Target-based Surrogates for Efficient Sequential Decision-making

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Based on work with Olivier Bachem, Simone Totaro, Robert Müller, Shivam Garg, Matthieu Geist, Marlos Machado, Pablo Samuel Castro, Jonathan Wilder Lavington, Reza Babanezhad, Mark Schmidt, Nicolas Le Roux

Microsoft Research, Montreal

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- Optimize functions with a composition structure $h(\theta) := \ell(f(\theta))$.
- Canonical example: Supervised learning where $\ell(z)$ is the loss function (squared loss, cross-entropy) and $z = f(\theta)$ is the model (linear model, neural network).

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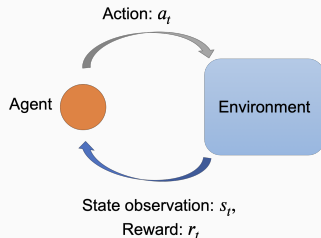
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Focus on problems in sequential decision-making where computing $\{\ell(z), \nabla_z \ell(z)\}$ can be much more computationally expensive compared to $\{f(\theta), \nabla_\theta f(\theta)\}$
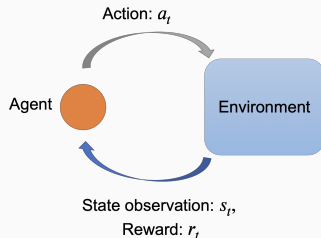
Objective: Given a Markov decision process (MDP) with state space $\mathcal{S}$ and action space $\mathcal{A}$, learn a policy $\pi : \mathcal{S} \to \Delta_A$ that maximizes the expected cumulative discounted reward $J(\pi) := \mathbb{E}[r_0 + \gamma r_1 + \gamma^2 r_2 + \ldots]$.

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State observation: s_t,
Reward: r_t

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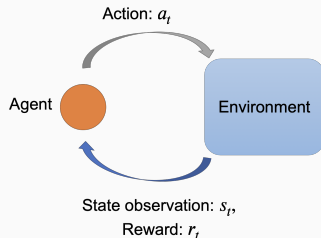
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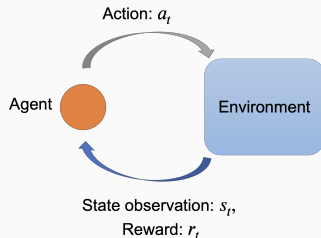
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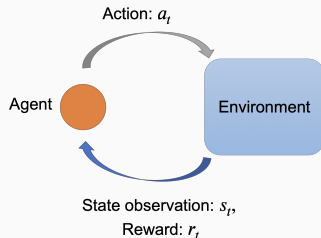
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    where Π_θ is the set of policies that can be expressed by the model.
- If $z = \pi$, $\mathcal{Z}_\theta = \Pi_\theta$, $\ell = -J$, equivalent to solving $\min_\theta h(\theta) = \ell(f(\theta))$.

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Motivating example: Online Imitation Learning

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    $\min_{\pi \in \Pi_\theta} \ell_t(\pi) := \mathbb{E}_{s \sim d^{\pi_t}} [D(\pi(\cdot|s)||\pi_e(\cdot|s))]$.
- If $z = \pi$, $\mathcal{Z}_\theta = \Pi_\theta$, equivalent to minimizing a sequence of functions of the form $h_t(\theta) := \ell_t(f(\theta))$.

Naive Idea: Parametric Gradient Descent

- Ignore the composition structure and optimize $h(\theta) = \ell(f(\theta))$ directly w.r.t θ.
- Parametric Gradient Descent: $\theta_{t+1} = \theta_t - \eta \nabla h(\theta_t)$; $z_{t+1} = f(\theta_{t+1})$.
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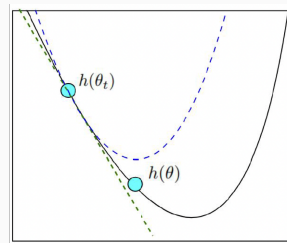- Idea: Form a surrogate function that exploits the composition structure and enables "reusing" the gathered data i.e can update the policy multiple times without computing $\nabla_z \ell(z)$.
- Example: In RL, methods such as TRPO/PPO construct such surrogate functions and update the policy to maximize the surrogates.

