Chair of Aerodynamics and Fluid Mechanics
Department of Mechanical Engineering
Technical University of Munich

Probabilistic Programming for Scientific Discovery

Lecture 1

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Lviv Data Science Summer School

July 29, 2020

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Course Outline

Example Applications of Probabilistic Programming
- ETALUMIS: Bringing Probabilistic Programming to Scientific Simulators at Scale
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Why Do We even Need Probabilistic Programming?

Underlying Theoretical Ideas

Different Types of Probabilistic Programming Systems

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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
- Different Types of Probabilistic Programming Systems

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

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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 [1]

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

[1] Ellis, K., Wong, C., Nye, M., Sable-Meyer, M., Cary, L., Morales, L., Hewitt, L., Solar-Lezama, A. and Tenenbaum, J.B., 2020. DreamCoder: Growing generalizable, interpretable knowledge with wake-sleep Bayesian program learning. arXiv preprint arXiv:2006.08381.

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 migh solve tasks in the domain

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

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

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

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DreamCoder

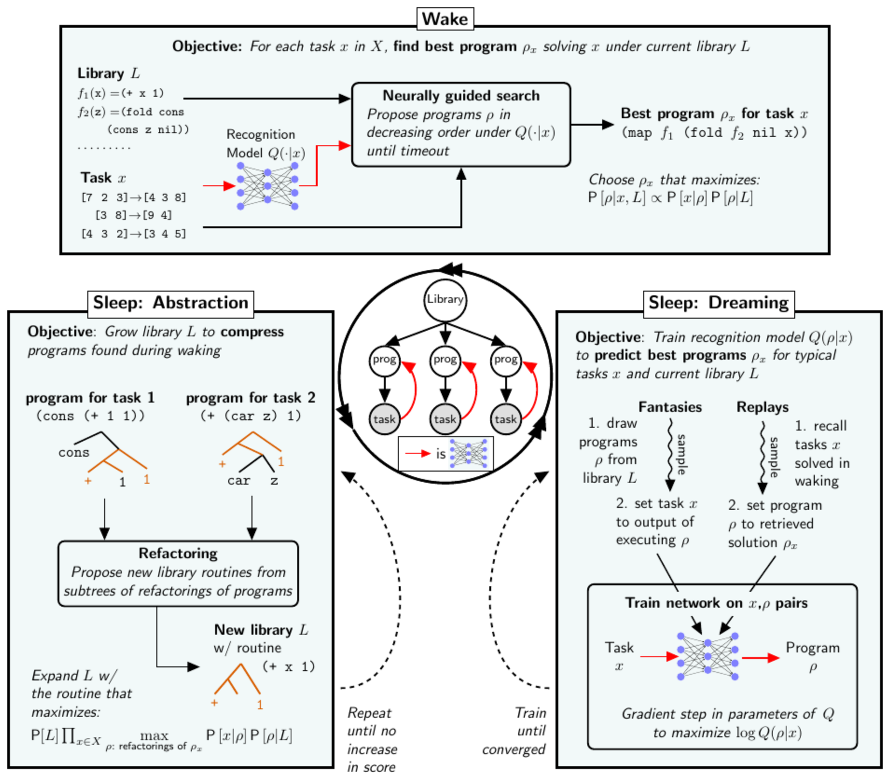

Figure: Algorithm Cycle of DreamCoder

DreamCoder

Algorithm 1 Full DreamCoder algorithm

