Tentative course schedule

Lecture	Topic	Reading
1	Introduction	White Chapter 2 Bishop Sections 1.0-1.1, 1.5.5 Goodfellow et al. Sections 5.0-5.4
2	Linear models for regression	White Chapter 3 Bishop Sections 3.0-3.2
3-4	Generalized linear models for classification	White Chapter 4 Bishop Sections 4.0-4.1, 4.2.0, 4.3.0-4.3.2
4-5	Nonparametric methods and ensemble learning	Bishop Sections 14.2-14.4 Murphy Chapter 18
6-7	Dimensionality reduction	Murphy Sections 7.5, 20.1, and 20.4 Goodfellow et al. Sections 2.8, 2.12, 5.8.1
7-8	Clustering	Murphy Sections 21.1-21.5
8	Discussion	Papers 1-2
9	Student presentations	Papers 3-4
10	Neural networks	White Chapter 6 Bishop Sections 5.0-5.1, 5.3.0-5.3.3, 5.5 Goodfellow et al. Chapters 6 and 7
11	Convolutional and graph architectures	White Chapters 7 and 8 Goodfellow et al. Sections 9.0-9.3
12-13	Student presentations	Papers 5-8
14-15	Equivariance	Paper 10
15-16	Attention and Transformers	3Blue1Brown DL5 and DL6 The Illustrated Transformer Understanding and Coding Self-Attention The Annotated Transformer Paper 17
17	Test	
18-20	Generative methods	White Chapters 14-15 Sections 1-2 of Paper 18 Papers 19-20
21-23	Student presentations	Papers 11-12, 14-15
24	Reinforcement learning	Sutton and Barto Sections 3.1-3.3, 4.1
25-27	Final project presentations	

Student presentation papers

1. Rogers D, Hopfinger AJ. Application of genetic function approximation to quantitative structure-activity relationships and quantitative structure-property relationships. Journal of Chemical Information and Computer Sciences. 1994 Jul;34(4):854-66.

2. Svetnik V, Liaw A, Tong C, Culberson JC, Sheridan RP, Feuston BP. Random forest: a classification and regression tool for compound classification and QSAR modeling. Journal

of Chemical Information and Computer Sciences. 2003 Nov 24;43(6):1947-58.

3. Rohrdanz MA, Zheng W, Maggioni M, Clementi C. Determination of reaction coordinates via locally scaled diffusion map. Journal of Chemical Physics. 2011 Mar 28;134(12): 124116.

4. Schultze S, Grubmüller H. Time-lagged independent component analysis of random walks and protein dynamics. Journal of Chemical Theory and Computation. 2021 Aug 27;17(9): 5766-76.

5. Rupp M, Tkatchenko A, Müller KR, Von Lilienfeld OA. Fast and accurate modeling of molecular atomization energies with machine learning. Physical Review Letters. 2012 Feb 3;108(5):058301.

6. Holley LH, Karplus M. Protein secondary structure prediction with a neural network. Proceedings of the National Academy of Sciences. 1989 Jan;86(1):152-6.

7. ~~Zhu RL, Jonas E. Rapid approximate subset-based spectra prediction for electron ionization-mass spectrometry. Analytical Chemistry. 2023 Jan 25;95(5):2653-63.~~

8. Gilmer J, Schoenholz SS, Riley PF, Vinyals O, Dahl GE. Neural message passing for quantum chemistry. In Proceedings of the 34th International Conference on Machine Learning, Proceedings of Machine Learning Research. 2017 Jul 17; 70:1263-1272.

9. ~~Behler J, Parrinello M. Generalized neural-network representation of high-dimensional po~~tential-energy surfaces. Physical Review Letters. 2007 Apr 6;98(14):146401.

10. Satorras VG, Hoogeboom E, Welling M. E (n) equivariant graph neural networks. In International Conference on Machine Learning, Proceedings of Machine Learning Research. 2021 Jul 1; 139:9323-9332.

11. Noé F, Olsson S, Köhler J, Wu H. Boltzmann generators: Sampling equilibrium states of many-body systems with deep learning. Science. 2019 Sep 6;365(6457):eaaw1147.

12. ~~Jumper J, Evans R, Pritzel A, Green T, Figurnov M, Ronneberger O, Tunyasuvunakool K, Bates R, Žídek A, Potapenko A, Bridgland A. et al. Highly accurate protein structure prediction with AlphaFold. Nature. 2021 Aug;596(7873):583-9.~~
The Illustrated AlphaFold: Group 1: Section 1; Group 2: Section 2; Group 3: Sections 3-4

13. ~~Zhong ED, Bepler T, Davis JH, Berger B. Reconstructing continuous distributions of 3D protein structure from cryo-EM images. arXiv preprint arXiv:1909.05215. 2019 Sep 11.~~

14. Wirnsberger P, Ballard AJ, Papamakarios G, Abercrombie S, Racanière S, Pritzel A, Jimenez Rezende D, Blundell C. Targeted free energy estimation via learned mappings. Journal of Chemical Physics. 2020 Oct 14;153(14).

15. Wang Y, Herron L, Tiwary P. From data to noise to data for mixing physics across temperatures with generative artificial intelligence. Proceedings of the National Academy of Sciences. 2022 Aug 9;119(32):e2203656119.

16. ~~Olivecrona M, Blaschke T, Engkvist O, Chen H. Molecular de-novo design through deep reinforcement learning. Journal of Cheminformatics. 2017 Dec;9(48):1-14.~~

17. Ying C, Cai T, Luo S, Zheng S, Ke G, He D, Shen Y, Liu TY. Do transformers really perform badly for graph representation? Advances in Neural Information Processing Systems. 2021 Dec 6;34:28877-88.

18. Kingma DP, Welling M. An introduction to variational autoencoders. Foundations and Trends in Machine Learning. 2019 Nov 27;12(4):307-92.

19. Gabrié M, Rotskoff GM, Vanden-Eijnden E. Adaptive Monte Carlo augmented with normalizing flows. Proceedings of the National Academy of Sciences. 2022 Mar 8;119(10):e2109420119.

20. Luo C. Understanding diffusion models: A unified perspective. arXiv preprint arXiv:2208.11970. 2022 Aug 25.