Nonparametric Stochastic Compositional Gradient Descent for Q-Learning in Continuous Markov Decision Problems

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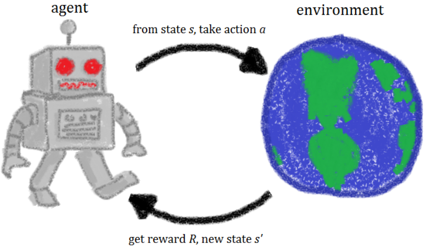
Markov Decision Problems



- At time t, agent is in state $\mathbf{s}_t$, select action $\mathbf{a}_t$.
- Transition from state $\mathbf{s}_t$ to $\mathbf{s}_{t+1}$, with $\mathbf{s}_{t+1} \sim \mathbb{P}(\cdot \mid \mathbf{s}_t, \mathbf{a}_t)$
  - Reward $r_t := r(\mathbf{s}_t, \mathbf{a}_t, \mathbf{s}_{t+1})$
- Markov Decision Process (MDP): $(\mathcal{S}, \mathcal{A}, \mathbb{P}, r, \gamma)$
  - State space $\mathcal{S}$, action space $\mathcal{A}$, discount factor $\gamma \in (0, 1)$
- Goal: find a policy $\pi \in \mathcal{S} \to \mathcal{A}$, a map from states to actions,
  - That maximizes the long-term reward accumulation

Reinforcement Learning

Goal: choose actions to maximize infinite discounted reward accumulation

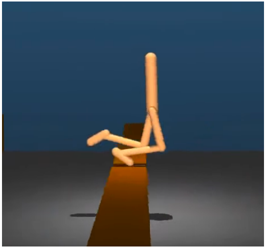
$$\max_{\{a_t\}} \sum_{t=0}^{\infty} \gamma^t r(s_t, a_t, s_{t+1})$$

Recent successes

- AlphaGo Zero (Silver, 2017)
- Bipedal walker on terrain (Heess, 2017)
- Personalized web services (Theocharous, 2015)

Remaining challenges in infinite spaces

- Reproducibility
- Lack of guarantees for function approx.



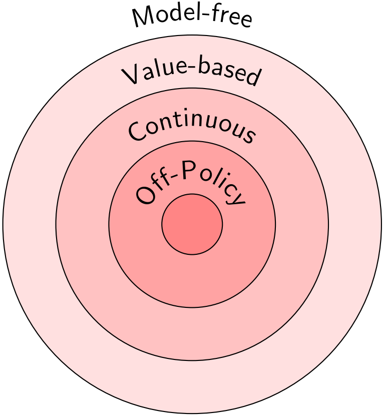
Our Approach

We develop the KQ-Learning algorithm:

- Formulate a stochastic program for off-policy Bellman loss
- Compute stochastic gradient
- Update the kernel model
- Sparsify the model

Our results provide:

- Convergence guarantees
- Experimental validation
- Low complexity solutions



Value Based Approaches

- Value function, expected reward accumulation given initial $\mathbf{s}$:
  - While following policy π

$$V^{\pi}(\mathbf{s}) := \mathbb{E}_{\mathbf{s}'}\left[\sum_{t=0}^{\infty}\gamma^{t} r(\mathbf{s}_t, \mathbf{a}_t, \mathbf{s}'_t) \mid \mathbf{s}_0 = \mathbf{s}, \mathbf{a}_t = \pi(\mathbf{s}_t)\right] \quad (1)$$

- Action-value function, the reward accumulation given initial $\mathbf{s}, \mathbf{a}$

$$Q^{\pi}(\mathbf{s}, \mathbf{a}) := \mathbb{E}_{\mathbf{s}'}\left[\sum_{t=0}^{\infty}\gamma^{t} r(\mathbf{s}_t, \mathbf{a}_t, \mathbf{s}'_t) \mid \mathbf{s}_0 = \mathbf{s}, \mathbf{a}_0 = \mathbf{a}, \mathbf{a}_t = \pi(\mathbf{s}_t)\right] \quad (2)$$