function DreamCoder(D, X):
Input: Initial library functions D, tasks X
Output: Infinite stream of libraries, recognition models, and beams
Hyperparameters: Batch size B, enumeration timeout T, maximum beam size M
$\theta \leftarrow$uniform distribution
$\mathcal{B}_x \leftarrow \varnothing, \forall x \in X$ ▷ Initialize beams to be empty
while true **do** ▷ Loop over epochs
    shuffle $\leftarrow$ random permutation of X ▷ Randomize minibatches
    while shuffle is not empty **do** ▷ Loop over minibatches
        batch $\leftarrow$ first B elements of shuffle ▷ Next minibatch of tasks
        shuffle $\leftarrow$ shuffle with first B elements removed
        $\forall x \in$ batch: $\mathcal{B}_x \leftarrow \mathcal{B}_x \cup \{\rho \mid \rho \in \text{enumerate}(\mathrm{P}[\cdot|D, \theta], T) \text{ if } \mathrm{P}[x|\rho] > 0\}$ ▷ Wake
        Train $Q(\cdot|\cdot)$ to minimize $\mathcal{L}^{\text{MAP}}$ across all $\{\mathcal{B}_x\}_{x \in X}$ ▷ Dream Sleep
        $\forall x \in$ batch: $\mathcal{B}_x \leftarrow \mathcal{B}_x \cup \{\rho \mid \rho \in \text{enumerate}(Q(\cdot|x), T) \text{ if } \mathrm{P}[x|\rho] > 0\}$ ▷ Wake
        $\forall x \in$ batch: $\mathcal{B}_x \leftarrow$ top M elements of $\mathcal{B}_x$ as measured by $\mathrm{P}[\cdot|x, D, \theta]$ ▷ Keep top M programs
        $D, \theta, \{\mathcal{B}_x\}_{x \in X} \leftarrow \textsc{Abstraction}(D, \theta, \{\mathcal{B}_x\}_{x \in X})$ ▷ Abstraction Sleep
        yield $(D, \theta), Q, \{\mathcal{B}_x\}_{x \in X}$ ▷ Yield the updated library, recognition model, and solutions found to tasks
    end while
end while

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DreamCoder

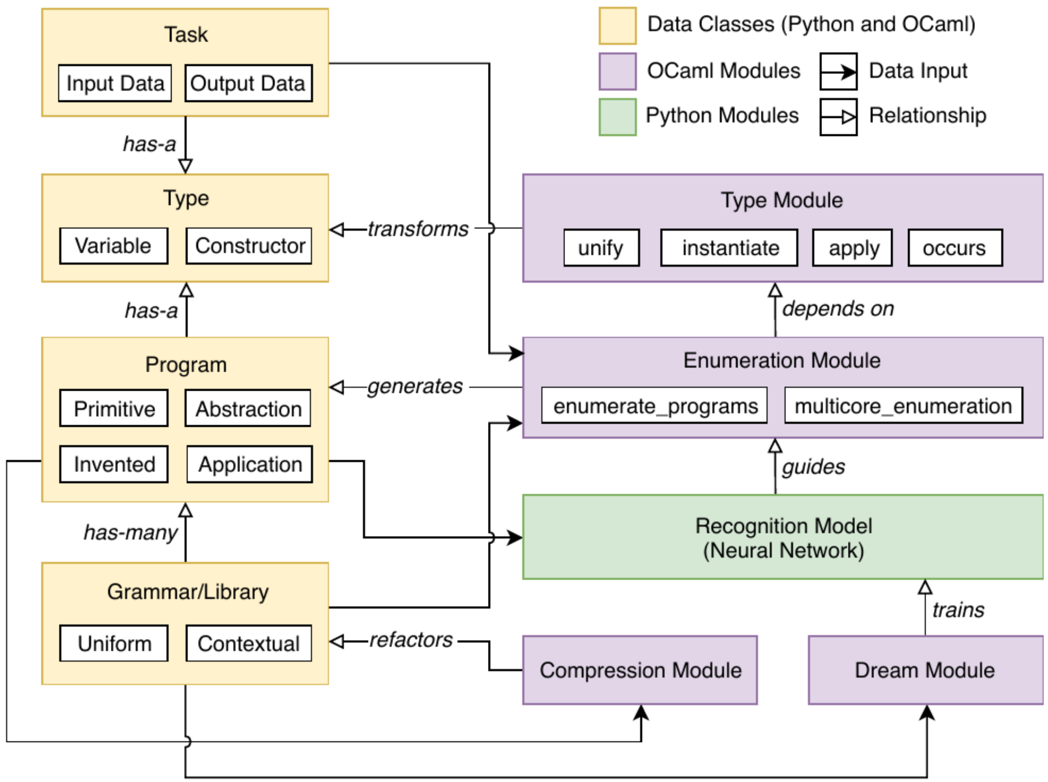

Figure: Different data-classes in DreamCoder.

