Pseudo-Bayesian Learning with Kernel Fourier Transform as Prior

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Introduction

We revisit **Rahimi and Recht (2007)**'s kernel random Fourier features (RFF) method through the lens of the PAC-Bayesian theory.

New perspective on RFF

- The Fourier transform is a *prior* distribution on trigonometric hypotheses.
- Then we learn a *pseudo-posterior* by minimizing PAC-Bayesian bounds.

Two learning approaches

- A kernel alignment algorithm.
- A landmarks-based similarity measure learning.

Random Fourier Features (RFF)

Let's consider a **translation invariant** kernel $k : \mathbb{R}^d \times \mathbb{R}^d \to \mathbb{R}$:

$$k(\mathbf{x}, \mathbf{x}') = k(\mathbf{x} - \mathbf{x}') = k(\boldsymbol{\delta}) \quad \text{with} \quad \boldsymbol{\delta} \coloneqq \mathbf{x} - \mathbf{x}'$$

Denote $p(\boldsymbol{\omega})$ the Fourier transform of $k(\boldsymbol{\delta})$,

$$p(\boldsymbol{\omega}) \;=\; \frac{1}{(2\pi)^d} \int_{\mathbb{R}^d} k(\boldsymbol{\delta})\, e^{-i\,\boldsymbol{\omega}\cdot\boldsymbol{\delta}} d\,\boldsymbol{\delta}$$

Thus,

$$\begin{aligned} k(\mathbf{x}-\mathbf{x}') = \int_{\mathbb{R}^d} p(\boldsymbol{\omega}) e^{i\,\boldsymbol{\omega}\cdot(\mathbf{x}-\mathbf{x}')} d\,\boldsymbol{\omega} \;&=\; \mathop{\mathbf{E}}_{\boldsymbol{\omega}\sim p} e^{i\,\boldsymbol{\omega}\cdot(\mathbf{x}-\mathbf{x}')} \\ &= \mathop{\mathbf{E}}_{\boldsymbol{\omega}\sim p} \Big[\cos\big(\boldsymbol{\omega}\cdot(\mathbf{x}-\mathbf{x}')\big) + i \sin\big(\boldsymbol{\omega}\cdot(\mathbf{x}-\mathbf{x}')\big) \Big] \\ &= \mathop{\mathbf{E}}_{\boldsymbol{\omega}\sim p} \cos\big(\boldsymbol{\omega}\cdot(\mathbf{x}-\mathbf{x}')\big) \end{aligned}$$

Example : Gaussian Kernel

The Gaussian kernel is given by

$$k_\sigma(\mathbf{x}, \mathbf{x}') = \exp\big(-\tfrac{1}{2\sigma^2}\|\mathbf{x}-\mathbf{x}'\|^2\big)$$

Its Fourier transform is

$$p_\sigma(\boldsymbol{\omega}) \;=\; \Big(\frac{\sigma^2}{2\pi}\Big)^{\frac{d}{2}} e^{-\frac{1}{2}\sigma^2\|\boldsymbol{\omega}\|^2} \;=\; \mathcal{N}(\boldsymbol{\omega}; \mathbf{0}, \tfrac{1}{\sigma^2}\mathbf{I})$$

PAC-Bayesian Theory

Given a data distribution $\mathcal{D}$, a training set $S = \{(\mathbf{x}_1, y_1), \ldots, (\mathbf{x}_n, y_n)\} \sim \mathcal{D}^n$, with $\mathbf{x}_i \in \mathbb{R}^d$ and $y_i \in \mathcal{Y} \subset \mathbb{N}$, a loss $\ell : \{-1, 1\}^2 \to [0, 1]$, a predictor $f \in F$:

$$\mathcal{L}_{\mathcal{D}}(f) \;=\; \mathop{\mathbf{E}}_{(\mathbf{x},y)\sim\mathcal{D}} \ell\Big(f(\mathbf{x}), y\Big) \qquad \textit{generalization loss}$$

$$\widehat{\mathcal{L}}_S(f) \;=\; \frac{1}{n}\sum_{i=1}^{n} \ell\Big(f(\mathbf{x}_i), y_i\Big) \qquad \textit{empirical loss}$$

PAC-Bayesian Theorem (Lever et al. 2013)

