Global Optimality Guarantees For Policy Gradient Methods

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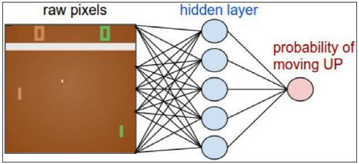
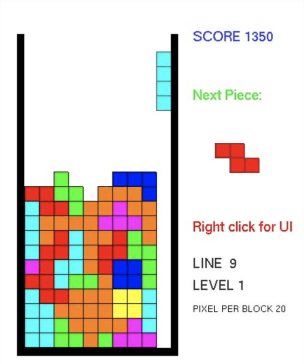
Policy Gradient Methods



REINFORCE:
Initialize policy parameters θ arbitrarily
for each episode $\{s_1, a_1, r_2, \cdots, s_{T-1}, a_{T-1}, r_T\} \sim \pi_\theta$ **do**
  for $t = 1$ to $T - 1$ **do**
    $\theta \leftarrow \theta + \alpha \nabla_\theta \log \pi_\theta(s_t, a_t) G_t$
  endfor
endfor
return θ

https://twitter.com/CovariantAI/status/1232396047948763136
https://youtu.be/kVmp0uGtShk

Policy Search In Tetris



- One approach is a Linear Approximation: $J(s) \approx \phi(s)^\top \theta$.
- $\phi(s)$ encodes features. E.g. column heights, inter-column height differences, max height etc.
- Each (s, a) associated with known successor state s'_a
- Could estimate θ, then play $\text{argmax}_a \, \phi(s'_a)^\top \theta$.
- Often better to directly search over the subclass of policies $\mu_\theta(s, a) \propto \exp(\phi(s'_a)^\top \theta)$

Policy Gradient Methods: Setup

Direct optimization over a policy class by local search.

- Cost-to-go function: $J_\mu(s) = \mathbb{E}_\mu \left[\sum_{t=0}^{\infty} \alpha^t g(s_t, \mu(s_t)) \mid s_0 = s\right]$
- Scalar loss: $\ell(\mu) = \mathbb{E}_{s\sim\nu}[J_\mu(s)]$.
  - Assume ν has full support. (*This is essential*!)
- Parameterized policies: $M_\Theta = \{\mu_\theta : \theta \in \Theta\} \subset M$.
  - $\Theta \subset \mathbb{R}^d$ is convex. $M = \{\text{Markov policies}\}$.
  - Overloaded notation: $\ell(\theta) \equiv \ell(\mu_\theta)$
- (Stochastic) Gradient Descent on $\ell(\cdot)$,

$$\theta_{t+1} = \theta_t - \gamma_t \left(\nabla \ell(\theta) + \text{noise}\right) \quad t = 1, 2, \ldots$$

Contrast to policy iteration

Policy gradient methods:

1. Make soft updates to policies
2. Aim to directly minimize a global loss function $\ell(\mu)$ rather than solve the changing surrogate problems $\min_u Q_{\mu_k}(s, u)$.
    - We'll see a connection, though, when we compute the gradients of $\ell(\cdot)$.
3. Approximation is through a policy class rather than a class of cost-to-go functions.
    - There is a connection to approximate PI when considering the set of policies that are (approximately) greedy with respect to a cost-to-go function. (See the tetris example above)
    - Actor-critic methods, which we'll get to later, are a hybrid.

Computing a stochastic gradient via simulation

Justified in the next two slides.

An unbiased estimate of $\nabla_\theta \ell(\mu_\theta)$ for a stochastic policy

Sample $T \sim \mathrm{Geometric}(1-\alpha)$.

Sample $s_0 \sim \nu$

Apply μ_θ for T periods from s_0.

Observe trajectory: $\tau = (s_0, u_0, c_0, \ldots, s_T, u_T, c_T, s_{T+1})$.

Observe total cost: $c(\tau) = c_0 + \cdots + c_T$.

