# **Entropy Regularization** in **RL** through **Interpolation**

**Riad Akrour** 

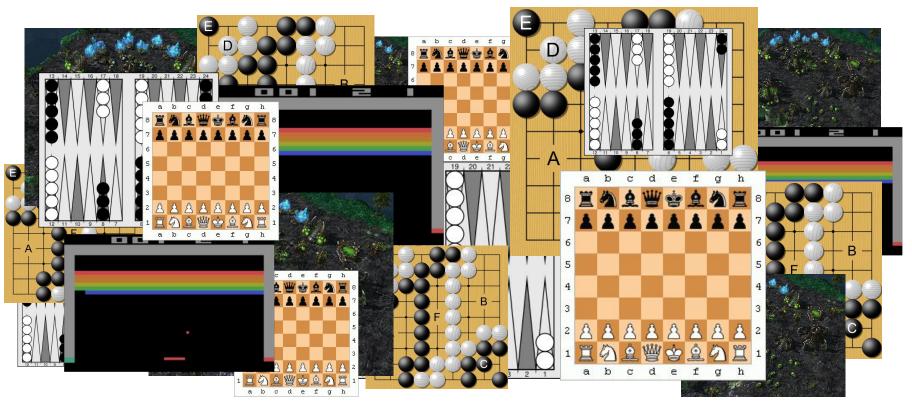


TECHNISCHE UNIVERSITÄT DARMSTADT

#### Outline

- Entropy Regularization in RL
  - Why it is important
  - How to solve the regularized problem
- Application: Explainable RL

#### Successes of RL



Entropy Regularization in RL through Interpolation

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## RL in the Physical World



- Small number of parameters (<20)
- Open loop policy

•

- Black-box optimization
- Requires expert demonstrations

**High Acceleration Reinforcement Learning for Real-World Juggling with Binary Rewards** K. Ploeger, M. Lutter, J. Peters CoRL20

#### Relative Entropy Policy Search (REPS)

• For Gaussian policies  $\pi_k(\theta) = \mathcal{N}(\theta | \mu_k, \Sigma_k)$ 

$$\max_{\pi_k} \quad \mathbb{E}_{\theta \sim \pi_k} \left[ R(\theta) \right]$$

s.t. 
$$\operatorname{KL}(\pi_k || \pi_{k-1}) \le \epsilon$$

• Closed-form solution

$$\pi_k \propto \pi_{k-1} \exp\left(\frac{R}{\eta}\right)$$

- Small number of parameters (<20)
- Open loop policy
- Black-box optimization
- Requires expert demonstrations

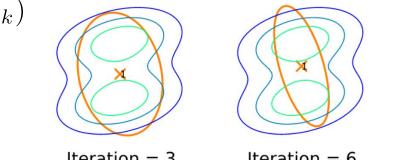
#### Outline

- Entropy Regularization in RL
  - How to solve this regularized problem
    - From black-box optimization
    - To Reinforcement Learning
    - To Deep RL
    - To convex optimization
  - Why it is important
- Application: Explainable RL

#### Model-based REPS (MORE)

For Gaussian policies  $\pi_k(\theta) = \mathcal{N}(\theta | \mu_k, \Sigma_k)$ 

 $\max_{\pi_k} \quad \mathbb{E}_{\theta \sim \pi_k} \left[ \hat{R}(\theta) \right]$ s.t.  $\operatorname{KL}(\pi_k || \pi_{k-1}) \leq \epsilon$  $\mathcal{H}(\pi_{k-1}) - \mathcal{H}(\pi_k) \le \beta$ 



Iteration = 3

Iteration = 6

Deisenroth et al.

