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

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- 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 1

- Example Applications of Probabilistic Programming
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    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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Outline

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

Etalumis

Bringing Probabilistic Programming to Scientific Simulators at Scale [2]

- Large scale inverse problem, where a particle simulator is inverted by probabilistically inferring all choices in the simulator given the desired outputs
  - Developed in the context of particle simulations at CERN
- First large-scale application of probabilistic programming to physical simulators in the quest to potentially unearth new physics [1]
- Largest-scale posterior inference with 25000 latent variables at the time
- Amount of compute required highly dependent on the specific approach to inference and the nature of the simulator, i.e. latent dimensionality and intensity of the compute routine
  - Only set to improve with the impeding exascale-era

[1] Cranmer, K., Brehmer, J. and Louppe, G., 2020. The frontier of simulation-based inference. Proceedings of the National Academy of Sciences.

[2] Baydin, A.G., Shao, L., Bhimji, W., Heinrich, L., Meadows, L., Liu, J., Munk, A., Naderiparizi, S., Gram-Hansen, B., Louppe, G. and Ma, M., 2019, November. Etalumis: Bringing probabilistic programming to scientific simulators at scale. In Proceedings of the International Conference for High Performance Computing, Networking, Storage and Analysis (pp. 1-24).

Etalumis

- Proposes a direct linking of particle physics simulators with probabilistic programming systems to trace the internal structure of the simulator
  - Probabilistic programming system controls the random number draws of the simulator akin to samples from prior distributions in Bayesian statistics
- Utilizing inference compilation with three-dimensional convolutional LSTMs to guide the inference procedure and amortize the high computational costs of training
  - Dynamic compilation, in which a core gets expanded with further neural network components as inference compilation proceeds
- Utilizes importance sampling in conjunction with inference compilation as approach to inference

Etalumis

Simulators as Probabilistic Programs

- A simulator execution is viewed as an execution trace, a single sample to the probabilistic programming system
  - I.e. sampling is taking place in the space of execution traces
- Abstracting the simulator in this way enables the following analysis
  - Compute likelihoods
  - Learn/construct surrogate models
  - Generate training data for inference compilation
  - Introduce other generative approaches into the loop
- Enables us to guide the simulation in an intelligent fashion, using the inference network, which acts as a kind of oracle

Etalumis

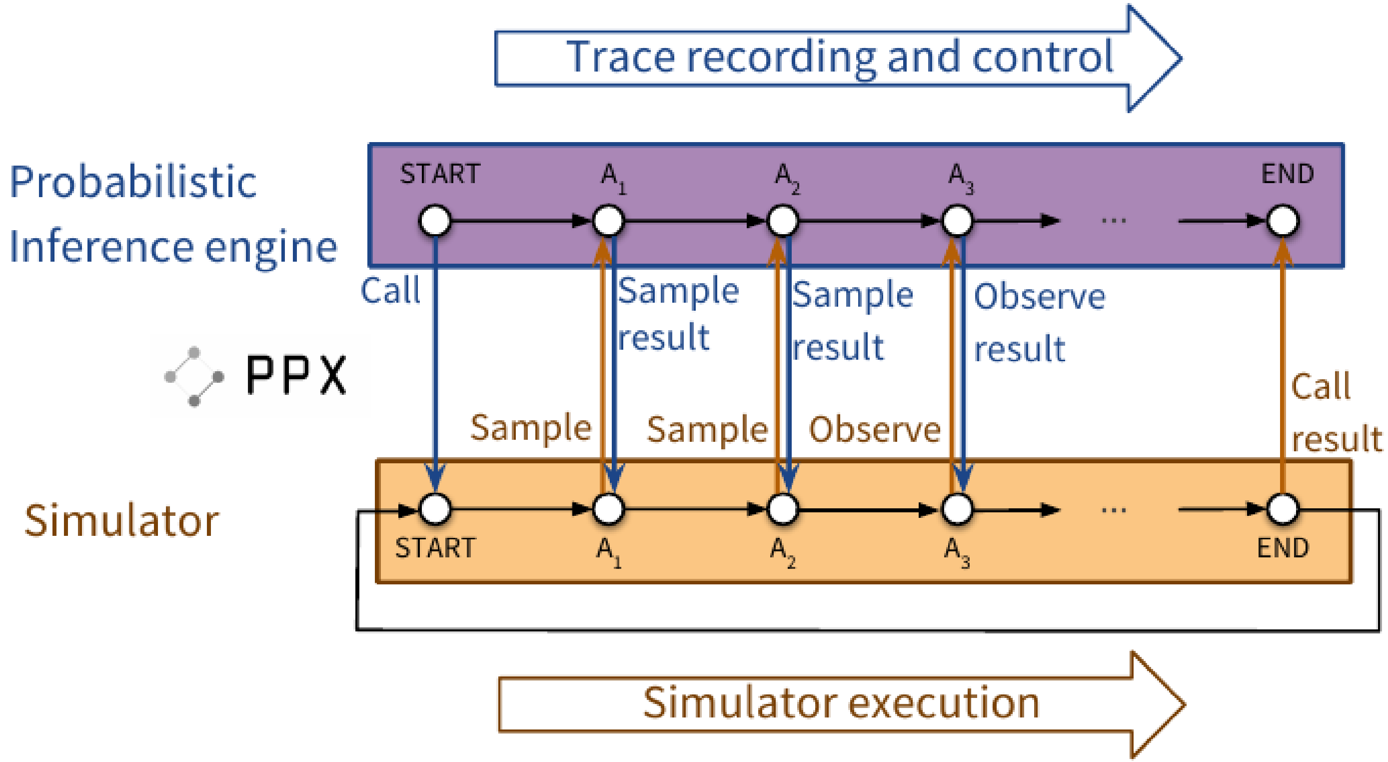

Figure: High-level view from the perspective of the probabilistic programming execution protocol (PPX).