Return $c(\tau) \sum_{t=0}^{T} \nabla_\theta \log \mu_\theta(u_t | s_t)$

Many variants and improvements:

- Infintesimal perturbation analysis
- Variance reduction by adding baselines
- Actor critic methods

Score function gradient estimator (Finite horizon case)

Consider a stochastic policy $\mu_\theta(u|s)$
For $\tau = (s_0, u_0, \cdots s_T, u_T)$, set $G(\tau) = \sum_{t=0}^{T} g(s_t, u_t)$
Let $P(\tau;\theta)$ denote its probability under μ_θ.

$$
\begin{aligned}
\nabla_\theta \, \mathbb{E}_\theta \left[\sum_{t=0}^{T} g(s_t, u_t) \right] &= \nabla_\theta \sum_\tau G(\tau) P(\tau;\theta) \\
&= \sum_\tau G(\tau) \nabla_\theta \nabla_\theta \, P(\tau;\theta) \\
&= \sum_\tau G(\tau) \left(\nabla_\theta \, \log P(\tau;\theta) \right) P(\tau;\theta) \\
&= \mathbb{E}_\theta \left[G(\tau) \left(\nabla_\theta \, \log P(\tau;\theta) \right) \right] \\
&= \mathbb{E}_\theta \left[G(\tau) \left(\nabla_\theta \, \log \prod_{t=0}^{T} \mu_\theta(u_t|s_t) P(s_{t+1}|u_t, s_t) \right) \right] \\
&= \mathbb{E}_\theta \left[G(\tau) \left(\sum_{t=0}^{T} \nabla_\theta \, \log \mu_\theta(u_t|s_t) \right) \right]
\end{aligned}
$$

Score function gradient estimator (infinite horizon case)

Take $T \sim \mathrm{Geom}(1-\alpha)$, so $\mathbb{P}(T \geq t) = \alpha^t$.

$$\ell(\theta) = \mathbb{E}_\theta \left[\sum_{t=0}^{\infty} \alpha^t g(s_t, u_t) \right] = \mathbb{E}_\theta \left[\sum_{t=0}^{\infty} \mathbb{P}(T \geq t) g(s_t, u_t) \right]$$
$$= \mathbb{E}_\theta \left[\sum_{t=0}^{T} g(s_t, u_t) \right]$$

One can show

$$\nabla \ell(\theta) = \mathbb{E}_\theta \left[\left(\sum_{t=0}^{T} g(s_t, u_t) \right) \left(\sum_{t=0}^{T} \nabla_\theta \log \mu_\theta(u_t | s_t) \right) \right]$$

You may encounter a slight improvement that recognizes some terms have mean zero and writes

$$\nabla \ell(\theta) = \mathbb{E}_\theta \left[\left(\sum_{t=0}^{T} \nabla_\theta \log \mu_\theta(u_t | s_t) \left(\sum_{i=t}^{T} g(s_t, u_t) \right) \right) \right]$$

Challenges with policy gradient methods

This class will cover issue (1). The rest next week.

1. Nonconvexity of the loss function $\ell(\mu)$.

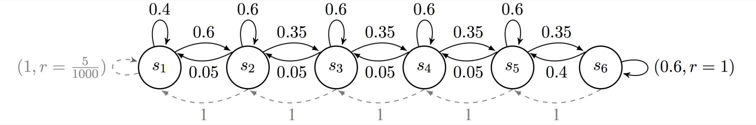
    Due to multi-period objective.

2. Unnatural policy parameterization $\theta \mapsto \mu_\theta$.

    Poor parameterization can lead to vanishing gradients in single period problems. Natural gradient methods are invariant to change of coordinates.

3. Insufficient exploration.

    We rely on the initial distribution $\nu(\cdot)$.



4. Large variance of stochastic gradients.

    Baselines and actor critic methods help.

