Advanced Policy Gradients - II

Easwar Subramanian

TCS Innovation Labs, Hyderabad

Email : easwar.subramanian@tcs.com / cs5500.2020@iith.ac.in

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Overview of this Lecture

Review

Policy Optimization Problem

The performance of a policy π_θ is given by

$$J(\theta) = V^{\pi_\theta}(s_0) = \mathbb{E}_{\pi_\theta}\left[\sum_{t=0}^{\infty} \gamma^t r_{t+1} | s_0 = s\right]$$

where $\gamma < 1$ is the discount factor of the MDP

General form for gradient of the performance measure is given by

$$\nabla_\theta J(\theta) = \mathbb{E}_{\pi_\theta}\left[\sum_{t=0}^{\infty} \nabla_\theta \log \pi_\theta(a_t|s_t)\Psi_t\right]$$

Disadvantages are :

- Sample Inefficiency : **on-policy expectation**
- Distance in parameter space $\neq$ policy space

Surrogate Loss Function

We recast the optimization problem using a **surrogate loss function**

$$\arg\max_{\pi'} J(\pi')$$

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We recast the optimization problem using a **surrogate loss function**

$$\arg\max_{\pi'} J(\pi') = \arg\max_{\pi'} \left[J(\pi') - J(\pi_0)\right] \approx \mathcal{L}_{\pi_0}(\pi')$$

where

$$\mathcal{L}_{\pi_0}(\pi') = \mathop{\mathbb{E}}_{\tau\sim\pi_0}\left[\sum_{t=0}^{\infty} \gamma^t \frac{\pi'(a_t|s_t)}{\pi_0(a_t|s_t)} A^{\pi_0}(s_t, a_t)\right]$$

The approximation is valid if policies π' and π_0 are **'close'** in terms of their KL divergence

Relative Policy Performance Bound

We can have a **relative policy performance bound** using KL divergence to measure the goodness of the approximation obtained

$$\left[J(\pi') - \left(J(\pi_0) + \mathcal{L}_{\pi_0}(\pi')\right)\right] \leq C\sqrt{\underset{s\sim d^{\pi_0}}{\mathbb{E}}\left[D_{KL}(\pi'||\pi_0)[s]\right]}$$

This gives rise to an optimization routine with the following iterative procedure with π_{k+1} and π_k are related by

$$\pi_{k+1} = \arg\max_{\pi'}\left[\mathcal{L}_{\pi_k}(\pi') - C\sqrt{\underset{s\sim d^{\pi_k}}{\mathbb{E}}\left[D_{KL}(\pi'||\pi_k)[s]\right]}\right]$$

Performance guarantee

$$[J(\pi_{k+1}) - J(\pi_k)] \geq 0$$

- C is quite high when γ is close to 1 and hence choosing step size becomes an issue

A First-Cut Algorithm

1: Initialize π_0
2: **for** $k = 0, 1, 2, \cdots$ until convergence **do**
3: Sample a trajectory τ from policy π_k
4: Compute advantage function $A^{\pi_{\theta_k}}(a_t, s_t)$ for all (s_t, a_t) pairs in the trajectory τ
5: Solve the optimization problem

$$\pi_{k+1} = \arg\max_{\pi'} L_{\pi_k}(\pi') - C\sqrt{\mathop{\mathbb{E}}_{s \sim d^{\pi_k}} \left[D_{KL}(\pi' || \pi_k)[s] \right]}$$

6: **end for**

A First-Cut Algorithm

Initialize π_0

for $k = 0, 1, 2, \cdots$ until convergence **do**

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  Compute advantage function $A^{\pi_{\theta_k}}(a_t, s_t)$ for all (s_t, a_t) pairs in the trajectory τ

