Machine Learning for Hard Optimization Problems in Computer System Design

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Facebook AI

2006 2008 2013 2015 2021 **PhD Waymo Facebook AI Research Computer Vision Reinforcement Learning**

Career Path

Reinforcement Learning

Go Chess Chess Shogi Shogi Poker

Big Success in Games

DoTA 2 StarCraft II

What is Reinforcement Learning?

What is Reinforcement Learning?

State: where you are?

Action: left/right/up/down

Next state: where you are after the action?

What is Reinforcement Learning?

State: $s=(x,y)=(6,0)$

Actions:

 $x \leftarrow x-1$ Left: Right: $x \leftarrow x + 1$ Up: $y \leftarrow y - 1$ Down: $y \leftarrow y + 1$

What is Reinforcement Learning? $\rightarrow x$ **Trajectory** s_{t+2} a_{t+1} s_{t+1} a_t St \dot{y}

Goal of Reinforcement Learning $\rightarrow x$ s_{t+2} a_{t+1} s_{t+1} a_t St \dot{y} Goal State

 $W^*(s)$ Maximal reward you can get starting from state s $Q^*(s, a)$ Maximal reward starting from s after taking action a Probability of taking action a given state s $\pi(a|s)$

 (S) Reward you can get, starting from s following policy π $Q^{\pi}(s, a)$ Reward starting from s after taking action a and following π

Bellman Equations

$$
Q^*(s, a) = r(s, a) + \gamma \max_{a'} Q^*(s'(s, a), a')
$$
\n
$$
V^*(s) = \max_{a} r(s, a) + \gamma V^*(s'(s, a))
$$
\n
$$
Q^*(s, a)
$$

As long as we can enumerate *all possible* states and actions

Q-learning

$$
Q^{(n)}(s_t, a_t) \leftarrow r(s_t, a_t) + \gamma \max_{a'} Q^{(n-1)}(s_{t+1}, a')
$$

 $Q_{\theta}(s, a)$ now have generalization capability

How could you take the gradient w.r.t θ ? Note that θ appears on both sides.

Q-learning

$$
Q_{\theta}(s_t, a_t) \leftarrow r(s_t, a_t) + \gamma \max_{a'} Q_{\theta'}(s_{t+1}, a')
$$

Old fixed parameters
Fixing RHS and learn θ from LHS.
Target network

Q-learning (make the target even smoother) Smoothing factor
 $Q_{\theta}(s_t, a_t) \leftarrow (1 - \alpha) Q_{\theta}(s_t, a_t) + \dot{\alpha} \left[r(s_t, a_t) + \gamma \max_{a'} Q_{\theta'}(s_{t+1}, a') \right]$ $\Delta Q_{\theta}(s_t, a_t) \propto r(s_t, a_t) + \gamma \max_{a'} Q_{\theta'}(s_{t+1}, a') - Q_{\theta}(s_t, a_t)$

Temporal Difference (TD) Error

facebook Artificial Intelligence

[*Mnih et al.* Human-level control through deep reinforcement learning*, Nature 2015]*

Multi-step Q-learning

Trajectories from **replay buffer**

Sample trajectories

Q-learning

$$
Q_{\theta}(s_t, a_t) \leftarrow r(s_t, a_t) + \gamma \max_{a'} Q_{\theta}(s_{t+1}, a')
$$

How could we sample a trajectory in the state space?

Dynamic "dataset": takes experience as input provide data for training

On-policy versus Off-policy approaches

Off-policy, sampled by some behavior policy $\beta(\cdot|s)$ Expert behaviors (imitation learning) Supervised learning

On-policy, sampled by the current models $Q(s, a)$ $\pi(\cdot|s)$

Agent not only learns from the data, but also chooses which data to learn.

Deep Q-Learning

Before training

What's Beyond Games?

GOOGLE TEACHES AI TO PLAY THE GAME OF CHIP DESIGN

February 20, 2020 Timothy Prickett Morgan

Several weeks with **human experts** in the loop

 \rightarrow

Fully automatic design in 6 hours

Optimization Problems

Wait…What?

- Many problems are NP-hard problems.
	- No good algorithm unless $P = NP$
- These guarantees are worst-case ones.
	- To prove a lower-bound, construct an adversarial example to fail the algorithm
- For specific distribution, there might be better heuristics.
	- Human heuristics are good but may not be suitable for everything

More Efficient Search for Optimization

Exhaustive search to get **a good solution**

More Efficient Search for Optimization

Exhaustive search to get **a good solution**

Efficient Search for Games

DarkForest (2015) AlphaGo (2016) AlphaZero (2017) OpenGo (2018)

Deep Blue (2002) AlphaZero (2017)

AlphaZero (2017)

Human Knowledge Machine learned models

Optimization \rightarrow Reinforcement Learning

Representation Matters!