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DreamCoder

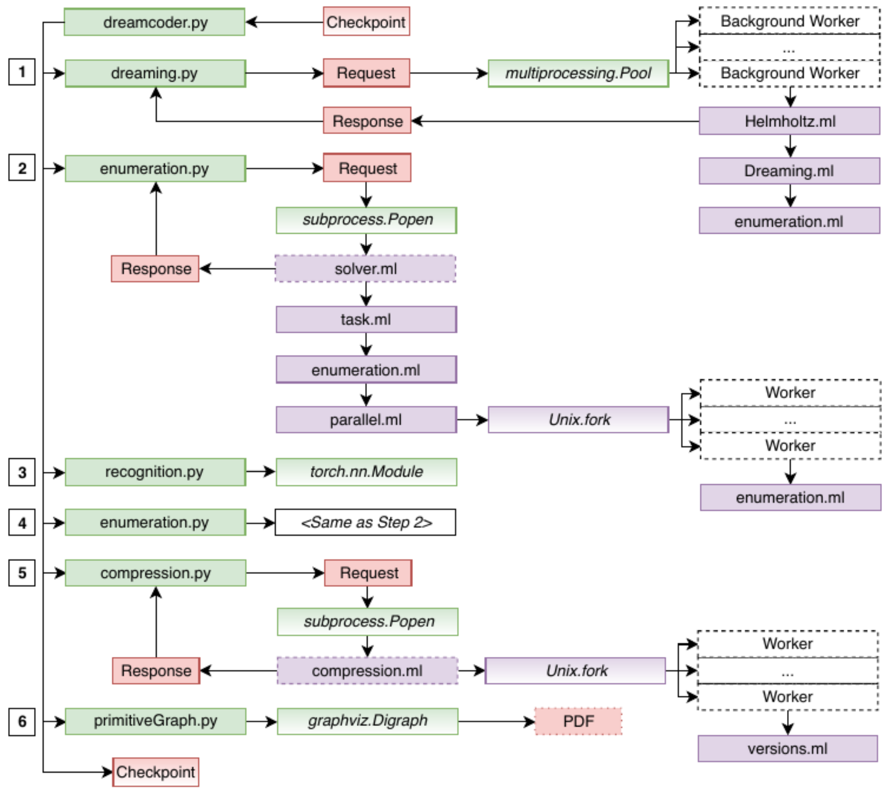

Figure: Program Flowchart: Phase 1, Dreaming. Phase 2, 1st Program Enumeration. Phase 3, Recognition Model Training. Phase 4, 2nd Program Enumeration. Phase 5, Abstraction (Compression). Phase 6, Library Visualization.

Recap: Helmholtz Machine [2] [3]

- Blub

[2] Graves, A., Wayne, G. and Danihelka, I., 2014. Neural turing machines. arXiv preprint arXiv:1410.5401.

[3] YouTube: DeepMind x UCL | Deep Learning Lectures | 8/12 | Attention and Memory in Deep Learning

Recap: Helmholtz Machine

- Blub 2

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Recap: Helmholtz Machine

- Blub 3

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Outlook: Differentiable Neural Computer [4]

- Differentiable Neural Computer

[4] Graves, A., Wayne, G., Reynolds, M., Harley, T., Danihelka, I., Grabska-Barwińska, A., Colmenarejo, S.G., Grefenstette, E., Ramalho, T., Agapiou, J. and Badia, A.P., 2016. Hybrid computing using a neural network with dynamic external memory. Nature, 538(7626), pp.471-476.

