Kernel Bayesian Inference with Posterior Regularization

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1. Introduction

Observations:

- Kernel methods can be used to embed a distribution to a Hilbert space and probability rules can be replaced by corresponding linear operators
- The kernel embedding of a conditional distribution has an optimizational formulation
- The posterior distribution in Bayes' rule has an optimizational formulation

Does the kernel embedding of a posterior distribution have an optimizational formulation?

Contributions:

- A theoretically justified affirmative answer to the question
- A simpler but faster regularization technique called thresholding regularization
- Posterior regularization for kernel Bayesian inference called kRegBayes, analogous to RegBayes

2. Preliminaries

Kernel embedding:

$$p_X \mapsto \mathbb{E}_{p_X}[\phi(X)] =: \mu_X \in \mathcal{H}_\mathcal{X},$$

where $\phi(X) := k(X, \cdot)$. (i) When p_X is a conditional distribution, μ_X is called *conditional embedding*. (ii) When p_X is a posterior distribution in a Bayesian setting, μ_X is called *posterior embedding*.

Optimizationl formulation of conditional embedding

$$\mu_{Y|X} = \arg\inf_\mu \mathcal{E}_s[\mu] = \arg\inf_\mu \mathbb{E}_{(X,Y)}[\|\psi(Y) - \mu(X)\|^2_{\mathcal{H}_\mathcal{Y}}]$$

Given i.i.d. samples $\{(x_1, y_1), \cdots, (x_n, y_n)\}$ from $p(X, Y)$, the *estimator* is

$$\widehat{\mathcal{E}}_s[\mu] = \frac{1}{n} \|\psi(y_i) - \mu(x_i)\|^2_{\mathcal{H}_\mathcal{Y}}$$

Optimizational formulation of posterior distribution

$$p(Y \mid X = x) = \arg\min_{q(Y)} \left\{ \mathrm{KL}(q(Y)\|\pi(Y)) - \int \log p(X = x \mid Y) dq(Y) \right\} \quad s.t. \quad q(Y) \in \mathcal{P}_{\text{prob}}$$

Posterior regularization for Bayesian inferece (RegBayes)

$$\min_{q(Y),\xi} \left\{ \mathrm{KL}(q(Y)\|\pi(Y)) - \int \log p(X = x \mid Y) dq(Y) + U(\xi) \right\} \quad s.t. \quad q(Y) \in \mathcal{P}_{\text{prob}}(\xi)$$

3. Posterior Embedding as a Regressor

Let $\pi(Y)$ be the prior, $p(X \mid Y)$ be the likelihood, $p^\pi(X, Y)$ be the joint distribution and suppose we have samples to directly estimate $\pi(Y)$ and $p(X \mid Y)$. The posterior embedding $\mu^\pi_{Y|X}$ is the same as conditional embedding

$$\mu^\pi_{Y|X} = \arg\inf_\mu \mathcal{E}_s[\mu] = \arg\inf_\mu \mathbb{E}_{(X,Y)}[\|\psi(Y) - \mu(X)\|^2_{\mathcal{H}_\mathcal{Y}}]$$

How to get a reasonable estimator of $\mathcal{E}_s$ when we do not have i.i.d. samples from $p^\pi(X, Y)$?

Assuming $f(x, y) = \|\psi(y) - \mu(x)\|^2_{\mathcal{H}_\mathcal{Y}} \in \mathcal{H}_\mathcal{X} \otimes \mathcal{H}_\mathcal{Y}$, we have

$$\mathcal{E}_s[\mu] = \mathbb{E}_{(X,Y)}[\|\psi(Y) - \mu(X)\|^2_{\mathcal{H}_\mathcal{Y}}] = \langle f, \mu_{(X,Y)} \rangle_{\mathcal{H}_\mathcal{X} \otimes \mathcal{H}_\mathcal{Y}}$$

We show in the paper that $\mu_{(X,Y)}$ can be estimated by $\sum_{i=1}^n \beta_i \psi(Y_i) \otimes \phi(X_i)$.

