

Probabilistic Programming for Scientific Discovery

Lecture 1

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Lviv Data Science Summer School

July 29, 2020

Table of Contents

Course Outline

Example Applications of Probabilistic Programming

ETALUMIS: Bringing Probabilistic Programming to Scientific Simulators at Scale

DreamCoder: Growing Generalizable, Interpretable Knowledge with Wake-Sleep Bayesian Program Learning

Why Do We even Need Probabilistic Programming?

Underlying Theoretical Ideas

Different Types of Probabilistic Programming Systems

Outline

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- 4 Lectures
 1. Foundational Knowledge
 2. Inference Engines & Introduction to Turing.jl
 3. Hierarchical Bayesian Approaches & Bayesian Deep Learning
 4. The Connection to Scientific Problems
- 3 Tutorials for Self-Paced Consumption
 1. In-Depth Introduction to Probabilistic Programming Systems with Turing.jl
 2. Bayesian Approaches in Probabilistic Programming
 - ▷ Bayesian Deep Learning
 - ▷ Hierarchical Bayesian Modelling
 3. Machine-Learning Based Design with Probabilistic Programming

Lecture 1

- Example Applications of Probabilistic Programming
 1. *ETALUMIS: Bringing Probabilistic Programming to Scientific Simulators at Scale*
 2. *DreamCoder: Growing Generalizable, Interpretable Knowledge with Wake-Sleep Bayesian Program Learning*
- Why do we even need Probabilistic Programming?
- Underlying Theoretical Ideas
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Lecture 2

- Approaches to Inference - the Inference Engine
- Practical Introduction to a Probabilistic Programming Framework
- Extending our learned ideas to a more complex example

Lecture 3

- Bayesian Hierarchical Approaches
- Bayesian Deep Learning, including but not limited to
 - Inference Networks
 - Uncertainty Quantification
- Marrying Deep Learning Frameworks with Probabilistic Programming for Type 2 Machine Learning

Lecture 4

- Interaction with Scientific Simulators
 - What types of simulators would I want to link to?
 - What are the hidden pitfalls?
- Areas of application
 - Robotics
 - Physics
 - Engineering
 - Machine-Learning Based Design
- Extensive Machine-Learning Based Design Example

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ETALUMIS

Bringing Probabilistic Programming to Scientific Simulators at Scale

- Blub

DreamCoder

Growing Generalizable, Interpretable Knowledge with Wake-Sleep Bayesian Program Learning

- Constructs domain-specific languages (DSLs) for scientific problems combined with a neural network, which embodies a learned domain-specific search strategy
 - Learns both the system prior and the needed inference algorithm
- Practically constructs a library of symbolic abstractions in a wake-sleep manner and applies said library to the solving of the chosen problem at hand
- Utilizes wake-sleep learning
 - During *sleep* the system consolidates its abstractions from the programs found during *wake* and improves upon the neural network recognition model by imagining new samples
 - During *wake* the generative model is exploited on the problem domain to find the programs with the highest posterior probability

DreamCoder

- Knowledge is accumulated in a multilayered hierarchy with knowledge and skills being successively learned over time, i.e. the knowledge is bootstrapped from very simple examples to ever more complex cases
- Can be broken down to a probabilistic inference procedure, i.e. observing task X and inferring program ρ_x to solve task $x \in X$ combined with a prior distribution over program, which might solve tasks in the domain

$$\rho_x = \underset{\substack{\rho: \\ Q(\rho|x) \text{ is large}}}{\arg \max} P[\rho|x, L] \propto P[x|\rho]P[\rho|L], \text{ for each task } x \in X \quad \textit{Wake}$$

$$L = \underset{L}{\arg \max} P[L] \prod_{x \in X} \max_{\rho \text{ a refactoring of } \rho_x} P[x|\rho]P[\rho|L] \quad \textit{Sleep : Abstraction}$$

$$\text{Train } Q(\rho|x) \approx P[\rho|x, L], \text{ where } x \sim X \text{ ('replay')} \text{ or } x \sim L \text{ ('fantasy')} \quad \textit{Sleep : Dreaming}$$