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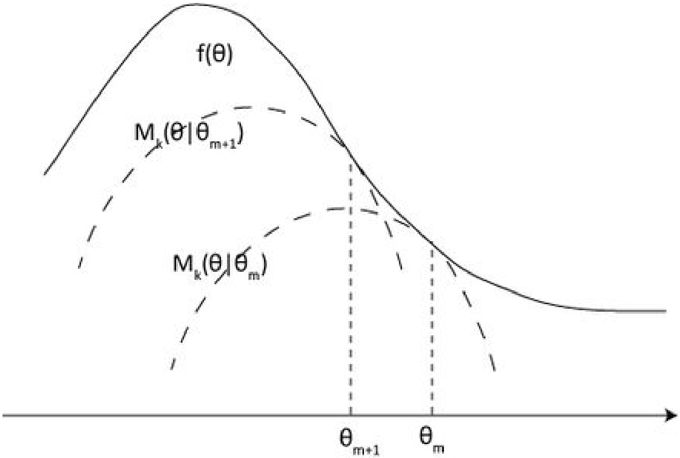
end for

Issues are :

- C is quite high when γ is close to 1 $\left(C = \frac{4\varepsilon\gamma}{1-\gamma^2}\alpha^2\right)$
- Consequently, step size becomes too small

Majorize Maximize Framework

Majorize-Maximize framework is used to solve the optimization step



Approximate Monotone Improvement

- Instead of KL penalty, use KL constraint
- Can control worst case error through constraint upper limit

$$
\begin{aligned}
\pi_{k+1} = \arg\max_{\pi'} &\left[L_{\pi_k}(\pi')\right] \\
\text{such that} \quad &\mathop{\mathbb{E}}_{s\sim d^{\pi_k}} D_{KL}(\pi' || \pi_k)[s] \leq \delta
\end{aligned}
$$

- From the constraint, **steps respect a notion of distance in policy space**
- Above constrained optimization is basis of many algorithms, Natural Policy Gradient (NPG), truncated NPG, TRPO and PPO
- The objective and the constraint can be estimated from the roll-out of old policies – **sample efficient**
- Update is **invariant** to parametrization

Natural Policy Gradient

Trust Region Formulation

We have the following optimization problem

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The constraint on the optimization problem is the trust region with size δ and some guarantees on performance improvement are there within the trust region

For parametrized policies the optimization can be written as

$$\pi_{\theta_{k+1}} = \arg\max_{\pi_\theta} \left[\mathcal{L}_{\pi_{\theta_k}}(\pi_\theta)\right]$$
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How do we solve it ?

- Linear approximation for the objective
- Quadratic approximation for the constraint

Approximation of Objective Function

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Taylor series expansion for function $f(x)$ around point a is given by

$$f(x) = f(a) + f'(a)(x-a) + \frac{1}{2}f''(a)(x-a)^2 + \cdots$$

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$$\mathcal{L}_{\pi_{\theta_k}}(\pi_\theta) \approx \cancelto{0}{\mathcal{L}_{\pi_{\theta_k}}(\pi_{\theta_k})} + g^T(\theta - \theta_k) \qquad \text{where } g \doteq \nabla_\theta \mathcal{L}_{\pi_{\theta_k}}(\pi_\theta)\,|_{\theta=\theta_k}$$

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- Recall that g is exactly the policy gradient (from previous lecture !)

$$\nabla_\theta \mathcal{L}_{\pi_{\theta_k}}(\pi_\theta)|_{\theta=\theta_k} = \mathop{\mathbb{E}}_{\tau \sim \pi_{\theta_k}} \left[\sum_{t=0}^{\infty} \nabla_\theta \log(\pi_{\theta_k}(a_t|s_t)|_{\theta=\theta_k} \ \gamma^t A^{\pi_{\theta_k}}(s_t, a_t) \right]$$

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- Objective function is simplified to

$$\theta_{k+1} = \arg\max_\theta g^T(\theta - \theta_k)$$

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The first order term $\nabla_\theta \bar{D}_{KL}(\pi_\theta||\pi_{\theta_k})$ evaluates to zero since the expectation of the score function is zero

$$\nabla_\theta \bar{D}_{KL}(\pi_\theta \,\|\, \pi_{\theta_k}) = \nabla_\theta \mathop{\mathbb{E}}_{\pi_\theta}[\log \pi_\theta] - \nabla_\theta \mathop{\mathbb{E}}_{\pi_\theta}[\log \pi_{\theta_k}] = \mathop{\mathbb{E}}_{\pi_\theta}[\nabla_\theta \log \pi_\theta] = 0$$