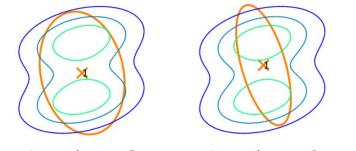
Closed-form solution in probability space

$$\pi_k \propto \pi_{k-1}^{\eta/(\eta+\omega)} \exp\left(\frac{\hat{R}}{\eta+\omega}\right)$$

Model-Based Relative Entropy Stochastic Search; A. Abdolmaleki, R. Lioutikov, N. Lau, L. Reis, J. Peters, G. Neumann; NeurIPS15

#### Model-based REPS (MORE)

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  - $\max_{\pi_k} \quad \mathbb{E}_{\theta \sim \pi_k} \left[ \hat{R}(\theta) \right]$ s.t.  $\operatorname{KL} \left( \pi_k || \pi_{k-1} \right) \leq \epsilon$   $\mathcal{H}(\pi_{k-1}) \mathcal{H}(\pi_k) \leq \beta$



Iteration = 3

Iteration = 6

Deisenroth et al.

Closed-form solution in probability space

$$\pi_k \propto \pi_{k-1}^{\eta/(\eta+\omega)} \exp\left(\frac{\hat{R}}{\eta+\omega}\right)$$

• Closed-form solution in parameter space for quad.  $\hat{R}$ 

Model-Based Relative Entropy Stochastic Search; A. Abdolmaleki, R. Lioutikov, N. Lau, L. Reis, J. Peters, G. Neumann; NeurIPS15

# Step-based MORE (MOTO)

• For linear-Gaussian policies  $\pi_k^t(a_t|s_t) = \mathcal{N}\left(a_t|K_ts_t, \Sigma_t\right)$ 

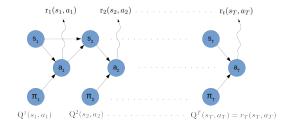
$$\max_{\substack{\pi_k^t \\ k}} \quad \mathbb{E}_{s \sim p_{k-1}^t, a \sim \pi_k^t(.|s)} \left[ \hat{Q}_{k-1}^t(s, a) \right]$$

$$s.t. \quad \mathbb{E}_{s \sim p_{k-1}^t} \left[ \text{KL} \left( \pi_k^t(.|s)| | \pi_{k-1}^t(.|s) \right) \right] \le \epsilon$$

$$\mathbb{E}_{s \sim p_{k-1}^t} \left[ \mathcal{H}(\pi_{k-1}^t(.|s)) - \mathcal{H}(\pi_k^t(.|s)) \right] \le \beta$$

• Closed-form solution in probability space

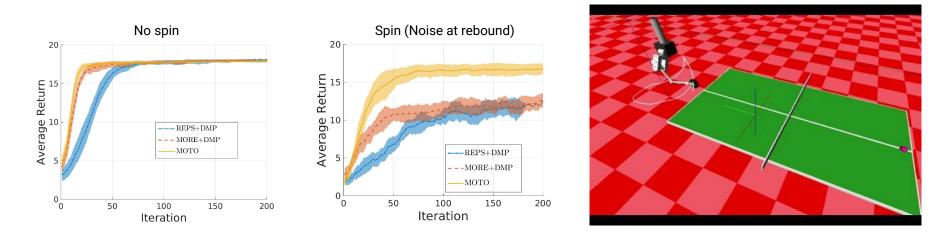
$$\pi_k^t(.|s) \propto \pi_{k-1}^t(.|s)^{\eta/(\eta+\omega)} \exp\left(\frac{\hat{Q}_{k-1}^t(s,.)}{\eta+\omega}\right)$$



- Closed-form solution in parameter space for quad.  $\hat{Q}$
- Additional Gaussian approx. of  $p_{k-1}^t$

#### Model-free Trajectory Optimization for Reinforcement Learning; R. Akrour, A. Abdolmaleki, H. Abdulsamad, G. Neumann; ICML16

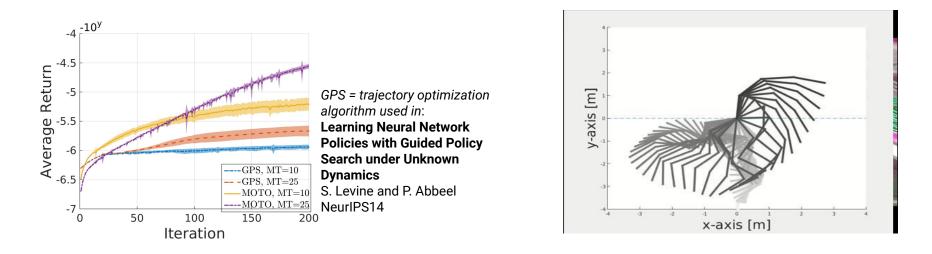
#### MOTO vs Black-box



- Comparable to black-box methods with open-loop policies despite much larger search space
- Closed-loop policy adapts to changes in the environment