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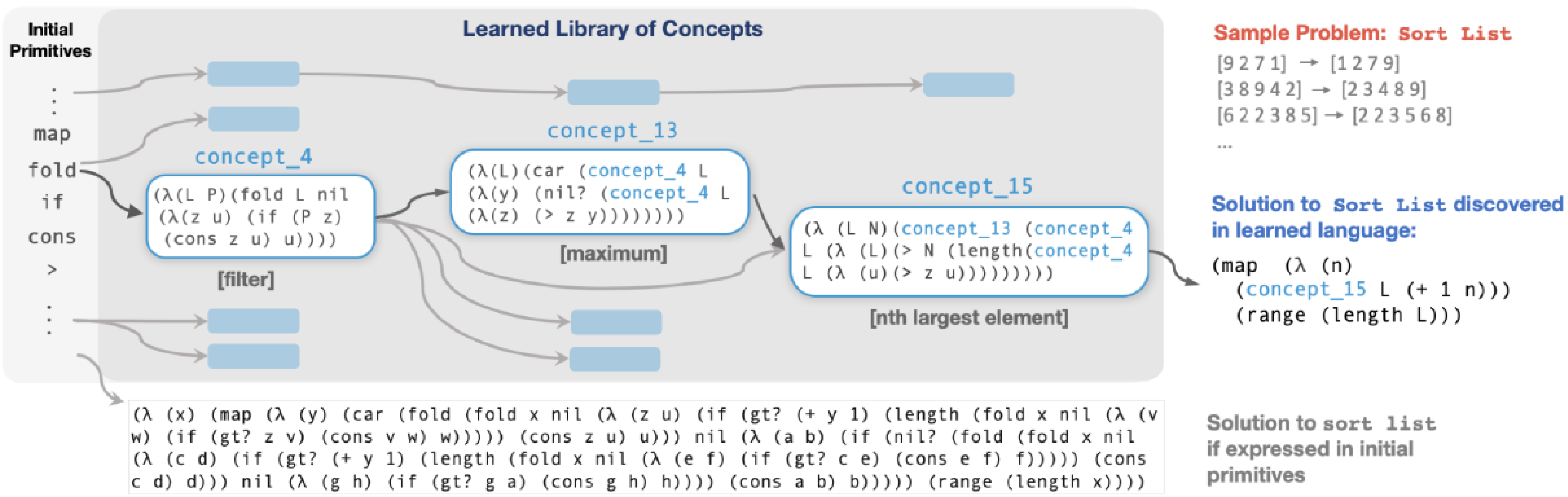
DreamCoder

