Hilbert Space Embeddings of POMDPs
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## Conditional Embedding Operators \& Kernel Bayes' Rule (KBR):

Let $\mathcal{H}_{\mathcal{X}}$ and $\mathcal{H}_{\mathcal{Y}}$ be RKHSs associated with $k_{\mathcal{X}}$ and $k_{\mathcal{Y}}$ over $\left(\mathcal{X}, \mathcal{B}_{\mathcal{X}}\right)$ and $\left(\mathcal{Y}, \mathcal{B}_{\mathcal{Y}}\right)$, respectively. Let $(X, Y)$ be a random variable taking values on $\mathcal{X} \times \mathcal{Y}$ with distribution $P$ and the density $p(x, y)$. The conditional density functions $\{p(Y \mid X=x) \mid x \in \mathcal{X}\}$ define a family of embeddings $\left\{\mu_{Y \mid x}\right\}$ in $\mathcal{H} \mathcal{Y}$. A mapping from $k_{\mathcal{X}}(x, \cdot) \in \mathcal{H}_{\mathcal{X}}$ to $\mu_{Y \mid x} \in \mathcal{H}_{\mathcal{Y}}$ for all $x \in \mathcal{X}$ can be characterized by conditional embedding operator $\mathcal{U}_{Y \mid X}: \mathcal{H}_{\mathcal{X}} \rightarrow \mathcal{H}_{\mathcal{Y}}$,

$$
\begin{equation*}
\mu_{Y \mid x}=\mathcal{U}_{Y \mid X} k_{\mathcal{X}}(x, \cdot)=C_{Y X} C_{X X}^{-1} k_{\mathcal{X}}(x, \cdot), \tag{2}
\end{equation*}
$$

where $C_{Y X}$ and $C_{X X}$ are uncentred covariance operators with respect to $P$ [?].
Since a posterior distribution is a conditional distribution, the embedding of a posterior can be expressed as a conditional embedding operator [?]. Let $\Pi$ be a prior distribution with density $\pi(x)$, and embedding of a posterior $q(\bar{X} \mid \bar{Y}=y)$ given $y$ is expressed by a conditional embedding operator $\mathcal{U}$

$$
\begin{equation*}
\mu_{\bar{X} \mid y}=\mathcal{U}_{\bar{X} \mid \bar{Y}} k_{\mathcal{Y}}(y, \cdot)=C_{\bar{X} \bar{Y}} C_{\bar{Y} \bar{Y}}^{-1} k_{\mathcal{Y}}(y, \cdot \cdot), \tag{3}
\end{equation*}
$$

## where $C_{\bar{X} \bar{Y}}$ and $C_{\bar{Y} \bar{Y}}$ are covariance operators with respect to $Q$.

## 3 Kernel POMDP (kPOMDP)

### 3.1 Kernel Bellman Equations (KBEs)

Let mean embeddings of relevant distributions $b(S), P\left(S^{\prime} \mid a ; b\right), P\left(O^{\prime} \mid a ; b\right), b^{a, o^{\prime}}\left(S^{\prime}\right)$ in the corresponding RKHSs $\mathcal{H}_{\mathcal{S}}, \mathcal{H}_{\mathcal{O}}$ be

$$
\begin{aligned}
& \mu_{S}=\mathbb{E}_{S \sim b(\cdot) \cdot(\varphi(S)],} \quad \quad \mu_{S^{\prime} \mid a ; \mu_{S}}=\mathbb{E}_{S^{\prime} \sim p(\cdot \mid a ; b)}\left[\varphi\left(S^{\prime}\right)\right], \\
& \mu_{O^{\prime} \mid a ; \mu_{S}}=\mathbb{E}_{O^{\prime} \sim(\cdot|\cdot| a ; b)}\left[\phi\left(O^{\prime}\right)\right], \quad \mu_{S^{\prime}}^{a, o^{\prime}}=\mathbb{E}_{S^{\prime} \sim \sigma^{a, o^{\prime}}(\cdot) \cdot}\left[\varphi\left(S^{\prime}\right)\right] .
\end{aligned}
$$

