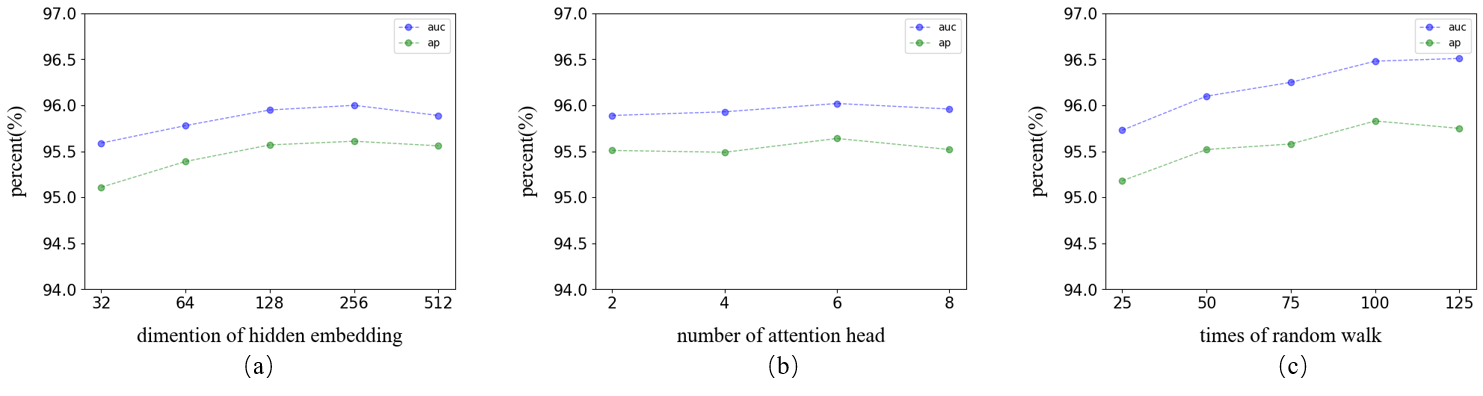
For the convenience of demonstration, random walk is performed only once in the above figure.



**Fig. 6.** Example of embedding representation of learned by single-head self-attention mechanism



**Fig. 7.** NIEE's performance in comparison to other benchmark models.



**Fig. 8.** Sensitivity analysis of parameters.

**Table 1.** 20 potential drugs for Alzheimer's disease predicted by NIEE.

|  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- |
| Rank | Predicted drugs | DrugBank ID | Evidence | Rank | Predicted drugs | DrugBank ID | Evidence |
| 1 | Seviteronel | DB12275 |  | 11 | Methylphenidate | DB00422 | CTD, [2,3] |
| 2 | Abarelix | DB00106 |  | 12 | Dopexamine | DB12313 |  |
| 3 | Aminoglutethimide | DB00357 | CTD | 13 | Lactitol | DB12942 |  |
| 4 | Volinanserin | DB16351 |  | 14 | Dopamine | DB00988 | CTD |
| 5 | Kynurenic Acid | DB11937 | CTD | 15 | Moxaverine | DB12251 |  |
| 6 | Ipragliflozin | DB11698 |  | 16 | Tetrabenazine | DB04844 | [4] |
| 7 | Tretazicar | DB04253 |  | 17 | Benfluorex | DB09022 |  |
| 8 | Metronidazole | DB00916 | CTD | 18 | Alprostadil | DB00770 | CTD |
| 9 | Racephedrine | DB14752 |  | 19 | Dexamethasone  acetate | DB14649 | CTD, [5] |
| 10 | Resveratrol | DB02709 | CTD, [1] | 20 | Methylprednisolone hemisuccinate | DB14644 | CTD, [5] |

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