Model-free Trajectory Optimization for Reinforcement Learning; R. Akrour, A. Abdolmaleki, H. Abdulsamad, G. Neumann; ICML16

#### MOTO vs trajectory optimization



• Back propagating approx. quad. Q functions > forward propagating approx. linear dynamics models

Model-free Trajectory Optimization for Reinforcement Learning; R. Akrour, A. Abdolmaleki, H. Abdulsamad, G. Neumann; ICML16

# Why does MOTO work?

• MOTO policy update

$$\max_{\pi_k^t} \quad \mathbb{E}_{s \sim p_{k-1}^t, a \sim \pi_k^t(.|s)} \left[ \hat{Q}_{k-1}^t(s, a) \right]$$

$$s.t. \quad \mathbb{E}_{s \sim p_{k-1}^t} \left[ \text{KL} \left( \pi_k^t(.|s) || \pi_{k-1}^t(.|s) \right) \right] \leq \epsilon$$

$$\mathbb{E}_{s \sim p_{k-1}^t} \left[ \mathcal{H}(\pi_{k-1}^t(.|s)) - \mathcal{H}(\pi_k^t(.|s)) \right] \leq \beta$$

- Strict compliance with KL-divergence cst. important in practice... why?
- Objective and constraints expressed in terms of  $p_{k-1}^t$ ... is it reasonable?

#### Policy improvement

- In tabular RL,  $\pi_k(s) = \arg \max Q_{k-1}(s, .)$ 
  - Take better action in **all states**
- Relaxation when using function approximators

$$\circ \quad \pi_k = \underset{\pi}{\operatorname{arg\,max}} \quad \mathbb{E}_{s \sim p_{k-1}, a \sim \pi(\cdot|s)} \left[ Q_{k-1}(s, a) \right]$$

- Take better actions in average of **previous state** distribution
- What about average under the **current state** distribution  $\mathbb{E}_{s \sim p_k, a \sim \pi(.|s)} [Q_{k-1}(s, a)]$ ?

•  $\Pi$  matrix representation of policy  $\pi$ 

•  $\prod$  matrix of size  $|\mathcal{S}| \times |\mathcal{S}| |\mathcal{A}|$  $\Pi_{(s,(s',a))} = \pi(a|s)$  if s = s', 0 else

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- $\Pi$  matrix representation of policy  $\pi$
- P transition matrix

• P matrix of size  $|\mathcal{S}||\mathcal{A}| imes |\mathcal{S}|$  $P_{((s,a),s')} = p(s'|s,a)$ 

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- $\Pi$  matrix representation of policy  $\pi$
- P transition matrix
- Value function  $V^{\pi} = \Pi R + \gamma \Pi P V^{\pi}$
- R matrix of size  $|\mathcal{S}||\mathcal{A}| imes 1$  $R_{((s,a),1)} = r(s,a)$ **Riad Akrour**

- $\Pi$  matrix representation of policy  $\pi$
- P transition matrix
- Value function  $V^{\pi} = \left(I \gamma \Pi P\right)^{-1} \Pi R$ 
  - Policy induced state distribution

$$(I - \gamma \Pi P)_{(s,s')}^{-1} = \sum_{t=0}^{\infty} \gamma^t (\Pi P)_{(s,s')}^t,$$
  
=  $\sum_{t=0}^{\infty} \gamma^t Pr(s_t = s' | s_0 = s; \pi),$ 

• We define  $\Pi_s = \left(I - \gamma \Pi P\right)^{-1}$ 

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- P transition matrix
- $\bullet \quad {\rm Value \ function} \ V^\pi = \Pi_s \Pi R$

