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

Problem Formulation

- 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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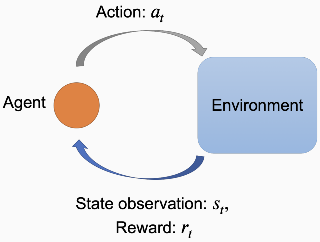
Focus on problems in sequential decision-making where computing $\{\ell(z), \nabla_z \ell(z)\}$ can be much more computationally expensive compared to $\{f(\theta), \nabla_\theta f(\theta)\}$

Motivating example: Policy Optimization in Reinforcement Learning

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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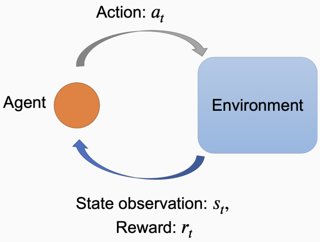

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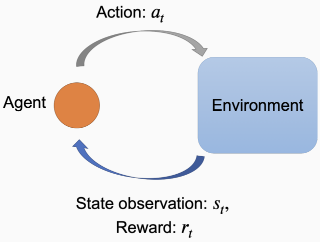

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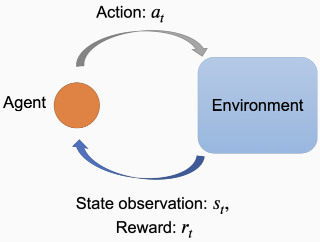

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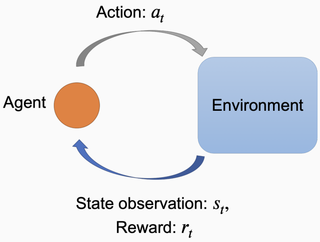

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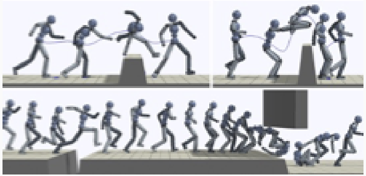
- If $z = \pi$, $\mathcal{Z}_\theta = \Pi_\theta$, $\ell = -J$, equivalent to solving $\min_\theta h(\theta) = \ell(f(\theta))$.

Motivating example: Online Imitation Learning

Objective: Learn a policy that tries to "imitate" the expert. E.g: Learning to control a robot from human supervision.



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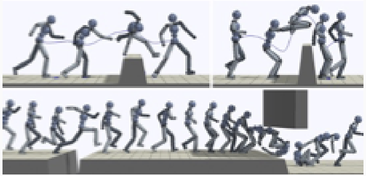

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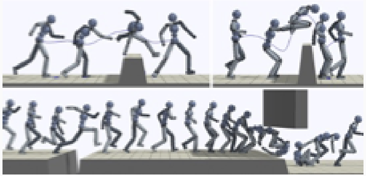

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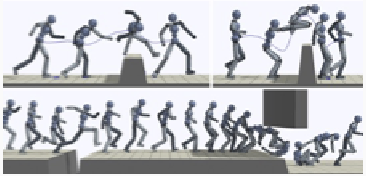

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  - Update the policy to minimize the discrepancy D to the expert policy π_e: $\min_{\pi \in \Pi_\theta} \ell_t(\pi) := \mathbb{E}_{s \sim d^{\pi_t}} \left[D(\pi(\cdot|s) || \pi_e(\cdot|s)) \right]$.

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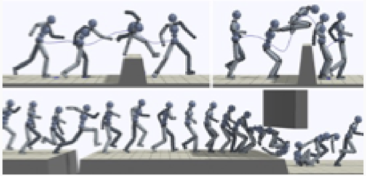

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- If $z = \pi$, $\mathcal{Z}_\theta = \Pi_\theta$, equivalent to minimizing a sequence of functions of the form $h_t(\theta) := \ell_t(f(\theta))$.

Outline

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

Naive Idea: Parametric Gradient Descent

- Ignore the composition structure and optimize $h(\theta) = \ell(f(\theta))$ directly w.r.t θ.
- Parametric Gradient Descent: $\theta_{t+1} = \theta_t - \eta \nabla h(\theta_t) \quad ; \quad z_{t+1} = f(\theta_{t+1})$.
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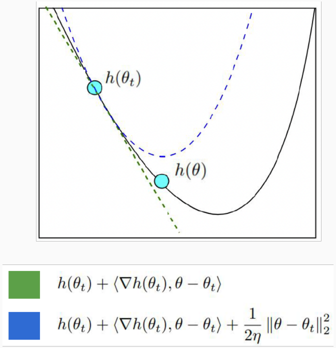
- × Each policy update requires computing $\nabla_\theta h(\theta) = \nabla_z \ell(z) \nabla_\theta f(\theta)$. Since computing $\nabla_z \ell(z)$ involves interacting with the environment, it is computationally expensive.
- Idea: Form a surrogate function that exploits the composition structure and 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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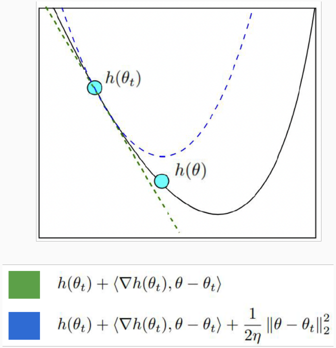