- At iteration t, gradient descent on a smooth (possibly non-convex) function $h(\theta)$ is equivalent to minimizing a local quadratic surrogate function around θ_t:

  $g_t(\theta) := h(\theta_t) + \langle \nabla h(\theta_t), \theta - \theta_t \rangle + \frac{1}{2\eta} \|\theta - \theta_t\|_2^2.$

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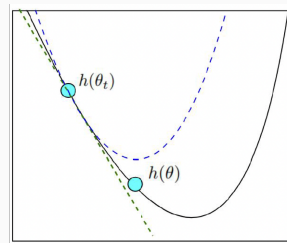

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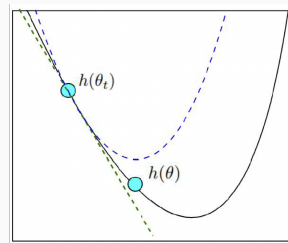

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- Algorithm: Iteratively form the surrogate $g_t(\theta)$ around θ_t and minimize it to update θ. Exactly gradient descent!

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- Equivalent to projected gradient descent in the target space: $z_{t+1} = \text{Proj}_{\mathcal{Z}_\theta}[z_t - \eta \nabla \ell(z_t)]$

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Input: θ_0 (initialization), T (number of iterations), m_t (number of inner-loops), η (step-size for the target space), α (step-size for the parametric space)

   for $t = 0$ to $T - 1$ **do**

      Access the gradient oracle to construct $g_t(\theta)$

      Initialize inner-loop: $\omega_0 = \theta_t$

      for $k \leftarrow 0$ to m_{t-1} **do**

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- Using $m = 1$ in the Alg 1. recovers parametric GD.

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- Hence, Alg. 1 with $m \in [1, \infty)$ interpolates between a first-order and second-order method without explicitly forming the Hessian.

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Theoretical Guarantees

Recall that $g_t(\theta) := \ell(f(\theta_t)) + \langle \nabla_z \ell(f(\theta_t)), f(\theta) - f(\theta_t) \rangle + \frac{1}{2\eta} \| f(\theta) - f(\theta_t) \|_2^2$

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- Other theoretical results:
  - Prove that Alg. 1 converges to a stationary point of $h(\theta)$ at an $O(1/T)$ rate.
  - For convex ℓ, prove convergence rates even when we only have access to a stochastic, unbiased gradient of $\ell(z)$.

Experiments – Imitation Learning
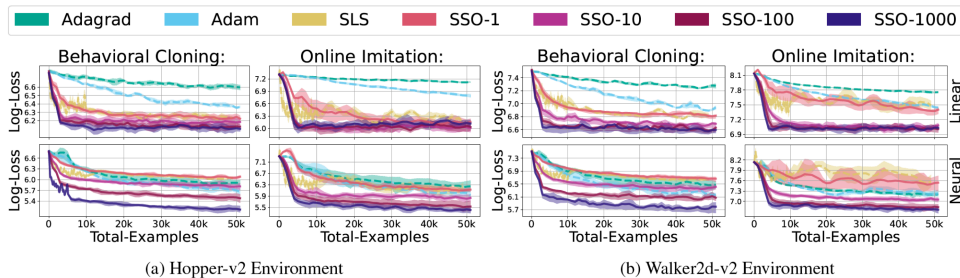
(a) Hopper-v2 Environment   (b) Walker2d-v2 Environment

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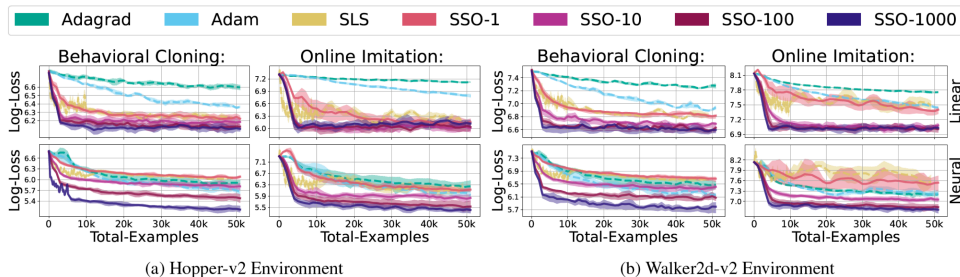
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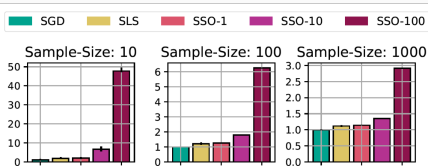
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✓ Constructed a sequence of surrogate functions that exploit the composition structure, and result in efficient updates for imitation learning.