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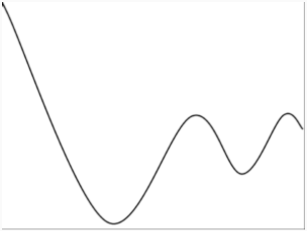
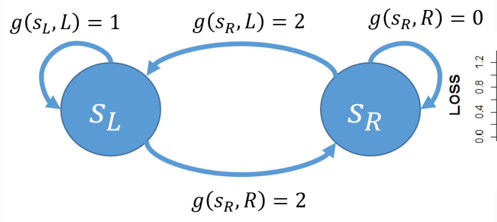
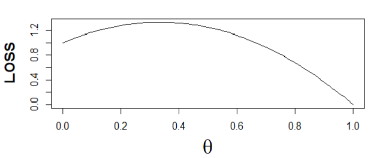
So we've reduced dynamic programming to black-box nonconvex optimization?

- PG is applicable to almost any decision problem.
- **But...** $\mu \mapsto \ell(\mu)$ is nonconvex.
  - Even for classical dynamic programming problems.
- Policy gradient is widely understood to converge toward first-order stationary points (i.e. w/ $\nabla_\theta \, \ell(\mu_\theta) = 0$).
  - Almost no guarantees on the quality of stationary points.
  - There are bad local minima in simple problems.



A Bad Example For Policy Gradient



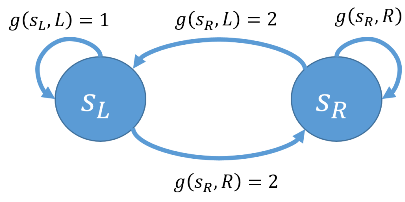


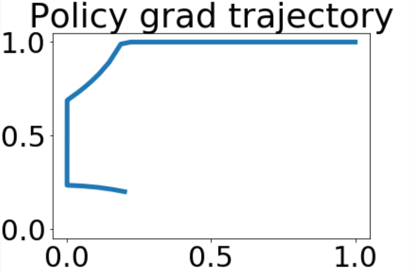
- $\mu_\theta(s_L) = \mu_\theta(S_R) = \theta =$ "Probability of Right."

Policy gradient gets stuck in a bad local minimum

Despite containing the optimal policy, the policy class is not rich enough to allow for a local improvement.

A Good Example For Policy Gradient





- $\mu_\theta(S_L) = \theta_L =$ "Probability of Right from left state."
- $\mu_\theta(S_R) = \theta_R =$ "Probability of Right from right state."

Policy gradient reaches the global optimum

The full policy class is rich enough to allow for local improvement... but this is unsatisfying.

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Warmup with the natural special case

- $\mathcal{S} = \{1, \cdots, n\}$ is a finite set.
- $U(s) = U = \Delta^{k-1}$ contains all probability distributions over k deterministic actions.
  - For $u \in U$, $g(s,u) = \sum_{i=1}^{k} g(s,i)$, $P_{ss'}(u) = \sum_{i=1}^{k} u_i P_{ss'}(i)$

Natural parameterization

- $\mu_\theta(s) = \theta_s \in \Delta^{k-1}$ associates each state with a probability distribution over actions.
- Drop the notational dependence on θ . . ., writing $\mu \in \mathbb{R}^{n \times k}$
- Stationary randomized policies: $M = \{\pi \in \mathbb{R}_{+}^{n \times k} : \sum_{i=1}^{k} \mu_{s,i} = 1 \ \forall s \in \{1, \cdots, n\}\}$.

First order methods

First order methods solve $\min_{\mu \in M} \ell(\mu)$ by iteratively minimizing (regularized) local linear approximations to $\ell(\cdot)$.

Example: Projected Gradient

$$\begin{aligned}\mu_{k+1} &= \Pi_{2,M}\left(\mu_k - \gamma_k \nabla \ell(\mu_k)\right) \\ &= \underset{\mu \in M}{\operatorname{argmin}} \;\; \ell(\mu_k) + \langle \nabla \ell(\mu_k)\,,\, \mu - \mu_k \rangle + \frac{1}{2\gamma_k}\left\|\mu - \mu_k\right\|_2^2\end{aligned}$$

Projection onto the probability simplex involves a simple soft-thresholding operation.

It is also natural to consider conditional gradient descent or exponentiated gradient descent (... a special case of mirror descent).

