Advanced Policy Gradient Methods: Natural Gradient, TRPO, and More

John Schulman

OpenAl

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Two Limitations of "Vanilla" Policy Gradient Methods



- Hard to choose stepsizes
 - ▶ Input data is nonstationary due to changing policy: observation and reward distributions change
 - ▶ Bad step is more damaging than in supervised learning, since it affects visitation distribution
 - ▶ Step too far → bad policy
 - Next batch: collected under bad policy
 - Can't recover—collapse in performance
- Sample efficiency
 - Only one gradient step per environment sample
 - Dependent on scaling of coordinates

Reducing reinforcement learning to optimization

- ▶ Much of modern ML: reduce learning to numerical optimization problem
 - Supervised learning: minimize training error
- ▶ RL: how to use all data so far and compute the best policy?
 - ► *Q*-learning: can (in principle) include all transitions seen so far, however, we're optimizing the wrong objective
 - ► Policy gradient methods: yes stochastic gradients, but no optimization problem*
 - This lecture: write down an optimization problem that allows you to do a small update to policy π based on data sampled from π (on-policy data)



OpenAl Baselines

https://blog.openai.com/openai-baselines-dqn/https://github.com/openai/baselines

- -A2C
- -ACFR
- -ACKTR
- -DDPG
- -DQN
- -PPO1 (Multi-CPU using MPI)
- -PPO2 (Optimized for GPU)
- -TRPO

What Loss to Optimize?

Policy gradients

$$\hat{g} = \hat{\mathbb{E}}_t \Big[
abla_{ heta} \log \pi_{ heta}(a_t \mid s_t) \hat{A}_t \Big]$$

► Can differentiate the following loss

$$L^{PG}(\theta) = \hat{\mathbb{E}}_t \Big[\log \pi_{\theta}(a_t \mid s_t) \hat{A}_t \Big].$$

but don't want to optimize it too far

Equivalently differentiate

$$L_{ heta_{ ext{old}}}^{IS}(heta) = \hat{\mathbb{E}}_t igg[rac{\pi_{ heta}(a_t \mid s_t)}{\pi_{ heta_{ ext{old}}}(a_t \mid s_t)} \hat{A}_t igg].$$

at $\theta= heta_{
m old}$, state-actions are sampled using $heta_{
m old}$. (IS = importance sampling)

Just the chain rule:
$$\nabla_{\theta} \log f(\theta) \big|_{\theta_{\text{old}}} = \frac{\nabla_{\theta} f(\theta) \big|_{\theta_{\text{old}}}}{f(\theta_{\text{old}})} = \nabla_{\theta} \Big(\frac{f(\theta)}{f(\theta_{\text{old}})} \Big) \big|_{\theta_{\text{old}}}$$



Surrogate Loss: Importance Sampling Interpretation

▶ Importance sampling interpretation

$$\begin{split} &\mathbb{E}_{s_t \sim \pi_{\theta_{\text{old}}}, a_t \sim \pi_{\theta}} \left[A^{\pi}(s_t, a_t) \right] \\ &= \mathbb{E}_{s_t \sim \pi_{\theta_{\text{old}}}, a_t \sim \pi_{\theta_{\text{old}}}} \left[\frac{\pi_{\theta}(a_t \mid s_t)}{\pi_{\theta_{\text{old}}}(a_t \mid s_t)} A^{\pi_{\theta_{\text{old}}}}(s_t, a_t) \right] \quad \text{(importance sampling)} \\ &= \mathbb{E}_{s_t \sim \pi_{\theta_{\text{old}}}, a_t \sim \pi_{\theta_{\text{old}}}} \left[\frac{\pi_{\theta}(a_t \mid s_t)}{\pi_{\theta_{\text{old}}}(a_t \mid s_t)} \hat{A}_t \right] \qquad \qquad \text{(replace A^{π} with estimator)} \\ &= \mathcal{L}_{\theta_{\text{old}}}^{IS}(\theta) \end{split}$$

- ▶ Kakade et al.¹ and S. et al.² analyze how L^{IS} approximates the actual performance difference between θ and θ_{old} .
- In practice, L^{IS} is not much different than the logprob version $L^{PG}(\theta) = \hat{\mathbb{E}}_t \left[\log \pi_{\theta}(a_t \mid s_t) \hat{A}_t \right]$, for reasonably small policy changes.