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✓ Black-box structure for stochastic optimization: Can use any stochastic optimization algorithm to form surrogates which can then be optimized using any deterministic optimization algorithm.

- Target-based Surrogate Optimization
- **Functional Mirror Ascent for Policy Gradient (FMA-PG)**
- Conclusions and Future Work

Motivation

- Policy gradient (PG) methods based on REINFORCE:
  - Each policy update requires recomputing the policy gradient.
  - ✓ Theoretical guarantees [Agarwal et al., 2020] with function approximation.
  - ✕ Each update requires computationally expensive interactions with the environment.

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- Methods such as TRPO, PPO and MPO:
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  No systematic way to design theoretically principled surrogate functions, or a unified framework to analyze their properties.

- **Functional representation**: Specifies a policy's sufficient statistics and is implicit.

  Examples:
  - *Direct functional representation*: Conditional distribution over actions $p^\pi(\cdot|s)$ for each s.
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- **Policy parameterization**: Practical realization of the sufficient statistics. Determines Π (the set of feasible policies). *Examples*:
  - *Tabular parameterization* for the direct functional representation: $p^\pi(a|s) = \theta(s,a)$.
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- **Standard PG approach**: Use a model (with parameters θ) to parameterize (the functional representation of) π and directly maximize $J(\pi(\theta))$ w.r.t. θ.

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- For a strictly convex, differentiable function Φ (*mirror map*), $D_\Phi(\pi, \pi')$ is the *Bregman divergence* between policies π and π'. $D_\Phi(\pi, \pi') := \Phi(\pi) - \Phi(\pi') - \langle \nabla\Phi(\pi'), \pi - \pi' \rangle$.
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In each iteration $t \in [T]$ of *functional mirror ascent* (FMA), with *step-size* η,

$$\pi_{t+1} = \arg \max_{\pi \in \Pi_\theta} \left[\langle \pi, \nabla_\pi J(\pi_t) \rangle - \frac{1}{\eta} D_\Phi(\pi, \pi_t) \right]$$

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Since $\pi \in \Pi_\theta$,

$$\pi_{t+1} = \pi(\theta_{t+1}) \quad ; \quad \theta_{t+1} = \arg\max_{\theta \in \mathbb{R}^d} \underbrace{\left[J(\pi(\theta_t)) + \langle \pi(\theta) - \pi(\theta_t), \nabla_\pi J(\pi(\theta_t)) \rangle - \frac{1}{\eta} D_\Phi(\pi(\theta), \pi(\theta_t)) \right]}_{\text{Surrogate function } g_t(\theta)}$$

Algorithm 1: Generic policy optimization

Input: π (functional representation), θ_0 (initial policy parameterization), T (PG iterations), m (inner-loops), η (step-size for functional update), α (step-size for parametric update)

for $t \leftarrow 0$ **to** $T - 1$ **do**
  Compute $\nabla_\pi J(\pi_t)$ and form the surrogate $g_t(\theta)$.
  Initialize inner-loop: $\omega_0 = \theta_t$
  for $k \leftarrow 0$ **to** m **do**
    $\omega_{k+1} = \omega_k + \alpha \nabla_\omega g_t(\omega_k)$ /* Off-policy actor updates */
  $\theta_{t+1} = \omega_m$
  $\pi_{t+1} = \pi(\theta_{t+1})$
Return θ_T

Algorithm 2: Generic policy optimization

Input: π (functional representation), θ_0 (initial policy parameterization), T (PG iterations), m (inner-loops), η (step-size for functional update), α (step-size for parametric update)

for $t \leftarrow 0$ to $T-1$ do

    Compute $\nabla_\pi J(\pi_t)$ and form the surrogate $g_t(\theta)$.

