MBM Essay 1: Human

Reverse-Engineering Brain Mechanisms through Explainable AI

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Part I

The Symbiotic Evolution of AI and Neuroscience: A Historical Perspective

1 Introduction

The human brain is the most complex computational machine known to mankind. As such, philosophers and scientists have been fascinated by it for centuries, and have put great effort into trying to understand how its billions of neurons, working together, can create thoughts, perceptions, and consciousness.

This essay will look at the closely connected history of Artificial Intelligence (AI) and Neuroscience, two symbiotic fields that often take inspiration from each other. From the earliest attempts to create computational models based on neural processes to the cutting-edge use of explainable neural networks to better our understanding of the brain's complex mechanisms, progress in one domain has consistently spurred innovation in the other. We will follow this shared evolution, looking at how ideas from Neuroscience have influenced AI designs, and how AI now gives us new tools and ways to think about reverse-engineering the brain. The discussion will culminate in a review of the current state-of-the-art in this field and a look towards future directions where this collaboration promises to yield even deeper understanding of both biological and artificial intelligence.

The essay is structured as follows: Part I will begin with a historical review, charting the dawn of AI and early neural models, the rise of connectionism, and the transformative impact of the deep learning revolution on neuroscience. Part II will delve into the "black box" problem inherent in many complex AI models and the subsequent birth of Explainable AI (XAI), detailing various methodologies and their crucial applications in closing the gap between AI performance and neuroscientific understanding. Finally, Part III will assess the current frontiers, discussing generative models, the shift beyond supervised learning, the rise of "Neuro-AI", and the use of large language models to simulate thought processes, while also considering the challenges, limitations, and ethical considerations inherent in this rapidly evolving field.

2 The Dawn of AI and Early Neural Models (1940s-1960s)

The foundational period of AI, spanning from the 1940s to the 1960s, was marked by pioneering efforts to conceptualize and model neural processes mathematically. A seminal contribution during this era was the McCulloch-Pitts neuron, introduced in 1943 [1]. This model presented a simplified, logical abstraction of a biological neuron, proposing that neurons could be understood as computational units performing logical operations. Although a simplification of true neuronal complexity, the McCulloch-Pitts neuron was a groundbreaking concept. It laid crucial groundwork for both the nascent field of AI, by suggesting that machines could, in principle, perform tasks analogous to human thought, and for computational neuroscience, by providing a formal framework to begin modeling neural activity and networks.

Building on the idea of interconnected processing units, Donald Hebb, in his influential 1949 work, "The Organization of Behavior" [2], proposed a mechanism for learning in the brain. His famous postulate, often summarized as "neurons that fire together, wire together," introduced the concept of synaptic plasticity. Hebbian learning suggested that the strength of a connection between two neurons increases when they are activated simultaneously. This principle was profoundly influential, offering a plausible biological basis for how learning and memory could arise from neural activity and directly inspiring early learning algorithms in artificial neural networks. It provided a dynamic element to the static connections of earlier models, suggesting

how networks could adapt and learn from experience.

Furthering the development of learning machines, Frank Rosenblatt introduced the Perceptron in 1958 [3]. The Perceptron was a more concrete implementation of a learning neural network, capable of learning to classify patterns by adjusting its synaptic weights based on errors. This invention generated considerable excitement, as it demonstrated a machine that could learn from data and perform pattern recognition tasks, a key aspect of intelligence. The Perceptron's architecture and learning rule were seen as analogous to early models of sensory processing in the brain, particularly in how simple features might be detected and combined to recognize more complex stimuli. It represented a significant step towards building practical AI systems inspired by neural principles.

Despite these early successes and the initial optimism, the field soon encountered significant challenges. In 1969, Marvin Minsky and Seymour Papert published "Perceptrons" [4], a detailed mathematical analysis that highlighted severe limitations of single-layer Perceptrons, most notably their inability to solve problems that were not linearly separable, such as the XOR problem. This critique, coupled with exaggerated claims and unmet expectations, led to a significant reduction in funding and interest in neural network research, a period often referred to as the first "AI winter." However, the foundational ideas laid during these early decades were not entirely abandoned. They simmered beneath the surface, awaiting new algorithmic breakthroughs and computational power that would eventually lead to a resurgence and the development of more powerful, multi-layered neural networks in the decades to follow.