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Therefore, we are left only with the second order term

$$\bar{D}_{KL}(\pi_\theta || \pi_{\theta_k}) \approx \frac{1}{2}(\theta - \theta_k)^T H \ (\theta - \theta_k) \qquad \text{where } H \doteq \nabla_\theta^2 \bar{D}_{KL}(\pi_\theta || \pi_{\theta_k})\ |_{\theta=\theta_k}$$

Natural Policy Gradient

The optimization problem is now simplified as

$$\theta_{k+1} = \arg\max_{\theta} g^T(\theta - \theta_k)$$

$$\text{such that } \frac{1}{2}(\theta - \theta_k)^T H \; (\theta - \theta_k) \leq \delta$$

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$$\boxed{\text{Linear objective with quadratic constraint}}$$

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Linear objective with quadratic constraint

Solution to the approximate problem obtained using Lagrange multiplier method

$$\theta_{k+1} = \theta_k + \sqrt{\frac{2\delta}{g^T H^{-1} g}} H^{-1} g$$

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The term $H^{-1}g$ is called the Natural gradient

Algorithm : Natural Policy Gradient

Algorithm Natural Policy Gradient

Initialize π_0
for $k = 0, 1, 2, \cdots$ **do**
    Collect trajectories D_k on policy $\pi_k = \pi_{\theta_k}$
    Estimate all advantages $A^{\pi_{\theta_k}}(s_t, a_t)$
    Form sample estimates for policy gradients $\hat{g}_k$ (using advantage estimates)
    Form sample estimates for the Hessian of KL divergence
    Compute the Natural Policy Gradient update

$$\theta_{k+1} = \theta_k + \sqrt{\frac{2\delta}{g_k^T H_k^{-1} g_k}} H_k^{-1} g_k$$

end for

Fisher Information Matrix and KL Divergence

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- Let $p(x|\theta)$ be a probability distribution parameterized by θ.
- Score function of a parameterized probability distribution is given by

$$s(\theta) = \nabla_\theta \log p(x|\theta)\,,$$

- For a parameter vector θ, Fisher Information Matrix is given by,

$$\mathrm{F} = \mathop{\mathbb{E}}_{p(x|\theta)}\left[\nabla_\theta \log p(x|\theta)\, \nabla_\theta \log p(x|\theta)^{\mathrm{T}}\right].$$

- The sample estimate of the above expectation is given by,

$$\mathrm{F} = \frac{1}{N}\sum_{i=1}^{N} \nabla_\theta \log p(x_i|\theta)\, \nabla_\theta \log p(x_i|\theta)^{\mathrm{T}}\,. \tag{1}$$

- **Claim** : Fisher Information Matrix F is the Hessian of KL-divergence between two probability distributions $p(x|\theta')$ and $p(x|\theta)$ evaluated at $\theta' = \theta$

$$\mathrm{KL}[p(x|\theta')\,\|\,p(x|\theta)] = \mathop{\mathbb{E}}_{p(x|\theta)}[\mathrm{H}_{\log p(x|\theta)}] = \mathrm{F}$$

Properties of Natural Policy Gradient

- Natural policy gradient algorithm gives an update-rule in which updates are pre-multiplied by H^{-1}
- The Hessian of the KL-divergence is the Fischer Information Matrix given by

$$\mathrm{F} = \mathop{\mathbb{E}}_{\pi_\theta}\left[\nabla \log \pi_\theta(\cdot|s)\, \nabla \log \pi_\theta(\cdot|s)^{\mathrm{T}}\right]$$

- The NPG direction $H^{-1}g$ is **co-variant**; i.e. it points in same direction irrespective of the parametrization that is used to compute it

Relationship of Natural Gradient to Policy Gradient

Policy Gradient Formulation

Consider the following optimization problem

$$\pi_{\theta_{k+1}} = \arg\max_{\pi_\theta} \left[\mathcal{L}_{\pi_{\theta_k}}(\pi_\theta)\right]$$
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After **linearising** the objective, the optimization problem is now,

$$\theta_{k+1} = \arg\max_{\theta} g^T(\theta - \theta_k) \text{ such that } (\theta - \theta_k)^2 \leq \delta$$

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This is the original policy gradient problem !!

