A Dual-Process Approach for Automated Knowledge Creation

Protocol Labs Research

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Abstract: Scientific knowledge growth combines elements of existing theories into new proposed models, which is combinatorially intractable. **Inspired by dual-system psychological theories, we conceptualize a knowledge creation process in two stages. Stage One** narrows the space of existing computational elements based on contextual queues, supplying components from which a new model will be proposed. It is trained on large datasets but is computationally inexpensive at runtime. **Stage Two** permutes these elements in accordance with their explicit constraints, resulting in a set of proposed computable theories. We have developed a system that implements Stage Two. This system provides robust infrastructure for expressing constraints imposed by scientific theories, supplying a framework relating theory sub-graphs to experimental datasets stored in relational databases. We demonstrate an implementation of this two-stage approach solving materials chemistry problems using experimental datasets.

1. An overview of Dual-Process Theories

Theories across several fields within psychology have identified two distinct types of cognitive process. Type I Processes are automatic, use implicit knowledge, operate quickly, and provide intuitive results based on subconscious cognition. Type II processes are deliberative, use explicit knowledge, operate slowly, and require conscious effort. These processes frequently work synergistically, but evidence of their distinct workings appears in situations where the two offer conflicting solutions. Type I processes frequently respond to complex tasks by using simple heuristics that often contradict deliberative Type II responses. By manipulating priming effects informing these heuristics, competing decision making processes can be assessed (Lucas 2005). Evidence for this dualism has been found in the study of reasoning (Wason 1974, Evans 2006), decision making (Van Gelder 2014, Motro 2018, Dhar 2013), learning and memory (Smith 2000), social psychology (Wilson 2000, Hochman 2015, Strack 2015), and the development of metacognition (Amsel 2008).

In this work we are inspired by the parallels between a generalized Type I psychological process and many existing machine learning approaches (see Table 1). However, corresponding representations of scientific theories analogous to Type II processes are undeveloped. The apparent utility of synergistic processing between the two psychological systems suggests that development of these "Stage II" approaches may allow interoperability between implicit and explicit theories when applying machine learning approaches to scientific datasets.

Type I Psychological Processes	Proposed Stage I	Type II Psychological Processes	Proposed Stage II
Unconscious mental processes	Neural Networks, Statistical Methods	Conscious mental processes	Explicit representations of theories
Evolutionarily old	Decades-old techniques	Evolutionarily Recent	General solutions non-existent
Fast, parallel	Fast at runtime	Slow, sequential, limited by working memory	Combinatorially limited
Inductive, Heuristic	Correlational	Deductive, Analytic	Logical
Implicit, Language-independent	'Black box'	Explicit, Language-based	Human-readable
Trained continuously over lifetime	Trained using large datasets	Models may be immediately remembered	Rules may be explicitly encoded
Shared with animals	Neural Networks	Distinctively human	?

Table 1: a comparison of dual-process theories in psychology with the proposed dual-stage automated knowledge generation system.

2. A Dual-Process Computational Approach for Science

In most scientific fields there is a **persistent computability gap** between the theories and models used in experimental design on one hand, and the datasets generated by these experiments on the other (figure 1). Explicit mental models are typically described in lab books and written documents but are rarely translated into a computable format.

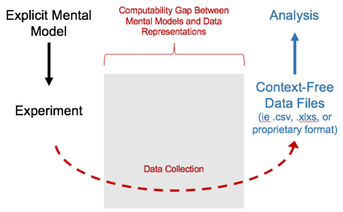


Figure 1: the computability gap in scientific datasets

Developing tools that allow researchers to easily input general mental models of experiments in a computable form has the potential to solve several important research problems by serving as a computable 'Type II' model. These problems include (1) improving the efficiency of data analysis by allowing improved search capabilities, (2) leveraging institutional knowledge across an organization and among distant collaborators, and (3) the potential for closed-loop automated knowledge generation processes that produce **cogent insights** rather than black-box correlational results.

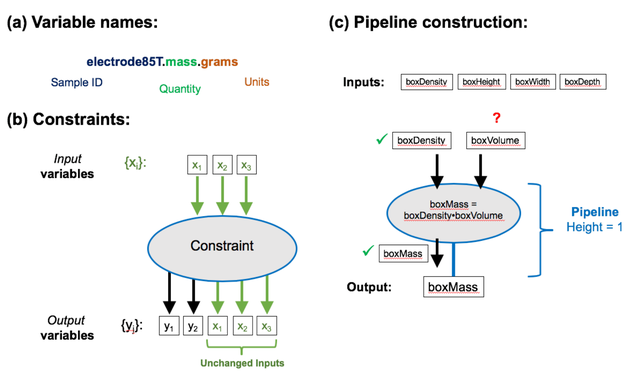


Figure 2: construction of pipelines to solve specific problems by leveraging constraints

3. Constraint-Pipeline Systems for Representing Explicit Knowledge

We have implemented a generalized system for representing scientific knowledge across domains shown in Figure 2. In this system, a **Schema** consists of a set of **Variables** representing quantities or abstract objects and **Constraints** representing relationships between these objects. **Variables** participate in a hierarchical namespace as shown in Figure 2 (a). **Constraints** relate a set of input ***Variables*** to a set of output **Variables** as shown in Figure 2 (b). These **Constraints** may correspond to simple algebraic operations or to any more abstract function. A problem may be posed to the **Schema** in the form of a set of input and output **Variables**. The function schema.plan() will then attempt to find a **Pipeline**, or a sequence of **Constraints**, that solves for the output **Variables** as a function of input **Variables** as illustrated in Figure 2 (c). **A list of successful pipelines representing this Schema's solutions to the posed problem, are exported as outputs. All of these objects can be exported and imported using JSON serialization**, in order to support efficient sharing and transfer between different solver implementations.