3 Connectionism and the Rise of Parallel Distributed Processing (1980s)

After the "AI winter," the 1980s witnessed a significant resurgence of interest in neural networks, largely fueled by the emergence of connectionism and the concept of Parallel Distributed Processing (PDP). Central to this revival was the work of the PDP Research Group, particularly David Rumelhart, Geoffrey Hinton, and James McClelland. Their influential two-volume book, "Parallel Distributed Processing: Explorations in the Microstructure of Cognition" [5], often referred to as the "Connectionist Bible," provided a comprehensive theoretical framework and compelling demonstrations of neural network capabilities. This work emphasized how complex cognitive phenomena could emerge from the parallel interactions of many simple processing units, akin to neurons. Connectionist models proposed that information was not stored in specific locations but distributed across connections, and that learning occurred through the modification of these connection strengths. This period also saw the popularization of ideas related to the capabilities of multi-layer networks.

A critical breakthrough that enabled the practical training of these more complex, multilayer networks was the popularization and refinement of the backpropagation algorithm, notably described by Rumelhart, Hinton, and Williams in 1986 [6]. While the core ideas of backpropagation had been explored earlier by others, their work made it accessible and demonstrated its power. Backpropagation provided an efficient method for calculating the gradient of the error function with respect to the network's weights, allowing for the systematic adjustment of these weights to minimize error. This meant that networks with hidden layers, which were previously difficult to train, could now learn complex input-output mappings. The ability to train multilayer networks was a game-changer, as these architectures could overcome the limitations of single-layer perceptrons identified by Minsky and Papert, enabling the modeling of non-linear relationships and, consequently, more sophisticated cognitive functions.

The advancements in network architectures and training algorithms led to a wave of early applications in cognitive science, where PDP models were used to simulate and offer insights into a variety of human cognitive processes. For instance, connectionist models were developed to explore language acquisition, demonstrating how networks could learn grammatical structures

and past tense formation from exposure to linguistic data. Other models addressed aspects of memory, such as pattern completion and content-addressable recall, showing how distributed representations could lead to robust and flexible memory systems. In the realm of perception, these models were applied to tasks like object recognition and speech perception, providing computational accounts of how the brain might process sensory information. These early applications, while often simplified, were crucial in demonstrating the potential of neural networks as tools for understanding the mind and brain, bridging the gap between abstract computational principles and observable cognitive phenomena [5].

4 The Deep Learning Revolution and its Impact on Neuroscience (2000s-Present)

The turn of the millennium marked the beginning of a new era for AI, largely characterized by the rise of deep learning. This revolution, which gained significant momentum from the 2000s onwards, has had a profound and reciprocal impact on neuroscience. The convergence of several key factors led to what some have termed the "unreasonable effectiveness" of deep learning models [7]. Firstly, the availability of massive datasets, such as ImageNet, provided the rich training material necessary for complex models to learn intricate patterns. Secondly, the parallel development and widespread adoption of powerful Graphics Processing Units (GPUs) offered the computational horsepower required to train these data-hungry and computationally intensive deep neural networks in a feasible timeframe. This combination of big data and powerful hardware unlocked the potential of deep learning architectures, allowing them to achieve state-of-the-art performance on a wide range of tasks, from image recognition to natural language processing, and in doing so, provided new, powerful tools for neuroscientific inquiry [8].

Among the most influential deep learning architectures for neuroscience have been Convolutional Neural Networks (CNNs). Initially inspired by the hierarchical processing observed in the mammalian visual cortex, particularly the work of Hubel and Wiesel on simple and complex cells, CNNs have demonstrated remarkable success in computer vision tasks. These networks typically consist of multiple layers, including convolutional layers that apply filters to input images to detect features, pooling layers that reduce dimensionality, and fully connected layers that perform classification. The hierarchical nature of CNNs, where early layers learn simple features like edges and textures, and deeper layers learn more complex and abstract representations like object parts and eventually whole objects, bears a striking resemblance to the processing stages in the primate visual pathway [9]. This architectural similarity has made CNNs invaluable tools for modeling the visual cortex. Neuroscientists have used them not only to predict neural responses to visual stimuli with unprecedented accuracy but also to generate hypotheses about how visual information is represented and transformed in the brain [10, 11]. By comparing the internal representations of CNNs trained on visual tasks with neural recordings from different stages of the visual system, researchers have found compelling correspondences, suggesting that these artificial models might capture fundamental principles of biological vision.

