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Towards Bayesian Symbolic Computational Graph Completion

A Roadmap for Scientific Knowledge Infusion into Symbolic Machine Learning

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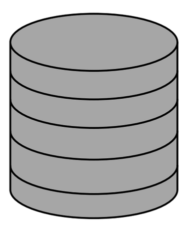
Recent progress in Machine Learning is great, but . . .

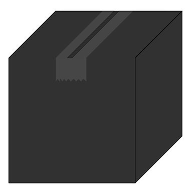
Current Machine Learning (ML) is often driven by large amounts of low quality internet data, yielding large, computationally expensive, *black box models* that provide little insight into the problem. When directly applied to *Scientific Domains*, such methods . . .

Big Data



. . . require a large amount of data to converge to a good solution. In many scientific domains only little data is available yielding to overfitting and unsatisfactory results.

Black Box Solutions



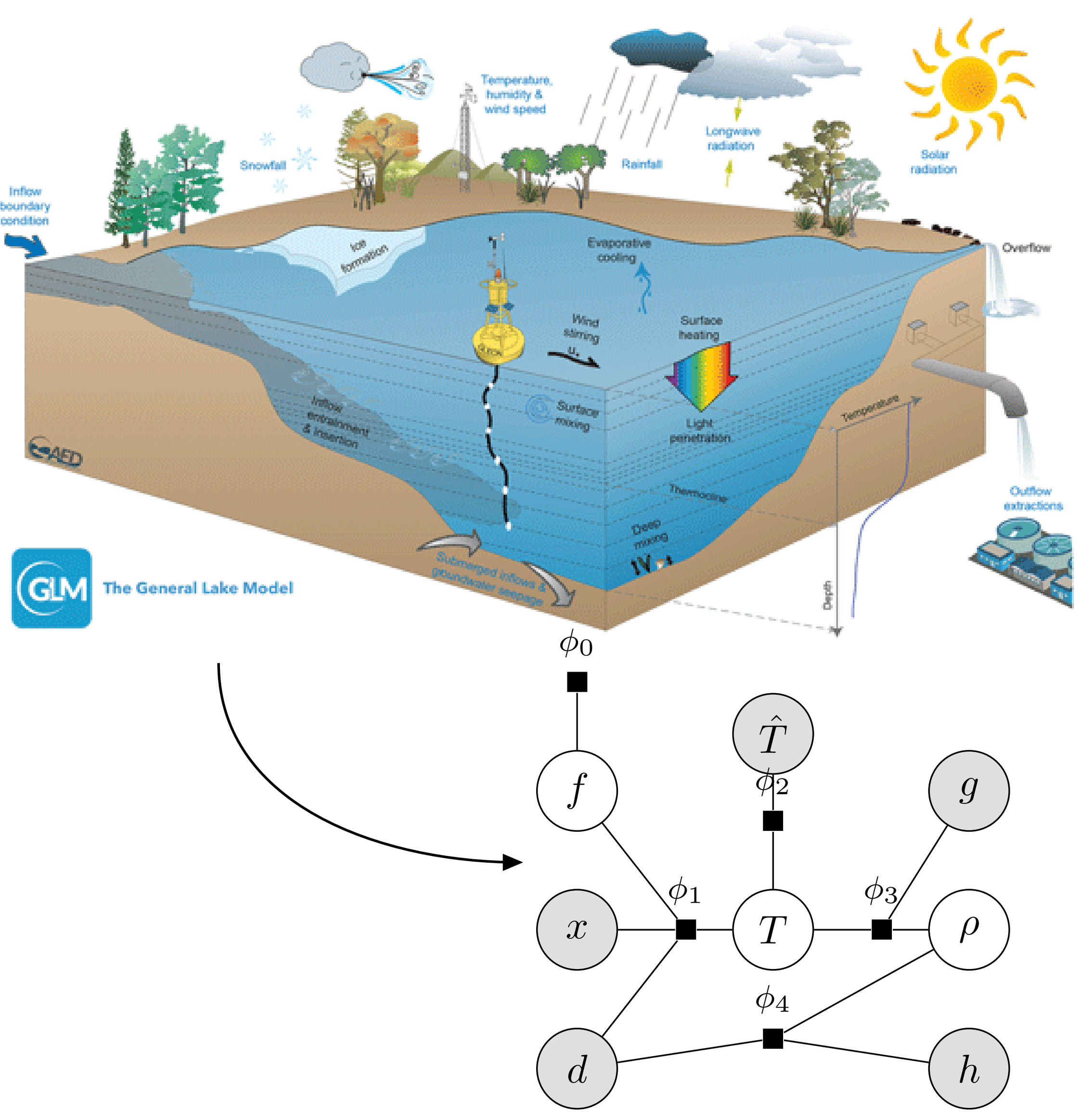
. . . provide black box solutions and therefore do not create new scientific hypothesis. But without the latter, ML only adds little value to the scientific domain research.

