NOTES

Chapter 1: Introduction: Prediction, Understanding, and Deep Neural Networks

1. Chris Anderson, "The End of Theory," *WIRED*, July 2008, 109.
2. Drew Conway, "The Hubris of 'The End of Theory'," June 25, 2008, Wayback Machine, Internet Archive, https://web.archive.org/web/20081013021957/http://blogs.nyu.edu/blogs/agc282/zia/2008/06/the_hubris_of_the_end_of_theor.html
3. Skullsinthestars, "Rant Time: The End of Theory? (Updated)," July 8, 2008, https://skullsinthestars.com/2008/07/08/rant-time-the-end-of-theory/
4. Massimo Pigliucci, "The End of Theory in Science?," *EMBO Reports*, 10, no. 6 (2008), 534.
5. Richard Van Noorden and Jeffrey M. Perkel, "AI and Science: What 1,600 Researchers Think," *Nature*, 621 (2023), 674.
6. Paul Humphreys, "Why Automated Science Should Be Cautiously Welcomed," in Marta Bertolaso and Fabio Sterpetti (eds.), *A Critical Reflection on Automated Science: Will Science Remain Human?* (Cham: Springer, 2020), pp. 11–26.
7. Tycho Brahe, *Tychonis Brahe Dani Opera omnia*, ed. J. L. E. Dreyer (Copenhagen: Libraria Gyldendaliana, 1913–1929).
8. Johannes Kepler, *Johannes Kepler: Gesammelte Werke*, vol. XVII (Munich: C. H. Beck, 1937), p. 327.
9. Johannes Kepler, *Admonitis ad astronomos de raris mirisque anni 1631 phaenomenis* (Frankfurt: Gottfried Tampach, 1630).
10. Edmond Halley, "Methodus singularis qua solis parallaxis sive distantia a terra," *Philosophical Transactions of the Royal Society*, 29, no. 348 (1716), 454–464.

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11. James Cook, *Captain Cook's Journal during His First Voyage Round the World Made in H.M. Bark "Endeavor" 1768–71*, ed. W. J. L. Wharton (London: Elliot Stock, 1893), p. 76.
12. Thomas Hornsby, "The Quantity of the Sun's Parallax, as Deduced from the Observations of the Transit of Venus, on June 3, 1769," *Philosophical Transactions of the Royal Society*, 61 (1771), 579.
13. Leo Breiman, "Statistical Modeling: The Two Cultures," *Statistical Science*, 16, no. 3 (2021), 199–215.
14. Henk W. de Regt and Dennis Dieks, "A Contextual Approach to Scientific Understanding," *Synthese*, 144, no. 1 (2005), 137–170.

Chapter 2: AlphaFold: Prediction without Understanding

1. Cade Metz, "London A.I. Lab Claims Breakthrough That Could Accelerate Drug Discovery," *The New York Times*, November 30, 2020.
2. Ian Sample, "DeepMind AI Cracks 50-Year-Old Problem of Protein Folding," *The Guardian*, November 30, 2020.
3. A. E. Mirsky and Linus Pauling, "On the Structure of Native, Denatured, and Coagulated Proteins," *Proceedings of the National Academy of Sciences*, 22, no. 7 (1936), 439–447.
4. C. B. Anfinsen, E. Haber, M. Sela, and F. H. White, Jr., "The Kinetics of Formation of Native Ribonuclease During Oxidation of the Reduced Polypeptide Chain," *Proceedings of the National Academy of Sciences*, 47, no. 9 (1961), 1309–1314.
5. Linus Pauling and Robert B. Corey, "Atomic Coordinates and Structure Factors for Two Helical Configurations of Polypeptide Chains," *Proceedings of the National Academy of Sciences*, 37, no. 5 (1951), 235–240; and Linus Pauling and Robert B. Corey, "The Pleated Sheet, a New Layer

