Random Fourier Features on Kernel Derivatives*

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Quick Summary

- Context: supervised learning with RKHSs (kernels).
- Scalability: random Fourier features (RFF) [2]
  - one of the most influential approach,
  - 10-year test-of-time award at NIPS-2017.
- Our motivation: tasks with function derivatives,

$$\min_{f\in\mathcal{H}_k} J(f) = \frac{1}{n}\sum_{i=1}^{n} V_i\left(y_i, \{\partial^{\mathbf{p}} f(\mathbf{x}_i)\}_{\mathbf{p}\in I_i}\right) + \lambda \|f\|^2_{\mathcal{H}_k}.$$

  Representer theorem ⇒ appr. of kernel derivatives.
- Goal: tight approximation guarantees on

$$\left\|\partial^{\mathbf{p},\mathbf{q}}k - \widehat{\partial^{\mathbf{p},\mathbf{q}}k}\right\|_{L^\infty(\mathcal{S}\times\mathcal{S})}.$$

Supervised Learning with Derivatives

- Task: given
  - samples $\{(x_i,y_i)\}_{i=1}^n \subset \mathcal{X}\times\mathbb{R}$,
  - $\mathcal{H}_k \subset \mathbb{R}^{\mathcal{X}}$ RKHS associated to kernel $k:\mathcal{X}\times\mathcal{X}\to\mathbb{R}$.
- Objective:

$$\min_{f\in\mathcal{H}_k} J(f) := \frac{1}{n}\sum_{i=1}^{n} V_i\left(y_i, \{\partial^{\mathbf{p}} f(\mathbf{x}_i)\}_{\mathbf{p}\in I_i}\right) + \lambda \|f\|^2_{\mathcal{H}_k}.$$

- Examples ($\mathbf{p}=\mathbf{q}=\mathbf{0}$):
  - kernel ridge regression (squared loss): $V(f(x_i),y_i) = [f(x_i)-y_i]^2$,
  - soft-classification (hinge loss): $V(f(x_i),y_i) = \max(1-y_i f(x_i), 0)$.
- Examples ($[\mathbf{p};\mathbf{q}]\neq 0$):
  - nonlinear variable selection,
  - semi-supervised or Hermite learning with gradient information,
  - fitting infinite-dimensional exponential families.
- Representer theorem [7]:

$$f(\cdot) = \sum_{j=1}^{n}\sum_{\mathbf{p}\in I_j} c_{j,\mathbf{p}}\partial^{\mathbf{p},\mathbf{0}}k(\cdot,\mathbf{x}_j), \quad (c_{j,\mathbf{p}}\in\mathbb{R}), \text{ and}$$

$$\min_{\mathbf{c}} \tilde{J}(\mathbf{c}) = \frac{1}{n}\sum_{i=1}^{n} V_i\left(y_i, \left\{\sum_{j=1}^{n}\sum_{\mathbf{p}\in I_j} c_{j,\mathbf{p}}\partial^{\mathbf{p},\mathbf{0}}k(\mathbf{x}_i,\mathbf{x}_j)\right\}_{\mathbf{p}\in I_i}\right) +$$

$$\lambda \sum_{i=1}^{n}\sum_{\mathbf{p}\in I_i}\sum_{j=1}^{n}\sum_{\mathbf{q}\in I_j} c_{i,\mathbf{p}}c_{j,\mathbf{q}}\partial^{\mathbf{p},\mathbf{q}}k(\mathbf{x}_i,\mathbf{x}_j),$$

where $\mathbf{c} = (c_{i,\mathbf{p}})_{i\in\{1,\ldots,n\},\mathbf{p}\in I_i} \in \mathbb{R}^{\sum_{i=1}^n |I_i|}$.

