AlphaD3M: Machine Learning Pipeline Synthesis

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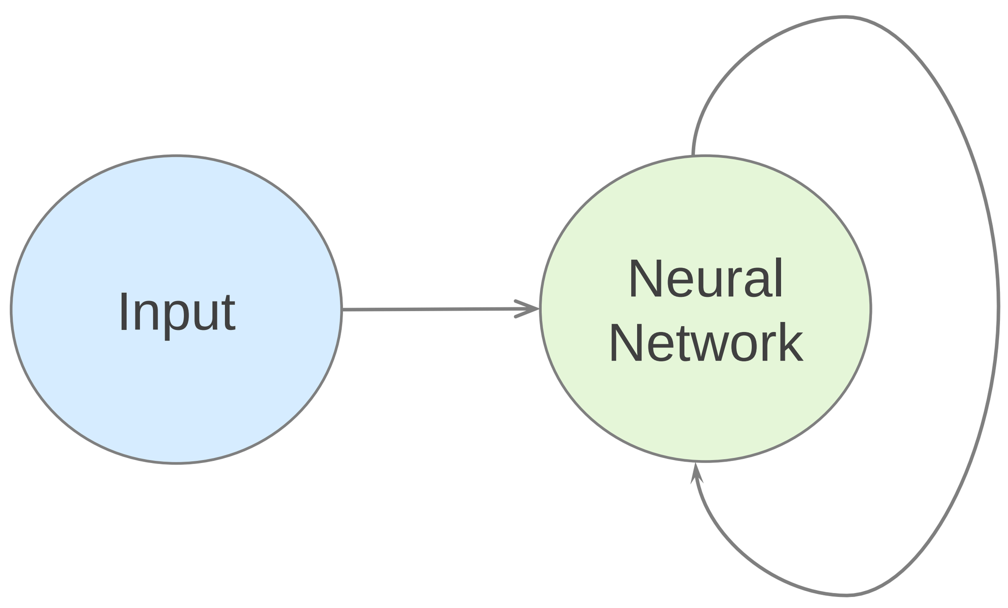
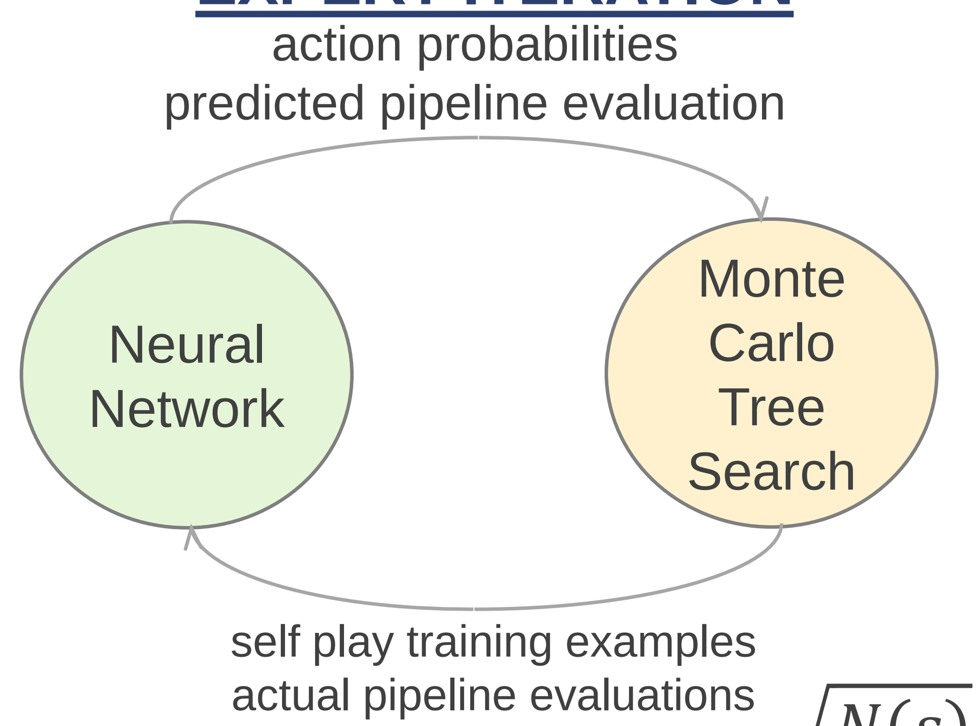
NEURAL NETWORK



$$L(\theta) = S \log R + (v - e)^2 + \alpha||\theta||_2 + \beta||S||_1$$

- Stochastic Gradient Descent (SGD), forward and backward passes
- Iterative Type 1 architecture
- Type 1: Optimize loss function by SGD for network parameter θ
- Make predicted model S match real world model R
- Make predicted evaluation v match real evaluation e