For $t > 0$, for any prior π on F, with probability $1-\varepsilon$ on the choice of $S \sim \mathcal{D}^n$, we have for all posterior distribution ρ on F :

$$\mathop{\mathbf{E}}_{f\sim\rho} \mathcal{L}_{\mathcal{D}}(f) \le \mathop{\mathbf{E}}_{f\sim\rho} \widehat{\mathcal{L}}_S(f) + \frac{1}{t}\left(\mathrm{KL}(\rho\|\pi) + \frac{t^2}{2n} + \ln\frac{1}{\varepsilon}\right)$$

Thus, the **optimal posterior distribution** ρ^* is :

$$\rho^*(f) \;=\; \frac{1}{Z}\pi(f)\,\exp\Big(-t\,\widehat{\mathcal{L}}_S(f)\Big)$$

PAC-Bayesian Theory for RFF

Idea : **See the Fourier transform of a kernel as a *prior* over predictors.**

$$\begin{aligned} k_p(\mathbf{x}-\mathbf{x}') &= \mathop{\mathbf{E}}_{\boldsymbol{\omega}\sim p} \cos\big(\boldsymbol{\omega}\cdot(\mathbf{x}-\mathbf{x}')\big) \\ &= \mathop{\mathbf{E}}_{\boldsymbol{\omega}\sim p} h_{\boldsymbol{\omega}}(\boldsymbol{\delta}) \qquad \text{with} \quad h_{\boldsymbol{\omega}}(\boldsymbol{\delta}) \coloneqq \cos(\boldsymbol{\omega}\cdot\boldsymbol{\delta}) \end{aligned}$$

Kernel alignment loss

Loss of a predictor $h_{\boldsymbol{\omega}}$ on $(\boldsymbol{\delta}, \lambda) \sim \Delta_{\mathcal{D}}$, given by two draws according to $\mathcal{D}$:

$$\ell\big(h_{\boldsymbol{\omega}}(\boldsymbol{\delta}), \lambda\big) \coloneqq \frac{1 - \lambda h_{\boldsymbol{\omega}}(\boldsymbol{\delta})}{2}, \quad \text{with } \lambda \coloneqq \begin{cases} 1 & \text{if } y = y', \\ -1 & \text{otherwise.} \end{cases}$$

Goal : **Learn a posterior q to minimize the loss of k_q.**

$$\mathcal{L}_{\mathcal{D}}(k_q) \;=\; \mathop{\mathbf{E}}_{\boldsymbol{\omega}\sim q} \mathop{\mathbf{E}}_{(\boldsymbol{\delta},\lambda)\sim\Delta_{\mathcal{D}}} \ell(h_{\boldsymbol{\omega}}(\boldsymbol{\delta}), \lambda) = \mathop{\mathbf{E}}_{\boldsymbol{\omega}\sim q} \mathcal{L}_{\mathcal{D}}(h_{\boldsymbol{\omega}})$$

Empirical loss estimation

Given $S \sim \mathcal{D}^n$, an *unbiased* second-order estimator of $\mathcal{L}_{\mathcal{D}}(k_q)$ is :

$$\widehat{\mathcal{L}}_S(k_q) \coloneqq \frac{1}{n(n-1)} \sum_{i,j=1, i\neq j}^{n} \ell\big(k_q(\boldsymbol{\delta}_{ij}), \lambda_{ij}\big)$$

Approach 1 : Kernel Alignment Algorithm

PAC-Bayesian Corollary

For $t > 0$ and a prior distribution p over $\mathbb{R}^d$, with probability $1-\varepsilon$, we have $\forall q$ on $\mathbb{R}^d$:

$$\mathcal{L}_{\mathcal{D}}(k_q) \le \widehat{\mathcal{L}}_S(k_q) + \frac{1}{t}\left(\mathrm{KL}(q\|p) + \frac{t^2}{2n} + \ln\frac{1}{\epsilon}\right)$$

