



## Advanced Policy Gradients - II

Easwar Subramanian

TCS Innovation Labs, Hyderabad

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

Novemer 20, 2021

### Overview of this Lecture



- Review
- 2 Approximations to Trust Region Formulation
- 3 Natural Policy Gradient
- Tisher Information Matrix and KL Divergence
- 6 Relationship of Natural Gradient to Policy Gradient
- 6 Other Algorithms
- Proximal Policy Optimization





### Review



## Policy Optimization Problem



The performance of a policy  $\pi_{\theta}$  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**
- $\triangleright$  Distance in parameter space  $\neq$  policy space



# Surrogate Loss Function



We recast the optimization problem using a surrogate loss function

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

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  $\pi'$  and  $\pi_0$  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  $\pi_{k+1}$  and  $\pi_k$  are related by

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

#### Performance guarantee

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

ightharpoonup C is quite high when  $\gamma$  is close to 1 and hence choosing step size becomes an issue

## A First-Cut Algorithm



- 1: Initialize  $\pi_0$
- 2: **for**  $k = 0, 1, 2, \cdots$  until convergence **do**
- 3: Sample a trajectory  $\tau$  from policy  $\pi_k$
- 4: Compute advantage function  $A^{\pi_{\theta_k}}(a_t, s_t)$  for all  $(s_t, a_t)$  pairs in the trajectory  $\tau$
- 5: Solve the optimization problem

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

#### 6: end for

#### Issues are:

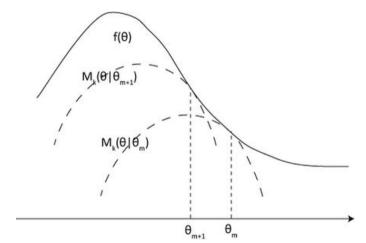
- ► C is quite high when  $\gamma$  is close to  $1\left(C = \frac{4\varepsilon\gamma}{1-\gamma^2}\alpha^2\right)$
- ► Consequently, step size becomes too small



### 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

$$\pi_{k+1} = \underset{\pi'}{\arg\max} \left[ L_{\pi_k}(\pi') \right]$$
  
such that 
$$\underset{s \sim d^{\pi_k}}{\mathbb{E}} D_{KL}(\pi'||\pi_k)[s] \le \delta$$

- ► 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





## Approximations to Trust Region Formulation

### Trust Region Formulation



We have the following optimization problem

$$\pi_{k+1} = \underset{\pi'}{\operatorname{arg\,max}} \left[ \mathcal{L}_{\pi_k}(\pi') \right]$$
  
such that  $\bar{D}_{KL}(\pi'||\pi_k) \leq \delta$ 

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

For parametrized policies the optimization can be written as

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

How do we solve it?

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



# Approximation of Objective Function



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

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

▶ Using Taylor series expansion on objective function  $\mathcal{L}_{\pi_{\theta_k}}(\pi_{\theta})$  around  $\theta_k$  (upto first order term) gives us

$$\mathcal{L}_{\pi_{\theta_k}}(\pi_{\theta}) \approx \mathcal{L}_{\pi_{\theta_k}}(\pi_{\theta_k}) + g^T(\theta - \theta_k) \quad \text{where } g \doteq \nabla_{\theta} \mathcal{L}_{\pi_{\theta_k}}(\pi_{\theta}) \mid_{\theta = \theta_k}$$

 $\triangleright$  Recall that q is exactly the policy gradient (from previous lecture!)

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

Objective function is simplified to

$$\theta_{k+1} = \underset{\theta}{\operatorname{arg max}} g^{T} (\theta - \theta_{k})$$

12 of 30



# Approximation of Trust Region Constraint



Using Taylor series expansion on the constraint (around  $\theta_k$ ; upto second order) gives us

$$\bar{D}_{KL}(\pi_{\theta}||\pi_{\theta_k}) \approx \bar{D}_{KL}(\pi_{\theta_k}||\pi_{\theta_k}) + \nabla_{\theta}\bar{D}_{KL}(\pi_{\theta}||\pi_{\theta_k})|_{\theta=\theta_k} + \nabla_{\theta}^2\bar{D}_{KL}(\pi_{\theta}||\pi_{\theta_k})|_{\theta=\theta_k}$$