- Goal: learn the optimal action-value function
  - Satisfying the Bellman optimality equation

$$Q^{*}(\mathbf{s}, \mathbf{a}) = \mathbb{E}_{\mathbf{s}'}[r(\mathbf{s}, \mathbf{a}, \mathbf{s}') + \gamma \max_{\mathbf{a}'} Q^{*}(\mathbf{s}', \mathbf{a}') \mid \mathbf{s}_0 = \mathbf{s}, \mathbf{a}_0 = \mathbf{a}] \quad (3)$$

  - Q-learning is an off-policy approach

Guarantees for Value Based Approaches

- Tabular Q-Learning (Dayan, 1992)
  - Off-policy observations in discrete state and action spaces
  - Convergence w.p. 1 when all states, actions observed i.o.
- Policy evaluation (Tsitsiklis, 1997)
  - Continuous state space with linear function approximation
  - Convergence a.s.
- Gradient Temporal Difference (Sutton, 2009)
  - Off-policy updates with linear function approximation
  - Convergence w.p. 1
- Policy evaluation (Koppel, 2017)
  - Continuous state space with non-parametric kernel methods
  - Convergence to the Bellman fixed point w.p. 1

Optimizing Bellman Loss

- Bellman optimality equation (Bertsekas, 2004)

$$Q^*(\mathbf{s},\mathbf{a}) = \mathbb{E}_{\mathbf{s}'}[r(\mathbf{s},\mathbf{a},\mathbf{s}') + \gamma \max_{\mathbf{a}'} Q^*(\mathbf{s}',\mathbf{a}')] \tag{4}$$

- Temporal difference for an observation $(\mathbf{s}, \mathbf{a}, \mathbf{s}')$:

$$\delta := r(\mathbf{s},\mathbf{a},\mathbf{s}') + \gamma \max_{\mathbf{a}'} Q(\mathbf{s}',\mathbf{a}') - Q(\mathbf{s},\mathbf{a}) \tag{5}$$

- Define an auxiliary function for the expected temporal difference:

$$f(Q;\mathbf{s},\mathbf{a}) := \mathbb{E}_{\mathbf{s}'}\delta = \mathbb{E}_{\mathbf{s}'}\left[r(\mathbf{s},\mathbf{a},\mathbf{s}') + \gamma \max_{\mathbf{a}'} Q(\mathbf{s}',\mathbf{a}') - Q(\mathbf{s},\mathbf{a}) \,\middle|\, \mathbf{s},\mathbf{a}\right]$$

- Reformulate Bellman optimality equation as comp. stochastic prog:

$$L(Q) = \frac{1}{2}\mathbb{E}_{\mathbf{s},\mathbf{a}}\left[f^2(Q;\mathbf{s},\mathbf{a})\right]. \tag{6}$$

- Q^* is a function that satisfies $f(Q;\mathbf{s},\mathbf{a}) = 0$ for all $(\mathbf{s},\mathbf{a})$.
  - A solution to the non-convex optimization problem

Reproducing Kernel Hilbert Spaces (RKHS)

- We restrict $Q \in \mathcal{H}$, a **Reproducing Kernel Hilbert space**
- An RKHS over $\mathcal{S} \times \mathcal{A}$ is equipped with a reproducing kernel (Norkin, 2009; Argyriou, 2009)
  - An inner product-like map, $\kappa : (\mathcal{S} \times \mathcal{A}) \times (\mathcal{S} \times \mathcal{A}) \to \mathbb{R}$:

$$\text{(i)}\langle Q, \kappa((\mathbf{s}, \mathbf{a}), \cdot)\rangle_{\mathcal{H}} = Q((\mathbf{s}, \mathbf{a})), \qquad \text{(ii)}\mathcal{H} = \text{span}\{\kappa((\mathbf{s}, \mathbf{a}), \cdot)\} \quad (7)$$

- A continuous function over a compact set may be approx. uniformly
  - In an RKHS equipped with a universal kernel (Michelli, 2006)
- We solve the regularized problem:

$$Q^* = \arg\min_{Q \in \mathcal{H}} J(Q) = \arg\min_{Q \in \mathcal{H}} L(Q) + \frac{\lambda}{2}\|Q\|^2_{\mathcal{H}}. \qquad (8)$$