- 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



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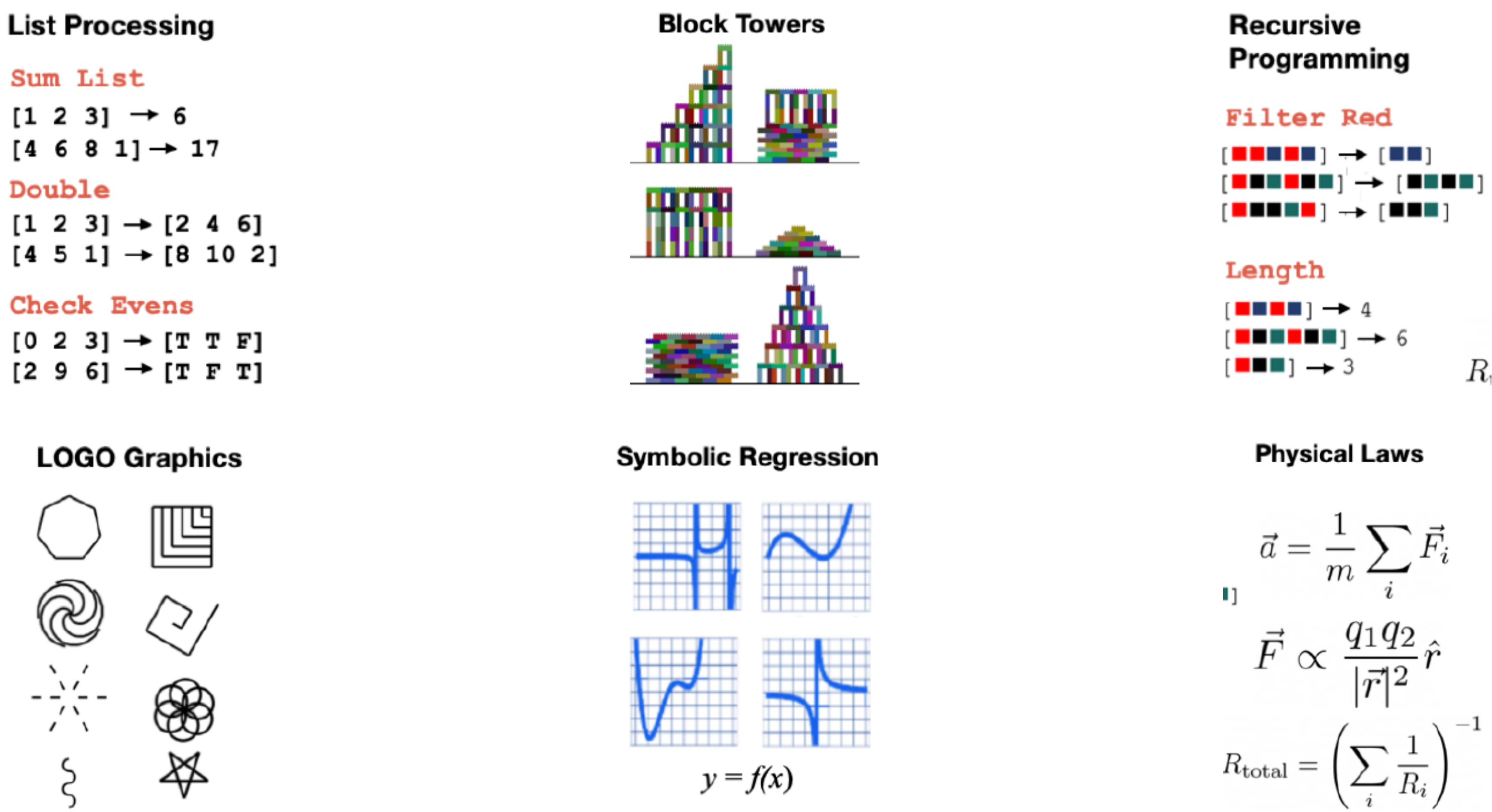
Applications