EXPERT ITERATION



$$U(s,a) = Q(s,a) + cP(s,a)\frac{\sqrt{N(s)}}{1 + N(s,a)}$$

- Type 2 using Type 1: MCTS calling NN action-value function
- $Q(s,a)$: expected reward for action a from state s
- $N(s,a)$: number of times action a was taken from state s
- $N(s)$: number of times state s was visited
- $P(s,a)$: estimate of NN probability of taking action a from state s
- c: constant determining amount of exploration

ALPHAD3M

AlphaD3M is based on Type2 architecture and **models meta data, task and a full pipeline chain as state** rather than individual primitives

Given datasets D, tasks T, and a set of pipelines $S = \{S_1, \ldots, S_n\}$ from available machine learning and pre-processing primitives

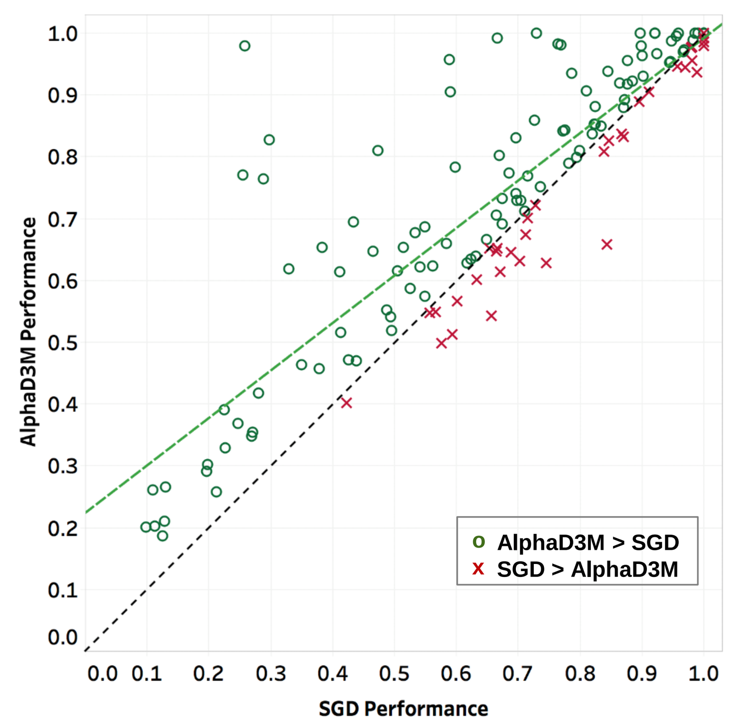
For each $D_i \in D$ and $T_j \in T$, to encode state at time t:

1. Encode dataset D_i as meta data features $f(D_i)$
2. Encode task T_j
3. Encode pipeline at time t by a vector S_t
4. Encode action $f_a(S_t)$, so policy π maps $\left(f(D_i), T_j, S_t\right)$ to $f_a(S_1), \ldots, f_a(S_n)$