Convergence to first order stationary points (1)

Definition: $\ell(\cdot)$ is L–smooth if $\nabla^2 \ell(\mu) \preceq L^2 I$

Informal Proposition (Asymptotic convergence)

If $\ell(\cdot)$ is L–smooth, and stepsizes are set appropriately, then for any limit point μ_∞ of $\{\mu_k\}$.

$$\langle \nabla \ell(\mu_k)\,,\, \mu - \mu_\infty \rangle \geq 0 \qquad \forall \mu \in M$$

Proposition (Convergence rate)

Set $e_k = \min_{\mu \in M} \langle \nabla \ell(\mu_k)\,,\, \mu - \mu_k \rangle$. If $\gamma_k = 1/L$ then,

$$\min_{k \leq K} |e_k| \leq \sqrt{\frac{\ell(\mu_0) - \ell(\mu^*)}{2LR^2K}}$$

where $R = \sup_{\mu, \mu'} \|\mu - \mu'\|_2$.

Similar guarantees apply with stochastic gradient evaluations

Proof of rate to reach approximate stationary point (1)

Descent Lemma

If $\ell(\cdot)$ is L smooth, then $\ell(\bar{\mu}) \leq \ell(\mu) + \langle \nabla \ell(\mu)\,,\, \bar{\mu} - \mu \rangle + \frac{L}{2}\|\bar{\mu} - \mu\|_2^2$

For $\gamma_k \leq \frac{1}{L}$, projected gradient descent *minimizes a quadratic upper bound* on $\ell(\cdot)$. We find

$$\ell(\mu_{k+1}) \leq \min_{\mu \in M} \ \ell(\mu_k) + \langle \nabla \ell(\mu_k)\,,\, \mu - \mu_k \rangle + \frac{1}{2\gamma_k}\|\mu - \mu_k\|_2^2$$

Take $\mu^+ = \operatorname{argmin}_{\mu \in M} \langle \nabla \ell(\mu_k)\,,\, \mu - \mu_k \rangle$ and pick $\gamma_k = 1/L$.
Minimizing only over the line segment connecting μ_k, μ^+ gives

$$\begin{aligned}
\ell(\mu_{k+1}) &\leq \min_{t \in [0,1]} \ell(\mu_k) + t\langle \nabla \ell(\mu_k)\,,\, \mu^+ - \mu_k \rangle + \frac{Lt^2}{2}\left\|\mu^+ - \mu_k\right\|_2^2 \\
&\leq \min_{t \in [0,1]} \ell(\mu_k) + t\langle \nabla \ell(\mu_k)\,,\, \mu^+ - \mu_k \rangle + \frac{t^2}{L2} R^2 \\
&= \ell(\mu_k) + \frac{1}{2LR^2}\left(\min_{\mu \in M} \langle \nabla \ell(\mu_k)\,,\, \mu - \mu_k \rangle\right)^2
\end{aligned}$$

Proof of rate to reach approximate stationary point (2)

Set $e_k = \min_{\mu \in M} \langle \nabla \ell(\mu_k)\,,\, \mu - \mu_k \rangle$ to be the distance from stationarity. We showed

$$\min_{k \leq K} e_k^2 \leq \frac{1}{K} \sum_{k=1}^{K} e_k^2 \leq \frac{2LR^2}{K} \sum_{k=1}^{K} \left(\ell(\mu_{k+1}) - \ell(\mu_k) \right) \leq \frac{\ell(\mu_0) - \ell(\mu^*)}{2LR^2 K}$$

Or

$$\min_{k \leq K} |e_k| \leq \sqrt{\frac{\ell(\mu_0) - \ell(\mu^*)}{2LR^2 K}}$$

Despite nonconvexity, there are suboptimal stationary points for policy gradient with a full policy class

If $\nu(s) > 0$ for all s the RHS is zero if and only if $J_\mu = TJ_\mu$.