Direct predicting solutions

[H. Mao et al, Resource Management with Deep Reinforcement Learning, ACM Workshop on Hot Topics in Networks, 2016*]*

[O. Vinyals. et al, Pointer Networks, NIPS 2015]

Local Rewriting Framework

Xinyun Chen Yuandong Tian

[X. Chen and Y. Tian, Learning to Perform Local Rewriting for Combinatorial Optimization, NeurIPS 2019]

Start from a feasible solution and iteratively converges to a good solution

Q-Actor-Critic Training

How to train two policies $\pi_{\omega}(\cdot | s_t)$ and $\pi_{\nu}(\cdot | s_t | \omega_t])$?

Learn Q to fit cumulative rewards:

$$
L_{\omega}(\theta) = \frac{1}{T} \sum_{t=0}^{T-1} \left(\sum_{t'=t}^{T-1} \gamma^{t'-t} r(s'_t, (\omega'_t, u'_t)) - Q(s_t, \omega_t; \theta) \right)^2
$$

 $\pi_{\omega}(\cdot | s_t)$: Q-learning with soft policy:

$$
\pi_{\omega}(\omega_t|s_t; \theta) = \frac{\exp(Q(s_t, \omega_t; \theta))}{\sum_{\omega_t} \exp(Q(s_t, \omega_t; \theta))}
$$

$$
\boldsymbol{\pi_u}(\cdot~|\boldsymbol{s_t}~[\boldsymbol{\omega_t}])\text{: Actor-Critic with learned Q:}\\\text{book Artificial Ir} \begin{equation} L_u(\phi) = -\sum_{t=0}^{T-1} \Delta(s_t,(\omega_t,u_t))\log\pi_u(u_t|s_t[\omega_t];\phi) \end{equation}
$$

facel

$$
\frac{\text{Advantage:}}{\Delta(s_t, (\omega_t, u_t))} \equiv \sum_{t=t'}^{T-1} \gamma^{t'-t} r(s'_t, (\omega'_t, u'_t)) - Q(s_t, \omega_t; \theta)
$$

Different Action Spaces for Different Applications

Online Job Scheduling

Graph representation

Online Job Scheduling

Structured Data

Delaunay triangulation timings (seconds)									
Number of points	10,000			100,000			1.000.000		
Point distribution	Uniform	Boundary	Tilted	Uniform	Boundary	Tilted	Uniform	Boundary	Tilted
Algonthin	Random	of Circle	Gnd	Random	of Circle	Grid	Random	of Circle	Grid
Div & Conq, alternating cuts									
robust	0.33	0.57	0.72	45	5.3	55	58	61	58
non-robust	0.30	0.27	0.27	4.0	4.0	35	53	56	44
Div & Conq, veitical cuts									
robust	0.47	1.06	0.96	6.2	9.0	7.6	79	98	85
non-robust	0.36	0.17	failed	5.0	2.1	42	64	26	failed
Sweepline									
non-robust	0.78	0.62	0.71	10.8	8.6	10.5	147	119	139
Incremental									
robust	1.15	3.88	2.79	24.0	112.7	101.3	545	1523	2138
non-robust	0.99	2.74	failed	213	94.3	failed	486	1327	failed
								39	

How to encode Structure Data

Child-Sum LSTM

$$
y_1 = f(y_2, y_3, x_1)
$$

[Improved Semantic Representation From Tree-Structured Long Short-Term Memory Networks. K. Tai et al]

f can be very complicated:

$$
\tilde{h}_j = \sum_{k \in C(j)} h_k,
$$
\n
$$
i_j = \sigma \left(W^{(i)} x_j + U^{(i)} \tilde{h}_j + b^{(i)} \right),
$$
\n
$$
f_{jk} = \sigma \left(W^{(f)} x_j + U^{(f)} h_k + b^{(f)} \right),
$$
\n
$$
o_j = \sigma \left(W^{(o)} x_j + U^{(o)} \tilde{h}_j + b^{(o)} \right),
$$
\n
$$
u_j = \tanh \left(W^{(u)} x_j + U^{(u)} \tilde{h}_j + b^{(u)} \right),
$$
\n
$$
c_j = i_j \odot u_j + \sum_{k \in C(j)} f_{jk} \odot c_k,
$$
\n
$$
h_j = o_j \odot \tanh(c_j),
$$

How to encode Structure data

• Graph Convolutional Network (GCN)