Ignores Scientific Knowledge

. . . ignore existing prior knowledge in the domain and learn everything from scratch often resulting in solutions that violate common knowledge.

To address these problems . . .

① Encode Prior Knowledge in a (Bayesian) Graph



- *computational graphs* [6] represent prior knowledge and relations between variables in computational tasks
- a *factor graph* [4] notation allows probabilities (=factors ϕ_i) for variables as well as knowledge like
  - equations and auxiliary variables [1]
  - differential equations [3]
  - structural priors (with grammars) [9]

- *Example:* 1*D* Lake Temperature Model

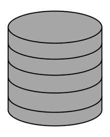
  Task: find the unknown function $f(x, d) = T$

  AND

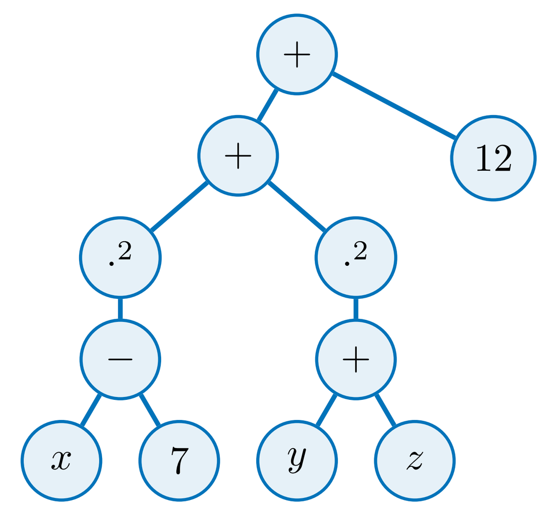
  "I know that temperature T is related to density ρ via g and the density monotony h holds with increasing depth d." (compare [1])

② Input Additional Data Evidence

- measurements or observations for certain variables in the graph



③ Output Symbolic Solution Candidates



- for the unknown functions in the graph
- composes complex expressions out of a *library* of known operations
- yields a *scientific hypothesis* that can be interpreted and debated
- can be found with Bayesian Symbolic Regression (BSR) [2] by performing MCMC steps in the space of symbolic representations.