¹S. Kakade and J. Langford. "Approximately optimal approximate reinforcement learning". ICML. 2002.

²J. Schulman, S. Levine, P. Moritz, M. I. Jordan, and P. Abbeel. "Trust Region Policy Optimization". ICML (£015). ⊕ ▶ ⟨ ₹ ▶ ⟨ ₹ ▶ ⟨ ₹ ⟩ ⟨ ? ♦ ⟨ ? ♦ ⟩ ⟨ ? ♦ ⟩ ⟨ ? ♦ ⟨ ? ♦ ⟩ ⟨ ? ♦ ⟩ ⟨ ? ♦ ⟨ ? ♦ ⟩ ⟨ ?

Simple Monte Carlo

- Statistical sampling can be applied to any expectation
- In general we can find the expectation of f(x) by sampling:

$$\int f(x)P(x)dx \approx \frac{1}{S} \sum_{s=1}^{S} f(x^{(s)}) \ x^{(s)} \sim P(x)$$

- The function f(x) is arbitrary, so this is very general
- Example: making predictions

$$P(x|\mathcal{D}) = \int P(x|\theta, \mathcal{D}) P(\theta|\mathcal{D}) d\theta$$

$$\approx \frac{1}{S} \sum_{s=1}^{S} P(x|\theta^{(s)}, \mathcal{D}) \quad \theta^{(s)} \sim P(\theta|\mathcal{D})$$

Properties of Monte Carlo

Estimator:

$$\int f(x)P(x)dx \approx \frac{1}{S} \sum_{s=1}^{S} f(x^{(s)}) \ x^{(s)} \sim P(x)$$

Estimator is unbiased

$$\mathbb{E}_{P(x^{(s)})}[\hat{f}] = \frac{1}{S} \sum_{s=1}^{S} \mathbb{E}_{P(x)}[f(x)] = \mathbb{E}_{P(x)}[f(x)]$$

• Variance shrinks $\propto 1/S$:

$$\operatorname{var}_{P(x^{(s)})}[\hat{f}] = \frac{1}{S^2} \sum_{s=1}^{S} \operatorname{var}_{P(x)}[f(x)] = \operatorname{var}_{P(x)}[f(x)]/S$$

Importance sampling

Computing both $\tilde{P}(x), \tilde{Q}(x)$ then throwing x away seems wasteful Instead rewrite the integral as an expectation under Q:

$$\int f(x)P(x)dx = \int f(x)\frac{P(x)}{Q(x)}Q(x)dx$$

$$\approx \frac{1}{S}\sum_{s=1}^{S} f(x^{(s)})\frac{P(x^{(s)})}{Q(x^{(s)})}$$

This is just simple Monte Carlo again, so it is unbiased

$$r^{(s)} = \frac{P(x^{(s)})}{Q(x^{(s)})}$$
 is called the importance weight

Importance sampling also applies when integral is not an expectation

Divide and multiply any integrand by a convenient distribution

Trust Region Policy Optimization

▶ Define the following trust region update:

$$\begin{array}{ll} \text{maximize} & \hat{\mathbb{E}}_t \bigg[\frac{\pi_{\theta}(a_t \mid s_t)}{\pi_{\theta_{\text{old}}}(a_t \mid s_t)} \hat{A}_t \bigg] \\ \text{subject to} & \hat{\mathbb{E}}_t [\mathsf{KL}[\pi_{\theta_{\text{old}}}(\cdot \mid s_t), \pi_{\theta}(\cdot \mid s_t)]] \leq \delta. \end{array}$$

Also worth considering using a penalty instead of a constraint

$$\max_{\theta} \text{maximize} \qquad \hat{\mathbb{E}}_t \left[\frac{\pi_{\theta}(a_t \mid s_t)}{\pi_{\theta_{\text{old}}}(a_t \mid s_t)} \hat{A}_t \right] - \beta \hat{\mathbb{E}}_t [\mathsf{KL}[\pi_{\theta_{\text{old}}}(\cdot \mid s_t), \pi_{\theta}(\cdot \mid s_t)]]$$