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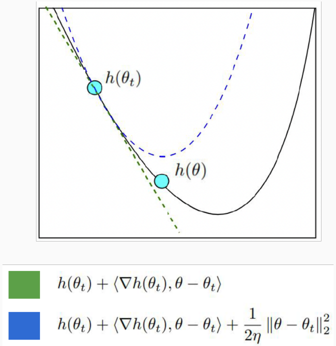

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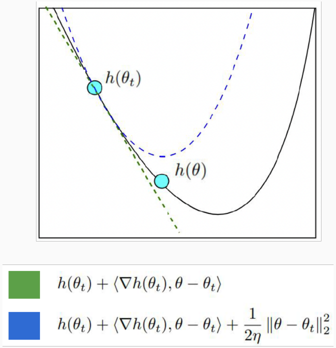

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- Algorithm: Iteratively form the surrogate $g_t(\theta)$ around θ_t and minimize it to update θ. Exactly gradient descent!

Target-based Surrogate Minimization

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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**
    $\omega_{k+1} = \omega_k - \alpha \nabla_\omega g_t(\omega_k)$
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- Using $m = 1$ in the Alg 1. recovers parametric GD.

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    for k ← 0 to m_{t−1} do
        ω_{k+1} = ω_k − α∇_ω g_t(ω_k)
    end for
    θ_{t+1} = ω_m    ;    z_{t+1} = f(θ_{t+1})
end for
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```

Target-based Surrogate Minimization – Example

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

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- Alg. 1 with $m = 1$ is equivalent to parametric GD: $\theta_{t+1} = \theta_t - \eta X^\top [X\theta_t - y]$
- Alg. 1 with $m = \infty$ and $\eta = 1$ is equivalent to Newton's method: $\theta_{t+1} = \theta_t - \eta (X^\top X)^{-1} [X^\top (X\theta_t - y)]$.

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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.

Theoretical Guarantees

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

- Property (i): For an appropriate η (set according to the smoothness of $\ell(z)$), $\forall \theta$, $g_t(\theta) \geq \ell(f(\theta)) = h(\theta)$ and $g_t(\theta_t) = \ell(f(\theta_t)) = h(\theta_t)$.

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- Property (ii): With an appropriate step-size α (set according to the smoothness of $g_t(\theta)$) and any value of m, GD on $g_t(\theta)$ ensures descent implying that $g_t(\theta_{t+1}) \leq g_t(\theta_t)$.

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- **Lemma**: $\ell(z_{t+1}) \overset{Def}{=} h(\theta_{t+1}) \overset{(i)}{\leq} g_t(\theta_{t+1}) \overset{(ii)}{\leq} g_t(\theta_t) \overset{Def}{=} h(\theta_t) \overset{Def}{=} \ell(z_t)$ meaning that Alg. 1 results in a decrease in $\ell(z)$ for any model f.

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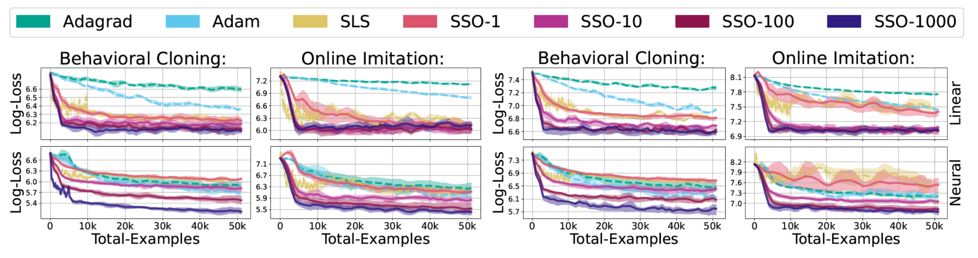
- Other theoretical results:
  - Prove that Alg. 1 converges to a stationary point of $h(\theta)$ at an $O(1/T)$ rate.
  - For convex ℓ, prove convergence rates even when we only have access to a stochastic, unbiased gradient of $\ell(z)$.

