Variational Inference for Policy Gradient

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Abstract

Inspired by the seminal work on Stein Variational Inference \cite{2} and Stein Variational Policy Gradient \cite{3}, we derived a method to generate samples from the posterior variational parameter distribution by explicitly minimizing the KL divergence to match the target distribution in an amortize fashion. Consequently, we applied this variational inference technique into vanilla policy gradient, TRPO and PPO with Bayesian Neural Network parameterizations for reinforcement learning problems.

1 Parametric Minimization of KL Divergence

Suppose we have a random sample from a base distribution $\xi \sim q_0(\xi)$, e.g. $q_0 = \mathcal{N}(0, I)$, we are able to generate an induced distribution $q_{\phi}(\theta)$ by the general invertible and differentiable transformation $\theta = h_\phi(\xi)$ (see Appendix A). Our goal is to regard $q_{\phi}(\theta)$ as a variational distribution to match the true distribution $p(\theta)$ such that $J = KL(q_{\phi}(\theta)||p(\theta))$ is minimized.

Lemma 1.

$$H(q) = H(q_0) + E_{\xi \sim q_0} \left( \log \det \left( \frac{\partial h_\phi(\xi)}{\partial \xi} \right) \right)$$  (1)

with (1), we can have the following identity for $KL(q_{\phi}(\theta)||p(\theta))$:

$$KL(q||p) = -H(q_0) - E_{\xi \sim q_0} \left( \log \det \left( \frac{\partial h_\phi(\xi)}{\partial \xi} \right) \right) - E_{\xi \sim q_0} (\log p(h_\phi(\xi)))$$

$$= -H(q_0) - E_{\xi \sim q_0} \left( \log \det \left( \frac{\partial h_\phi(\xi)}{\partial \xi} \right) + \log p(h_\phi(\xi)) \right)$$

Hence the gradient of $KL(q||p)$ with respect to the parameters of transformation mapping $\phi$ is:

$$\frac{\partial KL}{\partial \phi} = -E_{\xi \sim q_0} \left[ \frac{\partial \log p(h_\phi(\xi))}{\partial \phi} + \frac{\partial}{\partial \phi} \log \det \left( \frac{\partial h_\phi(\xi)}{\partial \xi} \right) \right]$$  (2)

Note that the first term is the usual log-likelihood term, and the second term serves as a repulsive force preventing all $\xi$’s from collapsing towards the
maximum likelihood estimation. We can perform stochastic gradient descent using (2) to find the optimal $\phi$. This method is related to the interesting and seminal Stein Variational Inference [1], the major difference is that the later one uses kernelized Stein variational gradient, while we use log determinate as the repulsive force.

2 Bayesian Formulation of Variational RL

We generate the policy distribution from Bayesian Neural Network. Suppose $\theta$ is the parameter of the policy network, the parameter is able to generated from a base distribution $\xi \sim N(0, I)$ with an invertible and differentiable transformation function $h_\phi(\xi)$. We may adopt complicated differentiable transformation functions $h_\phi(\xi)$. For a simple example, the weight for each connection of neuron could be $\theta_i = \mu_i + \sigma_i$. For each realized weight parameter $\theta$, we are able to generate a stochastic multi-modal policy distribution $\pi_\theta(a|s)$ represented as a Neural Network with several hidden layers.

$R(\theta)$ is the expected cumulative reward under policy $\pi_\theta$,

$$R(\theta) = E_{\pi_\theta} \left[ \sum_t \gamma^t r(s_t, a_t) \right]$$

$P$ is a distribution over $\theta$ and $H(P)$ is the Shannon entropy of $P$. We want to find $P$ to maximize the following objective:

$$\tilde{R} = \int R(\theta)dP(\theta) + \alpha H(P)$$

$$\tilde{R} = \alpha \int \left( \log \left( \frac{1}{p(\theta)} \right) + \frac{1}{\alpha} R(\theta) \right) dP(\theta)$$

$$= \int \log \left( \frac{\exp(\frac{1}{\alpha} R(\theta))}{p(\theta)} \right) dP(\theta)$$