- Goal: optimize $J(Q)$ over $\mathcal{H}$ given samples $(\mathbf{s}_t, \mathbf{a}_t, r_t, \mathbf{s}'_t)$
- First, differentiate $J(Q)$ w.r.t. Q. (Koppel, 2017)

$$\nabla_Q J(Q_t) = \mathbb{E}_{\mathbf{s}_t, \mathbf{a}_t}\Big[f(Q_t; \mathbf{s}_t, \mathbf{a}_t) \times \nabla_Q f(Q_t; \mathbf{s}_t, \mathbf{a}_t)\Big] + \lambda Q_t. \tag{9}$$

- Stoch. grad. unusuable since $\nabla_Q J(Q)$ has two expectations
- *Coupled* descent: estimate both terms in product-of-expectations
- Construct total mean of $\hat{\nabla}_Q f = [\gamma\kappa((\mathbf{s}'_t, \mathbf{a}'_t), \cdot) - \kappa((\mathbf{s}_t, \mathbf{a}_t), \cdot)]$?
  - Infinite complexity!
- Instead: build up expectation of scalar temporal difference δ

Stochastic Quasi-Gradient

- Goal: extend gradient temporal diff. (Sutton, 2009) to infinite MDPs
- Define a scalar fixed pt. recursion z_t to estimate average TD $\bar{\delta}$

$$\delta_t = r(\mathbf{s}_t, \mathbf{a}_t, \mathbf{s}') + \gamma \max_{a'} Q(\mathbf{s}'_t, \mathbf{a}') - Q_t(\mathbf{s}_t, \mathbf{a}_t),$$
$$z_{t+1} = (1 - \beta_t) z_t + \beta_t \delta_t$$

- $\delta_t \Rightarrow$ temporal difference; $\beta_t \in (0, 1) \Rightarrow$ step-size.
- $\mathbf{a}'_t = \arg\max_{\mathbf{a}'} Q(\mathbf{s}'_t, \mathbf{a}')$ can be replaced with a softmax
  - In practice, evaluated via simulated annealing
- Stoch. descent step: replace 1st term in expectation w/ estimate
  - $[\gamma\kappa((\mathbf{s}'_t, \mathbf{a}'_t), \cdot) - \kappa((\mathbf{s}_t, \mathbf{a}_t), \cdot)]$, evaluated at $(\mathbf{s}_t, \mathbf{a}_t, \mathbf{s}'_t, \mathbf{a}'_t)$
  - replace δ_t by $z_{t+1} \Rightarrow$ stoch. quasi-gradient (Ermoliev '83)

$$\hat{Q}_{t+1} = (1 - \alpha_t \lambda) \hat{Q}_t - \alpha_t z_{t+1} \left[\gamma\kappa((\mathbf{s}'_t, \mathbf{a}'_t), \cdot) - \kappa((\mathbf{s}_t, \mathbf{a}_t), \cdot)\right]$$

  - α_t is a second step-size

RKHS Parameterization

- If $Q_0 = 0 \in \mathcal{H}$, inductively applying Representer Thm. yields

$$Q_t(\mathbf{s},\mathbf{a}) = \sum_{n=1}^{2(t-1)} w_n \kappa((\mathbf{s}_n,\mathbf{a}_n),(\mathbf{s},\mathbf{a})) = \mathbf{w}_t{}^T \kappa_{\mathbf{X}_t}((\mathbf{s},\mathbf{a})) \qquad (10)$$

$$\begin{aligned} \mathbf{w}_t &= [w_1,\ldots,w_{2(t-1)}] \,, \\ \mathbf{X}_t &= [(\mathbf{s}_1,\mathbf{a}_1),(\mathbf{s}'_1,\mathbf{a}'_1),\ldots,(\mathbf{s}_{t-1},\mathbf{a}_{t-1}),(\mathbf{s}'_{t-1},\mathbf{a}'_{t-1})], \end{aligned} \qquad (11)$$