- $\Pi$  matrix representation of policy  $\pi$
- P transition matrix
- Value function  $V^{\pi} = \Pi_s \Pi R$
- Policy return  $J(\pi) = \mu^T V^\pi\,$  for initial state distribution matrix  $\mu$

• 
$$V^{\pi} - V^{\pi'} = \prod_{s} \prod A^{\pi'}$$

• 
$$V^{\pi} - V^{\pi'} = \prod_s \prod A^{\pi'}$$

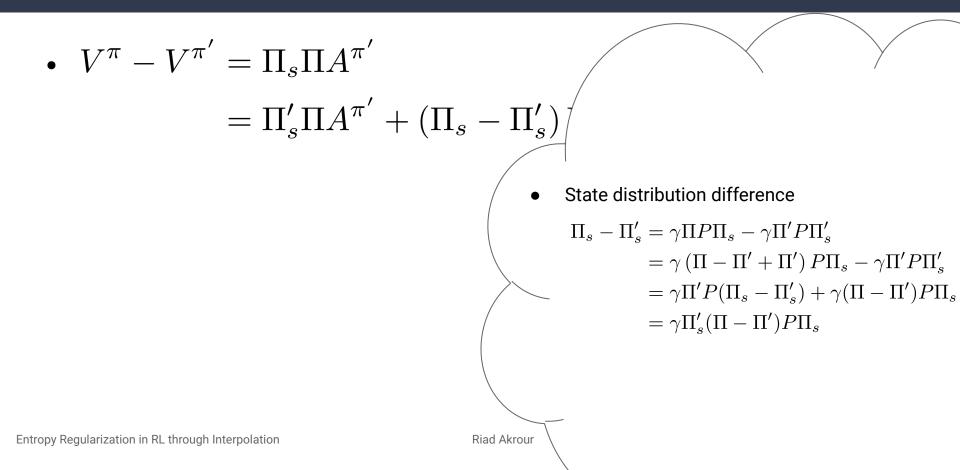
• Value difference

$$V^{\pi} - V^{\pi'} = \Pi \left( \mathcal{R} + \gamma P V^{\pi} \right) - V^{\pi'},$$
  
=  $\Pi \left( \mathcal{R} + \gamma P \left( V^{\pi} + V^{\pi'} - V^{\pi'} \right) \right) - V^{\pi'},$   
=  $\gamma \Pi P \left( V^{\pi} - V^{\pi'} \right) + \Pi \left( \mathcal{R} + \gamma P V^{\pi'} \right) - V^{\pi'},$   
=  $\gamma \Pi P \left( V^{\pi} - V^{\pi'} \right) + \Pi Q^{\pi'} - V^{\pi'},$   
=  $\gamma \Pi P \left( V^{\pi} - V^{\pi'} \right) + \Pi A^{\pi'},$   
=  $(I - \gamma \Pi P)^{-1} \Pi A^{\pi'}.$ 

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• 
$$V^{\pi} - V^{\pi'} = \Pi_s \Pi A^{\pi'}$$
  
=  $\Pi'_s \Pi A^{\pi'} + (\Pi_s - \Pi'_s) \Pi A^{\pi'}$ 



• 
$$V^{\pi} - V^{\pi'} = \Pi_s \Pi A^{\pi'}$$
  
=  $\Pi'_s \Pi A^{\pi'} + (\Pi_s - \Pi'_s) \Pi A^{\pi'}$   
=  $\Pi'_s \Pi A^{\pi'} + \gamma \Pi'_s (\Pi - \Pi') P \Pi_s \Pi A^{\pi'}$ 

- Expressed policy return as a function of old advantage under old state distribution
  - + term small when new policy is close to old one

- Previous expression contains  $\Pi_s$  which is hard to quantify
  - $\circ$  Prior work will mainly differ in bounding  $||\mu^T \left(\Pi_s \Pi_s'
    ight)||_{\infty}$