Experiments – Imitation Learning



(a) Hopper-v2 Environment (b) Walker2d-v2 Environment

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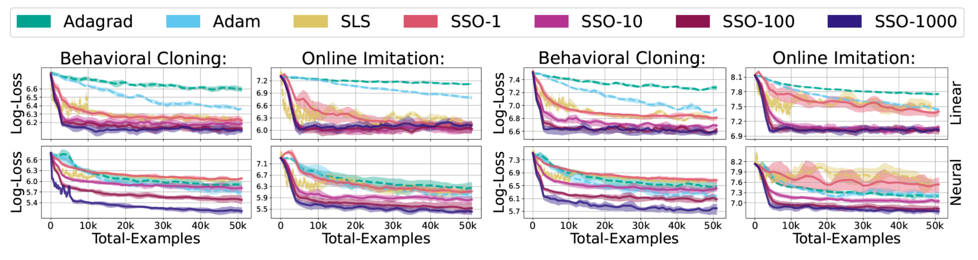

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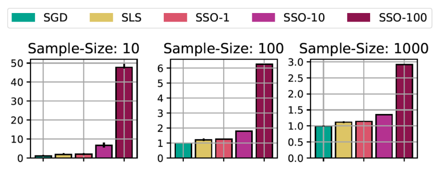

- Using a larger number of trajectories results in more computational cost for evaluating $\nabla \ell(z)$, amortizing the cost of multiple off-policy updates.

Conclusion

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- ✓ Proved that the resulting surrogate minimization algorithm will result in convergence to a stationary point.
- ✓ Strong empirical performance with better robustness towards hyper-parameters.
- ✓ 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.

Outline

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

Motivation

- Policy gradient (PG) methods based on REINFORCE:
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No systematic way to design theoretically principled surrogate functions, or a unified framework to analyze their properties.

Functional representation vs Policy parameterization

- **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.
  - *Softmax functional representation*: Logits $z^\pi(s, a)$ such that $p^\pi(a|s) = \frac{\exp(z^\pi(s,a))}{\sum_{a'} \exp(z^\pi(s,a'))}$.

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- **Policy parameterization**: Practical realization of the sufficient statistics. Determines Π (the set of feasible policies). *Examples*:
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- The functional representation of a policy is independent of its parameterization.
- **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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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 $\pi \in \Pi_\theta$,

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

FMA-PG Framework – Algorithm

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

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- 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.

Instantiating FMA-PG – Direct functional representation

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For the negative entropy mirror-map i.e. when $\phi(p^\pi(\cdot|s)) = \sum_a p^\pi(a|s)\log p^\pi(a|s)$,

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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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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 $\eta \leq \frac{(1-\gamma)^3}{2\gamma|A|}$.

× 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.

Instantiating FMA-PG – Softmax functional representation

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For the log-sum-exp mirror-map i.e. when $\phi_z(z(s,\cdot)) = \log\left(\sum_a \exp(z^\pi(s,a))\right)$,

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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 $\eta \leq 1 - \gamma$.

Instantiating FMA-PG – Softmax functional representation

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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- ✓ Above surrogate depends on the log of the importance sampling ratio.
- ✓ Surrogate involves the forward KL divergence making it *mode covering* encouraging exploration.

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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. $\mathbb{E}_{s\sim d^{\pi_t}}\,[\text{KL}(p^{\pi_t}(\cdot|s,\theta_t)||p^{\pi}(\cdot|s,\theta))] \leq \delta$,

- $g_t(\theta)$ 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 – Experimental Evaluation - Continuous control

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

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

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

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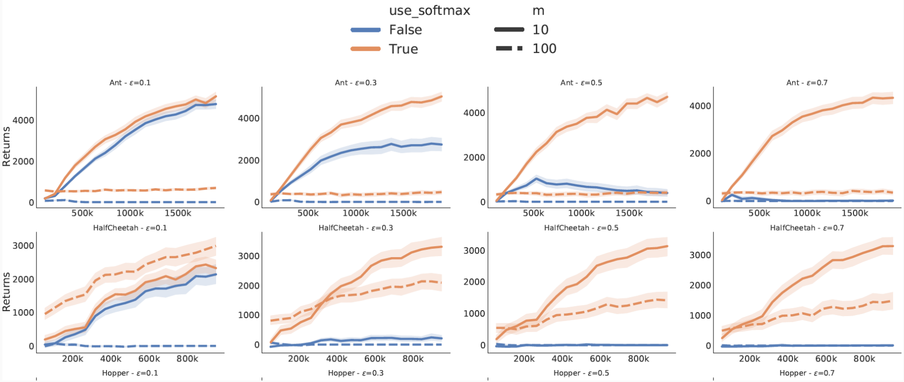

Outline

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

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- ✓ Show experimental evidence that on simple tabular MDPs, the algorithms instantiated with FMA-PG are competitive with popular PG algorithms such as TRPO, PPO. The framework suggests an alternative method, `sPPO` that out-performs PPO on the MuJoCo suite.