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Configuration of Polypeptide Chains," *Proceedings of the National Academy of Sciences*, 37, no. 5 (1951), 251–256.
6. Walter Kauzmann, "Some Factors in the Interpretation of Protein Denaturation," *Advances in Protein Chemistry*, 14 (1959), 1–63.
7. C. B. Anfinsen, "Studies on the Principles That Govern the Folding of Protein Chains," Nobel Lecture, December 11, 1972.
8. Cyrus Levinthal, "How to Fold Graciously," *Mössbauer Spectroscopy in Biological Systems Proceedings*, University of Illinois Bulletin, 67, no. 41 (1969), 22–24.
9. W. J. Browne et al., "A Possible Three-dimensional Structure of Bovine A-Lactalbumin Based on That of Hen's Egg-White Lysozyme," *Journal of Molecular Biology*, 42, no. 1 (1969), 71–86.
10. Mohammed AlQuraishi, "AlphaFold @ CASP13: 'What Just Happened?,'" Some Thoughts on a Mysterious Universe, December 9, 2018, https://moalquraishi.wordpress.com/2018/12/09/alphafold-casp13-what-just-happened/
11. John Jumper et al., "Highly Accurate Protein Structure Prediction with AlphaFold," *Nature*, 596 (2021), 583–589.
12. Brian Kuhlman et al., "Design of a Novel Globular Protein Fold with Atomic-Level Accuracy," *Science*, 302, no. 5649 (2003), 1364–1368.
13. Peter Haahr et al., "Actin Maturation Requires the ACTMAP/C19orf54 Protease," *Science*, 377, no. 6614 (2022), 1533–1537.
14. James P. Rooney and Sergey Ovchinnnikov, "State-of-the-Art Estimation of Protein Model Accuracy Using AlphaFold," *Physical Review Letters*, 129 (2022), 238101.
15. Google DeepMind, "AlphaFold: A Solution to a 50-Year-Old Grand Challenge in Biology," Google DeepMind blog, November 30, 2020, https://deepmind.google/blog/alphafold-a-solution-to-a-50-year-old-grand-challenge-in-biology/; Cade Metz, "London A.I. Lab Claims

Downloaded from https://www.cambridge.org/core. UNIVERSIDAD AUTONOMA METROPOLITANA, on 12 Nov 2026 at 08:19:31, subject to the Cambridge Core terms of use, available at https://www.cambridge.org/core/terms. https://www.cambridge.org/core/product/9C73F8F506E33BAAD682E48A61E510BA

Breakthrough That Could Accelerate Drug Discovery," *The New York Times*, November 30, 2020; Jonathan Chadwick, "50-Year-Old 'Protein Folding Problem' Is Finally SOLVED by Google-Owned AI in 'Stunning Advance' That Could Lead to Faster Drug Discoveries," *The Daily Mail*, December 1, 2020.

16. Ken A. Dill, S. Banu Ozkan, M. Scott Shell, and Thomas R. Weikl, "The Protein Folding Problem," *Annual Review of Biophysics*, 37 (2008), 289–316.
17. Gregory R. Bowman, "AlphaFold and Protein Folding: Not Dead Yet! The Frontier Is Conformational Ensembles," *Annual Review of Biomedical Data Science*, 7 (2024), 51–57.

Chapter 3: Physics: Learning from Networks

1. Mario Krenn et al., "Automated Search for New Quantum Experiments," *Physical Review Letters*, 16 (2016), 090405.
2. Mario Krenn, Jakob S. Kottmann, Nora Tischler, and Alán Aspuru-Guzik, "Conceptual Understanding Through Efficient Automated Design of Quantum Optical Experiments," *Physical Review X*, 11 (2021), 031044.
3. Mario Krenn et al., "On Scientific Understanding with Artificial Intelligence," *Nature Reviews Physics*, 4 (2022), 761–769.
4. Silviu-Marian Udrescu and Max Tegmark, "AI Feynman: A Physics-Inspired Method for Symbolic Regression," *Science Advances*, 6, no. 16 (2020), DOI: 10.1126/sciadv.aay2631
5. Miles Cranmer et al., "Discovering Symbolic Models from Deep Learning with Inductive Biases," 34th Conference on Neural Information Processing Systems, Vancouver, Canada, 2020, https://proceedings.neurips.cc/paper_files/paper/2020

Downloaded from https://www.cambridge.org/core. UNIVERSIDAD AUTONOMA METROPOLITANA, on 12 Nov 2026 at 08:19:31, subject to the Cambridge Core terms of use, available at https://www.cambridge.org/core/terms. https://www.cambridge.org/core/product/9C73F8F506E33BAAD682E48A61E510BA