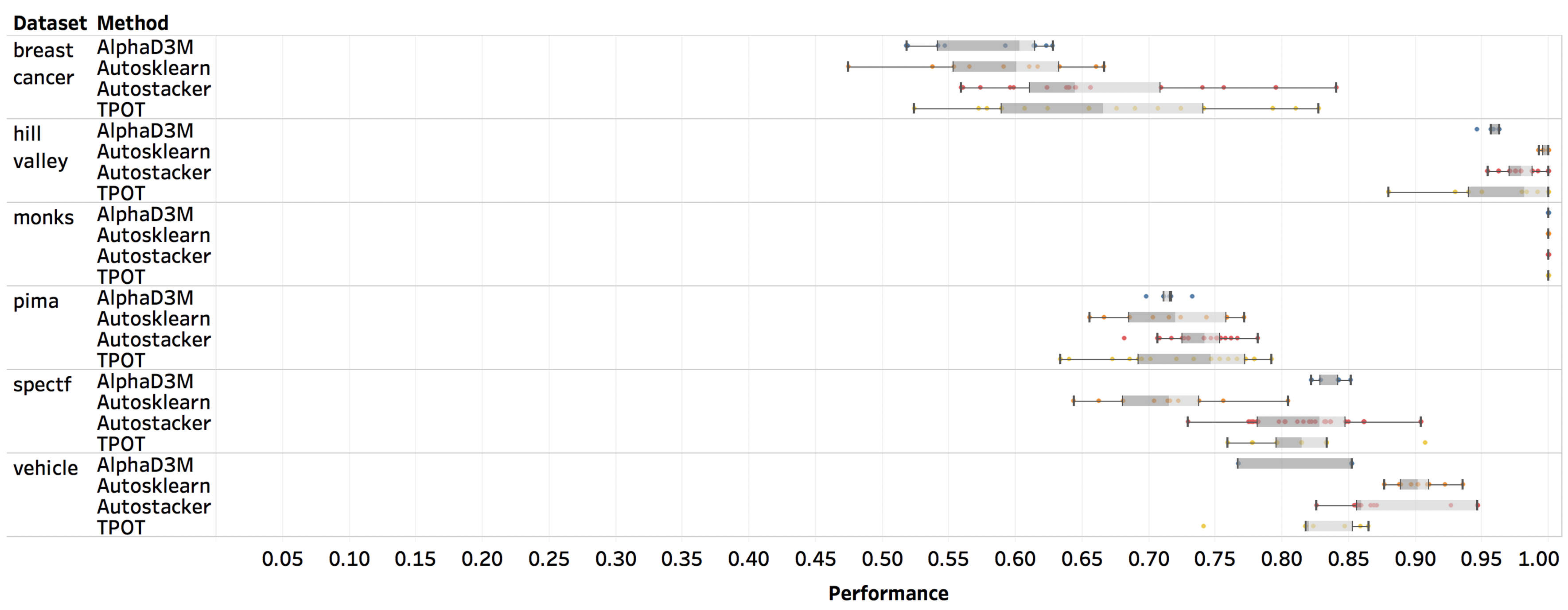
	AlphaZero	AlphaD3M
Game	Go, chess	AutoML
Unit	piece	pipeline, primitive
State	configuration	meta data, task, pipeline
Action	move	insert, delete, replace
Reward	win, lose, draw	pipeline performance

AlphaD3M single player representation

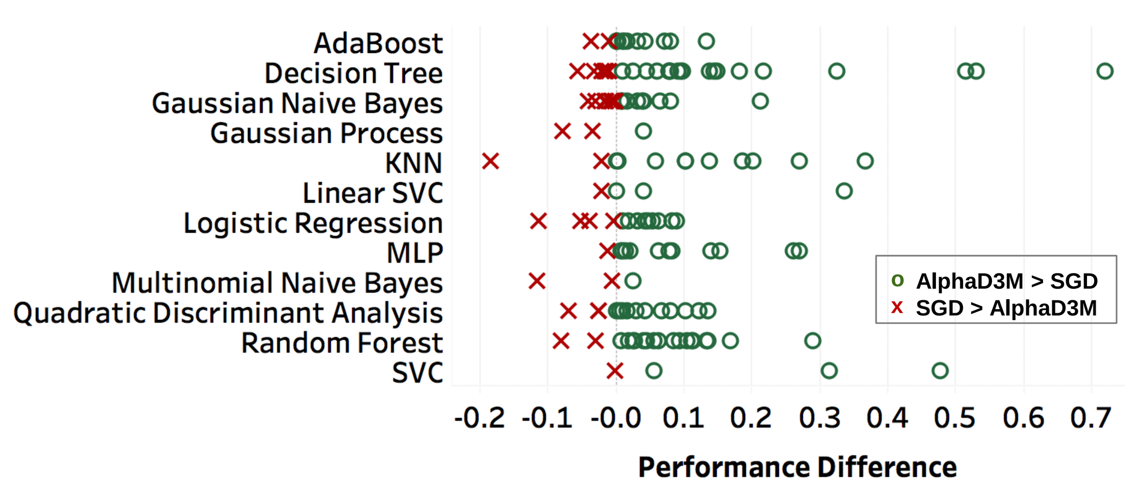
EXPERIMENT RESULTS



AlphaD3M vs SGD performance on OpenML



Comparison of AutoML methods on OpenML



AlphaD3M vs SGD for different estimators

Dataset/Method	TPOT	Autostacker(AS)	AlphaD3M	Speedup vs TPOT	Speedup vs AS
breast cancer	3366	1883	460	7.3	4
hill valley	17951	8411	556	32.2	15.1
monks	1517	1532	348	4.3	4.3
pima	5305	1940	619	8.5	3.1
spectf	4191	1673	522	8	3.2
vehicle	16795	4010	531	31.6	7.5

AlphaD3M running time comparison

ACKNOWLEDGEMENT

This work is funded by the Defense Advanced Research Projects Agency (DARPA) Data Driven Discovery (D3M) program