- Kernel expansion + together with FSQG $\Rightarrow$ parametric updates:

$$\begin{aligned} \mathbf{X}_{t+1} &= [\mathbf{X}_t,(\mathbf{s}_t,\mathbf{a}_t),(\mathbf{s}_t{}',\mathbf{a}_t{}')] \,, \\ \mathbf{w}_{t+1} &= [(1-\alpha_t\lambda)\mathbf{w}_t, \alpha_t z_{t+1}, -\alpha_t\gamma z_{t+1}] \end{aligned} \qquad (12)$$

- Intractable complexity intrinsic to RKHS optimization: $M_t = \mathcal{O}(t)$
- Solve via Kernel Orthogonal Matching Pursuit (KOMP) (Koppel, 2016)

KQ-Learning Algorithm

Require: $\{\mathbf{s}_t, \mathbf{a}_t, \mathbf{s}'_t, \alpha_t, \beta_t, \epsilon_t\}_{t=0,1,2,\ldots}$

initialize $Q_0(\cdot) = 0, \mathbf{D}_0 = [], \mathbf{w}_0 = [], z_0 = 0$

for $t = 0, 1, 2, \ldots$ **do**

Obtain trajectory realization $(\mathbf{s}_t, \mathbf{a}_t, \mathbf{s}'_t)$

Evaluate instantaneous maximizing action $\mathbf{a}'_t = \arg\max_{\mathbf{a}'} Q(\mathbf{s}'_t, \mathbf{a}')$

Compute temporal difference

$\delta_t = r(\mathbf{s}_t, \mathbf{a}_t, \mathbf{s}'_t) + \gamma \max_{\mathbf{a}'} Q_t(\mathbf{s}_t, \mathbf{a}') - Q_t(\mathbf{s}_t, \mathbf{a}_t)$

Update auxiliary sequence $z_{t+1} = (1 - \beta_t) z_t + \beta_t \delta_t$

Compute functional stochastic quasi-gradient step

$$\hat{Q}_{t+1}(\cdot) = (1 - \alpha_t \lambda) Q_t(\cdot) - \alpha_t z_{t+1} [\gamma \kappa((\mathbf{s}'_t, \mathbf{a}'_t), \cdot) - \kappa((\mathbf{s}_t, \mathbf{a}_t), \cdot)]$$

Revise dictionary $\hat{\mathbf{D}}_{t+1} = [\mathbf{D}_t, (\mathbf{s}_t, \mathbf{a}_t), (\mathbf{s}'_t, \mathbf{a}'_t)]$,

and weights $\hat{\mathbf{w}}_{t+1} = [(1 - \alpha_t \lambda) \mathbf{w}_t, \;\; \alpha_t z_{t+1}, -\alpha_t \gamma z_{t+1}]$

Project function $(Q_{t+1}, \mathbf{D}_{t+1}, \mathbf{w}_{t+1}) = \textbf{KOMP}(\hat{Q}_{t+1}, \hat{\mathbf{D}}_{t+1}, \hat{\mathbf{w}}_{t+1}, \epsilon_t)$

end for

Convergence w.p. 1 for Decreasing Step Sizes

Theorem

Consider the sequence z_t and $\{Q_t\}$ as stated in the KQ-Learning algorithm. Assume the regularizer is positive $\lambda > 0$, Assumptions 15-19 hold, and the step-size conditions hold, with $C > 0$ a positive constant:

$$\sum_{t=1}^{\infty} \alpha_t = \infty, \sum_{t=1}^{\infty} \beta_t = \infty, \sum_{t=1}^{\infty} \alpha_t^2 + \beta_t^2 + \frac{\alpha_t^2}{\beta_t} < \infty, \epsilon_t = C\alpha_t^2 \qquad (13)$$

Then $\|\nabla_Q J(Q)\|_{\mathcal{H}}$ **converges to null with probability 1***, and Q_t attains a stationary point of (8).*

- *The limit of Q_t achieves a Bellman fixed point in the RKHS.*
- *Proof uses existing results for compositional stochastic gradient descent (Wang, 2017)*