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Applications

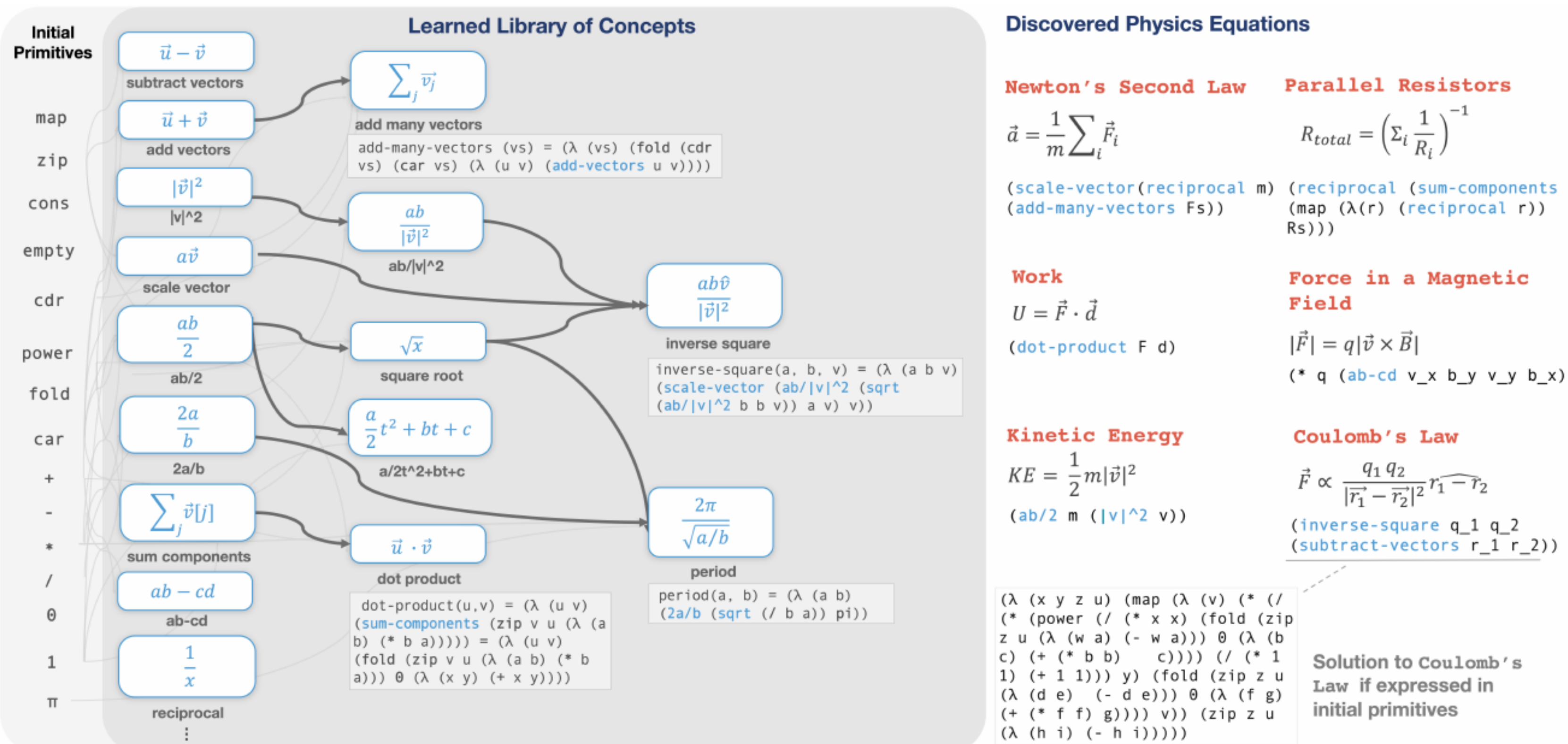

Figure: Learned library for physics equations.