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    ight)||_{\infty}$
- CPI (Kakade et al. ICML02):  $||\mu^T (\Pi_s \Pi'_s)||_{\infty} \leq \frac{2\alpha\gamma}{(1-\gamma)^2}$ 
  - Where  $\Pi = \alpha \Pi^g (1 \alpha) \Pi'$  mixes previous policy with policy maximizing old advantage
  - $\circ$  Improvement of policy return can be guaranteed for small enough lpha

$$J^{\pi} - J^{\pi'} \ge \frac{\left(\mu^T \Pi'_s \Pi^g A^{\pi'}\right)^2}{8}$$

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• USPI (Pirotta et al. ICML13): 
$$\|\mu^T (\Pi_s - \Pi'_s)\|_{\infty} \leq \frac{\gamma}{(1-\gamma)^2} \|\Pi - \Pi'\|_{\infty}$$
  
 $\circ \|\Pi - \Pi'\|_{\infty} = \max_{s \in \mathcal{S}} \sum_{a \in \mathcal{A}} |\pi(a|s) - \pi'(a|s)|$   
 $= 2 \max_{s \in \mathcal{S}} \operatorname{TV}(\pi(.|s) || \pi'(.|s))$ 

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$$||\mu^T (\Pi_s - \Pi'_s)||_{\infty} \leq \frac{2\gamma}{(1-\gamma)^2} \max_{s \in \mathcal{S}} \mathrm{TV}(\pi(.|s) \parallel \pi'(.|s))$$

• TRPO (Schulman et al. ICML15):  $\|\mu^T (\Pi_s - \Pi'_s)\|_{\infty} \leq \frac{2\gamma}{(1-\gamma)^2} \max_{s \in \mathcal{S}} \sqrt{\frac{1}{2}} \mathrm{KL}(\pi(.|s) \| \pi'(.|s))$ • Pinsker's inequality:  $\mathrm{TV} \leq \sqrt{\frac{1}{2}} \mathrm{KL}$ 

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• CPO (Achiam et al. ICML17): 
$$\|\mu^T (\Pi_s - \Pi'_s)\|_{\infty} \leq \frac{2\gamma}{(1-\gamma)^2} \mathbb{E}_{s \sim \pi'} [\operatorname{TV}(\pi(.|s) \parallel \pi'(.|s))]$$

#### Entropy Regularization in RL through Interpolation

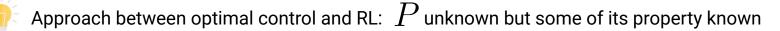
# Lower bounds for MOTO's setting

- Continuous state/action spaces
- We want to exploit specific model assumptions (Quad. Q and Gaussian state distributions)
- Same order of magnitude in terms of KL and discount in the lower bound
- As with prior work, lower bound too pessimistic to be used in practice
  - Despite using more specific assumptions on the MDP!

Model-Free Trajectory-based Policy Optimization with Monotonic Improvement; R. Akrour, A. Abdolmaleki, H. Abdulsamad, J. Peters, G. Neumann; JMLR18

#### Perspectives

- Progress can be made when bounding  $||(\Pi \Pi')P||_{\infty}$ 
  - Current work: same actions lead to same states
    - If action not supported by previous policy = maximum penalty
  - Transition function assumed completely unknown



- True for many physical systems (e.g. robots)
- Inject human knowledge to obtain more practical predictions of policy return
  - Useful for safety guarantees

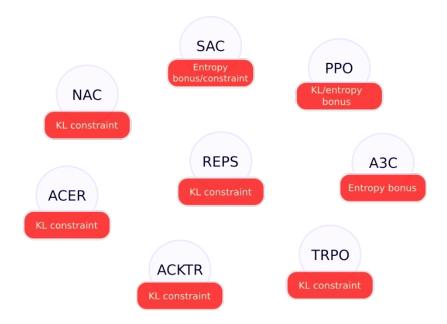
## Comparison to deep RL



- Specialized models of MOTO work well on control problems
- What if the state is high dimensional?

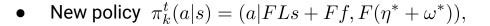
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# Entropy regularization in (deep) RL



• Can we transfer anything from the simpler setting of MOTO to deep RL?