- ▶ Method of Lagrange multipliers: optimality point of δ -constrained problem is also an optimality point of β -penalized problem for some β .
- ▶ In practice, δ is easier to tune, and fixed δ is better than fixed β

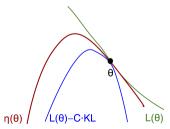


Monotonic Improvement Result

Consider KL penalized objective

$$\underset{\theta}{\mathsf{maximize}} \qquad \hat{\mathbb{E}}_t \bigg[\frac{\pi_{\theta}(\mathsf{a}_t \mid \mathsf{s}_t)}{\pi_{\theta_{\mathrm{old}}}(\mathsf{a}_t \mid \mathsf{s}_t)} \hat{A}_t \bigg] - \beta \hat{\mathbb{E}}_t [\mathsf{KL}[\pi_{\theta_{\mathrm{old}}}(\cdot \mid \mathsf{s}_t), \pi_{\theta}(\cdot \mid \mathsf{s}_t)]]$$

► Theory result: if we use max KL instead of mean KL in penalty, then we get a lower (=pessimistic) bound on policy performance





Trust Region Policy Optimization: Pseudocode

Pseudocode:

for iteration= $1, 2, \dots$ do

Run policy for T timesteps or N trajectories Estimate advantage function at all timesteps

$$\begin{array}{l} \text{maximize} \sum_{n=1}^{N} \frac{\pi_{\theta}(a_{n} \mid s_{n})}{\pi_{\theta_{\text{old}}}(a_{n} \mid s_{n})} \hat{A}_{n} \\ \text{subject to} & \overline{\text{KL}}_{\pi_{\theta_{\text{old}}}}(\pi_{\theta}) \leq \delta \end{array}$$

end for

- ► Can solve constrained optimization problem efficiently by using conjugate gradient
- ► Closely related to natural policy gradients (Kakade, 2002), natural actor critic (Peters and Schaal, 2005), REPS (Peters et al., 2010)



Solving KL Penalized Problem

- ightharpoonup maximize $_{\theta} L_{\pi_{\theta_{\mathrm{old}}}}(\pi_{\theta}) \beta \cdot \overline{\mathrm{KL}}_{\pi_{\theta_{\mathrm{old}}}}(\pi_{\theta})$
- lacktriangle Make linear approximation to $L_{\pi_{ heta_{
 m old}}}$ and quadratic approximation to KL term:

$$\begin{array}{ll} \text{maximize} & g \cdot (\theta - \theta_{\text{old}}) - \frac{\beta}{2} (\theta - \theta_{\text{old}})^{\mathsf{T}} F(\theta - \theta_{\text{old}}) \\ \\ \text{where} & g = \frac{\partial}{\partial \theta} \mathcal{L}_{\pi_{\theta_{\text{old}}}}(\pi_{\theta}) \big|_{\theta = \theta_{\text{old}}}, \quad F = \frac{\partial^2}{\partial^2 \theta} \overline{\text{KL}}_{\pi_{\theta_{\text{old}}}}(\pi_{\theta}) \big|_{\theta = \theta_{\text{old}}} \\ \end{aligned}$$

- Quadratic part of L is negligible compared to KL term
- ightharpoonup F is positive semidefinite, but not if we include Hessian of L
- Solution: $\theta \theta_{\text{old}} = \frac{1}{\beta} F^{-1} g$, where F is Fisher Information matrix, g is policy gradient. This is called the **natural policy gradient**³.