[Semi-Supervised Classification with Graph Convolutional Networks, T. Kipf and M. Welling, ICLR 2017]

How to encode Structure data

• Graph Convolutional Network (GCN)

A: Affinity matrix of a graph $\hat{A} = D^{-1/2} A D^{-1/2}$

Node embedding at layer *l*: $X_l \in \mathbb{R}^{n \times d_l}$

Node Embedding at layer *l+1*: $X_{l+1} = \text{ReLU}(\hat{A}X_lW)$

[Semi-Supervised Classification with Graph Convolutional Networks, T. Kipf and M. Welling, ICLR 2017]

Online Job Scheduling

Baselines:

Earliest Job First (EJF) Shortest Job First (SJF) Shortest First Search (SJFS) DeepRM

Google OR-tools (OR-tools) SJF-offline Offline baselines:

Online Job Scheduling: Ablation Study

The learned model can generalize to different job distributions.

Expression Simplification

Expression Simplification

Baselines:

Z3-simplify Z3-ctx-solver-simplify Heuristic Search Halide rules

Follow-up work: Getting rid of manually specified rules

[H. Shi et al., Deep Symbolic Superoptimization without Human Knowledge, ICLR 2020]

Capacitated Vehicle Routing

facebook Artificial Intelligence

Code is available: https://github.com/fa

Coda: An End-to-End Neural Program Decomplier

Cheng Fu¹, Huili Chen¹, Haolan Liu¹, Xinyun Chen³, Yuandong Tian², Farinaz Koushanfar¹, Jishen Zhao¹

1UC San Diego, 2Facebook AI Research, 3UC Berkeley

NeurIPS 2019

Background: Decompilation

- Goal of Decompilation
	- From Binary Execution to High-level program language

- Many hardware architectures (ISA): x86, MIPS, ARM
- Many Programming Languages (PL)
	- Extra Human effort to extend to the new version of the hardware architectures or programming languages
- Our goals:
	- Maintain both the functionality and semantics of the binary executables
	- Make the design process end-to-end (generalizable to various ISAs and PLs)

Leverage both syntax and dynamic information

Stage 1: Coda Sketch Generation

• Is Decompilation simply a translation problem?

More than a translation problem!

Stage 1: Coda Sketch Generation

• **Encoder**

- N-ary Tree Encoder to capture **inter** and **intra** dependencies of the low-level code.
- Opcode and its operands are encoded together
- Different encoder is used for different instruction types
	- memory (mem)
	- branch (br)
	- arithmetic (art).

5

Code **Sketch**

Stage 1: Coda Sketch Generation

• **Decoder**

- Generate Abstract Syntax Tree (AST)
- AST can be equivalently translated into its corresponding high level Program
- Advantages:
	- Prevent error propagation/ Preserve node dependency / capture PL grammar
	- Boundaries are more explicit (terminal nodes)
- Using Attention Mechanism

Stage 2: Iterative Error Correction

- The sketch generated in Stage 1 may contain errors:
	- mispredicted tokens, missing lines, redundant lines

Golden program If($a > c$) { $a = b + c * a$; $b = a - c$; } *Wrongly predicted* If($a > b$) { $a = b + c * a$; $b = a - b$ } *Missing lines* If($a > c$) { $a = b + c * a$; } *Redundant lines* If($a > c$) { $a = b + c * a$; $b = a$; $b = a$: }

Error Correction

Stage 2: Iterative Error Correction

Error **Correction**

- Correct the error by iterative Error Predictor (EP)
	- Iterative rewriting!
	- Spot errors in the generated assembly codes
	- Fix errors and recompile
	- Repeat 10 times

Experimental Setup

- Compiler configuration: Clang **–O0** (no code optimization)
- Benchmarks:
	- Synthetic programs:
		- **Karel library (Karel)** only function calls
		- **Math library (Math)** function calls with arguments
		- **Normal expressions (NE)** $(\hat{A}, \hat{B}, \hat{B}, -\hat{C}, \hat{C}, \hat{C}, -\hat{C}, -\hat{C}, -\hat{C}, -\hat{C})$
		- **Math library + Normal expressions (Math+NE)** replaces the variables in NE with a return value of math function.
- Metrics:
	- Token Accuracy
	- Program Accuracy

Result – Stage 1 Performance

• Token accuracy (%) across benchmarks

- Highest token accuracy across all benchmarks (96.8% on average) compared to baselines.
- 10.1% and 80.9% margin over a naive Seq2Seq model with and without attention.
- More tolerant to the growth of program length.