DreamCoder

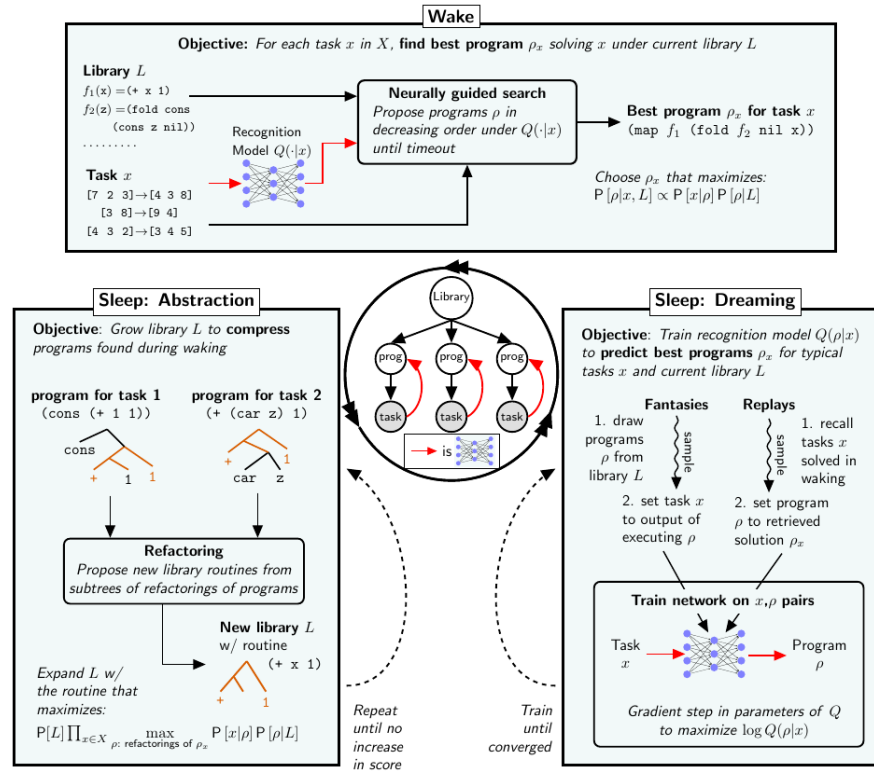
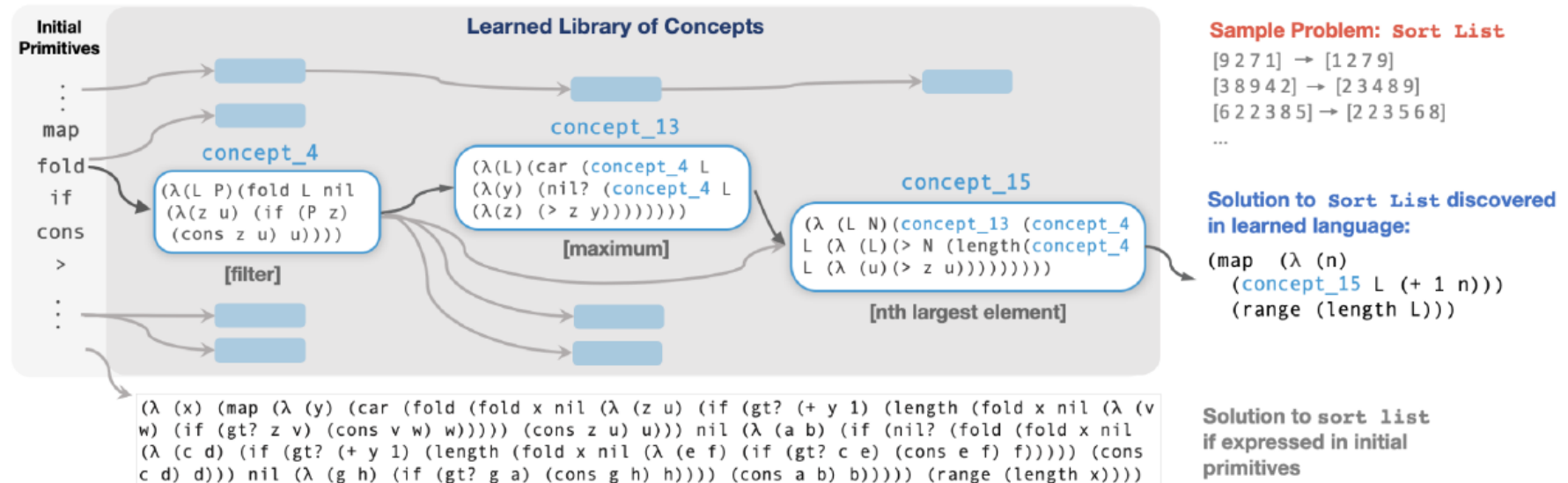


Figure: Algorithm Cycle of DreamCoder

DreamCoder

- Due to its compositional nature, representations of problems can be bootstrapped from earlier, simpler version of the scientific task to more and more complex settings



DreamCoder

- Applications from page 2

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Underlying Theoretical Ideas

Different Types of Probabilistic Programming Systems

Outline

Course Outline

Example Applications of Probabilistic Programming

ETALUMIS: Bringing Probabilistic Programming to Scientific Simulators at Scale

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Underlying Theoretical Ideas

Different Types of Probabilistic Programming Systems

Outline

Course Outline

Example Applications of Probabilistic Programming

ETALUMIS: Bringing Probabilistic Programming to Scientific Simulators at Scale

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Underlying Theoretical Ideas

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