Etalumis

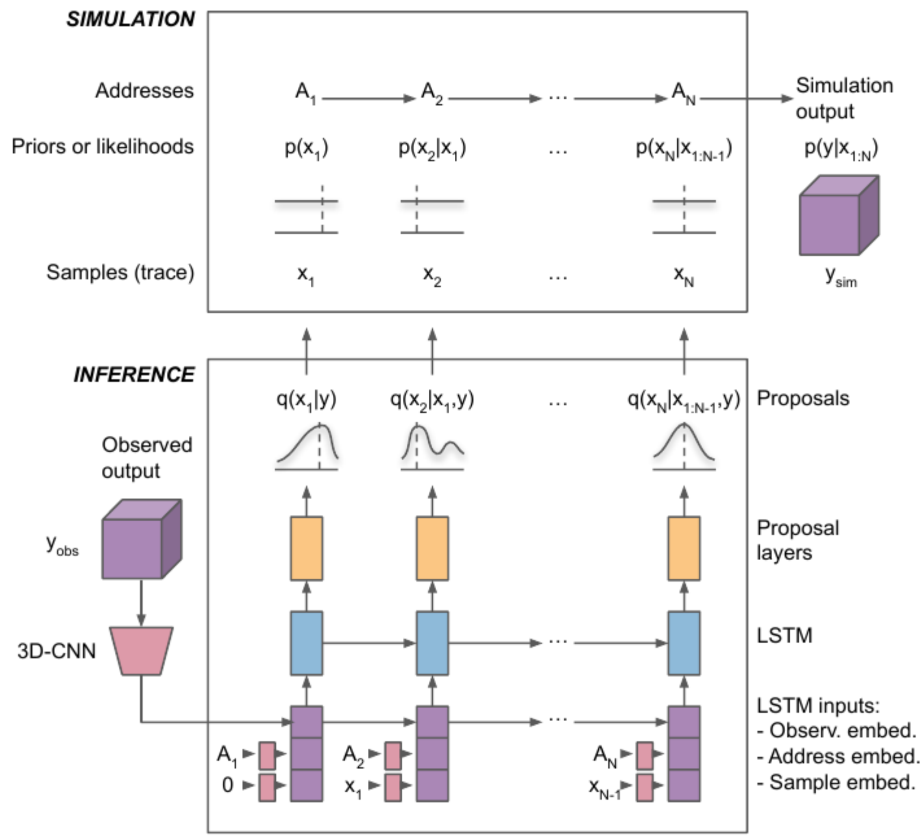

Figure: Detailed connection between simulation and inference in the probabilistic programming-based approach.

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Etalumis

Recap: Amortized Inference [3] [4]

- Blub 1

[3]Gershman, S. and Goodman, N., 2014. Amortized inference in probabilistic reasoning. In Proceedings of the annual meeting of the cognitive science society (Vol. 36, No. 36).

[4]Ritchie, D., Horsfall, P. and Goodman, N.D., 2016. Deep amortized inference for probabilistic programs. arXiv preprint arXiv:1610.05735.

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Etalumis

Recap: Amortized Inference

- Blub 2

Etalumis

Recap: Amortized Inference

- Blub 3

Etalumis

Outlook: Inference Compilation [5]

- Uses neural networks to construct a surrogate model for the probabilistic generative model, which is subsequently used at inference time as a custom proposal distribution to avoid sampling from the actual generative model
- Intuition is that the cost of constructing the surrogate can be amortized at inference time and be lower inference from the underlying generative model
  - Need to watch out for sample diversity and out-of-distribution samples
- Proposes adaptive neural network architecture with a recurrent core and embedding and proposal layers specified by the probabilistic program
- Approach is model-agnostic

[5] Le, T.A., Baydin, A.G. and Wood, F., 2017, April. Inference compilation and universal probabilistic programming. In Artificial Intelligence and Statistics (pp. 1338-1348).

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Etalumis

Outlook: Inference Compilation

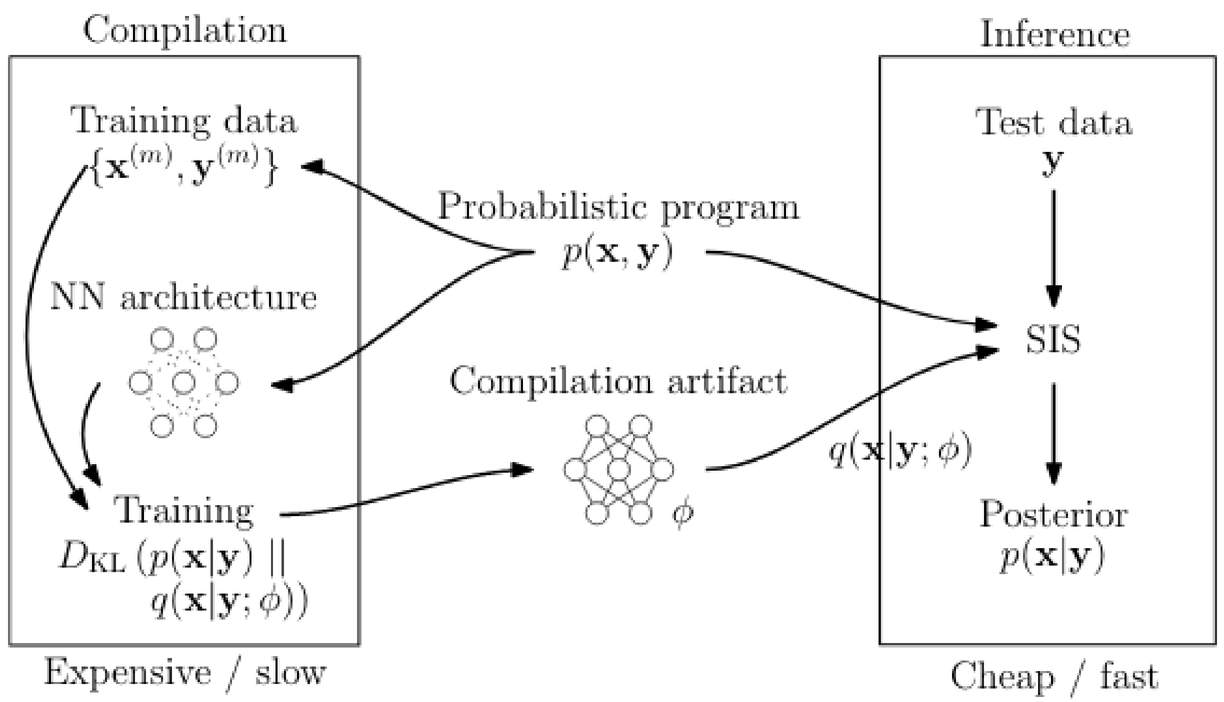

Figure: Automatic construction of a neural network surrogate, which is then trained with data generated by the probabilistic program to eventually act as the proposal distribution at inference time.

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Etalumis

Outlook: Inference Compilation

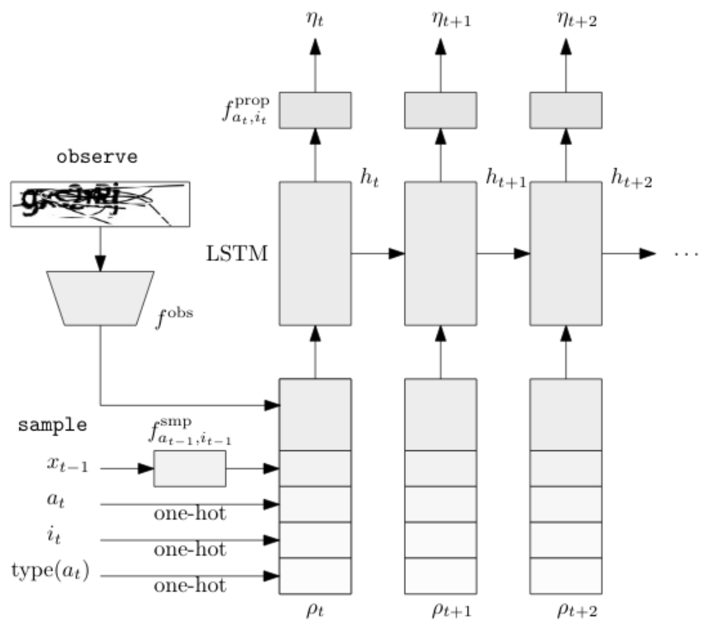

Figure: Example application for captcha solving based on probabilistic generative models for the captchas. With the LSTM at its core, required embeddings for the respective are attached adaptively.