We move a small distance in parameter space in the direction of the gradient

Natural Gradient Formulation

Natural policy gradient problem is given by,

$$\pi_{\theta_{k+1}} = \arg\max_{\pi_\theta} \left[\mathcal{L}_{\pi_{\theta_k}}(\pi_\theta) \right]$$
$$\text{such that } \bar{D}_{KL}(\pi_\theta || \pi_{\theta_k}) \leq \delta$$

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After **linearising** the objective and **quadratifying** the constraint, fhe optimization problem is then given by,

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- Vanilla policy gradient has the right objective but *"incorrect"* constraint (Euclidean penalty instead of KL penalty)
- Recall that, policy iteration (from MDP lectures) obtain policy improvement with no constraint

Other Algorithms

Truncated Natural Policy Gradient

- **Problem** : For neural networks, the dimensionality of parameter θ are high. High computational cost in inverting the matrix H

Truncated Natural Policy Gradient

- **Problem** : For neural networks, the dimensionality of parameter θ are high. High computational cost in inverting the matrix H
- **Solution** : Use the **conjugate gradient algorithm** to compute $H^{-1}g$ without inverting H
- Resultant algorithm : Truncated Natural Policy Gradient
- ACTKR algorithm uses KFAC technique to solve the inverse Hessian computation problem

Problems with Natural Policy Gradient Update

- Another problem with NPG update is that - might not be robust to trust region size δ
  - ★ δ may be too large in some iterations and can degrade the performance
- Because of quadratic approximation, the KL-divergence constraint may be violated
- Monotonic improvement may not occur in all iterations

TRPO : Line Search Algorithm

- Enforce improvement in surrogate (i.e. $\mathcal{L}_{\pi_{\theta_k}}(\pi_\theta) \geq 0$)
- Enforce KL constraint
- How ? Backtracking line search with exponential decay

Algorithm Line Search for TRPO

1: Compute the proposed policy step $\Delta_k = \sqrt{\frac{2\delta}{g_k^T H_k^{-1} g_k}} H_k^{-1} g_k$
2: **for** $j = 0, 1, 2, \cdots N$ **do**
3:     Compute proposed update $\theta = \theta_k + \alpha_j \Delta_k$
4:     **If** $\mathcal{L}_{\pi_{\theta_k}}(\pi_\theta) \geq 0$ and $\bar{D}_{KL}(\theta || \theta_k) \leq \delta$
5:         Accept the update $\theta = \theta_k + \alpha_j \Delta_k$
6:     **Else**
7:         Find another α_j (Reduce α_j)
8: **end for**

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6: Form sample estimates for the Hessian of KL divergence / FIM
7: Use conjugate gradient to obtain FIM estimate H^{-1}
8: Estimate step size α using backtracking line search to enforce KL constraint and monotonic improvement
9: Compute the Natural Policy Gradient update

$$\theta_{k+1} = \theta_k + \alpha \, \Delta_k$$

10: **end for**

Proximal Policy Optimization

Proximal Policy Optimization is a family of methods that approximately enforce without actually computing the natural gradient

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- **Adaptive KL Penalty**

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Penalty co-efficient β is changed between iterations to approximately enforce KL constraint

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  Penalty co-efficient β is changed between iterations to approximately enforce KL constraint

- **Clipped Objective** (Simpler to implement, no need to check KL constraint; works well)

$$\mathcal{L}^{CLIP}_{\pi_{\theta_k}}(\pi_\theta) = \mathbb{E}_{\tau \sim \pi_{\theta_k}} [\sum_{t=0}^{T} \min(r_t(\theta) A_t^{\pi_{\theta_k}}, clip(r_t(\theta), 1-\varepsilon, 1+\varepsilon) A_t^{\pi_{\theta_k}}]$$

  where $r_t(\theta)$ is the importance sampling ratio between target policy π_θ and behaviour policy π_{θ_k} and policy update takes place as

$$\pi_{\theta_{k+1}} = \arg\max_{\pi_\theta} \mathcal{L}^{CLIP}_{\pi_{\theta_k}}(\pi_\theta)$$

Gradient Descent and Parameterization

Probabilistic Models and Parameterization

Consider the following model that captures the joint distribution between two random variables x and y

$$p_\theta(x, y) = p(x)\mathcal{N}(y \mid \theta x + b, \sigma^2), \theta \in \mathbb{R},$$

where θ is a parameter and b and σ are constants.