Similarly, Recurrent Neural Networks (RNNs) have provided powerful models for understanding how the brain processes sequential data, such as language or temporal patterns in sensory input. Unlike feedforward networks like CNNs, RNNs possess connections that loop back on themselves, allowing them to maintain an internal state or "memory" of past inputs. This characteristic makes them well-suited for tasks where context and temporal dependencies are crucial. In neuroscience, RNNs have been employed to model various cognitive functions involving sequential processing, including working memory, decision-making over time, and motor control. For instance, they have been used to simulate how neural populations might integrate information over time to reach a decision or how motor commands are generated in a coordinated sequence. The ability of RNNs, particularly variants like Long Short-Term Memory (LSTM) networks and Gated Recurrent Units (GRUs) which can learn long-range dependen-

cies, to capture complex temporal dynamics has made them instrumental in exploring the neural mechanisms underlying time-sensitive cognitive processes [8]. The insights gained from these models are helping to bridge the gap between neural activity and dynamic cognitive behaviors.

Part II

The Black Box Dilemma and the Rise of Explainable AI (XAI)

5 The "Black Box" Problem in Deep Learning

- **Defining the Challenge:** While deep neural networks achieve impressive performance, their internal workings are often opaque and difficult to understand.
- Implications for Scientific Discovery: In the context of neuroscience, a "black box" model that mimics brain function without revealing *how* it does so offers limited scientific insight. The goal is not just to replicate but to understand the underlying principles.

6 A Taxonomy of Explainable AI Methods

- Post-hoc vs. Intrinsically Explainable Models: Differentiate between methods that analyze a trained model and those that are designed to be transparent from the outset.
- Feature Attribution Methods:
 - Saliency Maps: Visualizing which input features (e.g., pixels in an image) are most important for a model's prediction.
 - LIME (Local Interpretable Model-agnostic Explanations) and SHAP (SHapley Additive exPlanations): Explain how these methods build simpler, interpretable local models to approximate the behavior of the complex "black box" model.

• Model-based Interpretation:

- Analyzing Network Activations and Representations: Techniques for visualizing and understanding the features learned by different layers of a network.
- Causal Intervention and "Ablation" Studies: Simulating lesion studies in neuroscience by deactivating specific neurons or connections in the network to observe the effect on its output.

7 Explainable AI in Action: Bridging the Gap to Neuroscience

- Reverse-Engineering Sensory Systems:
 - Vision: Beyond object recognition, how XAI helps us understand how CNNs represent texture, shape, and motion, and how this compares to neural data from different visual areas.
 - Audition: Using deep learning models to understand the neural coding of sound, from the cochlea to the auditory cortex.
- **Decoding and Encoding Models:** Using explainable models to predict neural activity from stimuli (encoding) and to decode mental states or perceived stimuli from neural recordings (decoding).
- Understanding Higher Cognitive Functions:

- Language: Analyzing the representations within large language models (LLMs) like BERT and GPT, and comparing them to the brain's language processing centers (e.g., Broca's and Wernicke's areas).
- Decision-Making and Reinforcement Learning: How explainable reinforcement learning models can shed light on the neural circuits involved in reward, planning, and action selection.

Part III

The State of the Art and the Future of Brain-Inspired AI

8 Current Frontiers in Explainable Neural Networks for Neuroscience

- Generative Models and "In Silico" Experiments: Using generative adversarial networks (GANs) and other generative models to create stimuli that maximally activate specific neurons or brain regions, allowing for more targeted experiments.
- **Beyond Supervised Learning:** The role of self-supervised and unsupervised learning in creating models that learn more brain-like representations without requiring massive labeled datasets.
- The Rise of "Neuro-AI": The growing field of research that explicitly aims to build AI systems based on principles from neuroscience, creating a virtuous cycle of discovery.
- Thinking LLMs and Simulating Thought Processes: Discussing the emerging use of large language models to model and understand human-like reasoning, planning, and problem-solving.

9 Challenges, Limitations, and Ethical Considerations

- The "Simile" vs. "Model" Distinction: Emphasize that even the most brain-like ANNs are still simplifications. Discuss the key biological details they often omit (e.g., dendritic computation, neuromodulation).
- The Dangers of Over-interpretation: The risk of drawing premature or overly simplistic conclusions about the brain based on analogies with AI models.
- Data Privacy and Neuromarketing: Briefly touch on the ethical implications of being able to decode brain states with increasing accuracy.

10 Conclusion: The Future of a Fruitful Partnership

- Recap of the Main Arguments: Summarize the historical co-evolution and the current state of synergy between AI and neuroscience.
- Future Outlook: Project how this interdisciplinary collaboration will continue to unravel the complexities of the brain and, in turn, inspire more general and capable artificial intelligence. The ultimate goal: a unified theory of intelligence, both biological and artificial.
- Final Thought-Provoking Statement: Reiterate the profound potential of this research to not only advance science but also to fundamentally alter our understanding of ourselves.