6. Pablo Lemos et al., "Rediscovering Orbital Mechanics with Machine Learning," *Machine Learning: Science and Technology*, 4, no. 4 (2023), 045002.
7. Raban Iten, *Artificial Intelligence for Scientific Discoveries: Extracting Physical Concepts from Experimental Data Using Deep Learning* (Cham: Springer, 2023).
8. Raban Iten et al., "Discovering Physical Concepts with Neural Networks," *Physical Review Letters*, 124 (2020), 010508.
9. P. Baldi, P. Sadowski, and D. Whiteson, "Searching for Exotic Particles in High-Energy Physics with Deep Learning," *Nature Communications*, 5 (2014), 4308.
10. Philippe Gras et al., "Systematics of Quark/Gluon Tagging," *Journal of High Energy Physics*, (2017), 91.
11. Eric M. Metodiev and Jesse Thaler, "Jet Topics: Disentangling Quarks and Gluons at Colliders," *Physical Review Letters*, 120 (2018), 241602.
12. Patrick T. Komiske, Eric M. Metodiev, and Jesse Thaler, "Energy Flow Networks: Deep Sets for Particle Jets," *Journal of High Energy Physics* (2019), 121.
13. Andy Arditi et al., "Refusal in Language Models Is Mediated by a Single Direction," 38th Conference on Neural Information Processing Systems, Vancouver, Canada, 2024, https://proceedings.neurips.cc/paper_files/paper/2024
14. Adly Templeton et al., "Scaling Monosemanticity: Extracting Interpretable Features from Claude 3 Sonnet," Transformer Circuits Thread, 2024, https://transformer-circuits.pub/2024/scaling-monosemanticity/
15. Rio Alexa Fear et al., "Physics Steering: Causal Control of Cross-Domain Concepts in a Physics Foundation Model," arXiv, 2025, https://doi.org/10.48550/arXiv.2511.20798

Downloaded from https://www.cambridge.org/core. UNIVERSIDAD AUTONOMA METROPOLITANA, on 12 Nov 2026 at 08:19:31, subject to the Cambridge Core terms of use, available at https://www.cambridge.org/core/terms. https://www.cambridge.org/core/product/9C73F8F506E33BAAD682E48A61E510BA

16. Neel Nanda et al., "A Pragmatic Vision for Interpretability," AI Alignment Forum, December 1, 2025, www.alignmentforum.org/posts/StENzDcD3kpfGJssR/a-pragmatic-vision-for-interpretability
17. Keyon Vafa et al., "Evaluating the World Model Implicit in a Generative Model," 38th Conference on Neural Information Processing Systems, Vancouver, Canada, 2024, https://proceedings.neurips.cc/paper_files/paper/2024
18. Keyon Vafa, Peter G. Chang, Ashesh Rambachan, and Sendhil Mullainathan, "What Has a Foundation Model Found? Using Inductive Bias to Probe for World Models," arXiv, 2025, https://doi.org/10.48550/arXiv.2507.06952
19. Florian J. Boge and Henk W. de Regt, "Machine Learning Discoveries and Scientific Understanding in Particle Physics: Problems and Prospects," in Juan M. Durán and Giorgia Pozzi (eds.), *Philosophy of Science for Machine Learning: Core Issues and New Perspectives* (Cham: Springer, 2026), 403–434.
20. Cameron Buckner, "Understanding Adversarial Examples Requires a Theory of Artefacts for Deep Learning," *Nature Machine Intelligence*, 2 (2020), 731–736.
21. Christian Szegedy et al., "Intriguing Properties of Neural Networks," arXiv, 2014, https://doi.org/10.48550/arXiv.1312.6199
22. Ted Chiang, *Story of Your Life and Others* (New York: Vintage, 2016), 91–145.
23. Julius Adebayo et al., "Sanity Checks for Saliency Maps," 32nd Conference on Neural Information Processing Systems, Vancouver, Canada, 2018, https://proceedings.neurips.cc/paper_files/paper/2018
24. Lisa Schut et al., "Bridging the Human–AI Knowledge Gap Through Concept Discovery and Transfer in AlphaZero," *Proceedings of the National Academy of Sciences*, 122, no. 13 (2025), e2406675122.

Downloaded from https://www.cambridge.org/core. UNIVERSIDAD AUTONOMA METROPOLITANA, on 12 Nov 2026 at 08:19:31, subject to the Cambridge Core terms of use, available at https://www.cambridge.org/core/terms. https://www.cambridge.org/core/product/9C73F8F506E33BAAD682E48A61E510BA

25. Richard Sutton, "The Bitter Lesson," March 13, 2019, www.incompleteideas.net/IncIdeas/BitterLesson.html
26. Tess E. Smidt, Mario Geiger, and Benjamin Kurt Miller, "Finding Symmetry Breaking Order Parameters with Euclidean Neural Networks," *Physical Review Research*, 3 (2021), L012002.

Chapter 4: Neuroscience: Letting Go of the Dream

1. Alison Gopnik, "Explanation as Orgasm," *Minds and Machines*, 8 (1998), 101–118.
2. John M. Harlow, "Passage of an Iron Rod Through the Head," *The Boston Medical and Surgical Journal*, 34, no. 20 (1849), 389–393.
3. John M. Harlow, *Recovery from the Passage of an Iron Bar through the Head* (Boston: David Clapp & Son, 1869), p. 14.
4. Carl Craver, *Explaining the Brain: Mechanisms and the Mosaic Unity of Neuroscience* (Oxford: Oxford University Press, 2007).
5. Stephen W. Kuffler, "Discharge Patterns and Functional Organization of the Mammalian Retina," *Journal of Neurophysiology*, 16, no. 1 (1953), 37–68.
6. D. H. Hubel and T. N. Wiesel, "Receptive Fields of Single Neurones in the Cat's Striate Cortex," *The Journal of Physiology*, 148, no. 3 (1959), 574–591.
7. D. H. Hubel and T. N. Wiesel, "Receptive Fields, Binocular Interaction and Functional Architecture in the Cat's Visual Cortex," *The Journal of Physiology*, 160, no. 1 (1962), 106–154.
8. James J. Jun et al., "Fully Integrated Silicon Probes for High-Density Recording of Neural Activity," *Nature*, 551 (2017), 232–236.