#### MOTO's closed form solutions



 $\circ \quad F = (\eta^* \Sigma_t^{-1} - Q_{aa})^{-1}, \qquad \qquad L = \eta^* \Sigma_t^{-1} K_t + Q_{as},$  $f = \eta^* \Sigma_t^{-1} k_t + q_a.$ 

$$\neg \qquad \pi_{k-1}^{t}(a|s) \sim (K_{t}s + k_{t}, \Sigma_{t})$$

$$Q \text{ function}$$

$$\hat{Q}_{k-1}^{t}(s, a) = \frac{1}{2}a^{T}Q_{aa}a + a^{T}Q_{as}s + a^{T}q_{a} + q(s)$$

Old policy

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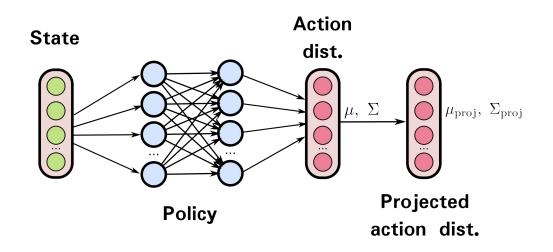
#### MOTO's closed form solutions

• New policy  $\pi_k^t(a|s) = (a|FLs + Ff, F(\eta^* + \omega^*)),$ 

$$\circ \quad F = (\eta^* \Sigma_t^{-1} - Q_{aa})^{-1}, \qquad \qquad L = \eta^* \Sigma_t^{-1} K_t + Q_{as}, f = \eta^* \Sigma_t^{-1} k_t + q_a.$$

- Dual param. entropy cst.  $\omega^*$ : scale covariance matrix
- Dual param. KL-divergence cst.  $\eta^*$ : interpolate params of policy and Q function
- Given an input covariance, can we compute in closed form the scaling satisfying an entropy constraint?

## Entropy projections



- Solve for  $\omega$ ,  $\mathcal{H}\left(\mathcal{N}\left(\mu,\omega\Sigma\right)\right)=\beta$
- Solve for  $\eta$ , KL  $(\mathcal{N}(\eta\mu + (1-\eta)\mu_{k-1}, \eta\Sigma + (1-\eta)\Sigma_{k-1}) | \mathcal{N}(\mu_{k-1}, \Sigma_{k-1})) = \epsilon$
- Closed form and differentiable solution => Use gradient descent to solve the policy update

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#### Entropy projections

- **Can solve** the entropy eq. in closed form
- **No closed** form solution for the KL (would require solving x + log x = a)
  - $\circ$  Replace with an upper bound of the KL, quadratic in  $\eta$
  - Similar approach for entropy/KL of soft-max distribution (discrete action space)

## Entropy projections

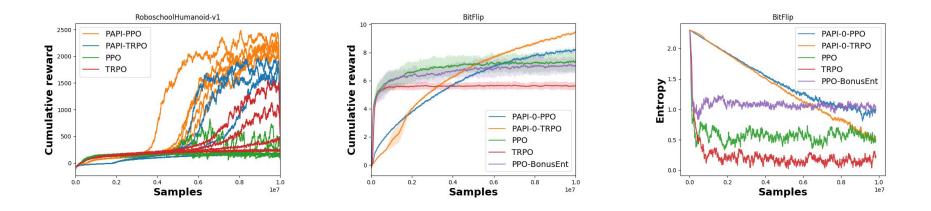
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Projections for Approximate Policy Iteration Algorithms; R. Akrour, J. Pajarinen,