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

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

Therefore, we are left only with the second order term

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





# Natural Policy Gradient



### Natural Policy Gradient



The optimization problem is now simplified as

$$\theta_{k+1} = \underset{\theta}{\arg\max} g^T(\theta - \theta_k)$$
  
such that  $\frac{1}{2}(\theta - \theta_k)^T H (\theta - \theta_k) \le \delta$ 

Linear objective with quadratic constraint

Solution to the approximate problem obtained using Lagrange multiplier method

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

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



### Algorithm: Natural Policy Gradient



### Algorithm Natural Policy Gradient

- 1: Initialize  $\pi_0$
- 2: **for**  $k = 0, 1, 2, \cdots$  **do**
- 3: Collect trajectories  $D_k$  on policy  $\pi_k = \pi_{\theta_k}$
- 4: Estimate all advantages  $A^{\pi_{\theta_k}}(s_t, a_t)$
- 5: Form sample estimates for policy gradients  $\hat{q}_k$  (using advantage estimates)
- 6: Form sample estimates for the Hessian of KL divergence
- 7: Compute the Natural Policy Gradient update

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

8: end for





Fisher Information Matrix and KL Divergence

### Fisher Information Matrix and KL Divergence



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

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

 $\triangleright$  For a parameter vector  $\theta$ , Fisher Information Matrix is given by,

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

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

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

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

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

(1)

## Properties of Natural Policy Gradient



- $\blacktriangleright$  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

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

▶ 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

$$\pi_{\theta_{k+1}} = \underset{\pi_{\theta}}{\arg\max} \left[ \mathcal{L}_{\pi_{\theta_k}}(\pi_{\theta}) \right]$$
  
such that  $\|\theta - \theta_k\|^2 \le \delta$ 

After linearising the objective, the optimization problem is now,

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

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,

$$\pi_{\theta_{k+1}} = \underset{\pi_{\theta}}{\operatorname{arg\,max}} \left[ \mathcal{L}_{\pi_{\theta_k}}(\pi_{\theta}) \right]$$
such that  $\bar{D}_{KL}(\pi_{\theta} || \pi_{\theta_k}) \le \delta$ 

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

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

### Relationship between Formulations



- ▶ 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  $\theta$  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



- $\blacktriangleright$  Another problem with NPG update is that might not be robust to trust region size  $\delta$ 
  - $\star$   $\delta$  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.  $\mathcal{L}_{\pi_{\theta_*}}(\pi_{\theta}) \geq 0$ )
- ► Enforce KL constraint
- ▶ How? Backtracking line search with exponential decay

### **Algorithm** Line Search for TRPO

- 1: Compute the proposed policy step  $\Delta_k = \sqrt{\frac{2\delta}{g_L^T H_b^{-1} g_k}} H_k^{-1} g_k$
- 2: **for**  $j = 0, 1, 2, \dots N$  **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  $\theta = \theta_k + \alpha_i \Delta_k$
- 6: **Else**
- 7: Find another  $\alpha_j$  (Reduce  $\alpha_j$ )
- 8: end for



### Algorithm: Trust Region Policy Optimization



### Algorithm Trust Region Policy Optimization

- 1: Initialize  $\pi_0$
- 2: **for**  $k = 0, 1, 2, \cdots$  **do**
- 3: Collect trajectories  $D_k$  on policy  $\pi_k = \pi_{\theta_k}$
- 4: Estimate all advantages  $A^{\pi_{\theta_k}}(s_t, a_t)$
- 5: Form sample estimates for policy gradients  $\hat{q}_k$  (using advantage estimates)
- 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  $\alpha$  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



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

#### ► Adaptive KL Penalty

$$\pi_{\theta_{k+1}} = \arg\max_{\pi_{\theta}} \left[ \mathcal{L}_{\pi_{\theta_k}}(\pi_{\theta}) - \beta \bar{D}_{KL}(\pi_{\theta}||\pi_{\theta_k}) \right]$$

Penalty co-efficient  $\beta$  is changed between iterations to approximately enforce KL constraint

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

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

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

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