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Applications

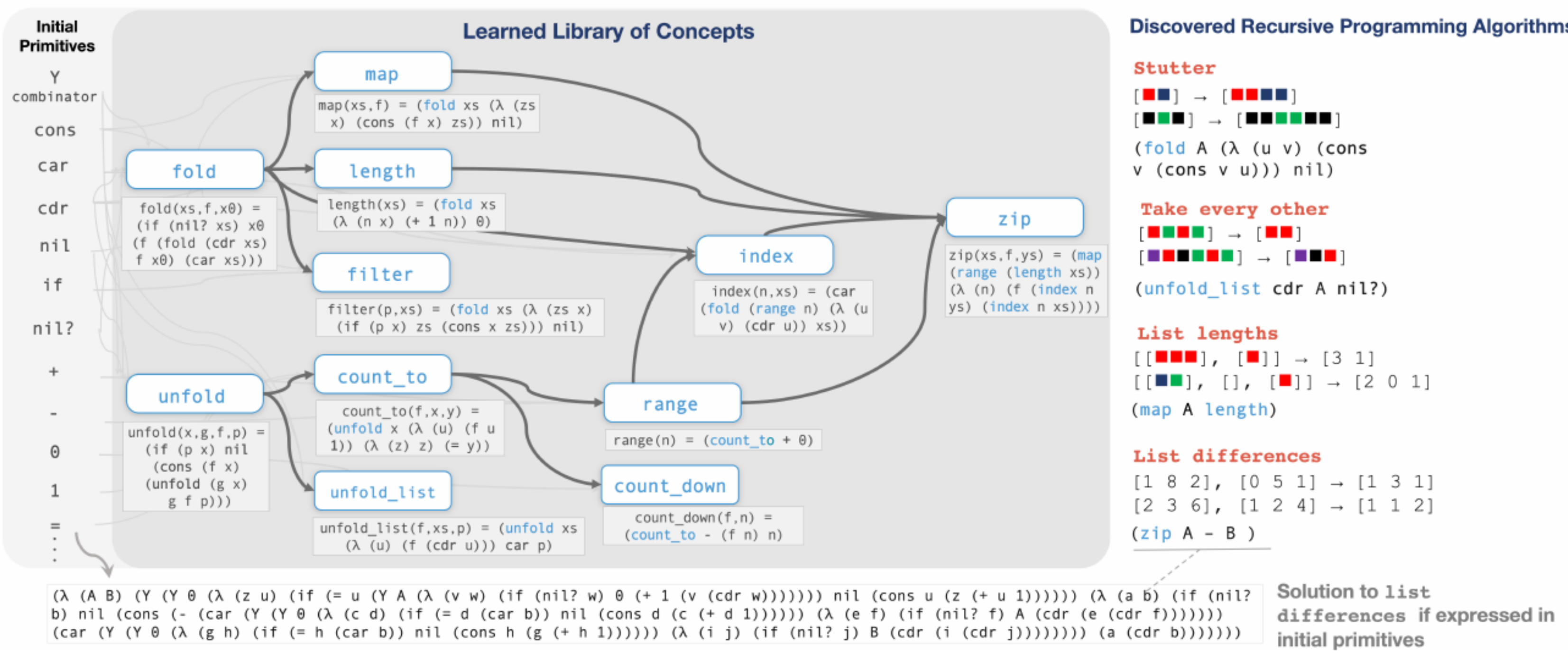

Figure: Learned library for recursive programming algorithm.