Solving KL Constrained Problem

- Method of Lagrange multipliers: solve penalized problem to get $\theta^*(\beta)$. Then substitute $\theta^*(\beta)$ into original problem and solve for β .
- \triangleright β only affects scaling of solution, not direction. Compute scaling as follows:
 - ▶ Compute $s = F^{-1}g$ (soln with $\beta = 1$)
 - Rescale $\theta \theta_{\rm old} = \alpha s$ so that constraint is satisfied. Quadratic approx $\overline{\mathrm{KL}}_{\pi_{\theta_{\rm old}}}(\pi_{\theta}) \approx \frac{1}{2}(\theta \theta_{\rm old})^T F(\theta \theta_{\rm old})$, so we want

$$\frac{1}{2}(\alpha s)^T F(\alpha s) = \delta$$
$$\alpha = \sqrt{2\delta/(s^T F s)}$$

▶ Even better, we can do a line search to solve the original *nonlinear* problem.

maximize
$$L_{\pi_{\theta_{\text{old}}}}(\pi_{\theta}) - \mathbf{1}[\overline{\mathrm{KL}}_{\pi_{\theta_{\text{old}}}}(\pi_{\theta}) \leq \delta]$$

Try $\alpha, \alpha/2, \alpha/4, \ldots$ until line search objective improves



"Proximal" Policy Optimization: KL Penalty Version

Use penalty instead of constraint

$$\underset{\theta}{\mathsf{maximize}} \sum_{n=1}^{N} \frac{\pi_{\theta}(a_n \mid s_n)}{\pi_{\theta_{\mathrm{old}}}(a_n \mid s_n)} \hat{A}_n - C \cdot \overline{\mathrm{KL}}_{\pi_{\theta_{\mathrm{old}}}}(\pi_{\theta})$$

Pseudocode:

for iteration=1,2,... do Run policy for T timesteps or N trajectories Estimate advantage function at all timesteps Do SGD on above objective for some number of epochs If KL too high, increase β . If KL too low, decrease β .

end for

ightharpoonup pprox same performance as TRPO, but only first-order optimization



Review

- ▶ Suggested optimizing surrogate loss L^{PG} or L^{IS}
- Suggested using KL to constrain size of update
- ightharpoonup Corresponds to natural gradient step $F^{-1}g$ under linear quadratic approximation
- ► Can solve for this step approximately using conjugate gradient method

Connection Between Trust Region Problem and Other Things

$$\begin{array}{l} \text{maximize} \sum_{n=1}^{N} \frac{\pi_{\theta}(a_{n} \mid s_{n})}{\pi_{\theta_{\text{old}}}(a_{n} \mid s_{n})} \hat{A}_{n} \\ \text{subject to} & \overline{\text{KL}}_{\pi_{\theta_{\text{old}}}}(\pi_{\theta}) \leq \delta \end{array}$$

- ► Linear-quadratic approximation + penalty ⇒ natural gradient
- ► No constraint ⇒ policy iteration
- ► Euclidean penalty instead of KL ⇒ vanilla policy gradient

Limitations of TRPO

- ► Hard to use with architectures with multiple outputs, e.g. policy and value function (need to weight different terms in distance metric)
- ► Empirically performs poorly on tasks requiring deep CNNs and RNNs, e.g. Atari benchmark
- ▶ CG makes implementation more complicated

Calculating Natural Gradient Step with KFAC

- Summary: do blockwise approximation to FIM, and approximate each block using a certain factorization
- Alternate expression for FIM as outer product (instead of second deriv. of KL):

$$\mathbb{\hat{E}}_t \big[\nabla_{\theta} \log \pi_{\theta} (a_t \mid s_t)^T \nabla_{\theta} \log \pi_{\theta} (a_t \mid s_t) \big]$$

Calculating Natural Gradient Step with KFAC

► Consider network with weight matrix W appearing once in network, with y = Wx. Then

$$\nabla_{W_{ij}} L = x_i \nabla_{y_j} L = x_i \overline{y}_j$$

$$F = \hat{\mathbb{E}}_t \left[\nabla_{W_{ij}} \log \pi_{\theta} (a_t \mid s_t)^T \nabla_{W_{ij}} \log \pi_{\theta} (a_t \mid s_t) \right]$$

$$F_{ij,i'j'} = \hat{\mathbb{E}}_t \left[x_i \overline{y}_j x_{i'} \overline{y}_{j'} \right]$$