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Etalumis

Algorithm 2 Distributed training with MPI backend. $p(\boldsymbol{x}, \boldsymbol{y})$ is the simulator and $\hat{G}(\boldsymbol{x}, \boldsymbol{y})$ is an offline dataset sampled from $p(\boldsymbol{x}, \boldsymbol{y})$

Require: OnlineData {True/False value}
Require: B {Minibatch size}
  Initialize inference network $q_\phi(\boldsymbol{x}|\boldsymbol{y})$
  $N \leftarrow$ number of processes
  for all $n \in \{1, \ldots, N\}$ **do**
    while Not Stop **do**
      if OnlineData **then**
        Sample $\mathcal{D}_n = \{(\boldsymbol{x}, \boldsymbol{y})_1, \ldots, (\boldsymbol{x}, \boldsymbol{y})_B\}$ from $p(\boldsymbol{x}, \boldsymbol{y})$
      else
        Get $\mathcal{D}_n = \{(\boldsymbol{x}, \boldsymbol{y})_1, \ldots, (\boldsymbol{x}, \boldsymbol{y})_B\}$ from $\hat{G}(\boldsymbol{x}, \boldsymbol{y})$
      end if
      Synchronize parameters (ϕ) across all processes
      $\mathcal{L}_n \leftarrow -\frac{1}{B} \sum_{(\boldsymbol{x}, \boldsymbol{y}) \in \mathcal{D}_n} \log q_\phi(\boldsymbol{x}|\boldsymbol{y})$
      Calculate $\nabla_\phi \mathcal{L}_n$
      Call `all_reduce` s.t. $\nabla_\phi \mathcal{L} \leftarrow \frac{1}{N} \sum_{n=1}^{N} \nabla_\phi \mathcal{L}_n$
      Update ϕ using $\nabla_\phi \mathcal{L}$ with e.g. ADAM, SGD, LARC, etc.
    end while
  end for

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Etalumis

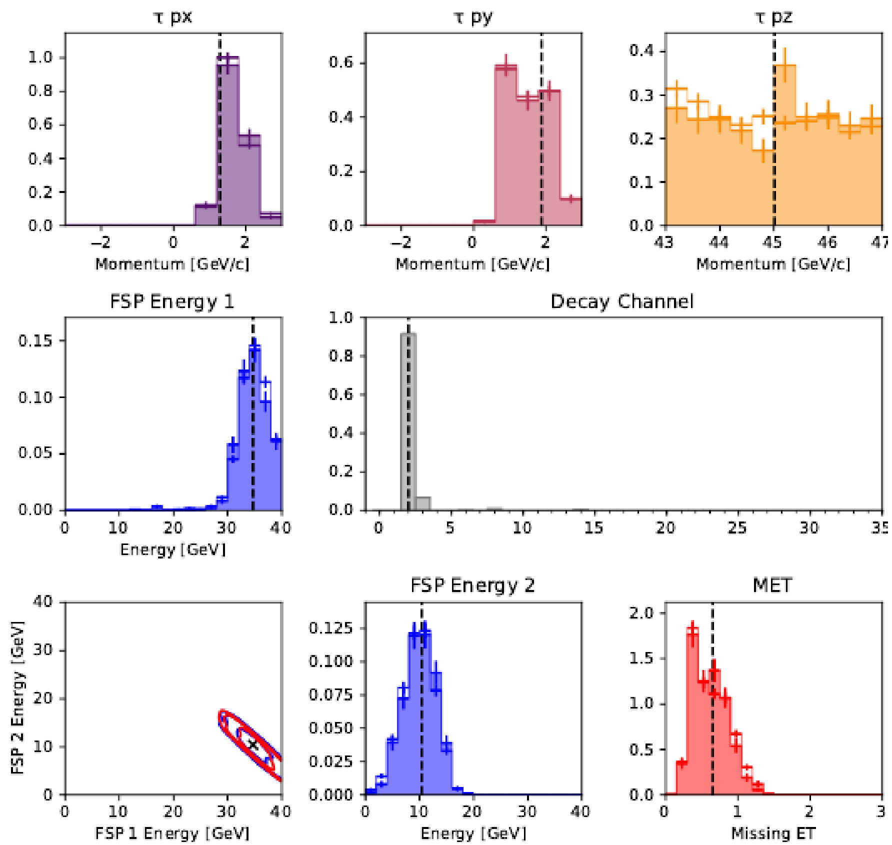

Figure: Posteriors obtained with random-walk Metropolis Hasting (filled histograms) and inference compilation (outline histograms) and ground truth values (dashed vertical lines).

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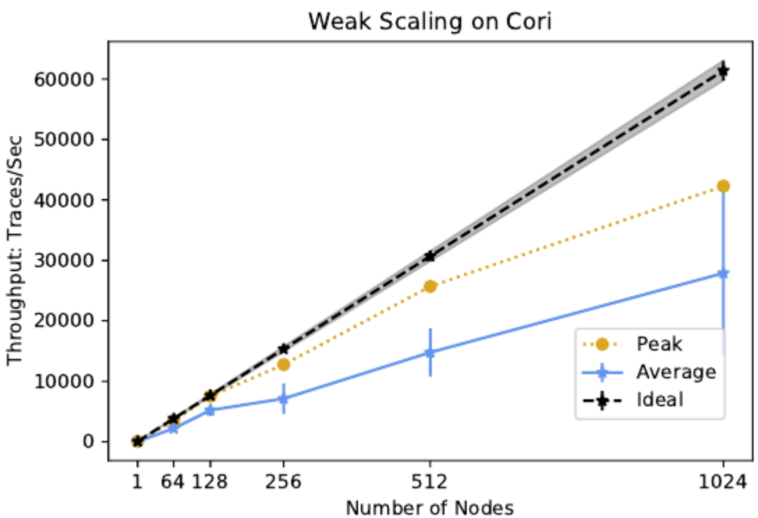
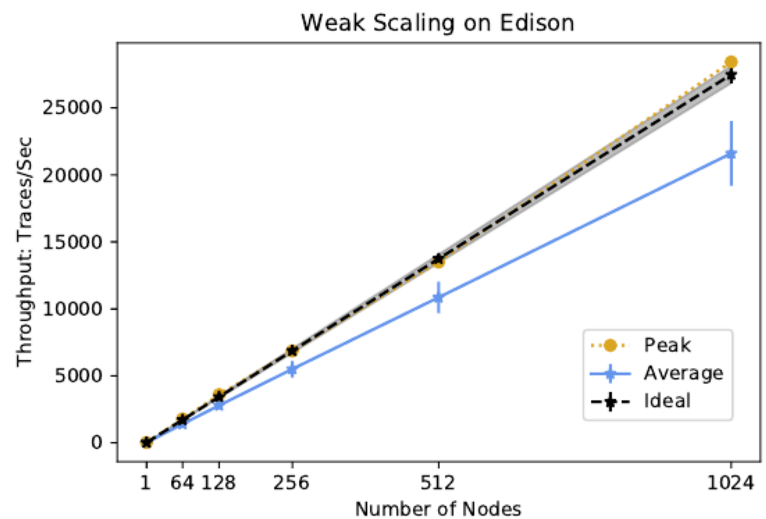
Etalumis





- Moving to supercomputer scale for massive-scale inference to be able to generate the necessary number of simulations for the inference compilation to be successful.

