

강의개요

Drug Target Prediction and Drug Repositioning with Graph Learning

약물-표적 관계 예측은 신약 개발 초기 단계에 필수적인 기술이며, 기존의 약물을 재활용하는 약물 재창출 분야에도 밀접한 관련이 있는 기술이다. 그렇다면, 약물의 표적은 어떻게 예측할 수 있을까? 이를 바탕으로 약물 재창출은 어떻게 할 수 있을까? *In silico* 기반의 약물-표적 관계 예측은 약물과 약물, 약물과 질병, 질병과 유전자 등 여러 가지 상호작용을 고려해야 하기에 많은 어려움이 따른다.

본 강의에서는 약물, 질병, 유전자 간 상호작용을 그래프로 학습하여 약물-표적 예측 및 약물 재창출을 설명한다. 먼저 Random walk, Network propagation, Graph neural network 등 기본적인 그래프 분석 기법들을 배우고, 이를 약물-표적 상관관계 분석/예측 및 약물 재창출 분야에서 효율적이고 효과적으로 활용한 최신 사례를 소개한다.

강의는 다음의 내용을 포함한다.

- 그래프 마이닝 알고리즘
- Graph neural network 기반의 딥러닝 기술
- 약물-표적 관계 예측(Drug-Target Interaction) 사례 및 기술
- 약물 재창출(Drug repositioning) 사례 및 기술

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* 강의 난이도: 중급

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Educational Experience

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Professional Experience

1998-2001 Senior Computer Scientist, DuPont Central Research
2001-2011 Assistant/Associate Professor, School of Informatics and Computing, Indiana University
2009-2011 Chair, School of Informatics and Computing, Indiana University
2011-2021 Director, Bioinformatics Institute, Seoul National University
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Selected Publications (5 maximum)

1. Lee, D., Yang, J., & Kim, S. (2022). Learning the histone codes with large genomic windows and three-dimensional chromatin interactions using transformer. *Nature Communications*, 13(1), 1-19.
2. Lim, S., Lu, Y., Cho, C. Y., Sung, I., Kim, J., Kim, Y., ... & Kim, S. (2021). A review on compound-protein interaction prediction methods: data, format, representation and model. *Computational and Structural Biotechnology Journal*, 19, 1541-1556.

3. Rhee, S., Seo, S., & Kim, S. (2018, July). Hybrid approach of relation network and localized graph convolutional filtering for breast cancer subtype classification. In Proceedings of the 27th International Joint Conference on Artificial Intelligence (pp. 3527-3534).
4. Seo, S., Oh, M., Park, Y., & Kim, S. (2018). DeepFam: deep learning based alignment-free method for protein family modeling and prediction. *Bioinformatics*, 34(13), i254-i262.
5. Jo, K., Jung, I., Moon, J. H., & Kim, S. (2016). Influence maximization in time bounded network identifies transcription factors regulating perturbed pathways. *Bioinformatics*, 32(12), i128-i136.

Curriculum Vitae

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Professional Experience

2020 Postdoctoral research fellow, SNU Bioinformatics Institute
2020-2021 Postdoctoral research fellow, SNU BK21 FOUR Intelligence Computing
2021- Postdoctoral research fellow, SNU Institute of Computer Technology

Selected Publications (5 maximum)

1. Lee, S., Lee, D., Piao, Y., & Kim, S. (2022). SPGP: Structure Prototype Guided Graph Pooling. NeurIPS 2022 Workshop New Frontiers in Graph Learning.
2. Piao, Y., Lee, S., Lee, D., & Kim, S. (2022, June). Sparse Structure Learning via Graph Neural Networks for Inductive Document Classification. In Proceedings of the AAAI Conference on Artificial Intelligence (Vol. 36, No. 10, pp. 11165-11173).
3. Lee, S., Lim, S., Lee, T., Sung, I., & Kim, S. (2020). Cancer subtype classification and modeling by pathway attention and propagation. Bioinformatics, 36(12), 3818-3824.
4. Lee, S., Lee, T., Noh, Y. K., & Kim, S. (2019). Ranked k-spectrum kernel for comparative and evolutionary comparison of exons, introns, and cpg islands. IEEE/ACM transactions on computational biology and bioinformatics, 18(3), 1174-1183.
5. Lee, S., Park, Y., & Kim, S. (2017). MIDAS: mining differentially activated subpaths of KEGG pathways from multi-class RNA-seq data. Methods, 124, 13-24.

