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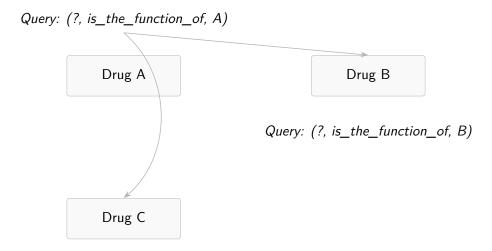
I Structure, 17

Part I Structure,

When modelling our surroundings, we construct concepts, judgments, and ourselves.

One key characteristic of intelligent behaviours is their structured nature – acting on groups of similar objects in systematic and consistent ways, assembling small actions into larger tasks, and producing controllable outcomes. In human cognition, structures allow us to efficiently organize, remember, and recall information about the reality that is important and interesting to our survival and well-being in the world. With structures, we can make valid logical inferences in similar scenarios and generate conclusions reliably given the same premises. Likewise in intelligent systems, understanding structures is essential because it underpins efficient knowledge representation, which allows composing complex reasoning chains with smaller ones, and producing reliable outcomes given repeatable queries. Recognizing the importance of structures for both human and machine intelligence, we now turn to the two main paradigms for constructing AI knowledge engines – structured and unstructured – which, as their names suggest, approach structures in fundamentally different ways.

Structured approaches, exemplified by knowledge graphs and expert systems, predefine structures by manually specifying how entities (subjects or objects) relate to one another with different relations (predicates). This allows the same predicates to be applied consistently across similar subject-object pairs, enabling systematic manipulation of entities and relations. For instance, if we want to infer the function of a drug A, we can query a knowledge graph with something akin to "(?, _is_the_function_of, A)." This query pattern can systematically be reused to search for the functions of other drugs, such as B, C, D, etc., simply by substituting the query object. In a nutshell, the knowledge graph approach is equivalent to manually *structuring* the reality of an artificial intelligence agent: it segments the reality into discrete units, conceptualizes them as named entities, and organizes these entities into hierarchies or relational networks.



Query: (?, is_the_function_of, C)

Figure 1: Knowledge graphs use predicates to define entity relationships, enabling the reuse of semantic structures like is_the_function_of across entities. This supports consistent inference over symbolic concepts.

On the other hand, the unstructured approaches, prominently featuring large language models (LLMs) trained on massive web corpora, do not prescribe any explicit structure. Continuing the drug search example above, in the unstructured approach, the relation "_is_the_function_of" can manifest in various forms with potential noise and lack a standarised reference identifier. Similarly, the drugs themselves do not adhere to a fixed or standardized naming structure. For instance, a drug search query posed to large language models might be expressed in natural and ambiguous terms: "Do you know when to use A-acid?". In this scenario, the model will retrieve information about the drug A through internal implicit associations, instead of utilizing a predefined predicate. The LLM (unstructured) approach, therefore, does not seem to *structure* reality in advance or impose standardised relation predicates to its training data.

However, this part of the thesis demonstrates that, regardless of whether a structure is predefined or not, training with a language modelling objective induces inherent structures within the final embedding-encapsulated model, which serves as the bedrock for both structured and unstructured approaches. These emergent structures enable the model to recover meaningful relational patterns¹ – pertaining to the realities underlying the data – solely based on the model's learned parameters. The following chapters dive into the details for both structured knowledge completion with language modelling and completion and structural pattern emergence in large language models. Concretely,

- 1. **Chapter 2**: We show how a language modelling objective can help recover the structure of knowledge graphs and predict the missing links, thereby completing the knowledge base and supporting downstream knowledge queries. The language modelling objective can thus be a good alternative to classic structural recovery objectives, like entity prediction.
- 2. **Chapter 3**: We demonstrate how similar language modelling objectives also induce structural patterns in transformer computation, which can then be extracted and applied to enhance interpretability, transparency and safety within foundational large language models.

By examining the effects of language modelling objectives on structure formation, we find that even models from unstructured approaches acquire structures about the realities underlying the data, supporting themselves to store knowledge and to behave in

¹Sequential patterns can be seen as hyper-relational edges on a graph.

the absence of predefined schematic structures. This connection between structured and unstructured approaches allows us to understand structure formation and highlight its particular role in achieving artificial intelligence, guiding our decisions on 1) when and why to incorporate structures – such as for the purpose of efficient knowledge representation, post-training interpretability, repeatable queries with consistent conclusions, and 2) how to induce structures – either explicitly through predefined structures in data for "shallow" model training or implicitly by training deep models on large corpora.

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