Etalumis

- First probabilistic programming system to link to scientific simulators at scale to enable large-scale posterior inference on a supercomputing-scale
  - Can only ever capture the processes encapsulated in the simulator
- Introduces a probabilistic programming execution protocol to link to scientific simulators
- To make inference tractable it needs to rely on techniques, such as amortization through inference compilation, which essentially constructs an oracle
- Pushes the frameworks to the extreme with communication requirements and data exchange between computing instances

DreamCoder [6]

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
- 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

[6] 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

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

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

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

DreamCoder

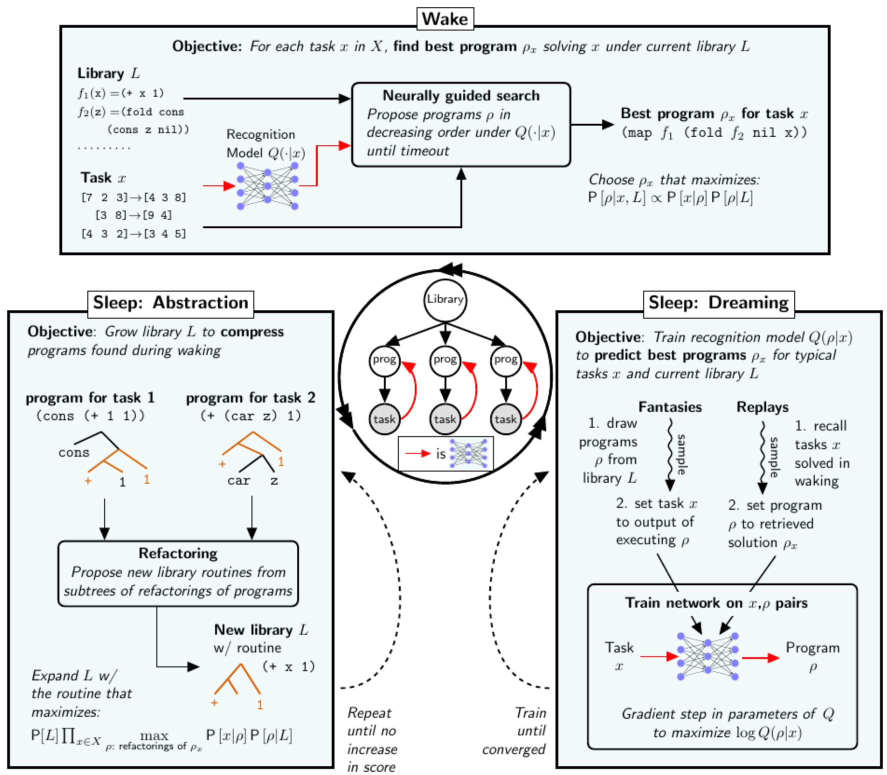


Figure: Algorithm Cycle of DreamCoder

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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: $\mathcal{B}_x \leftarrow \mathcal{B}_x \cup \{\rho \mid \rho \in$ enumerate$(\mathrm{P}[\cdot|D, \theta], T)$ 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: $\mathcal{B}_x \leftarrow \mathcal{B}_x \cup \{\rho \mid \rho \in$ enumerate$(Q(\cdot|x), T)$ 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
        $D, \theta, \{\mathcal{B}_x\}_{x \in X} \leftarrow$ABSTRACTION$(D, \theta, \{\mathcal{B}_x\}_{x \in X})$ ▷ Abstraction Sleep
        yield (D, θ), 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

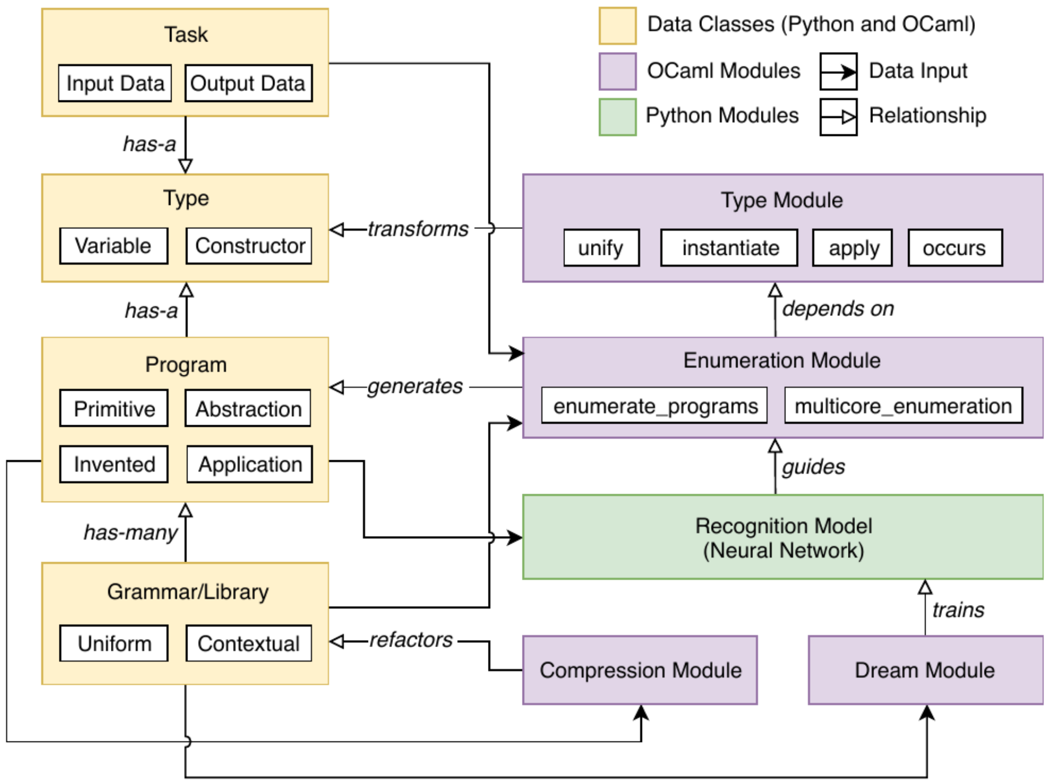

Figure: Different data-classes in DreamCoder.

