Project Example 1.

Flow Network based Generative Models ... Yoshua Bengio

Abstract

This paper is about the problem of learning a *stochastic policy* for generating an object (like a *molecular graph*) from a *sequence of actions*, such that the probability of generating an object is proportional to a given positive reward for that object. Whereas standard return maximization tends to converge to a single return-maximizing sequence, there are cases where we would like to sample a diverse set of high-return solutions. These arise, for example, in black-box function optimization when few rounds are possible, each with large batches of queries, where the batches should be diverse, e.g., in the design of new molecules. One can also see this as a problem of approximately converting an energy function to a generative distribution. While *MCMC* methods can achieve that, they are expensive and generally only perform local exploration. Instead, training a *generative policy amortizes the cost of search during training and yields to fast generation.* Using insights from Temporal Difference learning, we propose GFlowNet, based on a view of the generative process as a flow network, making it possible to handle the tricky case where different trajectories can yield the same final state, e.g., there are many ways to sequentially add atoms to generate some molecular graph. We cast the set of trajectories as a flow and co*nvert the flow consistency equations into a learning objective, akin to the casting of the Bellman equations into Temporal Difference* methods. We prove that any global minimum of the proposed objectives yields a policy which samples from the desired distribution, and demonstrate the improved performance and diversity of GFlowNet on a simple domain where there are many modes to the reward function, and on a molecule synthesis task.

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Topics:

- Theory: Reinforment Learning
- Application: Molecular graph
- Theory: MCMC
- Method:

Part 1.

Translation. Suppose we are doing regression. Then we are looking at two losses.

Quadratic: $(h - y)^2$

Log-Quadratic: $(\log h - \log y)^2$

Can we analyse those and make a conclusion?

Yes, see: https://en.wikipedia.org/wiki/Geometric_mean#Relationship_with_logarithms

Show that for a constant model, $h(x) = w$, with data $y = (y_1, \dots, y_m)$.

- Quadratic loss gives $w = AM(y) = \frac{1}{m} \sum y_i$
- Log-quadratic loss gives $GM(y) = (\Pi_i y_i)^{1/m}$

Interpretation:

E.g. $y = (1, 10^6)$, then

- $AM(y) \approx .5 * 10^6$ and errors are $\pm 10^6$
- $GM(y) = 10^3$ and relative ares are $10^3 : 1$ and $1 : 10^3$

But, does this explain "*equal gradient weighting to large and small magnitude predictions?*"

Idea: dig into this. Interpret that statement mathematically, and see if it holds.

Hint: $h(x) = wx$ what is gradient of loss of model now?

Hint: may need to change the statment.

Part 2

"To avoid this problem, we define the flow matching objective on a log-scale, where we match

not the incoming and outgoing flows but their logarithm... (equation 12) ... which gives equal gradient weighing to large and small magnitude predictions."

Interpret this. What is this theorem about? Is it just that there is a unique minimizer of the loss? Would this follow from textbook loss analysis? Or is there more?