Algorithm 2 API linear-Gaussian policy projection **Input:**  $A', \lambda, \lambda_{\text{off}}$ ,  $q(.|s) = (A_a^T \psi_a(s), \Sigma_a), A^T, \psi,$  $\epsilon$  and  $\beta$ **Output:**  $\pi(.|s) = \mathcal{N}(A'^T\psi(s), \Sigma)$  complying with KL (6) and entropy (7) constraints  $\Sigma = \text{Entropy_projection}(\lambda, \lambda_{\text{off_diag}}, \beta)$ if  $\mathbb{E}_s \mathrm{KL}(\mathcal{N}(A'^T \psi(s), \Sigma) \parallel q(.|s)) > \epsilon$  then  $\eta_q = \frac{\epsilon - m_q(A)}{m_q(A) + m_q(\Sigma) + e}$  $\Sigma = \eta_g \Sigma + (1 - \eta_a) \Sigma_a$ if  $\mathbb{E}_s \mathrm{KL}(\mathcal{N}(A'^T \psi(s), \Sigma) \parallel q(.|s)) > \epsilon$  then  $a = .5 \mathbb{E}_{s} ||A'^{T} \psi(s) - A^{T} \psi(s)||_{\Sigma_{a}^{-1}}^{2}$  $b = .5 \mathbb{E}_s [(A'^T \psi(s) - A^T \psi(s))^T]$  $\Sigma_a^{-1}(A^T\psi(s) - A_a^T\psi_a(s))]$  $c = m_q(A) + r_q(\Sigma) + e_a(\vec{\Sigma}) - \epsilon$  $A' = \eta_m A' + (1 - \eta_m).$ end if

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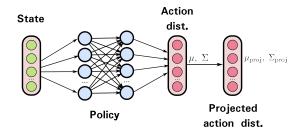
#### Results



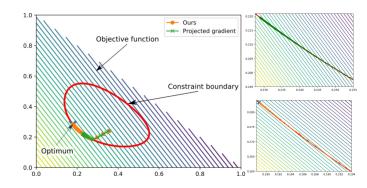
- **Pros**: entropy constraint (Gaussian and soft-max) very easy to implement and offers large gains
- **Caveat**: KL requires to store previous policies or only optimize last layer of the neural network

# Projection...?

- General algorithm: upper bound KL/entropy with a function 'simple' in an interpolation parameter
  - Solve for the interpolation parameter and return a distribution complying with cst.
- Is this a projection??
- What is the 'error' of the projection?
- Will gradient descent converge to a reasonable solution?



#### Convergence on toy problem



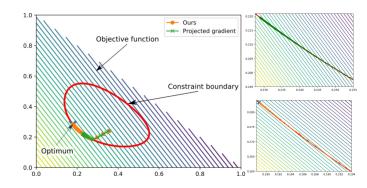
• Problem  $\max_{p \in \text{Simplex}} f(p) = c^T p$ 

s.t. 
$$\mathcal{H}(p) \ge \beta$$

• Projection g(p): solve for  $\eta$ 

$$\mathcal{H}(\eta p + (1 - \eta) \text{Unif.}) \ge \eta \mathcal{H}(p) + (1 - \eta) \mathcal{H}(\text{Unif.}) = \beta$$
$$\eta = \frac{\log |\mathcal{A}| - \beta}{\log |\mathcal{A}| - \mathcal{H}(p)}$$

#### Convergence on toy problem

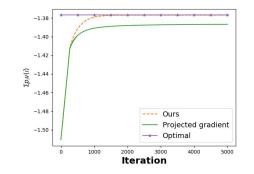


• Problem  $\max_{p \in \text{Simplex}} f(p) = c^T p$ 

s.t. 
$$\mathcal{H}(p) \ge \beta$$

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$$\mathcal{H}(\eta p + (1 - \eta) \text{Unif.}) \ge \eta \mathcal{H}(p) + (1 - \eta) \mathcal{H}(\text{Unif.}) = \beta$$
$$\eta = \frac{\log |\mathcal{A}| - \beta}{\log |\mathcal{A}| - \mathcal{H}(p)}$$