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DreamCoder

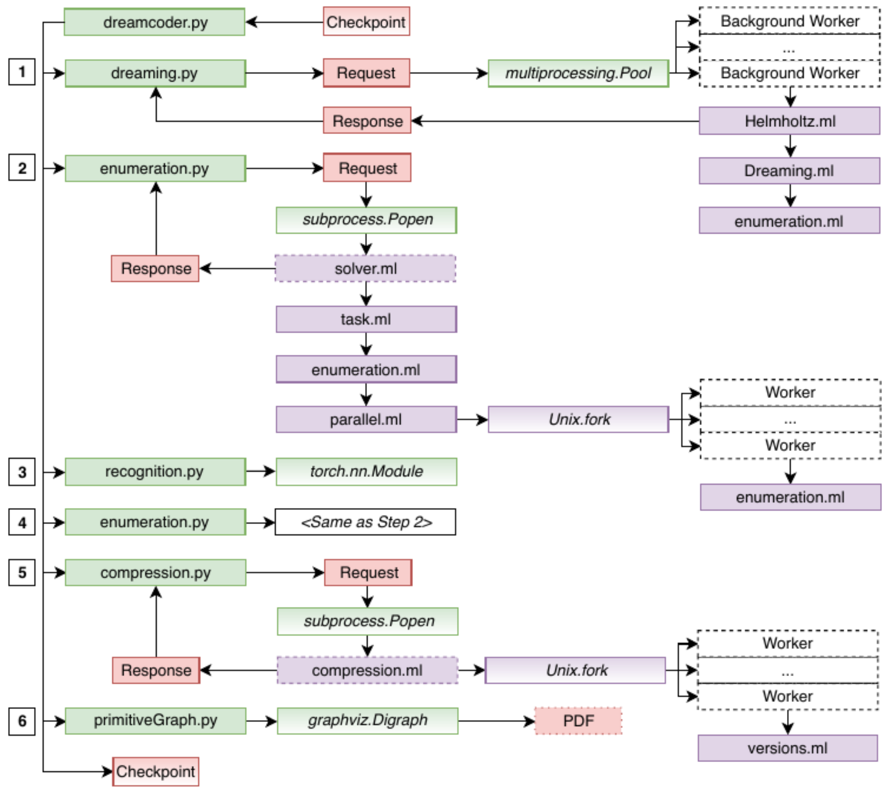
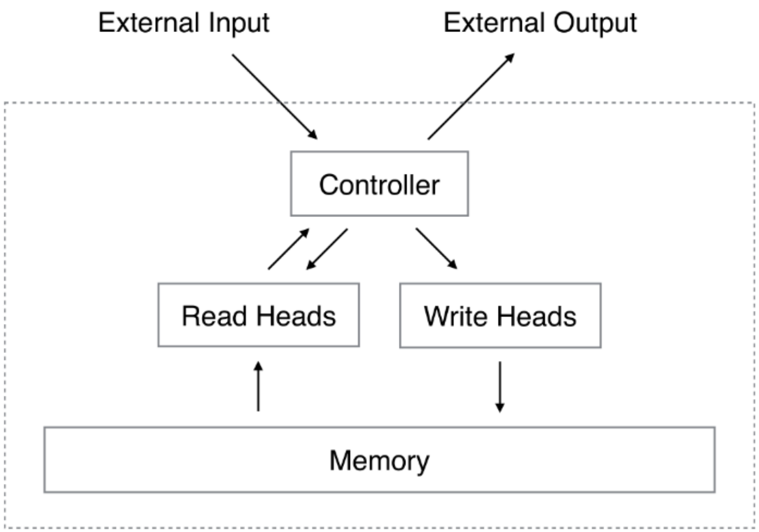


Figure: Program Flowchart: Phase 1, Dreaming. Phase 2, 1st Program Enumeration. Phase 3, Recognition Model Training. Phase 4, 2nd Program Enumeration. Phase 5, Abstraction (Compression). Phase 6, Library Visualization.

Recap: Helmholtz Machine [7] [8]

- Couples neural networks with external memory, which is accessed through an internal attention mechanism
  - Iteratively modify the state of the network through its memory mechanism
- Can infer simple algorithms from data
- Structure
  - Controller is a neural network
  - Heads select the part of the memory to access
  - Memory is essentially a large matrix



[7] Graves, A., Wayne, G. and Danihelka, I., 2014. Neural turing machines. arXiv preprint arXiv:1410.5401.
[8] YouTube: DeepMind x UCL | Deep Learning Lectures | 8/12 | Attention and Memory in Deep Learning

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Recap: Helmholtz Machine

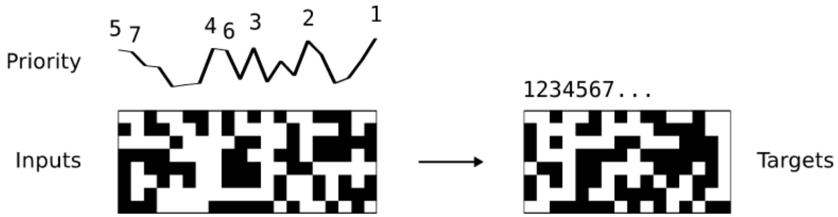
- Heavily relies on selection attention, whee the controller emits a distribution over the memory matrix, which then defines content- and location-based attention mechanisms [9]
- Content-based:
  - A key vector is compared to each memory location
- Location-based:
  - Use a shift kernel in conjunction with the weighting to shift to a new location in memory
- Results in three different interaction modes:
  1. Content key only
  2. Content and location
  3. Location only

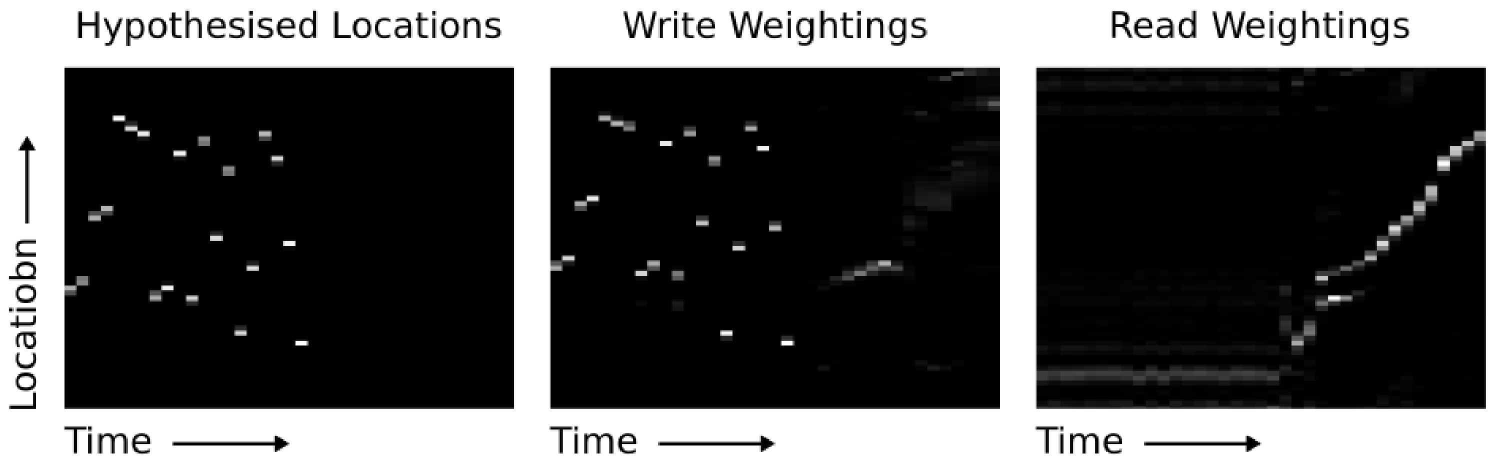
[9] Lilian Weng's review of attention: https://lilianweng.github.io/lil-log/2018/06/24/attention-attention.html

Recap: Helmholtz Machine

Example: Priority Sort

- Learns algorithm to sort data from a sequence of random binary vectors and their respective scalar priority rating