Lemma: If μ^+ is a policy iteration update to μ, then

$$\frac{d}{d\gamma}\ell(\mu + \gamma(\mu^+ - \mu))\Big|_{\gamma=0} \leq -\|J_\mu - TJ_\mu\|_{1,\nu}$$

Proof: Set $\mu_\gamma = \mu + \gamma(\mu^+ - \mu)$. One can show

$$T_{\mu_\gamma} J_\mu = (1-\gamma) T_\mu J_\mu + \gamma T_{\mu^+} J_\mu = J_\mu - \gamma \left(TJ_\mu - J_\mu \right) \preceq J_\mu$$

Monotonicity implies $J_{\mu_\gamma} \preceq \cdots \preceq T_{\mu_\gamma} J_\mu \preceq J_\mu$. Hence,

$$\frac{J_{\mu_\gamma} - J_\mu}{\gamma} \preceq \frac{T_{\mu_\gamma} J_\mu - J_\mu}{\gamma} = TJ_\mu - J_\mu$$

Left multiplying by ν, and using $TJ_\mu \preceq J_\mu$

$$\frac{\ell(\mu_\gamma) - \ell(\mu)}{\gamma} \leq \|TJ_\mu - J_\mu\|_{1,\nu}$$

Taking $\gamma \to 0$ gives the result.

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Weighted policy iteration

Policy iteration is

$$\mu_{k+1} \in \operatorname*{argmin}_{\mu \in M} T_\mu J_{\mu_k},$$

where the minimization is performed elementwize. As long as $w(s) > 0$, policy iteration can be written minimizing a scalarized objective:

$$\mu_{k+1} \in \operatorname*{argmin}_{\mu \in M} w \left(T_\mu J_{\mu_k} \right)$$

Define the weighted policy iteration cost function

$$\mathcal{B}(\bar{\mu}|w, J_\mu) = w T_{\bar{\mu}} J_\mu = \sum_s w(s)(T_{\bar{\mu}} J_\mu)(s) = \sum_s w(s) Q_\mu(s, \bar{\mu}(s))$$

We will connect policy gradient to the constrained policy iteration scheme

$$\mu_{\theta_{k+1}} = \operatorname*{argmin}_{\mu_\theta \in M_\Theta} \mathcal{B}(\mu_\theta | w, J_{\mu_{\theta_k}})$$

that restricts to the parameterized policy class when minimizing.

A policy gradient formula

*Overload notation: $\mathcal{B}(\bar{\theta}|\nu, J) \equiv \mathcal{B}(\mu_\theta|\nu, J)$.,
and $\nu_\mu := \sum_{k=0}^{\infty} \alpha^k \nu P_\mu^k$.

Under appropriate smoothness conditions

$$\nabla \ell(\theta) = \nabla_{\bar{\theta}} \mathcal{B}(\bar{\theta}|\nu_{\mu_\theta}, J_{\mu_\theta})\Big|_{\bar{\theta}=\theta} = \mathbb{E}_{s\sim\nu_{\mu_\theta}}\left[\nabla_{\bar{\theta}} Q_{\mu_\theta}(s, \mu_{\bar{\theta}}(s))\Big|_{\bar{\theta}=\theta}\right]$$

Policy gradient is the iteration

$$\theta_{i+1} = \theta_i - \nabla_{\bar{\theta}} \mathcal{B}(\bar{\theta}|\nu_{\mu_{\theta_i}}, J_{\mu_{\theta_i}})\Big|_{\bar{\theta}=\theta_i}$$

This is similar to weighted PI restricted to M_Θ, except:

1. PG takes incremental gradient steps rather than solving $\min_{\bar{\theta}} \mathcal{B}(\bar{\theta}|w, J_{\mu_{\theta_i}})$ to optimality.
2. PG uses state-relevance weights $\nu_{\mu_{\theta_i}}$ induced by applying μ_{θ_i}.

Deriving the policy gradient formula

A first-order approximation to J_{μ_θ}

Under appropriate smoothness conditions

$$J_{\mu_{\bar\theta}} = J_{\mu_\theta} + (I - \alpha P_{\mu_\theta})^{-1} \left(T_{\mu_{\bar\theta}} J_{\mu_\theta} - J_{\mu_\theta}\right) + O(\|\bar\theta - \theta\|_2^2),$$

Proof Set $T_\theta \equiv T_{\mu_\theta}$, $P_\theta \equiv P_{\mu_\theta}$, $g_\theta \equiv g_{\mu_\theta}$.