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Let $\theta = 2\mu$. We can rewrite the above model in terms of new parameter μ as

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Note that even if $p_\theta(x, y)$ and $p_\mu(x, y)$ have different analytical forms, they represent the same (family) distribution. Specifically,

$$p_{\theta=a}(x, y) \equiv p_{\mu=a/2}(x, y), \text{ for any } a \in \mathbb{R}$$

Gradient Descent and Parameterization

Construct a negative log-likelihood as loss function for the distribution $p(x, y)$ as

$$
\begin{aligned}
\mathcal{L}(p(x,y)) &= -[\log p(x,y)] \\
&= \left[\frac{1}{2\sigma^2}(\theta x + b - y)^2 + \log \sqrt{2\pi}\sigma\right] \quad (\text{for } p_\theta(x,y)) \\
&= \left[\frac{1}{2\sigma^2}(2\mu x + b - y)^2 + \log \sqrt{2\pi}\sigma\right] \quad (\text{for } p_\mu(x,y))
\end{aligned}
$$

Gradient Descent and Parameterization

- For $p_\theta(x, y)$ the update rule is given by $\theta_{t+1} = \theta_t - \alpha \nabla_{\theta_t} \mathcal{L}(p_{\theta_t}(x, y))$ where α is the step size with

$$\nabla_{\theta_t} \mathcal{L}(p_{\theta_t}(x, y)) = \left[\frac{x}{\sigma^2} (\theta_t x + b - y) \right]$$

- For $p_\mu(x, y)$ the update rule is given by $\mu_{t+1} = \mu_t - \alpha \nabla_{\mu_t} \mathcal{L}(p_{\mu_t}(x, y))$ where α is the step size with

$$\nabla_{\mu_t} \mathcal{L}(p_{\mu_t}(x, y)) = \left[\frac{2x}{\sigma^2} (2\mu_t x + b - y) \right]$$

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we will have,

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\theta_{t+1} &= \theta_t - \alpha \nabla_{\theta_t} \mathcal{L}(p_{\theta_t}(x, y)) \\
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- Hence the $t + 1$-th optimization step will result in different probabilistic models $p_{\theta_{t+1}}(x, y) \neq p_{\mu_{t+1}}(x, y)$

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- Hence, requires carefully choosing the parameterization to avoid hindering optimization
- Not all optimization procedures are parameterization dependent. For example, the Newton-Raphson method is invariant to affine transformations of model parameters
- Natural gradient methods are invariant to arbitrary differentiable transformations of model parameters when the learning rate is small enough

Sanity Check : Natural Gradients

Recall that the natural gradient of a loss function is given by,

$$\widetilde{\nabla}_\theta \mathcal{L}(p_\theta(x,y)) := \mathbf{F}_\theta^{-1} \nabla_\theta \mathcal{L}(p_\theta(x,y)),$$

where

$$[\mathbf{F}_\theta]_{i,j} := \mathbb{E}_{p_\theta(x,y)}\left[\left(\frac{\partial}{\partial\theta_i}\log p_\theta(x,y)\right)\left(\frac{\partial}{\partial\theta_j}\log p_\theta(x,y)\right)\right],$$

For different parameterizations of Gaussian conditional distributions, the derivatives of the log densities are respectively

$$\begin{aligned}
\frac{\partial}{\partial\theta}\log p_\theta(x,y) &= \frac{(y-\theta x-b)x}{\sigma^2} \\
\frac{\partial}{\partial\mu}\log p_\mu(x,y) &= \frac{2(y-2\mu x-b)x}{\sigma^2}
\end{aligned}$$

With $\theta_t = 2\mu_t$, we can conclude that $\mathbf{F}_{\mu=\mu_t} = 4\mathbf{F}_{\theta=\theta_t}$. Using

$$\widetilde{\nabla}_\mu \mathcal{L}(p_\mu(x,y))|_{\mu=\mu_t} = \frac{1}{2}\widetilde{\nabla}_\theta \mathcal{L}(p_\theta(x,y))|_{\theta=\theta_t}$$

we can conclude that, $\theta_{t+1} = 2\mu_{t+1}$

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