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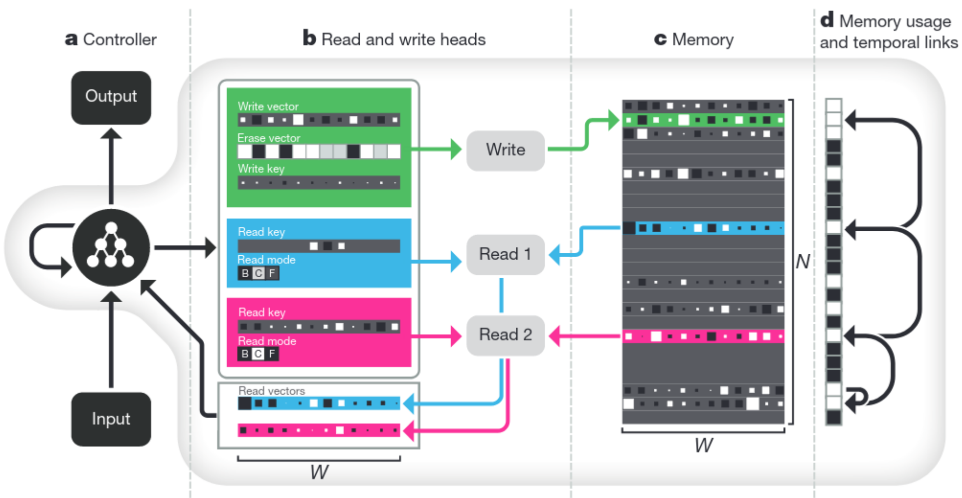
Outlook: Differentiable Neural Computer [10]

- Successor architecture to the neural turing machine with new attention mechanisms
- Specifically geared towards applications in graphs ⟶ more on this later!



[10] 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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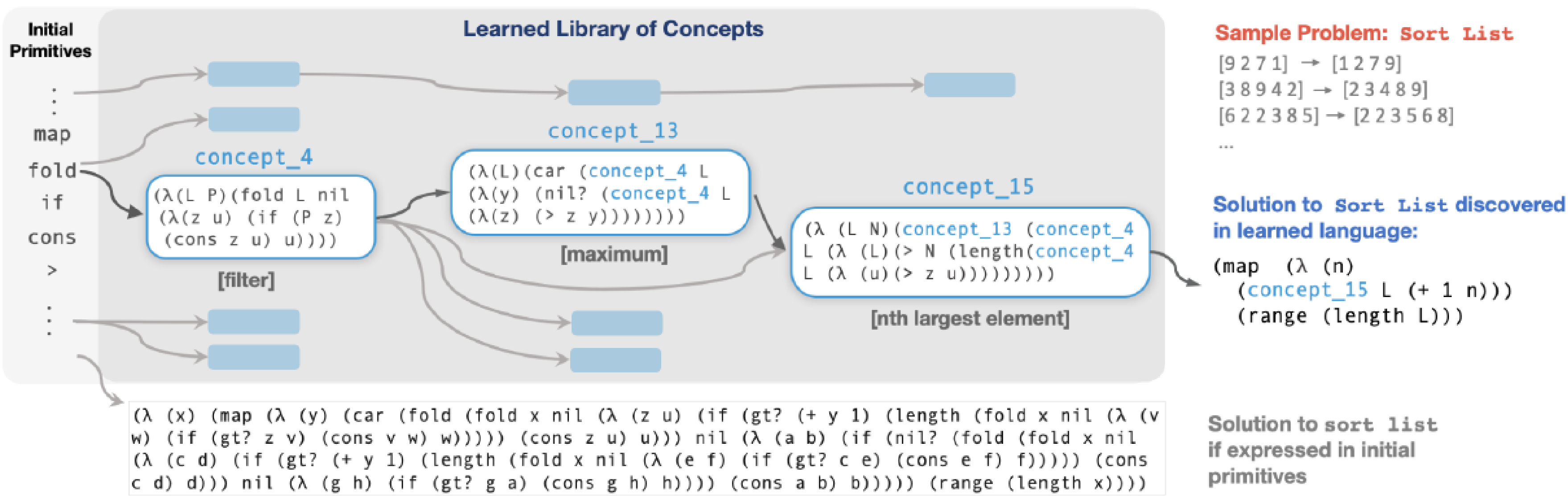
DreamCoder

- 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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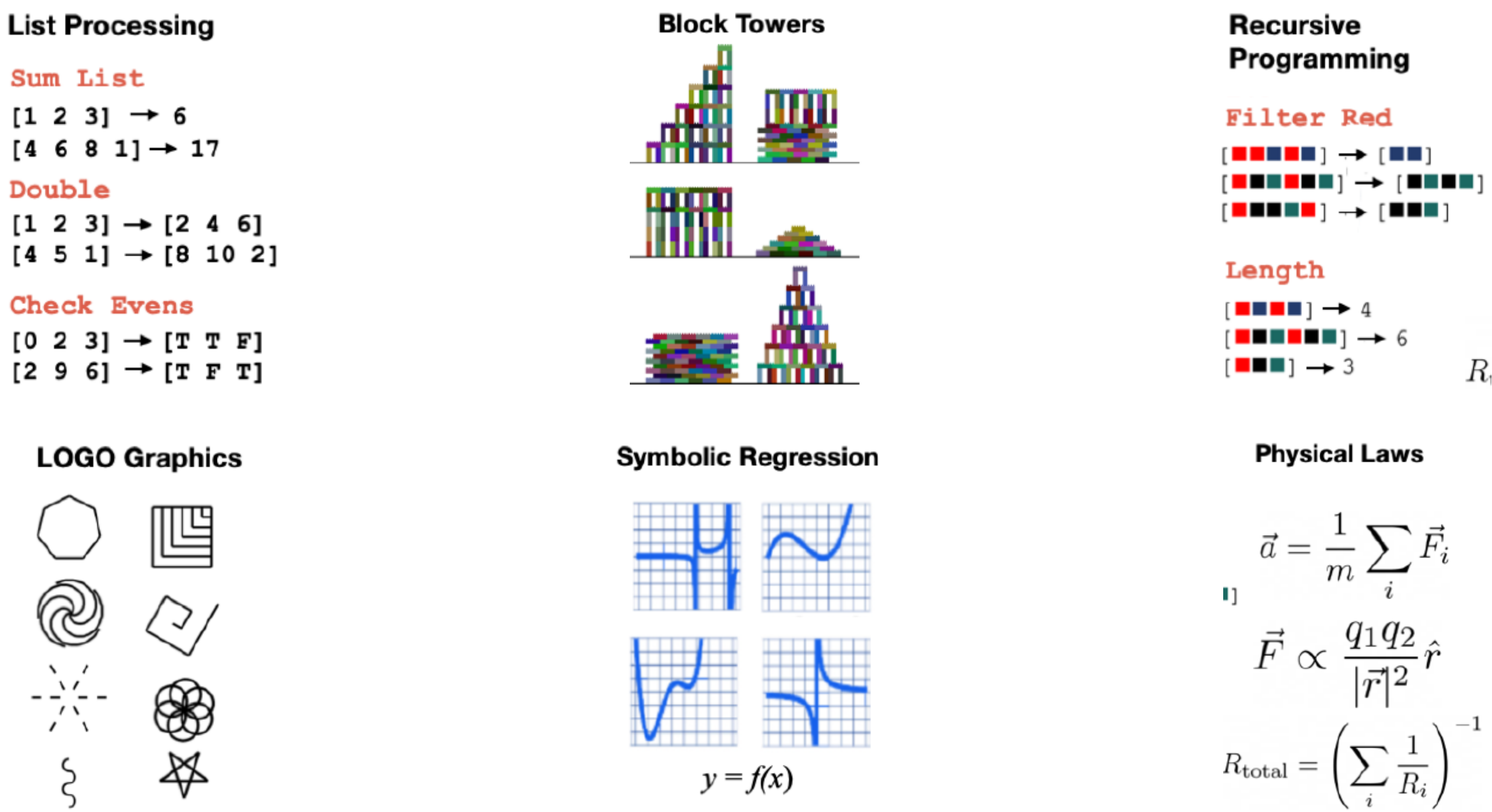
DreamCoder