    Initialize inner-loop: $\omega_0 = \theta_t$

    for $k \leftarrow 0$ to m do

        $\omega_{k+1} = \omega_k + \alpha \nabla_\omega g_t(\omega_k)$ /* `Off-policy actor updates` */

    $\theta_{t+1} = \omega_m$

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Return θ_T

- If we can guarantee that (i) $g_t(\theta) \leq J(\pi(\theta))$ and (ii) $g_t(\theta_{t+1}) \geq g_t(\theta_t)$, then the above algorithm results in monotonic policy improvement regardless of the policy parameterization.

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Instantiating FMA-PG – Direct functional representation

- Policy is represented by distributions $p^\pi(\cdot|s)$ over actions for each state $s \in \mathcal{S}$.
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For the negative entropy mirror-map i.e. when $\phi(p^\pi(\cdot|s)) = \sum_a p^\pi(a|s) \log p^\pi(a|s)$,

$$g_t(\theta) = \mathbb{E}_{(s,a)\sim\mu^{\pi_t}} \left[\left(Q^{\pi_t}(s, a) \frac{p^\pi(a|s, \theta)}{p^\pi(a|s, \theta_t)} \right) \right] - \frac{1}{\eta} \mathbb{E}_{s\sim d^{\pi_t}} \left[\mathsf{KL} \left(p^\pi(\cdot|s, \theta) || p^\pi(\cdot|s, \theta_t) \right) \right] + C.$$

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Setting η for the direct functional representation with negative entropy mirror map

For any policy parameterization, $\forall \theta$, $J(\pi(\theta)) \geq g_t(\theta)$ for $\eta \leq \frac{(1-\gamma)^3}{2\gamma|A|}$.

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For any policy parameterization, $\forall \theta$, $J(\pi(\theta)) \geq g_t(\theta)$ for $\eta \leq \frac{(1-\gamma)^3}{2\gamma|A|}$.

- × Involves the importance-sampling ratio $\frac{p^{\pi}(a|s,\theta)}{p^{\pi}(a|s,\theta_t)}$ that could be potentially large.
- × Involves the reverse KL divergence making it *mode seeking* hindering exploration.

- Policy is represented by the logits $z^\pi(s, a)$ such that $p^\pi(a|s) \propto \exp(z^\pi(s, a))$ for each state.

Instantiating FMA-PG – Softmax functional representation

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$$g_t(\theta) = E_{(s,a) \sim \mu^{\pi_t}} \left[A^{\pi_t}(s, a) \, z^\pi(s, a|\theta_t) \right] - \frac{1}{\eta} \sum_s d^{\pi_t}(s) \, D_{\phi_z} \left(z^\pi(s, \cdot|\theta), z^\pi(s, \cdot|\theta_t) \right) + C.$$

Instantiating FMA-PG – Softmax functional representation

- Policy is represented by the logits $z^\pi(s, a)$ such that $p^\pi(a|s) \propto \exp(z^\pi(s, a))$ for each state.
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For the log-sum-exp mirror-map i.e. when $\phi_z(z(s, \cdot)) = \log\left(\sum_a \exp(z^\pi(s, a))\right)$,

$$g_t(\theta) = E_{(s,a) \sim \mu^{\pi_t}} \left[\left(A^{\pi_t}(s, a) + \frac{1}{\eta}\right) \log \frac{p^\pi(a|s, \theta)}{p^\pi(a|s, \theta_t)}\right] + C.$$

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Setting η for the softmax functional representation with log-sum-exp mirror map

For any policy parameterization, $\forall \theta$, $J(\pi(\theta)) \geq g_t(\theta)$ for $\eta \leq 1 - \gamma$.