Random Fourier Features

- $k:\mathbb{R}^d\times\mathbb{R}^d\to\mathbb{R}$ continuous bounded shift-invariant.
- By the Bochner theorem:

$$\begin{aligned} k(\mathbf{x},\mathbf{y}) &= \int_{\mathbb{R}^d} \cos\left(\boldsymbol{\omega}^T(\mathbf{x}-\mathbf{y})\right) \mathrm{d}\Lambda(\boldsymbol{\omega}) \\ &= \int_{\mathbb{R}^d} \langle\phi_{\boldsymbol{\omega}}(\mathbf{x}),\phi_{\boldsymbol{\omega}}(\mathbf{y})\rangle_{\mathbb{R}^2}\,\mathrm{d}\Lambda(\boldsymbol{\omega}), \text{ where} \\ \phi_{\boldsymbol{\omega}}(\mathbf{x}) &= \left[\cos\left(\boldsymbol{\omega}^T\mathbf{x}\right);\sin\left(\boldsymbol{\omega}^T\mathbf{x}\right)\right], \\ \partial^{\mathbf{p},\mathbf{q}}k(\mathbf{x},\mathbf{y}) &= \int_{\mathbb{R}^d} \langle\partial^{\mathbf{p}}\phi_{\boldsymbol{\omega}}(\mathbf{x}),\partial^{\mathbf{q}}\phi_{\boldsymbol{\omega}}(\mathbf{y})\rangle_{\mathbb{R}^2}\,\mathrm{d}\Lambda(\boldsymbol{\omega}). \end{aligned}$$

- RFF idea [2] ($[\mathbf{p};\mathbf{q}]=\mathbf{0}$): change Λ to Λ_m

$$\begin{aligned} \hat{k}(\mathbf{x},\mathbf{y}) &= \int_{\mathbb{R}^d} \langle\phi_{\boldsymbol{\omega}}(\mathbf{x}),\phi_{\boldsymbol{\omega}}(\mathbf{y})\rangle_{\mathbb{R}^2}\,\mathrm{d}\Lambda_m(\boldsymbol{\omega}), \\ \widehat{\partial^{\mathbf{p},\mathbf{q}}k}(\mathbf{x},\mathbf{y}) &= \int_{\mathbb{R}^d} \langle\partial^{\mathbf{p}}\phi_{\boldsymbol{\omega}}(\mathbf{x}),\partial^{\mathbf{q}}\phi_{\boldsymbol{\omega}}(\mathbf{y})\rangle_{\mathbb{R}^2}\,\mathrm{d}\Lambda_m(\boldsymbol{\omega}). \end{aligned}$$

Related Work

- Kernel values [5]:

$$\|k-\hat{k}\|_{L^\infty(\mathcal{S}_m\times\mathcal{S}_m)} = O_{a.s.}\left(\sqrt{\log|\mathcal{S}_m|}/\sqrt{m}\right).$$

- Kernel ridge regression [3, 1], kernel PCA [4, 6].

Our Result

Finite sample guarantee for kernels satisfying the Bernstein condition: $\exists K\geq 1$

$$\int_{\mathbb{R}^d} \frac{|\boldsymbol{\omega}^{\mathbf{p}+\mathbf{q}}|^n}{(\sigma_{\mathbf{p},\mathbf{q}})^n}\mathrm{d}\Lambda(\boldsymbol{\omega}) \leq \frac{n!}{2}K^{n-2}, \quad n=2,3,\ldots,$$

where $\sigma_{\mathbf{p},\mathbf{q}} = \sqrt{\int_{\mathbb{R}^d}|\boldsymbol{\omega}^{\mathbf{p}+\mathbf{q}}|^2\,\mathrm{d}\Lambda(\boldsymbol{\omega})}$. Specifically,

$$\boxed{\left\|\partial^{\mathbf{p},\mathbf{q}}k - \widehat{\partial^{\mathbf{p},\mathbf{q}}k}\right\|_{L^\infty(\mathcal{S}_m\times\mathcal{S}_m)} = O_{a.s.}\left(\sqrt{\log(|\mathcal{S}_m|)}/\sqrt{m}\right).}$$

Our result implies that

$$\left\|\partial^{\mathbf{p},\mathbf{q}}k - \widehat{\partial^{\mathbf{p},\mathbf{q}}k}\right\|_{L^\infty(\mathcal{S}_m\times\mathcal{S}_m)} \xrightarrow{a.s.} 0 \text{ if } |\mathcal{S}_m| = e^{o(m)}.$$

Bernstein requirement: For $f_\Lambda(\omega)\propto e^{-\omega^{2\ell}}$, $p+q\leq 2\ell$: ✓

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