Applications



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Applications

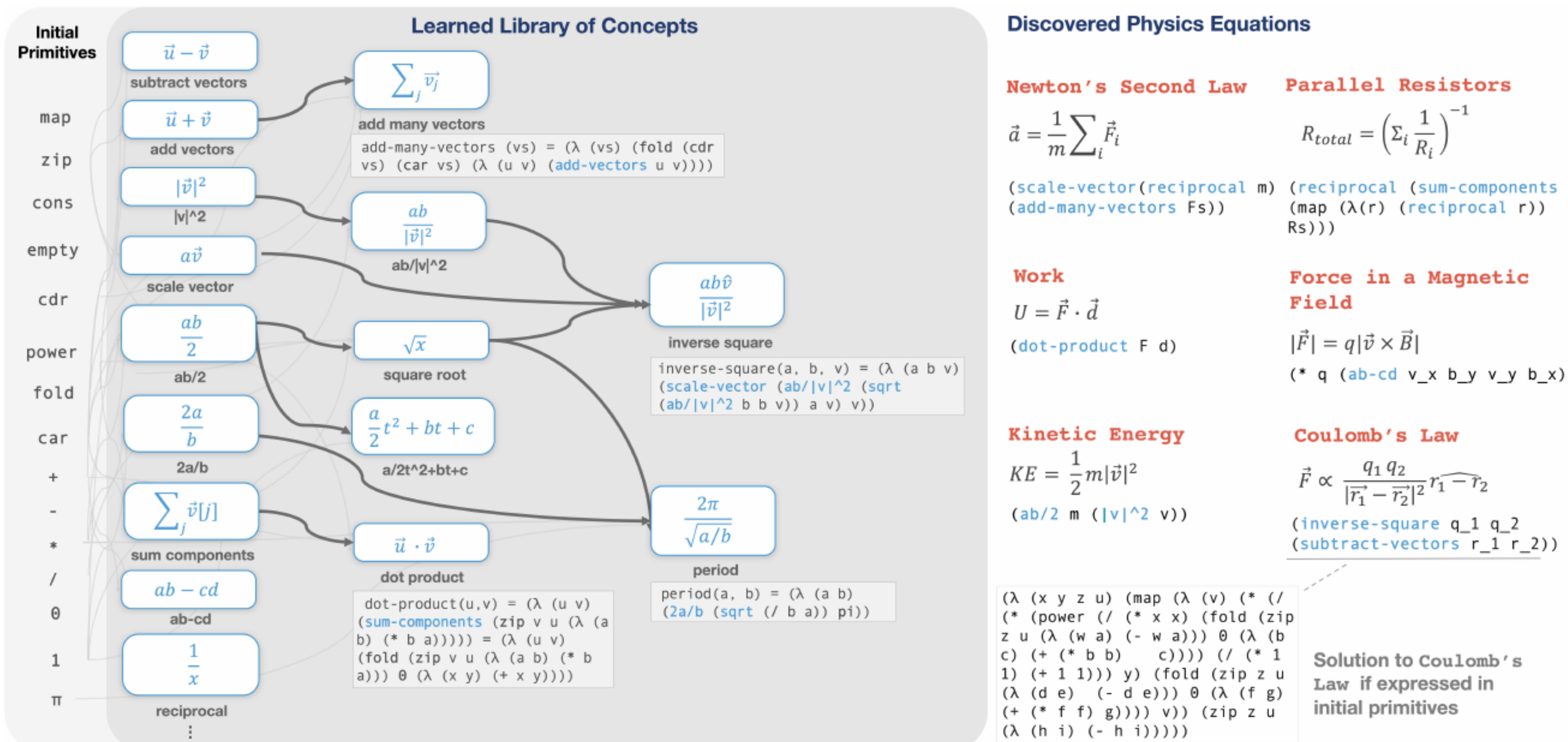

Figure: Learned library for physics equations.

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Applications

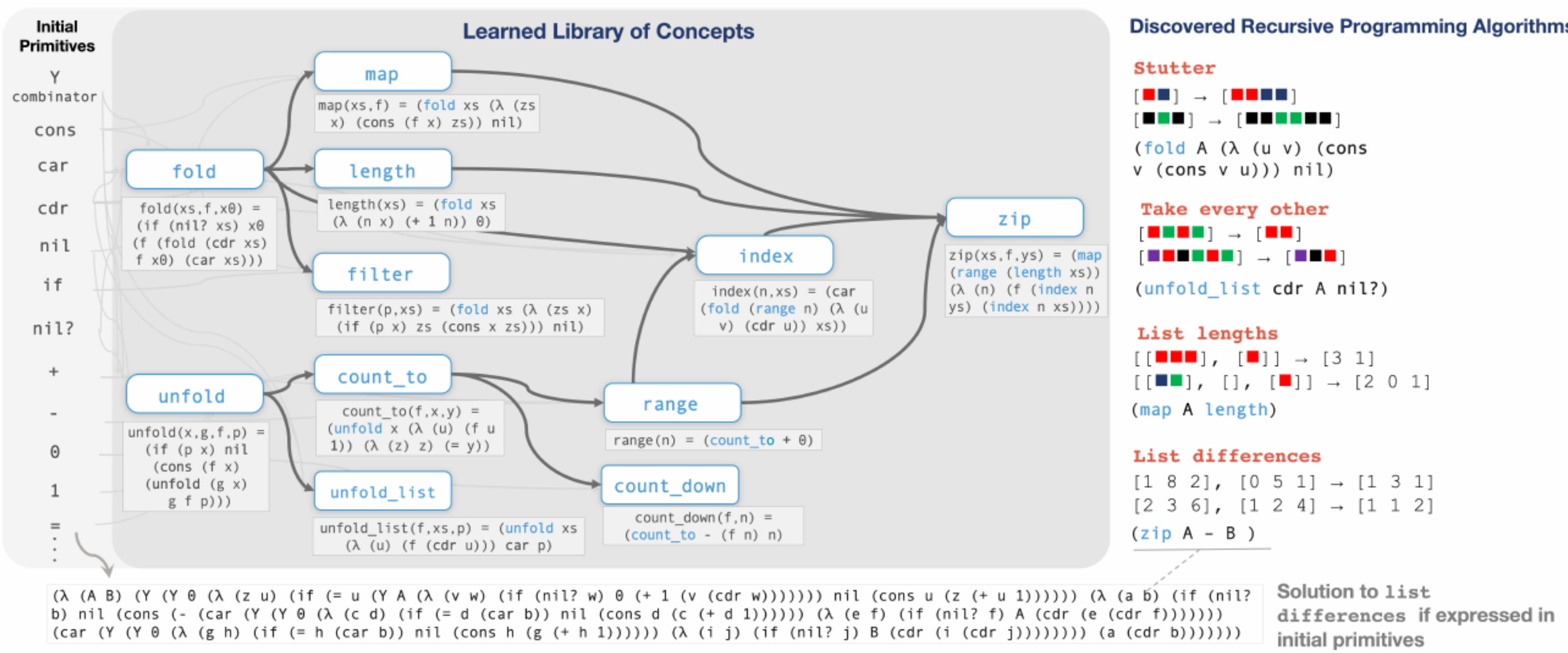

Figure: Learned library for recursive programming algorithm.