Consider a uniform prior P on N *random features* drawn according to p, then learn $Q(h_m)$ for $m = 1, \ldots, N$:

$$Q(h_m) \;=\; \frac{1}{Z}\exp\Big(-t\,\widehat{\mathcal{L}}_S(h_m)\Big)$$

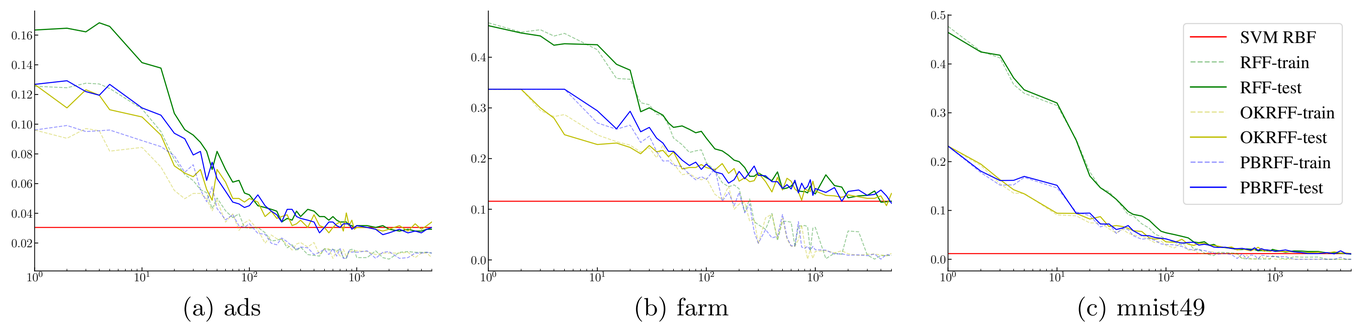
We then sample $D < N$ features according to Q and execute an SVM using the learned kernel

$$\widehat{k}_Q(\mathbf{x}, \mathbf{x}') \coloneqq \frac{1}{D}\sum_{i=1}^{D} h_i(\mathbf{x} - \mathbf{x}')$$

Also in the paper

A general PAC-Bayesian theorem for $\mathcal{L}_{\mathcal{D}}(k_q)$, where $\mathrm{KL}(q\|p)$ can be replaced by other f-divergences. As a special case, it provides a justification to the *Optimal Kernel (OK) alignment algorithm* of Sinha and Duchi (2016).

Experiments



(a) ads (b) farm (c) mnist49

Figure 1: Train and test error of the kernel learning approaches according to the number of random features D.

Approach 2 : Similarity Measure Learning

For a **subset of landmarks** $L = \{(\mathbf{x}_l, y_l)\}_{l=1}^{|L|} \subseteq S$ chosen such that $(\mathbf{x}_i, y_i) \in S$:

$$\mathcal{L}^l_{\mathcal{D}}(k_q) \coloneqq \mathop{\mathbf{E}}_{(\mathbf{x},y)\sim\mathcal{D}} \ell\Big(k_q(\mathbf{x}_l - \mathbf{x}), \lambda(y_l, y)\Big), \; \widehat{\mathcal{L}}^l_S(k_q) \coloneqq \frac{1}{n-1}\sum_{j=1, j\neq l}^{n} \ell\Big(k_q(\mathbf{x}_l - \mathbf{x}_j), \lambda(y_l, y_j)\Big)$$

PAC-Bayesian Corollary

For $t > 0$, $l \in \{1, \ldots, |L|\}$, and a prior distribution p over $\mathbb{R}^d$, with probability $1-\varepsilon$, we have $\forall q$ on $\mathbb{R}^d$:

$$\mathcal{L}^l_{\mathcal{D}}(k_q) \le \widehat{\mathcal{L}}^l_S(k_q) + \frac{1}{t}\left(\mathrm{KL}(q\|p) + \frac{t^2}{2(n-1)} + \ln\frac{1}{\varepsilon}\right)$$

For all $\mathbf{x}_l \in L$, consider a uniform prior P on D *random features* drawn according to p, then learn $Q^l(h^l_m)$

$$Q^l(h^l_m) \;=\; \frac{1}{Z_l}\exp\Big(-t\,\widehat{\mathcal{L}}^l_S(h^l_m)\Big)$$

Then execute an SVM on the following mapping

$$\mathbf{x} \mapsto \Big(\widehat{k}_{Q^1}(\mathbf{x}_1, \mathbf{x}), \widehat{k}_{Q^2}(\mathbf{x}_2, \mathbf{x}), \ldots, \widehat{k}_{Q^{|L|}}(\mathbf{x}_{|L|}, \mathbf{x})\Big)$$

Experiments

- Intuition of the method with toy problem :