Theorem 1 (Proof in Appendix)**.** *Under some conditions (details in paper), we have the following consistent estimator of $\mathcal{E}_s[\mu]$:*

$$\widehat{\mathcal{E}}_s[\mu] = \sum_{i=1}^n \beta_i \|\psi(y_i) - \mu(x_i)\|^2_{\mathcal{H}_\mathcal{Y}},$$

where $\boldsymbol{\beta} = (\beta_1, \cdots, \beta_n)^\intercal$ is given by $\boldsymbol{\beta} = (G_Y + n\lambda I)^{-1} \tilde{G}_Y \tilde{\boldsymbol{\alpha}}$, where $(G_Y)_{ij} = k_\mathcal{Y}(y_i, y_j)$, $(\tilde{G}_Y)_{ij} = k_\mathcal{Y}(y_i, \tilde{y}_j)$, and $\tilde{\boldsymbol{\alpha}} = (\tilde{\alpha}_1, \cdots, \tilde{\alpha}_l)^\intercal$.

What if some β_i's are negative and $\widehat{\mathcal{E}}_s[\mu]$ has no minima?

Under some conditions, $\widehat{\mathcal{E}}^+_s[\mu] = \sum_{i=1}^n \beta^+_i \|\psi(y_i) - \mu(x_i)\|^2_{\mathcal{H}_\mathcal{Y}}$, where $\beta^+_i = \max(0, \beta_i)$ is also consistent. This is called *thresholding regularization*.

Finally, we can establish the consistency of $\widehat{\mu}_{\lambda,n} = \arg\inf_\mu \widehat{\mathcal{E}}_{\lambda,n}[\mu]$, where

$$\widehat{\mathcal{E}}_{\lambda,n}[\mu] = \sum_{i=1}^n \beta^+_i \|\psi(y_i) - \mu(x_i)\|^2_{\mathcal{H}_\mathcal{Y}} + \lambda \|\mu\|^2_{\mathcal{H}_K}.$$

4. kRegBayes

$$\mathcal{L} := \underbrace{\sum_{i=1}^m \beta^+_i \|\mu(x_i) - \psi(y_i)\|^2_{\mathcal{H}_\mathcal{Y}} + \lambda \|\mu\|^2_{\mathcal{H}_K}}_{\widehat{\mathcal{E}}_{\lambda,n}[\mu]} + \delta \underbrace{\sum_{i=m+1}^n \|\mu(x_i) - \psi(t_i)\|^2_{\mathcal{H}_\mathcal{Y}}}_{\text{The regularization term}},$$

where $\{(x_i, y_i)\}_{i=1}^m$ is the sample used for *representing likelihood*, $\{(x_i, t_i)\}_{i=m+1}^n$ is the sample used for nonparametric *posterior regularization*. $\psi(t_i)$ is the kernel embedding of $\delta(Y = t_i)$ and encourages $p(Y \mid X = x_i)$ to be close to $\delta(Y = t_i)$.

5. Experiments

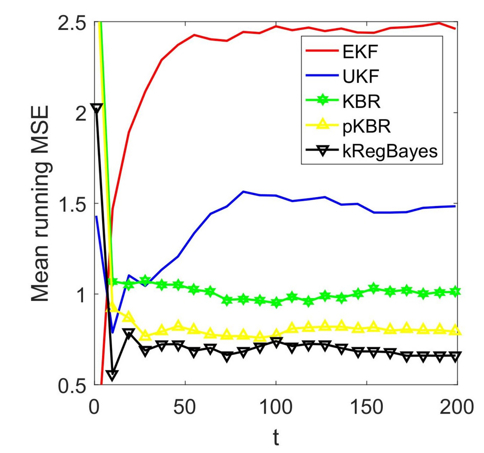
We apply the framework to state-space filtering tasks, since Bayesian inference is a key element of filtering.

Toy dynamics

- We compare results of EKF, UKF, KBR (kernel Bayes' rule), pKBR (KBR with thresholding regularization) and kRegBayes
- The data points $\{(\theta_t, x_t, y_t)\}$ are generated from the dynamics

$$\theta_{t+1} = \theta_t + 0.4 + \xi_t \pmod{2\pi}, \quad \begin{pmatrix} x_{t+1} \\ y_{t+1} \end{pmatrix} = (1 + \sin(8\theta_{t+1})) \begin{pmatrix} \cos\theta_{t+1} \\ \sin\theta_{t+1} \end{pmatrix} + \zeta_t$$

- Use samples from the true dynamics as regularization for kRegBayes.