Downloaded from https://www.cambridge.org/core. UNIVERSIDAD AUTONOMA METROPOLITANA, on 12 Nov 2026 at 08:19:31, subject to the Cambridge Core terms of use, available at https://www.cambridge.org/core/terms. https://www.cambridge.org/core/product/9C73F8F506E33BAAD682E48A61E510BA

9. Sven Dorkenwald et al., "Neuronal Wiring Diagram of an Adult Brain," *Nature*, 634 (2025), 124–138.
10. Eric Jonas and Konrad Paul Kording, "Could a Neuroscientist Understand a Microprocessor?," *PLOS Computational Biology*, 13 no. 1 (2017), e1005268.
11. Bruno A. Olshauen and David J. Field, "What Is the Other 85 Percent of V1 Doing?," in J. Leo van Hemmen and Terrence J. Sejnowski (eds.), *23 Problems in Systems Neuroscience* (Oxford: Oxford University Press, 2006), pp. 182–212.
12. Shinji Nishimoto et al., "Reconstructing Visual Experiences from Brain Activity Evoked by Natural Movies," *Current Biology*, 21 (2011), 1641–1646.
13. Maitreyee Wairagkar et al., "An Instantaneous Voice-Synthesis Neuroprosthesis," *Nature*, 644 (2025), 145–152.
14. Frank Rosenblatt, "The Perceptron: A Probabilistic Model for Information Storage and Organization in the Brain," *Psychological Review*, 65, no. 6 (1959), 386–408.
15. Daniel L. K. Yamins et al., "Performance-Optimized Hierarchical Models Predict Neural Responses in Higher Visual Cortex," *Proceedings of the National Academy of Sciences*, 111 no. 23 (2014), 8619–8624.
16. Seyed-Mahdi Khaligh-Razavi and Nikolaus Kriegeskorte, "Deep Supervised, But Not Unsupervised, Models May Explain IT Cortical Representation," *PLOS Computational Biology*, 10, no. 11 (2014), e1003915.
17. Pouya Bashivan, Kohitij Kar, and James J. DiCarlo, "Neural Population Control Via Deep Image Synthesis," *Science*, 364 (2019), eaav9436.
18. Bashivan, Kar, and DiCarlo, "Neural Population Control," 1.
19. Blake A. Richards et al., "A Deep Learning Framework for Neuroscience," *Nature Neuroscience*, 22 (2019), 1761–1770.

Downloaded from https://www.cambridge.org/core. UNIVERSIDAD AUTONOMA METROPOLITANA, on 12 Nov 2026 at 08:19:31, subject to the Cambridge Core terms of use, available at https://www.cambridge.org/core/terms. https://www.cambridge.org/core/product/9C73F8F506E33BAAD682E48A61E510BA

20. Eva Dyer and Blake Richards, "Accepting 'the Bitter Lesson' and Embracing the Brain's Complexity," *The Transmitter*, March 26, 2025.
21. Eric Y. Wang et al., "Foundation Model of Neural Activity Predicts Response to New Stimulus Types," *Nature*, 640 (2025), 470–477.

Chapter 5: Conclusion: The Rise of AI Scientists

1. Federico Bianchi et al., "Exploring the Use of AI Authors and Reviewers at Agents4Science," *Nature Biotechnology*, 44 (2026), 11–14.
2. David Adam, "The AI Co-scientist Is Here," *Nature Medicine*, 32 (2026), 772.
3. Matthew Schwartz, "Vibe Physics: The AI Grad Student," Anthropic, March 23, 2026, www.anthropic.com/research/vibe-physics
4. Ted Chiang, "Catching Crumbs from the Table," *Nature*, 405 (2000), 517.

Downloaded from https://www.cambridge.org/core. UNIVERSIDAD AUTONOMA METROPOLITANA, on 12 Nov 2026 at 08:19:31, subject to the Cambridge Core terms of use, available at https://www.cambridge.org/core/terms. https://www.cambridge.org/core/product/9C73F8F506E33BAAD682E48A61E510BA