- GD on composition  $p_{k+1} = p_k \alpha \nabla f \circ g(p_k)$ 
  - converges

$$\succ$$
 PGD  $p_{k+1} = g(p_k - \alpha \nabla f(p_k))$ 

 No convergence because not an orthogonal projection

#### Convergence in a convex optimization setting

• Problem:  $\min_{x \in \mathbb{R}^d} \quad f(x) = c^T x,$ s.t.  $h(x) \le 0.$ 

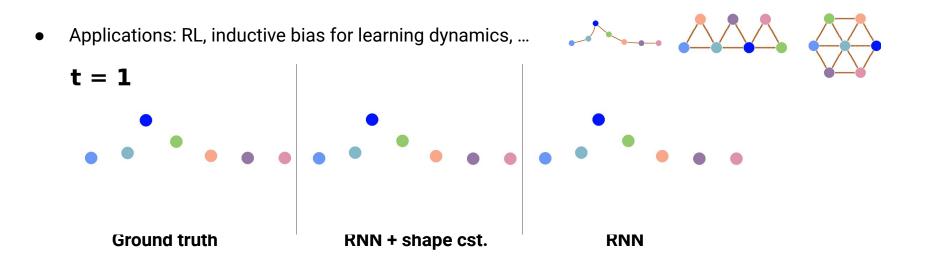
• Projection: 
$$g(x) = \begin{cases} x & \text{if } h(x) \leq 0, \\ \eta_x x + (1 - \eta_x) x_0 & \text{else,} \end{cases}$$
 with  $\eta_x = \frac{h(x_0)}{h(x_0) - h(x)}$  and  $h(x_0) < 0$ 

• Algorithm: 
$$x_{k+1} = x_k - \alpha \nabla f \circ g(x_k)$$
, with gradient  $\nabla f \circ g(x_k) = \eta_k \left( \nabla f(g(x_k)) + \frac{\nabla f(g(x_k))^T(g(x_k) - x_0)}{h(x_0)} \nabla h(x_k) \right)$ 

• Convergence rate  $\mathcal{O}(\frac{1}{\sqrt{K}})$  (interpolation is non-smooth)

Convex Optimization with an Interpolation-based Projection and its Application to Deep Learning; R. Akrour, A. Atamna, J. Peters; MACH (submitted)

# Applications of the interpolation projection

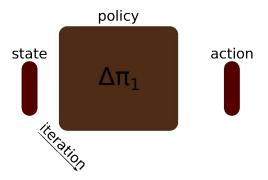


• About x200 faster than orthogonal projection layers (Differentiable Convex Optimization Layers; Agrawal et al.; NeurIPS19)

Convex Optimization with an Interpolation-based Projection and its Application to Deep Learning; R. Akrour, A. Atamna, J. Peters; MACH (submitted)

#### Perspectives

- Non i.i.d. RL setting alternates data collection and model update
  - Very important to update the policy gracefully
    - Doable with linear policies, trees (MCTS), not so much with NNs
- Updating all NN params. at once **not reasonable**?
  - Incremental construction of the policy
    - Stack smaller **policy 'delta'** networks at each update
      - Easy to control KL/TV
    - How to forget?



## Examples of explainable RL policies

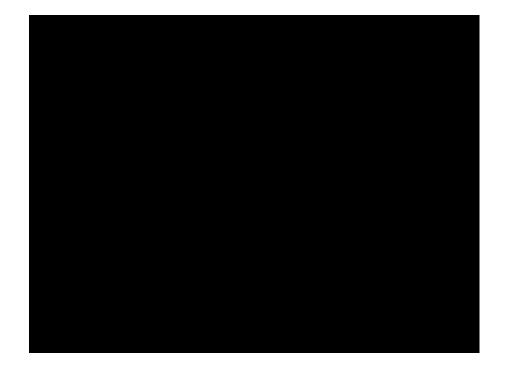
- **Example of an interpretable policy**: solving the Rubik's cube
- **Policy structure**: IF State similar to Prototype DO Action
- Can we extract similar policies for other decision problems?



# Limits of differentiable programming?

• IF State similar to Prototype DO Action

- Naive approach: differentiable policy with prototypical states = basis functions
- Hard to relate cluster centers and behavior



#### **Proposed solution**

- Stay in the **manifold** of (interpretable) states
- **Pick prototypes** from trajectory data (non-differentiable operation)
- Mixture of discrete optimization (search heuristics) and continuous optimization (gradient descent + interpolation projections)



Reinforcement Learning from a Mixture of Interpretable Experts; R. Akrour, D. Tateo, J. Peters; TPAMI (submitted)

#### Perspectives

- **Limitation**: similarity to prototype based on Euclidean distance
  - How to scale to more complex inputs and keep the similarity function interpretable?



Perspective 1: Ensure temporal coherency

• Higher similarity between states occurring closely after each other in the MDP