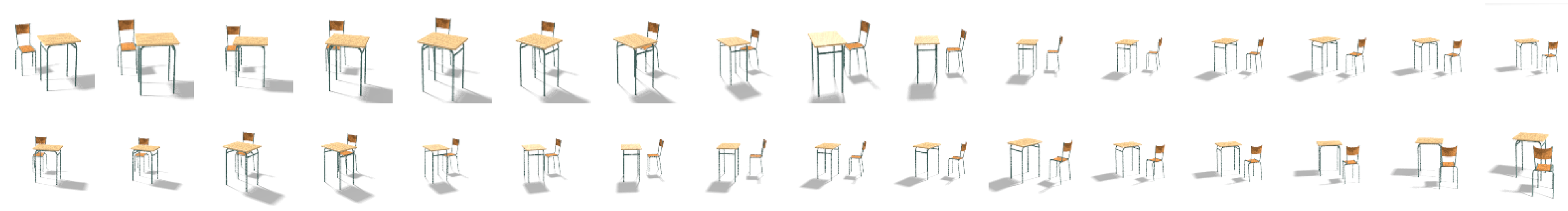
Results for toy dynamics

Camera position recovery

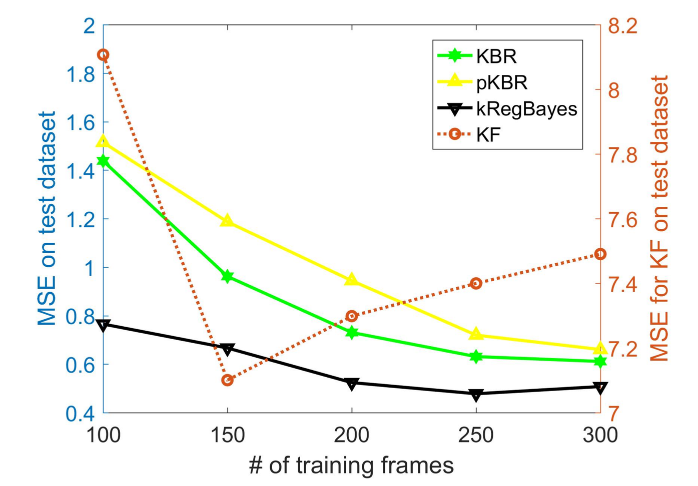
- We compare results of KF, KBR, pKBR and kRegBayes
- The camera has a fixed height and is in a circular region with bounded radii.
- The dynamics is

$$\theta_{t+1} = \theta_t + 0.2 + \xi_\theta, \quad r_{t+1} = \max(R_2, \min(R_1, r_t + \xi_r)), \quad x_{t+1} = \cos\theta_{t+1}, \quad y_{t+1} = \sin\theta_{t+1}$$

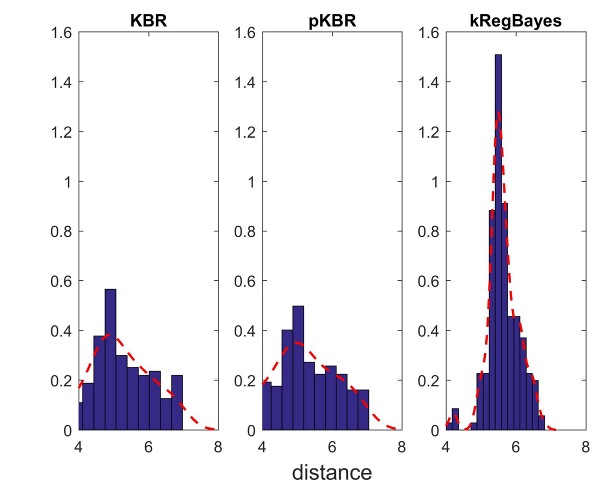
- During training we choose $R_1 = 0$ and $R_2 = 10$ while during testing we use $R_1 = 5$ and $R_2 = 7$.
- We generate positions with radii 6 and use them as the regularization for kRegBayes.



First several training and testing frames for camera position recovery



MSEs for camera position recovery



Probability histograms of distances