By the variational form of Bellman's equation,

$$\begin{aligned} J_{\bar\theta} =& J_\theta + \left(I - \alpha P_{\bar\theta}\right)^{-1} \left(T_{\bar\theta} J_\theta - J_\theta\right) \\ =& J_\theta + \left(I - \alpha P_\theta\right)^{-1} \left(T_{\bar\theta} J_\theta - J_\theta\right) + e_\theta \end{aligned}$$

where

$$\begin{aligned} e_\theta &= \left(\left[I - \alpha P_{\bar\theta}\right]^{-1} - \left[I - \alpha P_\theta\right]^{-1}\right) \left(T_{\bar\theta} J_\theta - J_\theta\right) \\ &= \left(\left[I - \alpha P_{\bar\theta}\right]^{-1} - \left[I - \alpha P_\theta\right]^{-1}\right) \left(g_{\bar\theta} - g_\theta + \alpha \left[P_{\bar\theta} - P_\theta\right] J_\theta\right) \end{aligned}$$

is $O(\|\bar\theta - \theta\|_2^2)$ assuming $\theta \mapsto P_\theta$ and $\theta \mapsto g_\theta$ are differentiable.

Deriving the policy gradient formula (2)

Under appropriate smoothness conditions

$$J_{\mu_{\bar{\theta}}} = J_{\mu_\theta} + (I - \alpha P_{\mu_\theta})^{-1} \left(T_{\mu_{\bar{\theta}}} J_{\mu_\theta} - J_{\mu_\theta} \right) + O(\|\bar{\theta} - \theta\|_2^2),$$

Left multiplying each side by ν gives the following:

Under appropriate smoothness conditions

$$\ell(\bar{\theta}) = \ell(\theta) + \nu_{\mu_\theta} \left(T_{\mu_{\bar{\theta}}} J_{\mu_\theta} - J_{\mu_\theta} \right) + O(\|\bar{\theta} - \theta\|_2^2),$$

Differentiating with respect to $\bar{\theta}$ gives,

$$\nabla \ell(\theta) = \nabla_{\bar{\theta}} \nu_{\mu_\theta} \left(T_{\mu_{\bar{\theta}}} J_{\mu_\theta} \right) \Big|_{\bar{\theta}=\theta} = \nabla_{\bar{\theta}} \mathcal{B}(\bar{\theta} | \nu_{\mu_\theta}, J_{\mu_\theta}) \Big|_{\bar{\theta}=\theta}$$

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Main insight of Bhandari and Russo (2020)

Two conditions ensure $\ell(\cdot)$ has no suboptimal stationary points

1. The policy class is closed under policy improvement
   - A PI update to $\mu \in M_\Theta$ can be solved within the policy class:

$$\min_{\mu_\theta \in M_\Theta} \mathcal{B}(\mu_\theta | \nu, J_\mu) = \min_{\bar{\mu} \in M} \mathcal{B}(\bar{\mu} | \nu, J_\mu)$$

   - A sense in which the policy class is sufficient for control.
   - Much weaker than requiring it represents (nearly) all policies
   - Necessarily stronger than requiring $\mu^* \in M_\Theta$.

2. First order methods can solve the PI problem
   - $\theta \mapsto \mathcal{B}(\mu_\theta \mid \nu, J_\mu)$ has no suboptimal stationary points.
   - E.g. this single period objective is often convex...

Example: linear quadratic control (deterministic for this talk)

States $s_t \in \mathbb{R}^n$ and actions $a_t \in \mathbb{R}^k$

$$\text{Minimize} \quad \sum_{t=0}^{\infty} \alpha^t \left(s_t^\top R s_t + a_t^\top U a_t \right)$$

$$\text{Subject to} \quad s_t = A s_{t-1} + B a_{t-1}$$

Linear policies: $\mu_\theta(s) = \theta s$.