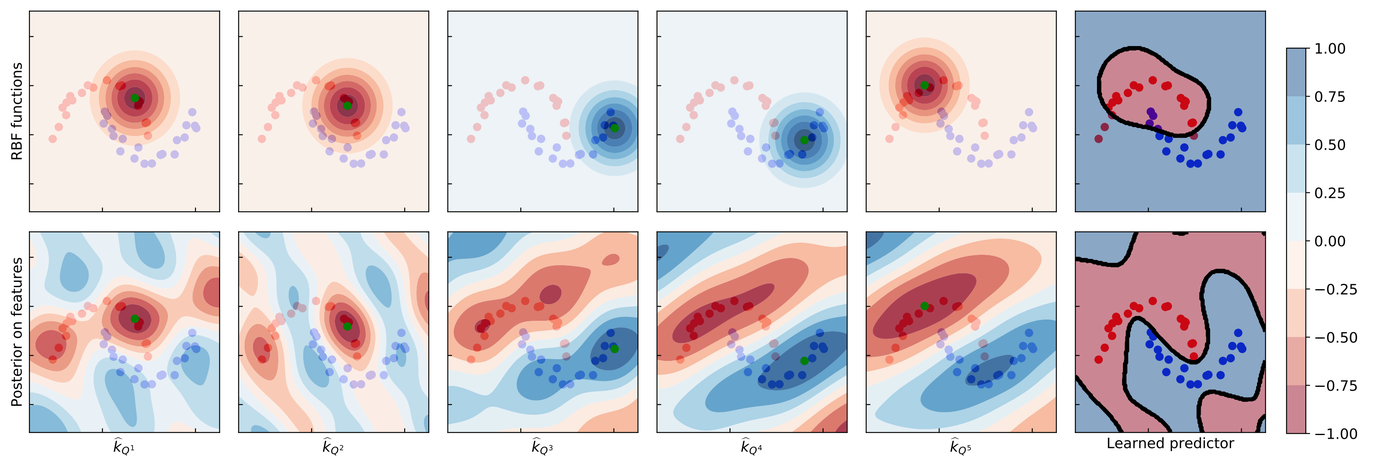


Figure 2: From a RBF prior on 5 randomly selected landmarks (1st row), PB-Landmarks (2nd row) successfully finds a representation from which the linear SVM can predict well.

- Real data results :

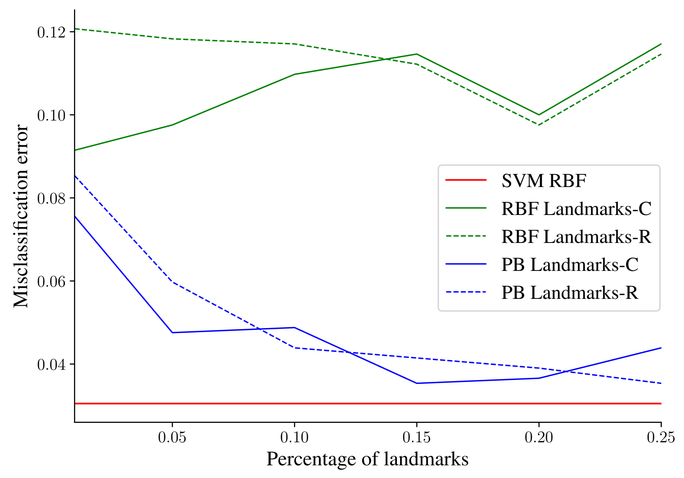


Figure 3: Behavior of the landmarks-based approach according to the percentage of landmarks on the dataset "ads".

Table 1: Test error of the landmarks-based approach.

Dataset	SVM	landmarks-based RBF	PB	$\mathrm{PB}_{t=\sqrt{n}}$	$\mathrm{PB}_{D=64}$
ads	3.05	10.98	**4.88**	5.12	5.00
adult	19.70	19.60	**17.99**	**17.99**	**17.99**
breast	4.90	6.99	3.50	3.50	**2.80**
farm	11.58	17.47	15.73	**14.19**	15.73
mnist17	0.34	0.74	0.42	**0.32**	**0.32**
mnist49	1.16	2.26	**1.80**	2.09	2.50
mnist56	0.55	**0.97**	1.06	1.55	1.03

Contact : gael.letarte.1@ulaval.ca
Code : github.com/gletarte/pbrff

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