

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

*교육생준비물: X (이론강의)

* 강의 난이도: 중급

* 강의: 김선 교수 (서울대학교 컴퓨터공학부) / 이상선 컴퓨터공학 박사

Curriculum Vitae

Speaker Name: Sun Kim, Ph.D.



► Personal Info

Name Sun Kim
Title Professor
Affiliation Seoul National University (SNU)

► Contact Information

Address Department of Computer Science and Engineering, 301-421,
Seoul National University, 1, Gwanak-ro, Gwanak-gu, Seoul, 08826
Email sunkim.bioinfo@snu.ac.kr

Research interest : Machine Learning, Deep Learning, Multi-omics, Bioinformatics, AI-drug discovery

Educational Experience

1985 B.S., Computer Science, Seoul National University
1987 M.S., Computer Science, KAIST
1997 Ph.D., Computer Science, University of Iowa

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
2011- Professor, Department of Computer Science and Engineering & Interdisciplinary Program in Bioinformatics, Seoul National University
2022- Research Director, MOGAM Institute for Biomedical Research

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

Speaker Name: Sangseon Lee, Ph.D.



► Personal Info

Name Sangseon Lee
Title Post-doc research fellow
Affiliation Institute of Computer Technology,
Seoul National University

► Contact Information

Address 220-653, Seoul National University, 1, Gwanak-ro, Gwanak-gu,
Seoul, 08826
Email sangseon486@snu.ac.kr

Research interest : Translational bioinformatics, Machine learning and computational genomics

Educational Experience

2013 B.S. in Computer Engineering, Seoul National University, Korea
2020 Ph.D. in Computer Engineering, Seoul National University, Korea

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.