Total cost $\ell(\mu_\theta) = \mathbb{E}_{s_0 \sim \nu}[J_{\mu_\theta}(s_0)]$ is messy and nonconvex:

$$\begin{aligned} J_{\mu_\theta}(s_0) &= \sum_{t=0}^{\infty} \alpha^t \left(s_t^\top R s_t + s_t^\top \theta^\top U \theta s_t \right) \\ &= s_0^\top \underbrace{\left(\sum_{t=0}^{\infty} \alpha^t \left[(A + B\theta)^t \right]^\top \left(R + \theta^\top U \theta \right) \left[(A + B\theta)^t \right] \right)}_{K_\theta} s_0 \end{aligned}$$

since $s_t = A s_{t-1} + B\theta s_{t-1} = \cdots = (A + B\theta)^t s_0$

Policy iteration for LQ control –Kleinman (1968)

The policy improvement objective is quadratic in a:

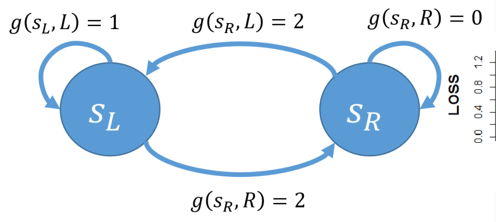
$$Q_{\mu_\theta}(s,a) = a^\top U a + \alpha(As+Ba)^\top K_\theta (As+Ba)$$

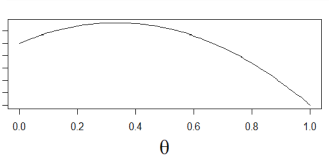
Condition 1: The policy class M_Θ is closed under PI updates?

- Yes. $\bar{\theta}s = \mathrm{argmin}_a\, Q(s,a)$ for all s
  (Updated parameter is $\bar{\theta} = \alpha\left(U + \alpha B^\top K_\theta B\right)^{-1} B^\top K_\theta A$)

Condition 2 The PI obj. has no suboptimal stationary points?

- Holds since $\bar{\theta} \mapsto \mathbb{E}_{s\sim\nu}\left[Q_{\mu_\theta}(s, \bar{\theta}s)\right]$ is quadratic





- $\mu_\theta(s_L) = \mu_\theta(S_R) = \theta =$ "Probability of Right."

The parameterized policy class is not closed

For $\theta = .1$,

$$L = \operatorname*{argmin}_{a \in \{L,R\}} Q_{\mu_\theta}(S_L, a)$$

whereas

$$R = \operatorname*{argmin}_{a \in \{L,R\}} Q_{\mu_\theta}(S_R, a)$$

Approximation with rich policy classes?

Punchline: if the policy iteration problem can be nearly solved within the policy class, then stationary points of the PG objective are nearly optimal.

Approximation with rich policy classes

- **Condition 1b**: Policy class is closed under approximate PI

$$\text{For any } \mu \in M_\Theta, \quad \min_{\mu_\theta \in M_\Theta} \mathcal{B}(\mu_\theta|\nu, J_\mu) \leq \min_{\bar{\mu} \in M} \mathcal{B}(\bar{\mu}|\nu, J_\mu) + \epsilon$$

- **Condition 2a** The PI objective has no suboptimal stationary points
  - $\theta \mapsto \mathbb{E}_{s\sim\nu}\left[Q_\mu(s, \mu_\theta(s))\right]$ has no suboptimal stationary points for any distribution ν over $\mathcal{S}$.

Theorem (Informal)

Under conditions 1b and 2a (and mild regularity conditions), if θ is a stationary point of $\ell(\cdot)$ then

$$\ell(\mu_\theta) \leq \min_{\mu \in M} \ell(\mu) + \frac{\kappa_\nu}{(1-\alpha)^2} \cdot \epsilon$$

where

$$k_\nu = \sup_{J_\mu \,:\, \mu \in M_\Theta} \frac{\|J_\mu - TJ_\mu\|_{1,\nu_{\mu^*}}}{\|J_\mu - TJ_\mu\|_{1,\nu}}$$