References

- [1] Warren S McCulloch and Walter Pitts. "A logical calculus of the ideas immanent in nervous activity". In: *The bulletin of mathematical biophysics* 5.4 (1943), pp. 115–133.
- [2] Donald Olding Hebb. The organization of behavior: A neuropsychological theory. Wiley, 1949.
- [3] Frank Rosenblatt. "The perceptron: a probabilistic model for information storage and organization in the brain". In: *Psychological review* 65.6 (1958), p. 386.
- [4] Marvin Minsky and Seymour Papert. Perceptrons: An introduction to computational geometry. MIT press, 1969.
- [5] James L McClelland, David E Rumelhart, and PDP Research Group. *Parallel distributed processing: Explorations in the microstructure of cognition, vol. 2.* MIT press, 1986.
- [6] David E Rumelhart, Geoffrey E Hinton, and Ronald J Williams. "Learning representations by back-propagating errors". In: *Nature* 323.6088 (1986), pp. 533–536.
- [7] Yann LeCun, Yoshua Bengio, and Geoffrey Hinton. "Deep learning". In: *Nature* 521.7553 (2015), pp. 436–444.
- [8] Blake A Richards et al. "A deep learning framework for neuroscience". In: *Nature neuroscience* 22.11 (2019), pp. 1761–1770.
- [9] Daniel L Yamins and James J DiCarlo. "Using goal-driven deep learning models to understand sensory cortex". In: *Nature neuroscience* 19.3 (2016), pp. 356–365.
- [10] Nikolaus Kriegeskorte and Pamela K Douglas. "Cognitive computational neuroscience". In: *Nature Neuroscience* 21.9 (2018), pp. 1148–1160.
- [11] Neil Savage. "How AI is helping to explain the brain". In: Nature 571.7766 (2019), S16–S18.
- [12] Marco Tulio Ribeiro, Sameer Singh, and Carlos Guestrin. "Why should I trust you?": Explaining the predictions of any classifier". In: *Proceedings of the 22nd ACM SIGKDD international conference on knowledge discovery and data mining.* 2016, pp. 1135–1144.
- [13] Scott M Lundberg and Su-In Lee. "A unified approach to interpreting model predictions". In: Advances in neural information processing systems. 2017, pp. 4765–4774.
- [14] Chris Olah et al. "The building blocks of interpretability". In: Distill 3.3 (2018), e10.
- [15] Finale Doshi-Velez and Been Kim. "Towards a rigorous science of interpretable machine learning". In: arXiv preprint arXiv:1702.08608 (2017).
- [16] Tim Miller. "Explanation in artificial intelligence: Insights from the social sciences". In: *Artificial Intelligence* 267 (2019), pp. 1–38.
- [17] Patrick McClure and Nikolaus Kriegeskorte. "How to compare representations in brains and machines". In: bioRxiv (2024), pp. 2024–01.
- [18] Ruth C Fong and Andrea Vedaldi. "Interpretable explanations of black boxes by meaningful perturbation". In: *Proceedings of the IEEE international conference on computer vision*. 2017, pp. 3429–3437.
- [19] David Bau et al. "Network dissection: Quantifying interpretability of deep visual representations". In: *Proceedings of the IEEE conference on computer vision and pattern recognition*. 2017, pp. 6541–6549.
- [20] Martin Schrimpf et al. "Brain-Score: A framework for comparing computational models of the brain". In: bioRxiv (2020).

- [21] Mariya Toneva and Leila Wehbe. "Interpreting and improving natural language processing models for neuro-imaging analyses". In: Advances in Neural Information Processing Systems. 2019, pp. 14382–14392.
- [22] Charlotte Caucheteux and Jean-R'emi King. "Brains and algorithms partially converge in natural language processing". In: Communications Biology 5.1 (2022), pp. 1–12.
- [23] Jason Wei et al. "Chain of thought prompting elicits reasoning in large language models". In: arXiv preprint arXiv:2201.11903 (2022).
- [24] Marcel Binz and Eric Schulz. "Using cognitive psychology to understand large language models". In: *Nature Reviews Psychology* 2.7 (2023), pp. 385–386.
- [25] Kyle Mahowald et al. "Dissociating language and thought in large language models: a cognitive perspective". In: arXiv preprint arXiv:2301.06627 (2023).