The optimal $P$ is:

$$p(\theta) \propto \exp \left( \frac{1}{\alpha} R(\theta) \right) \quad (3)$$

This formulation is originally proposed in [3]. The difficulty of this formulation is calculating the normalization factor $\int \exp(\frac{1}{\alpha} R(\theta))d\theta$. We are able to bypass it by calculating the gradient of the its log-probability which was a exciting idea from Stein variational inference [2] and similarly, here we can use Eq. [2]. Suppose we generate sample of $\theta$ by transforming random noise $\xi$ using $h_\phi(\xi)$. Let $q_\phi(\theta)$ be the induced variational distribution from the transformation. Our optimization objective is to match the induced variational distribution and the
'true' policy parameter distribution by minimizing $KL(q||p)$. The gradients for the parameters ($\phi$) of policy distribution are,

$$-\frac{\partial KL}{\partial \phi} = E_{\xi \sim q_0} \left[ \frac{1}{\alpha} \frac{\partial R(\theta)}{\partial \theta} + \frac{\partial}{\partial \phi} \log \det \left( \frac{\partial h_\phi(\xi)}{\partial \xi} \right) \right]$$

(4)

where $\frac{\partial R}{\partial \theta}$ can be calculated using the standard policy gradient formula,

$$\frac{\partial R(\theta)}{\partial \theta} = E_{\pi_\theta} \left[ \sum_t \frac{\partial}{\partial \theta} \log \pi_\theta(a_t|s_t) \frac{\partial h(\theta)}{\partial \theta} A(s_t, a_t) \right]$$

(5)

We can sample different $\theta$ for exploration in different sessions. We may want to decrease $\alpha$ during the training to anneal the temperature to stationary parameter distributions.

$A(s_t, a_t)$ is the advantage function, it can be estimated as $A(s_t, a_t) = Q(s_t, a_t) - b(s_t)$ or let baseline $b(s_t) = V(s_t)$, or $A(s_t, a_t) = r(s_t, a_t) + V(s_t) - V(s_{t+1})$, and $Q(s_t, a_t)$ is the state-action $Q$ value and $V(s_t)$ is the value function. For more sophisticated estimation, we can use GAE (Generalized Advantage Estimation, [5]).

**Example 1:** For a simple transformation of the following form:

$$\theta_i = \mu_i + \sigma_i \xi_i$$

the sample gradient estimation w.r.t $\mu_i$ and $\sigma_i$ is:

$$\frac{\partial KL}{\partial \mu_i} = \frac{1}{\alpha} \frac{\partial R(\theta)}{\partial \theta_i}$$

$$\frac{\partial KL}{\partial \sigma_i} = \frac{1}{\alpha} \xi_i \frac{\partial R(\theta)}{\partial \theta_i} + \frac{1}{\sigma_i}$$

3 Variational Policy Gradient with Transformation

We introduce our varational inference into vanilla policy gradient REINFORCE [7]. Given a realization of network parameter $\theta$, in order to generate a stochastic policy distribution, we introduce another random noise $\zeta \sim \pi_0(\cdot)$. With the second invertible and differentiable transformation $a = g_\theta(s, \zeta)$, it induces a stochastic policy distribution $a \sim \pi_\theta(a|s)$ in the closed form,

$$\pi_\theta(a_t|s_t) = \frac{\pi_0(g_\theta^{-1}(a_t, s_t))}{\det \left( \frac{\partial g_\theta(s_t, \zeta)}{\partial \zeta} \right)}$$

(6)

Hence, the policy gradient is,

$$E_{\pi_\theta} \left\{ \sum_t \left[ \frac{\partial}{\partial \theta} \log \pi_0(g_\theta^{-1}(a_t, s_t)) - \frac{\partial}{\partial \theta} \log \det \left( \frac{\partial g_\theta(s_t, \zeta)}{\partial \zeta} \right) \right] A(s_t, a_t) \right\}$$

(7)
When the inverse of transformation \( \zeta = g^{-1}_\theta(a, s) \) is difficult to calculate, we could use \( g_\theta(s, \zeta) \) directly,

\[
\frac{\partial R(\theta)}{\partial \theta} = E_{\pi_\theta} \left\{ \sum_t \left[ \frac{\partial}{\partial \zeta} \log \pi_0(\zeta) \cdot \frac{\partial \zeta}{\partial g_\theta(s_t, \zeta)} - \frac{\partial}{\partial \theta} \log \det \left( \frac{\partial g_\theta(s_t, \zeta)}{\partial \zeta} \right) \right] A(s_t, a_t) \right\}
\]