Let $\mathcal{U}_{S^{\prime} \mid S, A}$ and $\mathcal{U}_{O \mid S}$ be conditional embedding operators for transition model $T$ and observation model $Z$, respectively, $\mathcal{U}_{\bar{S} \mid O}^{\left(a, \mu_{S}\right)}$ be a posterior embedding operator with a prior embedding $\mu_{S^{\prime} \mid a ; \mathcal{S}_{S}}$, corresponding to eq.(3). These embedding operators yield relations
$\mu_{S^{\prime} \mid a ; \mu_{S}}=\mathcal{U}_{S^{\prime} \mid S, A} \mu_{S} \otimes k_{A}(a, \cdot), \mu_{O^{\prime} a ; \mu_{S}}=\mathcal{U}_{O \mid S} \mu_{S^{\prime} \mid a ; \mu_{S}}, \mu_{S^{\prime}}^{a, o^{\prime}}=\mathcal{U}_{\bar{S} \mid O}^{\left(a, \mu_{S}\right)} k_{O}\left(o^{\prime}, \cdot\right)$. Let $\mathcal{P}_{\mathcal{S}}$ be the set of beliefs and $\mathcal{I}_{\mathcal{S}}$ be the set of embeddings of $\mathcal{P}_{\mathcal{S}}$ in $\mathcal{H}_{\mathcal{S}}$.
Claim 1. Let $R(\cdot, a) \in \mathcal{H}_{\mathcal{S}}$ and $V^{*}\left(\mu_{S^{\prime}}^{a, \cdot(\cdot)}\right) \in \mathcal{H}_{\mathcal{O}}$ for all $a \in \mathcal{A}$ and $\mu_{S} \in \mathcal{I}_{\mathcal{S}}$. The kernel Bellman optimality equations on $R K H S \mathcal{H}_{\mathcal{S}}$ may be

$$
\begin{aligned}
V^{*}\left(\mu_{S}\right) & =\max _{a \in \mathcal{A}} Q^{*}\left(\mu_{S}, a\right), \quad \pi^{*}\left(\mu_{S}\right)=\underset{a \in \mathcal{A}}{\arg \max } Q^{*}\left(\mu_{S}, a\right) \\
Q^{*}\left(\mu_{S}, a\right) & =\left\langle\mu_{S}, R(\cdot, a)\right\rangle_{\mathcal{H}_{s}}+\gamma\left\langle\mu_{O^{\prime} \mid a ; \mu_{S}}, V^{*}\left(\mu_{S^{\prime}}^{a,()}\right)\right\rangle_{\mathcal{H}_{o}}
\end{aligned}
$$

## Empirical Expression

Training samples are a set of $D_{n}=\left\{\left(\tilde{s}_{i}, \tilde{o}_{i}\right), \tilde{a}_{i}, \tilde{R}_{i},\left(\tilde{s}_{i}^{\prime}, \tilde{o}_{i}^{\prime}\right)\right\}_{i=1}^{n}$ according to a POMDP. We assume Traning samples are a set of $D_{n}=\left\{\left(\tilde{s}_{i}, o_{i}\right), a_{i}, \tilde{R}_{i},\left(s_{i}, o_{i}\right)\right\}_{i=1}$ according to a POMDP. We ass
that the true state samples $\left\{\left\{\tilde{s}_{i}, \tilde{s}_{i}^{\prime}\right)\right\}$ are available for training, but not during the test phase. Belief Embedding Update Rule:
Empirical estimates $\hat{\mu}_{S}, \hat{\mu}_{O^{\prime}\left(a ; \hat{\mu}_{S}\right.}, \hat{\mu}_{S^{\prime}}^{a, o^{\prime}}$ take respective forms $\hat{\mu}_{S}=\Upsilon \boldsymbol{\alpha}, \hat{\mu}_{O^{\prime} \mid a ; \mu_{S}}=\Phi \boldsymbol{\beta}_{a ; \boldsymbol{\alpha}}^{\prime}, \mu_{S^{\prime}}^{a, o^{\prime}}=$
 matrix