Proposed Framework: Symbolic Computational Graph Completion

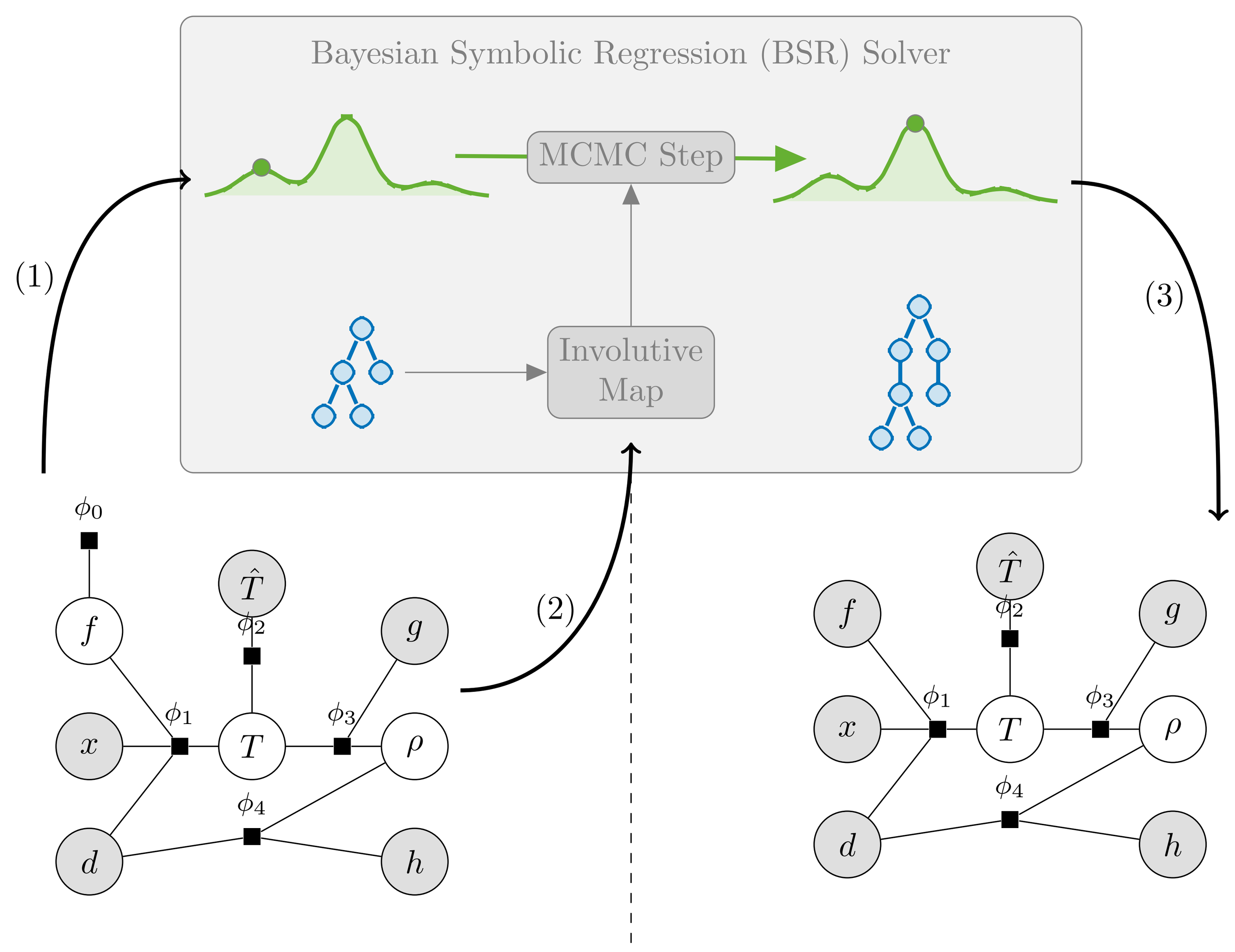


Figure: Overview of the proposed framework for Symbolic Computational Graph Completions

Our Approach

- Encode the problem as well as all prior knowledge in a *computational (factor) graph* representation.
- Fill in symbolic solutions with data and *Bayesian Reasoning*.

Scientific Knowledge Exploitation

Hereby, the framework considers *three steps* that exploit the prior knowledge in the graph:

(1) *Unnormalized Posterior:*
use the graph to evaluate the unnormalized posterior distribution of potential symbolic expressions in order to sample from it using MCMC (see [2])

(2) *Informed Sampler:*
involutive maps [5] encode additional information about the problem to design informed samplers that produce samples of high likelihood. Especially learned maps [8] allow a connection to recent advances in deep learning (e.g. [7]).

(3) *Graph Update:*
The Bayesian solver yields symbolic hypothesis that enables a *human researcher* to
- accept one of the hypothesis / candidates or
- come up with new prior knowledge in the graph

References

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