### 3.1 Simple Policy Network Parameterization

We adopt a very simple yet general representative generative model. The policy parameter is generated from noise \( \xi \) with transformation \( h_\phi(s, \xi) \), which is a neural network parameterized with \( \phi \). With another noise \( \zeta \), we generate the action \( a \) by another transformation \( g_\theta(s, \zeta) \), parameterized with \( \theta \), from policy network distribution.

\[
\xi \sim N(0, I), \zeta \sim N(0, I)
\]

\[
\theta = h_\phi(s, \xi) = \mu_\phi(s) + \xi \cdot \sigma_\phi(s)
\]

\[
a = g_\theta(s, \zeta) = \theta(s, \xi) + \zeta
\]

This induces a simple policy distribution,

\[
\pi_\theta(a|s, \theta) \propto \exp \left( -0.5 \cdot (a - \theta)^T (a - \theta) \right)
\]

\( \mu_\phi(s) \) and \( \sigma_\phi(s) \) are mean and variance networks, with weight parameter \( \phi \), they are used to generate the posterior distribution of action mean \( \theta \). For continuous control problems, we use MLP (multilayer perceptron) to represents the mean and variance networks. Then we can find the variational policy parameter distribution by minimizing the KL divergence between the variation distribution \( q_\phi(\theta) \) generated based on the transformation \( h_\phi(s, \xi) \) and the optimal posterior parameter distribution \( p(\theta) \) (energy-based model, Eq. 3) as \( KL(q_\phi(\theta)|| \exp \{ R(\theta) \} ) \).

From the full complete gradient of Eq. (4), we have,

\[
-\frac{\partial KL}{\partial \phi} = E_{\xi \sim q_0} \left[ \frac{1}{\alpha} \frac{\partial R(\theta)}{\partial \theta} \frac{\partial h_\phi(s, \xi)}{\partial \phi} + \sum_{i=0}^{d} \frac{\partial \log \sigma^i_\phi(s)}{\partial \phi} \right]
\]

It is straightforward to auto diff \( \frac{\partial R(\phi)}{\partial \phi} \) and \( \frac{\partial \log \sigma_\phi(s)}{\partial \phi} \). \( \frac{\partial \log \sigma_\phi(s)}{\partial \phi} \) is the backprop of variance network \( \sigma_\phi \), for the simplest example, let \( \sigma_\phi(s) = \sigma(w^T s) \) a sigmoid function, we have,

\[
\sum_{i=0}^{d} \frac{1}{\sigma^i_\phi(s)} \frac{\partial \sigma^i_\phi(s)}{\partial \phi} = \sum_{i=0}^{d} (1 - \sigma^i_\phi(w^T s)) s
\]
3.2 Auxiliary Policy Network Parameterization

For a more general parameterization of the policy, instead of regarding $\theta$ as a parameter of policy, we can take $\theta$ as a random variable, and introduce the auxiliary network parameter $\Psi$, then the action $a$ is generated from noise $\zeta$ by transformation $g_\Psi(s, \theta, \zeta)$, it induces the corresponding policy distribution $\pi(a|s, \theta, \Psi)$. An example of $g_\Psi(s, \theta, \zeta)$ could be a MLP as,

$$g_\Psi(s, \theta, \zeta) = \text{MLP}_\Psi(\theta(s, \xi), s) + \zeta$$

Similarly, the posterior of $\theta$ is,

$$p(\theta) \propto p_0(\theta) \exp\left\{ \frac{1}{\alpha} R_\Psi(\theta) \right\}$$

here the cumulative rewards,

$$R_\Psi(\theta) = E_{\pi(\theta, \Psi)} \left[ \sum_t \gamma^t r(s_t, a_t) \right]$$

This gives us a more general representation of the policy, compared to the previous formulation in Section 3.1. Furthermore, it is easy to introduce multimodal distribution for the stochastic actions.

The gradient of KL divergence between the variational distribution and posterior $p(\theta)$ is Eq. 4. In addition, we need to learn network parameter $\Psi$,

$$\frac{\partial R_\Psi(\theta)}{\partial \Psi} = E_{\pi(\theta, \Psi)} \left[ \sum_t \frac{\partial \log \pi(\theta, \Psi)(a_t|s_t)}{\partial \Psi} A(s_t, a_t) \right]$$

4 Connection to TRPO

The motivation is to combine fast convergence with sample efficiency of TRPO \[4\] and the exploration introduced by variational inference of posterior policy parameter distribution.