$$
\begin{equation*}
L_{O \mid S, a}=\left(G_{S}+\varepsilon_{S} n I_{n}\right)^{-1} G_{S S^{\prime}}\left(G_{(S, A)}+\varepsilon_{(S, A)} n I_{n}\right)^{-1} G_{(S, A)(S, a)} \tag{5}
\end{equation*}
$$

with $G_{S S^{\prime}}:=\Upsilon^{\top} \Upsilon^{\prime}, G_{(S, A)(S, a)}:=D\left(\mathbf{k}_{A}(a)\right) G_{S,}$, and $\mathbf{k}_{A}(a)=\Psi^{\top} \psi(a)$. Update rule $\boldsymbol{\beta}_{a ; \boldsymbol{\alpha}}^{\prime} \mapsto \boldsymbol{\alpha}_{a, o^{\prime}}^{\prime}$ is a transformation $\boldsymbol{\alpha}_{a, \prime^{\prime}}^{\prime}=R_{S \mid O}\left(\hat{\boldsymbol{\beta}}_{a ; \alpha}^{\prime}\right) \mathbf{k} O\left(o^{\prime}\right)$ with a non-negative vector $\hat{\boldsymbol{\beta}}_{a ; \boldsymbol{\alpha}}^{\prime}$ and $n \times n$ matrix

$$
R_{S \mid O}\left(\hat{\boldsymbol{\beta}}_{a ; \boldsymbol{\alpha}}^{\prime}\right)=\left(D\left(\hat{\boldsymbol{\beta}}_{a ; \boldsymbol{\alpha}}^{\prime}\right) G_{O}+\epsilon n I_{n}\right)^{-1} D\left(\hat{\boldsymbol{\beta}}_{a ; \boldsymbol{\alpha}}^{\prime}\right) .
$$

Claim 2. Given samples $D_{n}$, the empirical expression of the kernel Bellman optimality equation (Claim 1) is
$\hat{V}^{*}(\boldsymbol{\alpha})=\max _{a \in \mathcal{A}} \hat{Q}^{*}(\boldsymbol{\alpha}, a), \hat{\pi}^{*}(\boldsymbol{\alpha})=\underset{a \in \mathcal{A}}{\arg \max } \hat{Q}^{*}(\boldsymbol{\alpha}, a), \hat{Q}^{*}(\boldsymbol{\alpha}, a)=\boldsymbol{\alpha}^{\top} \boldsymbol{R}_{a}+\gamma \boldsymbol{\beta}_{a ; \boldsymbol{\alpha}}^{\top} \mathrm{V}^{*}\left(\boldsymbol{\alpha}_{a, \mathcal{O}_{0}}^{\prime}\right)$,
where $\mathbf{R}_{a}=\left(R\left(\tilde{s}_{1}, a\right), \ldots, R\left(\tilde{s}_{n}, a\right)\right)^{\top} \in \mathbb{R}^{n}$ is the reward vector on samples $\mathcal{S}_{0}$ for action a and
$\hat{\mathbf{V}}^{*}$
samples
$\left.\mathcal{O}_{a, 0, \mathcal{O}_{0}}^{\prime}\right)=\left(\hat{V}^{*}\left(\boldsymbol{\alpha}_{a, \tilde{0}_{1}}^{\prime}\right), \ldots, \hat{V}^{*}\left(\boldsymbol{\alpha}_{a, \tilde{n}_{n}}^{\prime}\right)\right)^{\top} \in \mathbb{R}^{n}$ is the posterior belief value vector on
Kernel Value Iteration Algorithm:
$\hat{V}_{d}=\hat{H}_{n} \hat{V}_{d-1}(d \geq 1)$, where $\hat{H}_{n}$ is the kernel Bellman operator

$$
\begin{equation*}
\left(\hat{H}_{n} V\right)(\boldsymbol{\alpha})=\max _{a \in \mathcal{A}}\left[\boldsymbol{\alpha}^{\top} \boldsymbol{R}_{a}+\gamma \boldsymbol{\beta}_{a ; \boldsymbol{\alpha}}^{\top} \mathbf{V}\left(\boldsymbol{\alpha}_{a, \mathcal{O}_{0}}^{\prime}\right)\right] . \tag{7}
\end{equation*}
$$