Conclusion

- ✓ Used functional mirror ascent to propose FMA-PG, a systematic way to define surrogate functions for generic policy optimization. Ensures monotonic policy improvement for arbitrary policy parameterization.
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- ✓ Show experimental evidence that on simple tabular MDPs, the algorithms instantiated with FMA-PG are competitive with popular PG algorithms such as TRPO, PPO. The framework suggests an alternative method, `sPPO` that out-performs PPO on the MuJoCo suite.
- ✓ 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?

Papers: https://arxiv.org/abs/2108.05828, https://arxiv.org/abs/2302.02607

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Backup Slides

FMA-PG – Experimental Evaluation - Tabular MDP

- 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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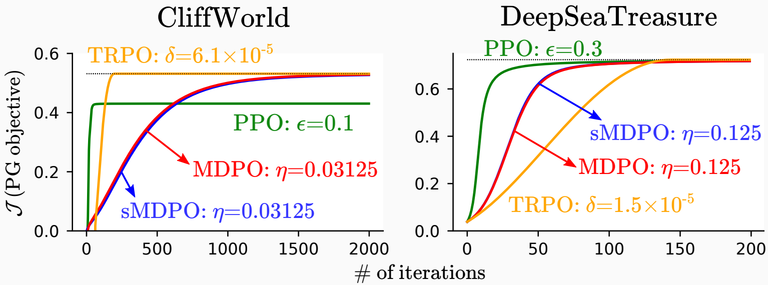

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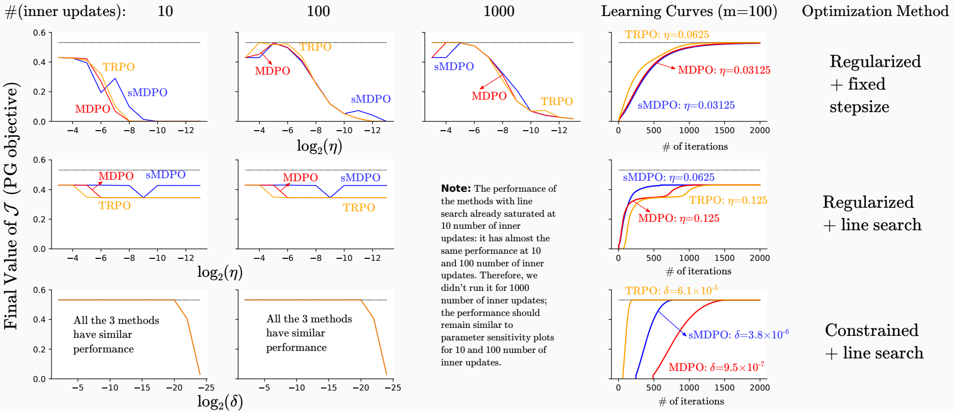

FMA-PG – Experimental Evaluation - Continuous control

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

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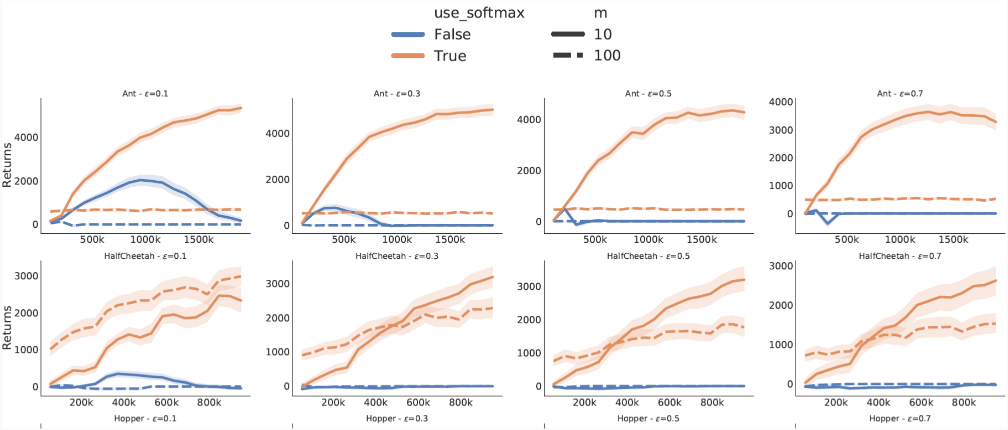

Extra Slides

Instantiating FMA-PG – Direct functional representation

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

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- With the tabular parameterization,
  - similar to uniform TRPO [Shani et al., 2020] and Mirror Descent Modified Policy Iteration [Geist et al., 2019].
  - with $m = \infty$ (exact maximization of the surrogate), and,
    (i) squared Euclidean distance mirror map, same as REINFORCE [Williams and Peng, 1991]
    (ii) negative entropy mirror map, same as natural policy gradient [Kakade, 2001].

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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.