KFAC approximation:

$$F_{ij,i'j'} = \hat{\mathbb{E}}_t \big[x_i \overline{y}_j x_{i'} \overline{y}_{j'} \big] \approx \hat{\mathbb{E}}_t [x_i x_{i'}] \hat{\mathbb{E}}_t \big[\overline{y}_j \overline{y}_{j'} \big]$$

- ▶ Approximating Fisher block as tensor product $A \otimes B$, where A is $nin \times nin$ and B is $nout \times nout$. $(A \otimes B)^{-1} = A^{-1} \otimes B^{-1}$ and we can compute matrix-vector product without forming full matrix.
- Maintain running estimate of covariance matrices $\hat{\mathbb{E}}_t[x_i x_j], \hat{\mathbb{E}}_t[\overline{y}_{i'} \overline{y}_{j'}]$ and periodically compute matrix inverses (small overhead)

ACKTR: Combine A2C with KFAC Natural Gradient

- ► Combined with A2C, gives excellent on Atari benchmark and continuous control from images⁴.
- Note: we're already computing $\nabla_{\theta} \log \pi_{\theta}(a_t \mid s_t)$ for policy gradient: no extra gradient computation needed
- Matrix inverses can be computed asynchronously
- Limitation: works straightforwardly for feedforward nets (including convolutions), less straightforward for RNNs or architectures with shared weights

⁴Y. Wu, E. Mansimov, S. Liao, R. Grosse, and J. Ba. "Scalable trust-region method for deep reinforcement learning using Kronecker-factored approximation". (2017).

Proximal Policy Optimization: KL Penalized Version

▶ Back to penalty instead of constraint

$$\underset{\theta}{\mathsf{maximize}} \sum_{n=1}^{N} \frac{\pi_{\theta}(\mathsf{a}_{n} \mid \mathsf{s}_{n})}{\pi_{\theta_{\mathrm{old}}}(\mathsf{a}_{n} \mid \mathsf{s}_{n})} \hat{A}_{n} - C \cdot \overline{\mathrm{KL}}_{\pi_{\theta_{\mathrm{old}}}}(\pi_{\theta})$$

Pseudocode:

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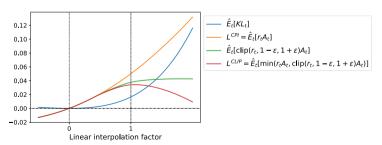
Proximal Policy Optimization: Clipping Objective

▶ Recall the surrogate objective

$$L^{IS}(\theta) = \hat{\mathbb{E}}_t \left[\frac{\pi_{\theta}(a_t \mid s_t)}{\pi_{\theta_{\text{old}}}(a_t \mid s_t)} \hat{A}_t \right] = \hat{\mathbb{E}}_t \left[r_t(\theta) \hat{A}_t \right]. \tag{1}$$

▶ Form a lower bound via clipped importance ratios

$$L^{CLIP}(\theta) = \hat{\mathbb{E}}_t \left[\min(r_t(\theta) \hat{A}_t, \text{clip}(r_t(\theta), 1 - \epsilon, 1 + \epsilon) \hat{A}_t) \right]$$
 (2)



Forms pessimistic bound on objective, can be optimized using SGD



Proximal Policy Optimization

► Pseudocode:

```
for iteration=1,2,... do Run policy for T timesteps or N trajectories Estimate advantage function at all timesteps Do SGD on L^{CLIP}(\theta) objective for some number of epochs end for
```

- ▶ A bit better than TRPO on continuous control, much better on Atari
- Compatible with multi-output networks and RNNs

Further Reading

- S. Kakade. "A Natural Policy Gradient." NIPS. 2001
- S. Kakade and J. Langford. "Approximately optimal approximate reinforcement learning". ICML. 2002
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- Y. Wu, E. Mansimov, S. Liao, R. Grosse, and J. Ba. "Scalable trust-region method for deep reinforcement learning using Kronecker-factored approximation". (2017)
- J. Schulman, F. Wolski, P. Dhariwal, A. Radford, and O. Klimov. "Proximal Policy Optimization Algorithms". (2017)
- blog.openai.com: recent posts on baselines releases

That's all. Questions?