$\hat{H}_{n}$ can be enforced to be isotonic and contractive by replacing above weight vectors with probability vectors $\hat{\boldsymbol{\alpha}}, \widehat{\boldsymbol{\beta}}_{a ; \boldsymbol{\alpha}}^{\prime}, \hat{\boldsymbol{\alpha}}_{a, o^{\prime}}^{\prime}$ as $\hat{w}_{i}=\frac{\max \left\{\left\{{ }^{2}, 0,\right\}\right.}{\sum_{i=1}^{m} \max \left\{w_{i}, 0\right\}}$ for weights $\boldsymbol{w}$, proposed in [?].
5 Experiments
5.1 Sets $\mathcal{S}, \mathcal{O}, \mathcal{A}$ are Finite

$10 \times 10$ Gridworld (naive extension of $4 \times 4$ Gridworld), Network, and Hallway 1 benchmark problems from left to right. Plots are averaged discounted sum of rewards earned in test experiments (vertical) against the number of training samples $n$ (horizontal). Training samples are collected by uniform random actions. Parameters are within the title $(\gamma, \mathrm{S}, \mathrm{A}, \mathrm{O}, \mathrm{I}, \mathrm{N})=(\gamma,|\mathcal{S},| \mathcal{A}, \mathcal{O}, \mathcal{I}, ~ N)$,
where $T$ and $N$ indicates that one episode consists of $T$ steps and results are averaged over $N$ trials. kPOMDP are compared with hitogram methods, in which transition and observation matrices are naively estimated by histograms.

### 5.2 Sets $\mathcal{S}, \mathcal{O}$ are Euclidian spaces $\mathbb{R}^{d}$



An inverted pendulum problem, where hidden state $s$ is angular and angular velocity $(\theta, \dot{\theta})$, and angular $\theta$ is only observed. All the points (colored by RGBY) in the three 3D plots indicate training samples on hidden states $\mathcal{S}$, and $z$ axis indicates beief embedding weights $\boldsymbol{\alpha}$ on their samples (after
normalization). The true hidden state is marked by the black point in each 3D plot. Since $\dot{\theta}$ is normalization). The true hidden state is marked by the black point in each 3D plot. Since $\dot{\theta}$ is
uncertain at the initial point, positive weights spread in the direction of $\dot{\theta}$ axis in the middle 3D figure. uncertain at the initial point, positive weights spread in the direction of $\theta$ axis in the middle 3D figure.
The left and right 3D figures show that $\dot{\theta}$ is well estimated by the kPOMDPs dynamics for both of executed actions $a_{1}$ and $a_{2}$.

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Mean Embedding: The mean embedding of distribution $P$ in $\mathcal{H}_{\mathcal{X}}$ is the mean features of $P$, i.e., the RKHS element $\mu_{X}=\mathbb{E}_{X \sim P}\left[k_{\mathcal{\chi}}(X, \cdot)\right] . \quad\left\langle\mu_{X}, f\right\rangle_{\mathcal{H}_{X}}=\mathbb{E}_{X \sim P}[f(X)]$ holds for all $f \in \mathcal{H} \mathcal{H}$. Empirical estimate $\hat{\mu}_{X}$ has a form $\hat{\mu}_{X}=\Upsilon \boldsymbol{\Upsilon} \boldsymbol{\alpha}$, where $\Upsilon=\left(k_{\mathcal{X}}\left(\cdot, X_{1}\right), \ldots, k_{\mathcal{X}}\left(\cdot, X_{n}\right)\right)$ is a feature matrix and nonparametrically estimated by $\left\langle\hat{\mu}_{X}, f\right\rangle_{\mathcal{H}_{x}}=\boldsymbol{\alpha}^{\top} \mathbf{f}$, where $\mathbf{f}=\left(f\left(X_{1}\right), \ldots, f\left(X_{n}\right)\right)^{\top}$ is the sample vector of $f$.