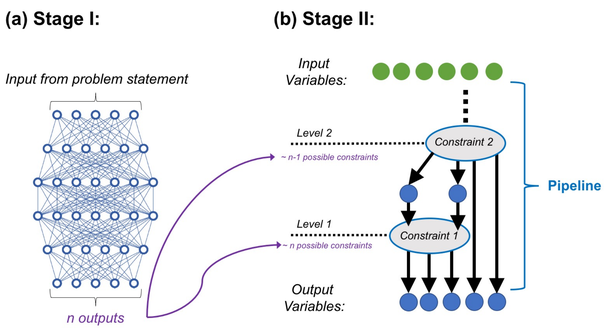


Figure 3 (above): (a-b) A comparison of the first and second stages in the proposed dual-stage process. (c) A comparison of this process to a heuristic-analytic dual process model from the literature (Evans, 2006).

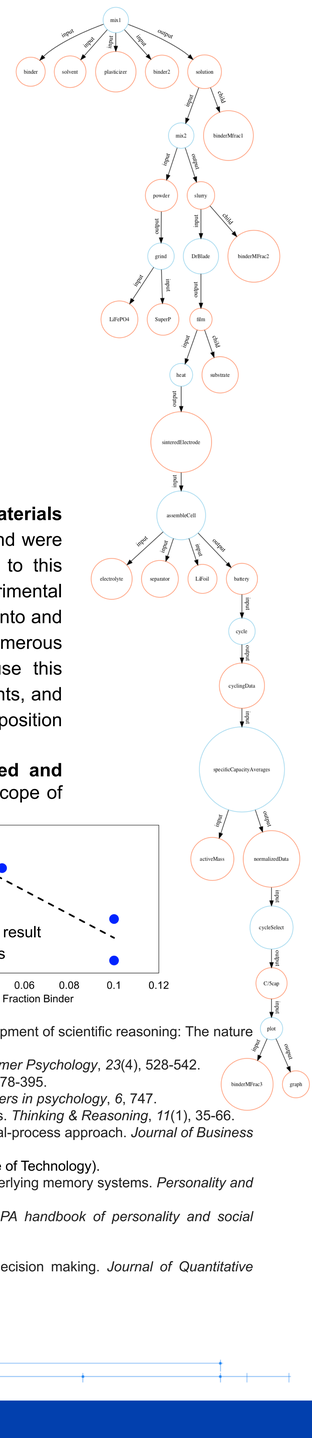
4. Computational Benefits of a Dual-Process Approach

An analysis of the computational complexity of single and dual stage approaches to novel theory generation provides a theoretical justification for the dual-stage approach (Figure 3).

The role of deductive reasoning in the scientific method, analogous to Stage II in our proposed approach, is to combine previously established theories and principles in novel ways to generate candidate explanations for observed phenomena. One might imagine a database consisting of a large number n of individual constraints representing the totality of known theory in a subfield. As n increases, the number of possible permutations of these constraints increases proportionally to the factorial of n. Thus, **an algorithm that tests all possible pipelines constructed from n constraints would exhibit complexity of O(n!).** By contrast, **a Stage I neural network trained to classify n constraints as relevant or irrelevant exhibits polynomial complexity of O(n^p)**, where the value of p depends on the network architecture.

A dual-process approach, then, would use Stage I to winnow the space of relevant constraints from a large number n down to a small number which is independent of n. Different sets of a constraints would be sequentially suggested by Stage I until Stage II is able to generate an accepted pipeline. In this way, **dual stage processes are hypothesized to realize the benefits of Type-II reasoning while countering its O(n!) computational inefficiency through the use of O(n^p) Type I processes.**

Figure 4 (below): Graph of experimental procedure to produce and process battery data varying novel binder content



5. Application to Materials Chemistry

We demonstrated the relevance of our approach by applying our Stage II system to materials chemistry datasets. These datasets evaluated a novel binder material for Lithium-Ion Batteries, and were obtained by following a complex synthesis procedure (Ransil 2018). The graph corresponding to this procedure is shown in figure 4, in which samples are outlined in blue and constraints, experimental processes and data analysis steps are outlined in orange. All objects in this graph can be imported into and exported from the analysis engine schema using the JSON format discussed in section 3 (with numerous edges and constraints omitted from the graph for clarity). The analysis engine is able to use this representation to solve for experimentally relevant results due to explicit representations of constraints, and perform data processing as well as planning subsequent experiments. A graph of the effect of composition on battery capacity is shown in figure 5.

This proof of concept shows that materials chemistry data can be usefully represented and processed using the proposed Stage II system. Subsequent effort will go into broadening the scope of this system to other fields and demonstrating integration with Type I processes.

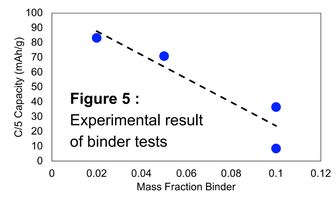


Figure 5 : Experimental result of binder tests

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