Category Theory in Machine Learning

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Machine Learning in Industry

- Almost every sufficiently large software system today involves some Machine Learning
- Many engineers view Machine Learning as a black box component of the system

Machine Learning Research

- Many of the largest and most sophisticated research ML systems are poorly understood
- Small details like the default way of rounding numbers or the random seed can dramatically impact performance
- Reinforcement learning systems are among the worst offenders

Machine Learning as Alchemy

- Without our knowledge of modern chemistry chemistry and physics, alchemists attempted to find an elixir for immortality, and cure any disease
- Could we be in a similar situation with Machine Learning?

Machine Learning Today

- Individual components are very well understood
- Composition and combinations of models are poorly understood
- State of the art results come from heuristics about what works well in practice

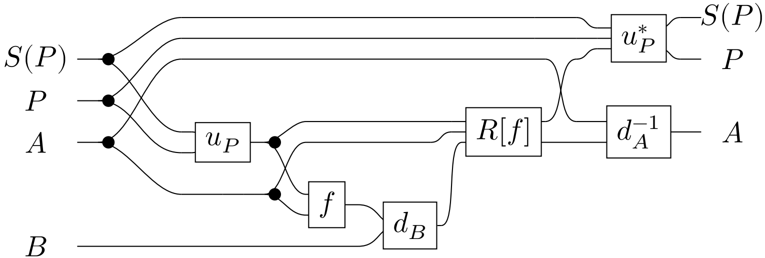
Category Theory in Machine Learning

- **Gradient-based methods** Building from the foundations of automatic differentiation to neural network architectures, loss functions and model updates.
- **Probabilistic methods** Building from the foundations of probability to simple Bayesian models.
- **Invariant and Equivariant Learning** Characterizing the invariances and equivariances of unsupervised and supervised learning algorithms.

Gradient-based methods

- Given a differentiable loss function $l : X \to \mathbb{R}$, the gradient descent algorithm finds $x \in X$ that minimizes $l(x)$ by setting x_0 and repeating $x_{t+1} = x_t - \alpha \nabla l(x)$
- Many researchers have explored generalizations of the derivative in terms of the primitives of Cartesian categories.
- We can use these generalized derivatives to study the structure of gradient-based optimization

Gradient-based methods



Category Theoretic Probability

A popular strategy is to treat the notion of a random variable as a fundamental one, equivalent to notions such as space, group, or function.

Probabilistic methods: Synthetic probability theory

The systemization of basic concepts from probability theory into an axiomatic framework based in Category Theory. This enables understanding of joint distributions, marginalization, conditioning, Bayesian inverses, and more, purely in terms of interaction of morphisms.

Probabilistic methods: Probabilistic Machine Learning

Study categories in which morphisms represent inference/sampling maps that allow us to update a distribution and reason about uncertainty

$$
\begin{tikzcd}
1 \arrow[d, "P \sim \mathcal{GP}(m,k)"] \arrow[dr, "P_{ev_{\mathbf{x}}^{-1}} \sim \mathcal{N}(m(\mathbf{x}),k(\mathbf{x},\mathbf{x}))"] & \\
Y^X \arrow[r, shift left, "\mathcal{S}^{\mathbf{x}} = \delta_{ev_{\mathbf{x}}}"] & Y \arrow[l, shift left, "\mathcal{I}^{\mathbf{x}}"]
\end{tikzcd}
$$

Probability Monads

Base category	Monad D	$Kl(D)$	Has all conditionals?
Set	Distribution	- [6]	?
Meas	Giry	**Stoch**	? (Fritz, 2020, Ex. 11.7)
FinMeas	Giry	**FinStoch**	(Fritz, 2020, Ex. 11.6)
CGMeas	Giry	**CGStoch**	(Fong, 2013, Def. 3.4)
Pol	Giry	**BorelStoch**	(Fritz et al., 2020, Ex. 2.4)
QBS	- [6]	- [6]	?
CHaus	Radon	- [6]	X (Fritz, 2020, Ex. 11.4)

Invariant and Equivariant Learning

- Many powerful machine learning algorithms are invariant or equivariant to certain kinds of dataset transformations.
- Understanding these properties allows us to better understand how algorithms separate signal from noise.
- By characterizing an algorithm as a functor or natural transformation we can encode these invariances and equivariances in the morphisms of the source and target category.

Example: Unsupervised Learning

- Unsupervised learning algorithms extract insights from data without explicit supervision
- The output of the algorithm must be somewhat in line with the structure of that data
- If we cast these algorithms as various kinds of functors we can characterize this property in term of functoriality

Thank You