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DreamCoder

Applications

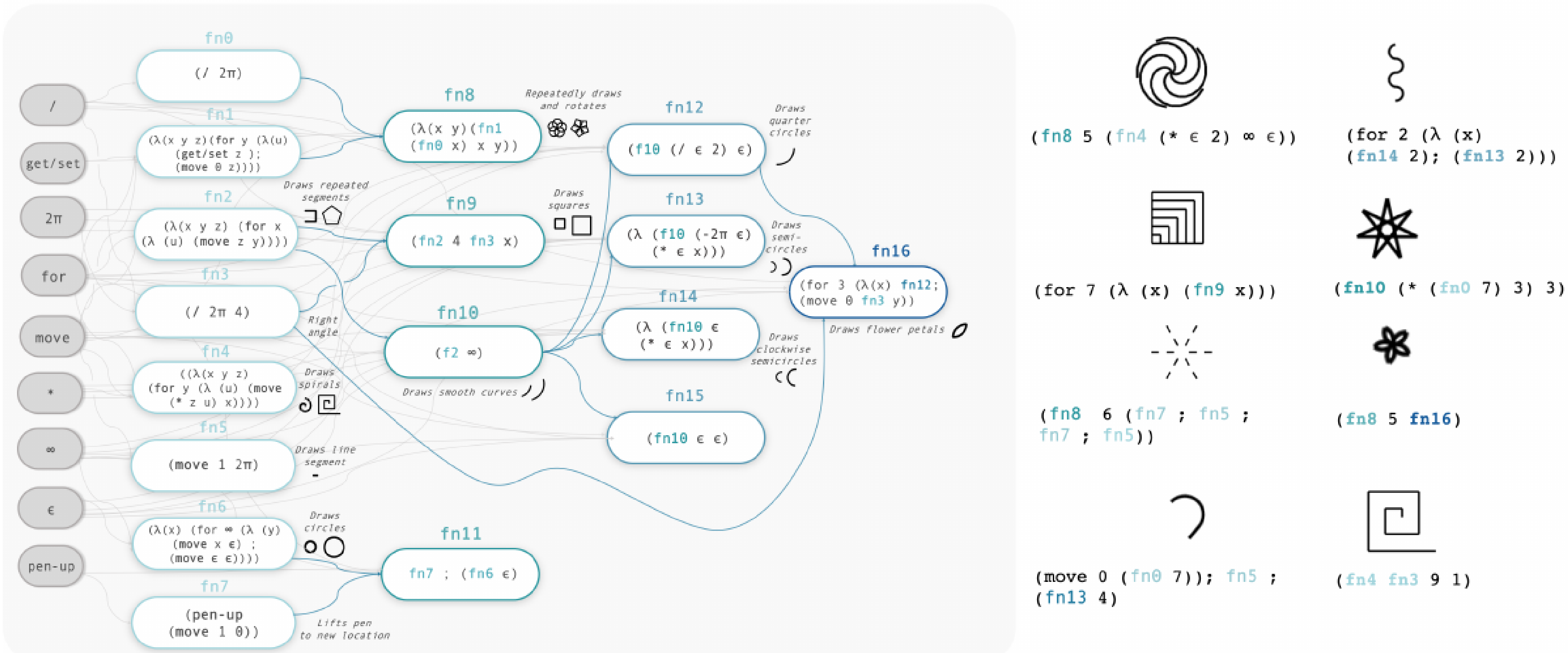

Figure: Learned library for LOGO graphics.

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DreamCoder

Applications

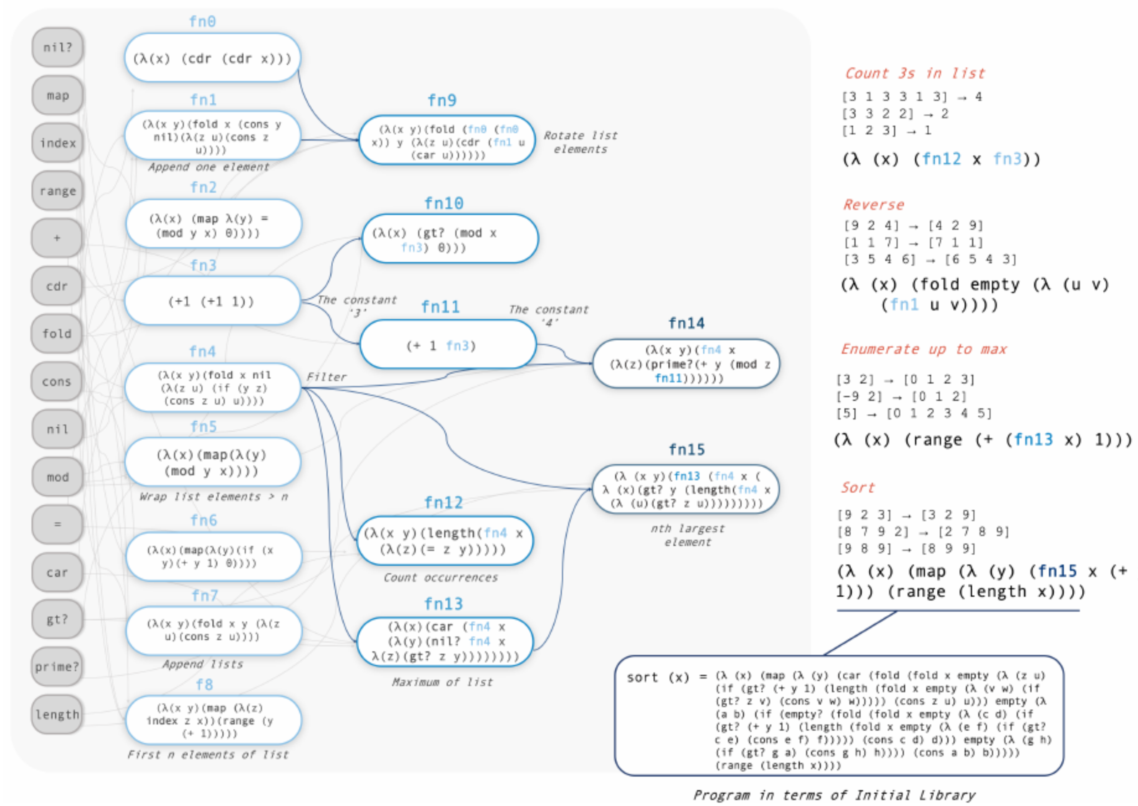

Figure: Learned library for list processing.

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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Outline

Why Do We Need Probabilistic Programming?

- Blub 1

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Why Do We Need Probabilistic Programming?

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Why Do We Need Probabilistic Programming?

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Why Do We Need Probabilistic Programming?

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Why Do We Need Probabilistic Programming?

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Why Do We Need Probabilistic Programming?

- Blub 8

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