The surrogate can be rewritten as

$$g_t(\theta) = \mathbb{E}_{s \sim d^{\pi_t}} \left[\mathbb{E}_{a \sim p^{\pi_t}} \left(A^{\pi_t}(s,a) \log \frac{p^\pi(a|s,\theta)}{p^\pi(a|s,\theta_t)} \right) - \frac{1}{\eta} \mathrm{KL}(p^\pi(\cdot|s,\theta_t) || p^\pi(\cdot|s,\theta)) \right] + C.$$

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Compared to TRPO: $\max_{\theta \in \mathbb{R}^d} \mathbb{E}_{(s,a) \sim \mu^{\pi_t}}[A^{\pi_t}(s,a)\frac{p^\pi(a|s,\theta)}{p^\pi(a|s,\theta_t)}]$ s.t. $\mathbb{E}_{s \sim d^{\pi_t}}[\mathsf{KL}(p^{\pi_t}(\cdot|s,\theta_t)||p^\pi(\cdot|s,\theta))] \leq \delta$,

- $g_t(\theta)$ involves the log of the importance sampling ratio, and enforces proximity between policies using a regularization (with parameter $1/\eta$) rather than a constraint.

- we ensure monotonic policy improvement for any policy parameterization.

- FMA-PG with the softmax representation suggests sPPO with the following surrogate:

$$g_t(\theta) = \mathbb{E}_{(s,a)\sim\mu^{\pi_t}} \left[A^{\pi_t}(s, a) \log \left(\text{clip} \left(\frac{p^\pi(a|s,\theta)}{p^\pi(a|s,\theta_t)}, \frac{1}{1+\epsilon}, 1+\epsilon \right) \right) \right]$$

.
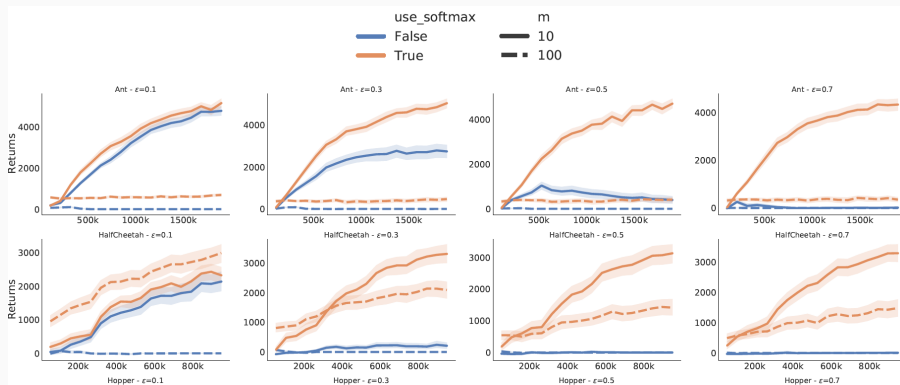- Compare to PPO on standard Mujoco tasks, with both algorithms using a critic.

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- Target-based Surrogate Optimization
- Functional Mirror Ascent for Policy Gradient (FMA-PG)
- **Conclusion**

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✓ Recent work [Vaswani et al., 2023]: Generalized FMA-PG to design a decision-aware actor-critic framework where the actor and critic are trained cooperatively to optimize a joint objective.

Questions?

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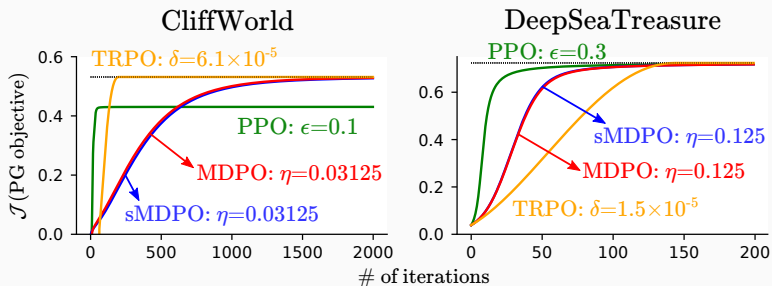
Backup Slides