The TRPO objective,

$$L(\theta) = E_{\theta_{old}} \frac{\pi(\theta|a|s)}{\pi_{old}(\theta|a|s)} A_{\pi_{old}}(a|s)$$

s.t. $D_{KL}(\pi_\theta, \pi_{old}) \leq \delta$

The TRPO Variational Policy Gradient,

$$-\frac{\partial KL}{\partial \phi} = E_{q_0} \left[ \frac{1}{\alpha} \frac{\partial L(\theta)}{\partial \theta} \frac{\partial }{\partial \phi} + \frac{\partial }{\partial \phi} \log \det \left( \frac{\partial h_\phi(\xi)}{\partial \xi} \right) \right]$$

TRPO Variational Policy Update:

$$\phi \leftarrow \phi - \eta H^{-1}(\theta) \nabla_{\phi} KL$$
Another important point is how to calculate the KL divergence between the current and previous policies efficiently?

\[
D_{KL}(\pi_\theta(\cdot|s), \pi_{\theta,old}(\cdot|s))) = KL(\mu_\theta(s), \mu_{\theta,old}(s))
\]

\[
\approx \frac{1}{2}(\theta - \theta_{old})^T H(\theta_{old})(\theta - \theta_{old})
\]

To get the Fisher information matrix, first method is to compute the Hessian of averaged KL divergence,

\[
H(\theta_{old})_{i,j} = E_s \left[ \frac{\partial^2}{\partial \theta_i \partial \theta_j} D_{KL}(\pi_\theta(\cdot|s), \pi_{\theta,old}(\cdot|s))) \right]
\]

This is equivalent to calculate the second derivative of \( KL(\mu_\theta(s), \mu_{\theta,old}) \) w.r.t. \( \theta \).

The other method is using Covariance matrix,

\[
H(\theta_{old}) = E_s \left[ \frac{\partial}{\partial \theta} \log \pi_\theta(\cdot|s) \left( \frac{\partial}{\partial \theta} \log \pi_\theta(\cdot|s) \right)^T \right]
\]

5 Connection to PPO

It is natural to adopt our variational inference method to PPO (Proximal Policy Optimization) \[6\]. The objective function of PPO to be maximized is,

\[
J_{ppo}(\theta) = E_{old_s} \left[ \pi_\theta(a|s) Q^\pi(a|s) - \lambda KL(\pi_{old}, \pi_\theta) \right]
\]

where \( KL(\pi_{old}, \pi_\theta) = E_{\pi_{old}}[KL(\pi_{old}(\cdot|s), \pi_\theta(\cdot|s))] \)

PPO Variational Policy Gradient,

\[
\frac{\partial KL}{\partial \phi} = E_{\xi \sim q_\phi} \left[ \frac{1}{\alpha} \frac{\partial J_{ppo}(\theta)}{\partial \theta} \frac{\partial \theta}{\partial \phi} + \frac{\partial}{\partial \phi} \log \det \left( \frac{\partial h_\phi(\xi)}{\partial \xi} \right) \right]
\]

The PPO Variational Policy Update is,

\[
\phi \leftarrow \phi - \eta \nabla_\phi KL
\]

A random variable transformation

Given random variable \( X \), we introduce the transformation function \( Y = f(X) \) to generate random variable \( Y \). The transformation function,

\[
f : \mathcal{R} \rightarrow \mathcal{R}
\]

\( f \) needs to be invertible, the inverse image of \( f \) of set \( A \),

\[
f^{-1}(A) = \{ x \in \mathcal{R}, f(x) \in A \}
\]

The inverse image also needs to satisfy the following requirements.
1. $f^{-1}(\mathcal{R}) = \mathcal{R}
2. f^{-1}(A^c) = f^{-1}(A)^c
3. f^{-1}(\bigcup_{\lambda} A_{\lambda}) = \bigcup_{\lambda} f^{-1}(A_{\lambda})$, for any sets $\{A_{\lambda}, \lambda \in \Omega\}$

Assume the distribution of r.v. $X$ and $Y$ are $p_X(x)$ and $p_Y(y)$, we have,

$$p_Y(y) = p_X(f^{-1}(y)) \det \left( \frac{\partial f^{-1}(y)}{\partial y} \right)$$

(13)

References

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