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Applications

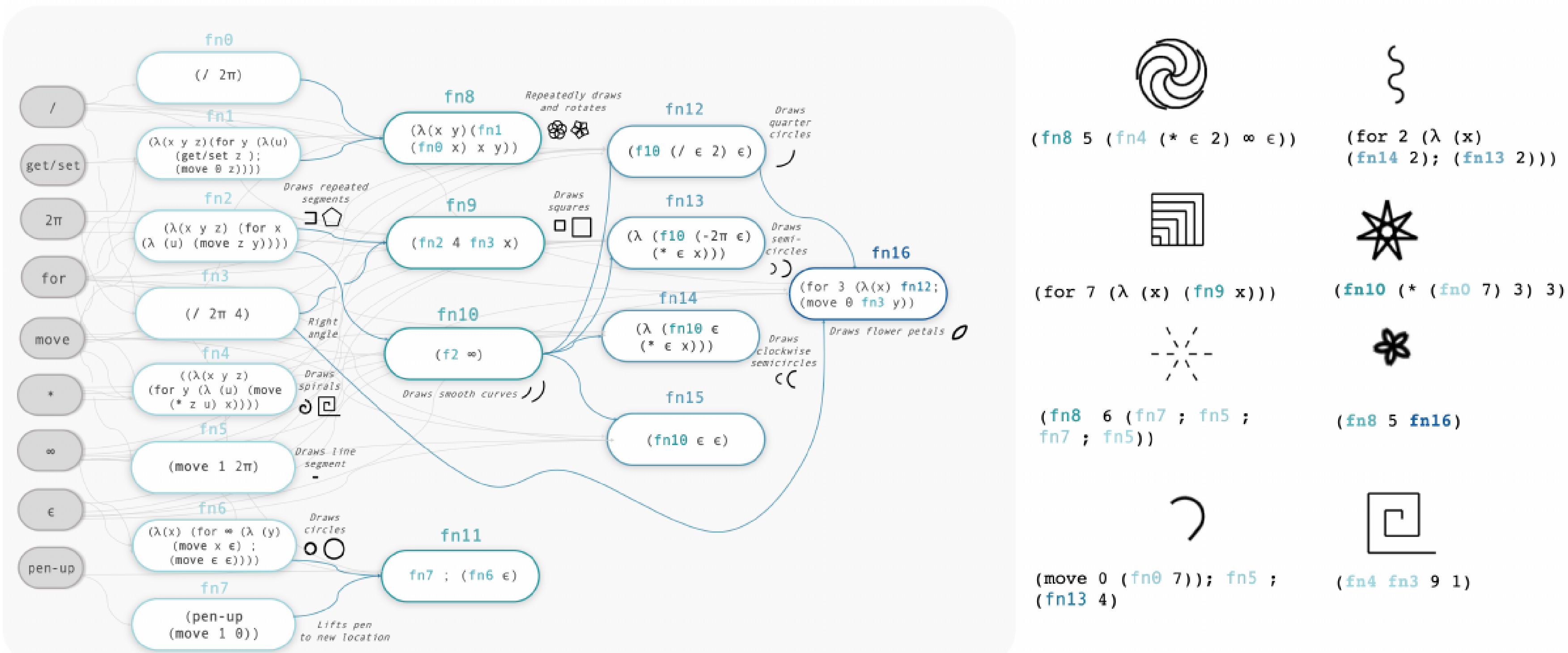

Figure: Learned library for LOGO graphics.

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Applications

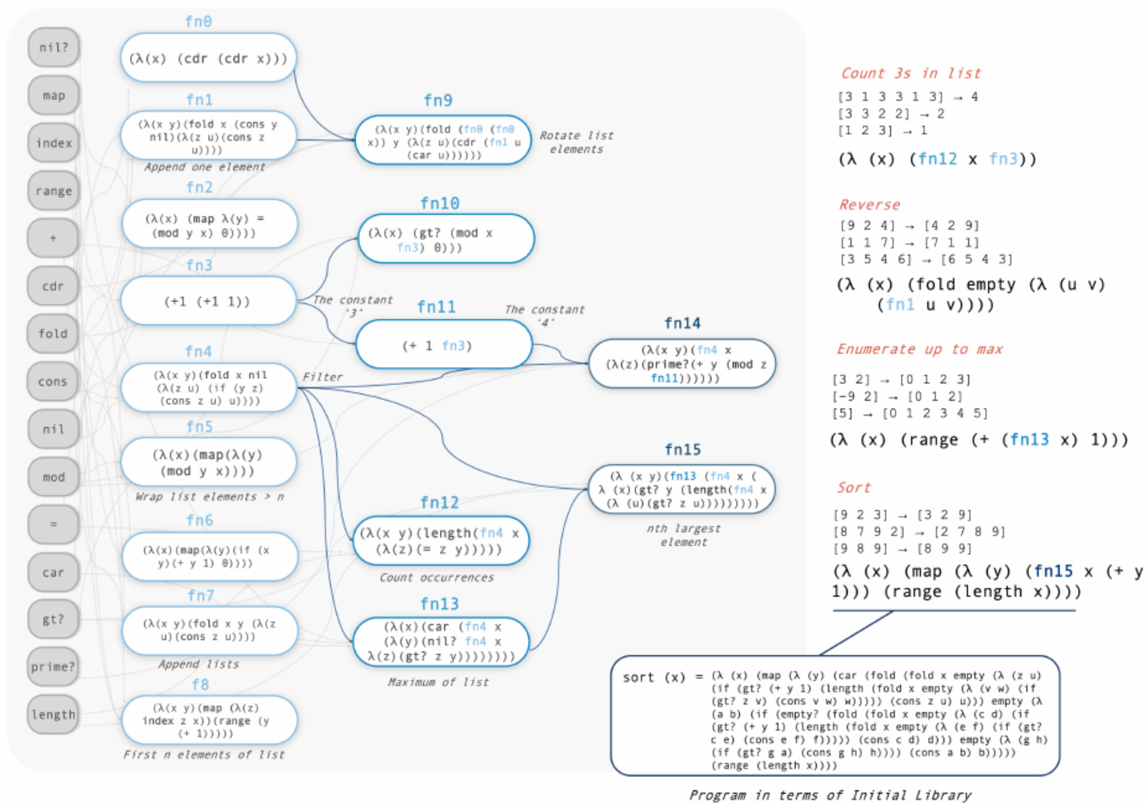

Figure: Learned library for list processing.

DreamCoder

Take-Aways

- Combining probabilistic programming with a DSL-learning procedure and novel probabilistic inference procedure to iteratively learn to represent a problem's domain allows one to gain the ability to solve a problem
- Such applications require highly complex codebase structures across multiple languages
- For more complex examples reliant on a highly efficient inference procedure

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