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| 文章名Prediction of Drug–Target Interaction Networks from the Integration of Protein Sequences and Drug Chemical Structures | |
| 中文译名 | 结合蛋白序列和药物化学结构预测药物靶点相互作用网络 |
| 网址 |  |
| 关键词 | DTI; RVM; BIGP; PCA  Bi-gram probabilities (BIGP)  Position Specific Scoring Matrix (PSSM)  Principal Component Analysis(PCA)  Relevance Vector Machine (RVM)关联向量机 |
| 摘要 | Acc高。与支持向量机做了比较。（有对比实验） |
| 启发 | 1，五折交叉验证，分蛋白类别。  2，the correct choice of feature extraction method and classifier带来了更优的结果。  3，Bi-gram probability，提取了更具有代表性的特征，降低了稀疏性，  4，随机选取负样本，做训练。 |
| 摘录 | 评价体系： |
| 相关论文 | **We can freely obtain some of them from the public sector, such as SuperTarget and Matador [6], Kyoto Encyclopedia of Genes and Genomes (KEGG) [7], DrugBank [8,9], Therapeutic Target Database (TTD) [10,11], etc.**  **数据获取来源**  **Günther, S. SuperTarget and Matador: Resources for exploring drug-target relationships. Nucleic Acids Res.**  **2008, 36, 919–922. [CrossRef] [PubMed]**  **7. Kanehisa, M.; Goto, S.; Hattori, M.; Aokikinoshita, K.F.; Itoh, M.; Kawashima, S.; Katayama, T.; Araki, M.;**  **Hirakawa, M. From genomics to chemical genomics: New developments in KEGG. Nucleic Acids Res. 2005,**  **34, 354–357. [CrossRef] [PubMed]**  **8. Wishart, D.S. DrugBank: A knowledgebase for drugs, drug actions and drug targets. Nucleic Acids Res. 2008,**  **36, D901–D906. [CrossRef] [PubMed]**  **9. Wishart, D.S.; Knox, C.; Guo, A.C.; Shrivastava, S.; Hassanali, M.; Stothard, P.; Chang, Z.; Woolsey, J.**  **DrugBank: A comprehensive resource for in silico drug discovery and exploration. Nucleic Acids Res. 2006,**  **34, 668–672. [CrossRef] [PubMed]**  **10. Chen, X.; Ji, Z.L.; Chen, Y.Z. TTD: Therapeutic Target Database. Nucleic Acids Rese. 2002, 30, 412. [CrossRef]**  **11. Zhu, F.; Han, B.C.; Kumar, P.; Liu, X.H.; Ma, X.H.; Wei, X.N.; Huang, L.; Guo, Y.F.; Han, L.Y.; Zheng, C.J.**  **Update of TTD: Therapeutic Target Database. Nucleic Acids Res. 2010, 38, D787. [CrossRef] [PubMed]**  **[18]-[24]介绍了很多当前人们的研究。**  18. Yang, K.; Bai, H.; Ouyang, Q.; Lai, L.; Tang, C. Finding multiple target optimal intervention in disease-related molecular network. *Mol. Syst. Biol.* **2008**, *4*, 228. [CrossRef] [PubMed] 19. Niu, Y.Q. Supervised prediction of drug-target interactions by ensemble learning. *J. Chem. Pharm. Res.* **2014**, *6*, 1991–1999. 20. Kuang, Q.; Xu, X.; Li, R.; Dong, Y.; Li, Y.; Huang, Z.; Li, Y.; Li, M. An eigenvalue transformation technique for predicting drug-target interaction. *Sci. Rep.* **2015**, *5*, 13867. [CrossRef] [PubMed] 21. Bharadwaja, A. Similarity Based Learning Method for Drug taRget Interaction Prediction. M.Sc. Thesis, University of Windsor, Windsor, ON, Canada, 2014. 22. Peng, L.; Liao, B.; Zhu, W.; Li, K. Predicting Drug-Target Interactions with Multi-information Fusion. *IEEE J. Biomed. Health Inform.* **2015**, *21*, 561–572. [CrossRef] [PubMed] 23. Wang, Y.Y.; Nacher, J.C.; Zhao, X.M. Predicting drug targets based on protein domains. *Mol. Biosyst.* **2012**, *8*, 1528–1534. [CrossRef] [PubMed] 24. Zhang, R. *An Ensemble Learning Approach for Improving Drug–Target Interactions Prediction*; Springer International Publishing: New York, NY, USA, 2015; pp. 433–442.  **现有的四个DTI预测算法**  **DBSI [26], Yamanishi [27], KBMF2K [28], and NetCMP [29] on enzyme, ion channel, GPCR, and nuclear receptor datasets, respectively.**  27. Yamanishi, Y.; Araki, M.A.; Honda, W.; Kanehisa, M. Prediction of drug-target interaction networks from the integration of chemical and genomic spaces. *Bioinformatics* **2008**, *24*, i232–i240. [CrossRef] [PubMed] 28. Gönen, M. Predicting drug-target interactions from chemical and genomic kernels using Bayesian matrix factorization. *Bioinformatics* **2012**, *28*, 2304–2310. [CrossRef] [PubMed] 29. Zong, W.; Huang, G.B.; Chen, Y. Weighted extreme learning machine for imbalance learning. *Neurocomputing* **2013**, *101*, 229–242. [CrossRef]  **想要看的论文：**  **23，蛋白质域怎么确定的？** |

体会：一段中连着3句都用”however”，估计作者脑子被驴踢了

数据集，使用的是之前见过的黄金数据集。

突出的特点是：对数据的表示进行了优化Bi-gram probability等，，使用了新的方法“关联向量机”

论文感觉写颠倒了，应该先介绍数据集和实验方法，后介绍成绩。

收获：找到了一些相关论文，将要逐一查看。

2篇远古论文：pssm，PSI-blast

1篇，看起来是处理不平衡数据的算法论文。

1篇，介绍蛋白质域预测DTI的论文。

除此之外，我发现了该领域，目前还没有针对作用位点的预测。

下次找论文，要找“深度学习”和“作用位点”相关的论文。