Result – Stage 2 Performance

• Program accuracy (%)

s2s = sequence-to-sequence with attention I2a = instruction encoder to AST decoder with attention

Result – Overall

- Coda vs. traditional decompiler (RetDec)
	- Lines of code: ~10K vs. ~500K **-- 50x reduction**
	- Toolkit size: ~10MB Neural network size vs. ~5GB toolkit size **-- 500x reduction**
- Summary:
	- First neural-based decompiler
		- Generative models with iterative error corrections.
	- Significantly outperforms seq2seq models.

Predefined Action Space

Fixed action space = R^{361}

[B. Zoph and Q. Le, Neural Architecture Search with Reinforcement Learning, 2016]

[G. Malazgirt, TauRieL: Targeting Traveling Salesman Problem with a deep reinforcement learning inspired architecture]

Predefined Action Space

Fixed action space = R^{361}

[G. Malazgirt, TauRieL: Targeting Traveling Salesman Problem with a deep reinforcement learning inspired architecture]

S₃

 S_1

 $S₃$

Why Predefined Action Space?

We only care the final solution

We don't care how we get it.

Different Representation matters

Depth = $\{1, 2, 3, 4, 5\}$ Channels = $\{32, 64\}$ KernelSize = $\{3x3, 5x5\}$

1364 networks.

#samples

Goal: Find the network with the best accuracy using fewest trials.

Representation of action space

Sequential = { add a layer, set K, set C }

Global = { Set depth, set all K, set all C }

The Meaning of Learning Action Space

Not allowed in games, but doable in optimization.

Learning Action Space

[L. Wang, R. Fonseca, Y. Tian, **Learning Search Space Partition for Black-box Optimization using Monte Carlo Tree Search***, NeurIPS 2020]*

[L. Wang, S. Xie, T. Li, R. Fonseca, Y. Tian, **Sample-Efficient Neural Architecture Search by Learning Action Space***, TPAMI 2021]*

$Different$ Partition \rightarrow Different Value Distribution

facebook Artificial Intelligence

Accuracy

Learn action space

facebook Artificial Intelligence

[L. Wang, et al, Learning Search Space Partition for Black-box Optimization using MCTS, NeurIPS 2020]

Fixed action branches (but not action space) (a) Train the action space.

(b) Search using learned action space until a fixed #rollouts are used.

> Monte Carlo Tree Search (MCTS)

Getting the true quality $f(x)$ for the solution x

Monte Carlo Tree Search

Search towards the good nodes while keeping exploration in mind

Why Exploration is Important

- Bad solution
- OK solution \bullet
	- Optimal solution

OK solutions but not optimal Most solutions are bad but there exists an optimal one

NASNet Search Space

Customized dataset: LSTM-10K (PTB)

Customized dataset: ConvNet-60K (CIFAR-10, VGG style models)

Performance

NASBench-101 (CIFAR-10, 420k models, NASNet Search Space)

Each curve is repeated 100 times. We randomly pick 2k models to initialize.

M: number of samples selected.

Open Domain

La-MCTS as a meta method $x^* = \arg\min_{x \in \Omega} f(x)$

Optimizing linear policy for Mujoco tasks

Limitations

N/A stands for not reaching reward threshold.

 r_{best} stands for the best reward achieved by LA-MCTS under the budget in Fig. 3.

Too many explorations might hurt in Mujoco tasks.

Multi-Objective Optimization

Code is public now!

https://github.com/facebookresearch/LaMCTS

Both 3rd and 8th teams in NeurIPS 2020 Black-box optimization competition use our method!

https://github.com/facebookresearch/CompilerGym

Robust, high-performance reinforcement learning environments for compiler optimization tasks facebook Artificial Intelligence

An iterative decision-making process **And iterative decision-making process** Challenges

- 1. Huge state and action space
- 2. Many irrelevant actions
- 3. Graph-structured observations
- 4. Learned policy needs to transfer well

Goals

- 1. Lower the barrier to entry to AI for compilers res
- 2. Provide common benchmarks for compiler optin
	- o e.g. "ImageNet for Compilers", CodeXGLUE for pe
- 3. Advance the state-of-the-art in AI for compilers

Long term

- 1. Enable every single compiler decision to be cont
- 2. Build a family of "SysML Gyms" and tools for ma

There are a lot of Programs available

Leader Board

LLVM Instruction Count

Summarization and Future Works

• Summary

- Machine Learning can be used to learn heuristics for optimization problems.
- Many system problem are optimization problems
- Use ML to make the system smarter \odot
- Many Challenges ahead
	- Huge state / action space.
	- Irrelevant actions
	- Slow evaluation (sim2real problem)