- Compare MDPO (direct + negative entropy mirror map), sMDPO (softmax + logsumexp mirror map), PPO, TRPO with access to exact Q^π, A^π values (no function approximation).
- Use best-tuned values of the functional step-size η for MDPO and sMDPO, clipping value ϵ for PPO and KL constraint value δ for TRPO. Using best-tuned α for each method.
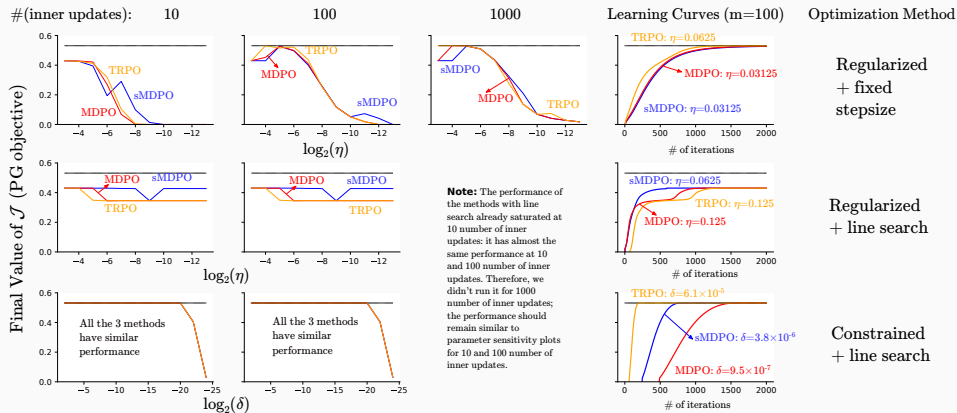
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CliffWorld

$\mathcal{J}$ (PG objective)

TRPO: $\delta=6.1\times10^{-5}$

PPO: $\epsilon=0.1$

MDPO: $\eta=0.03125$

sMDPO: $\eta=0.03125$

DeepSeaTreasure

PPO: $\epsilon=0.3$

sMDPO: $\eta=0.125$

MDPO: $\eta=0.125$

TRPO: $\delta=1.5\times10^{-5}$

# of iterations

- Ablation study on MDPO, sMDPO, TRPO to evaluate the effect of m, algorithm hyperparameters (η, δ) and design decisions – line-search in the inner-loop and using a constraint vs regularization.

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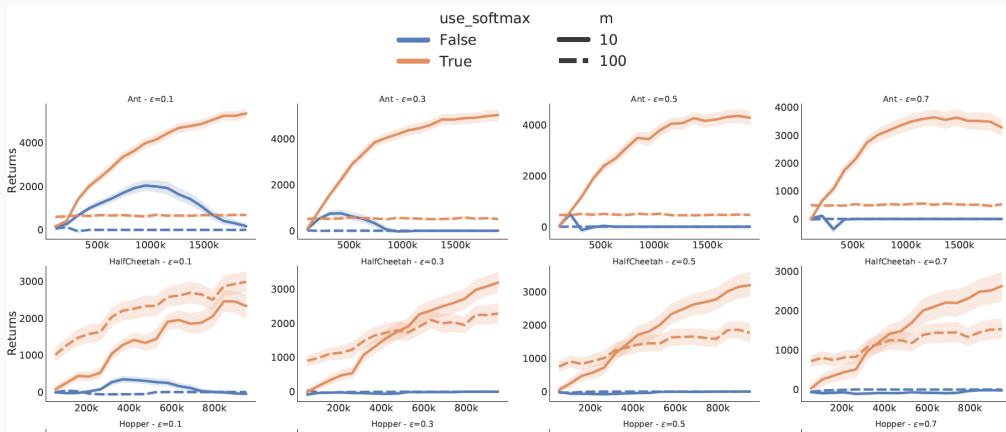
- Ablation study on sPPO, PPO disabling both learning rate decay and gradient clipping.

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Extra Slides

Recall that $g_t(\theta) = \mathbb{E}_{(s,a)\sim\mu^{\pi_t}}\left[\left(Q^{\pi_t}(s,a)\frac{p^\pi(a|s,\theta)}{p^\pi(a|s,\theta_t)}\right)\right] - \frac{1}{\eta}\mathbb{E}_{s\sim d^{\pi_t}}\left[\mathsf{KL}\left(p^\pi(\cdot|s,\theta)||p^\pi(\cdot|s,\theta_t)\right)\right] + C$.

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- For gradient-based maximization of the surrogate, the resulting update is the same as Mirror Descent Policy Optimization [Tomar et al., 2020], but we set the step-sizes that ensure monotonic policy improvement for any policy parameterization and any number of inner-loops.