Convergence for Constant Step Sizes

Theorem

Consider the sequence z_t and $\{Q_t\}$ as stated in the KQ-Learning algorithm. Assume the regularizer is positive $\lambda > 0$, Assumptions 15-19 hold, and the step-sizes are chosen as constant such that $0 < \alpha < \beta < 1$, with $\epsilon = C\alpha^2$ and the parsimony constant $C > 0$ is positive.
Then **Bellman error converges to a neighborhood in expectation***:*

$$\liminf_{t\to\infty} \mathbb{E}[J(Q_t)] \leq \mathcal{O}\left(\frac{\alpha\beta}{\beta-\alpha}\left[1+\sqrt{1+\frac{\beta-\alpha}{\alpha\beta}\left(\frac{1}{\beta}+\frac{\beta^2}{\alpha^2}\right)}\right]\right) \quad (14)$$

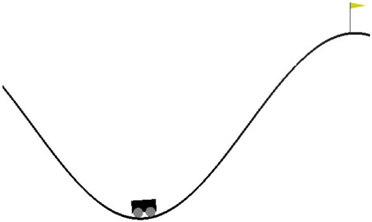
Summary of Results

	Diminishing	Constant
Learning rate	$\sum_{t=1}^{\infty} \alpha_t^2 + \beta_t^2 + \frac{\alpha_t^2}{\beta_t} < \infty$	$0 < \alpha < \beta < 1$
Compression	$\epsilon_t = \mathcal{O}(\alpha_t^2)$	$\epsilon = \mathcal{O}(\alpha^2)$
Regularization	$0 < \lambda$	$0 < \lambda$
Convergence	$\|\nabla_Q J(Q_t)\|_{\mathcal{H}} \to 0$ a.s.	$\liminf_t \mathbb{E}[J(Q_t)] = R(\alpha, \beta)$
Model Order	Infinite	Finite

- $R(\alpha, \beta) = \mathcal{O}\left(\frac{\alpha\beta}{\beta-\alpha}\left[1+\sqrt{1+\frac{\beta-\alpha}{\alpha\beta}\left(\frac{1}{\beta}+\frac{\beta^2}{\alpha^2}\right)}\right]\right)$
- Exact solution requires infinite memory
- **Approximate, but accurate solution with finite memory**

Continuous Mountain Car

- Open AI Gym benchmark problem
- State is 2-dimensional: position and velocity
- Action is 1-dimensional: force within a continuous interval $[-1, 1]$
- Reward is 100 at goal position, and $-0.1a^2$ for actions a



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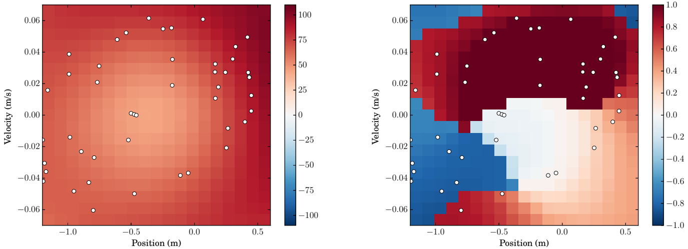
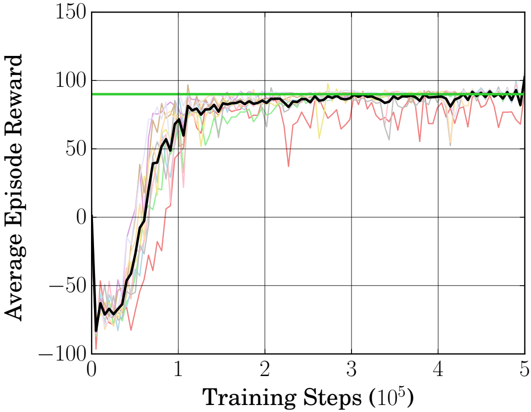


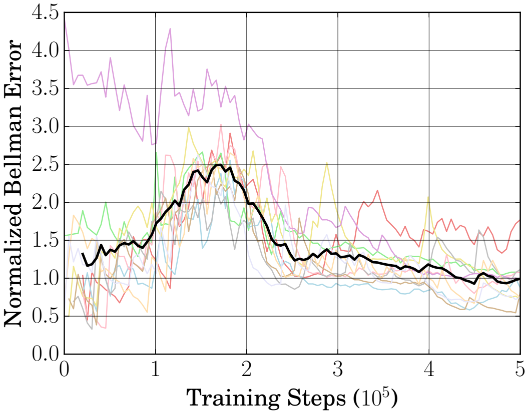
- Visualization of the learned value function and policy
  - Grid color - value,policy
  - White circles - kernel dictionary elements

Continuous Mountain Car



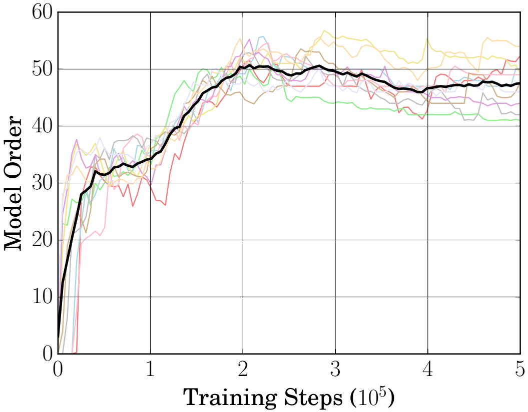
- Reward above 90 (green line) is considered solved

Continuous Mountain Car



- Corroborated by Q function converging to stationarity
- Bellman error $J(Q)$ normalized by $\|Q\|_{\mathcal{H}}$

Continuous Mountain Car



- This is done with an automatic sparse parameterization of Q
  - Directly in a continuous space
  - Model order stabilizes between 45-55

Conclusions

- Contributions
  - KQ-learning approach using non-parametric RKHS representations
  - Convergence guarantees for the KQ-Learning algorithm
- Demonstration on the Mountain Car benchmark problem
  - High reproducibility of results
  - Low complexity of solutions
- Future work
  - Applications in higher-dimensional problems
  - Robotics applications
  - Policy and actor-critic based approaches

Thank you!

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Technical Setting for KQ-Learning

- The state space $\mathcal{S} \subset \mathbb{R}^p$ and action space $\mathcal{A} \subset \mathbb{R}^q$ are compact.
- The reproducing kernel map is **bounded**:

$$\sup_{\mathbf{s} \in \mathcal{S}, \mathbf{a} \in \mathcal{A}} \sqrt{\kappa((\mathbf{s}, \mathbf{a}), (\mathbf{s}, \mathbf{a}))} = S < \infty \tag{15}$$

- The temporal difference δ and z satisfy, for $\bar{\delta} = \mathbb{E}[\delta | \mathbf{s}, \mathbf{a}]$,

$$\mathbb{E}[\delta | \mathbf{s}, \mathbf{a}] = \bar{\delta}, \ \ \mathbb{E}[(\delta - \bar{\delta})^2] \leq \sigma_\delta^2, \ \ \ \mathbb{E}[z^2 | \mathbf{s}, \mathbf{a}] \leq G_\delta^2 \tag{16}$$

- The quasi-gradient is an **unbiased estimate** for $\nabla_Q J(Q)$:

$$\mathbb{E}[(\gamma \kappa((\mathbf{s}_t', \mathbf{a}_t'), \cdot) - \kappa((\mathbf{s}_t, \mathbf{a}_t), \cdot))\bar{\delta}] = \nabla_Q J(Q) \tag{17}$$

- The difference of reproducing kernels has **finite cond. variance**:

$$\mathbb{E}[\| \gamma \kappa((\mathbf{s}_t', \mathbf{a}_t'), \cdot) - \kappa((\mathbf{s}_t, \mathbf{a}_t), \cdot) \|_{\mathcal{H}}^2 | \mathcal{F}_t] \leq G_Q^2 \tag{18}$$

- The projected functional gradient has **finite cond. 2$^{\text{nd}}$ moments**:

$$\mathbb{E}[\| \tilde{\nabla}_Q J(Q_t z_{t+1}; \mathbf{s}_t, \mathbf{a}_t, \mathbf{s}_t') \|_{\mathcal{H}}^2 \mid \mathcal{F}_t] \leq \sigma_Q^2 \tag{19}$$