Consistency of Orlicz Random Fourier Features

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Joint work with:

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Focus (high level)

- Task: speed up kernel machines on $\mathbb{R}^d$.
- Technique: random Fourier features.
- Interest: high-order derivatives.

Kernel k, RKHS $\mathcal{H}_k \leftarrow$ generalization of $\mathbf{a}^T\mathbf{b}$

Given: $\mathcal{X}$ set. $\mathcal{H}$(ilbert space).

- Kernel:

$$k(a,b) = \langle \varphi(a), \varphi(b) \rangle_{\mathcal{H}}, \quad (\forall a, b \in \mathcal{X}).$$

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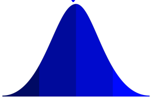
- Reproducing kernel of a $\mathcal{H} \subset \mathbb{R}^{\mathcal{X}}$:

$$\underbrace{k(\cdot, a)} \in \mathcal{H}, \qquad \underbrace{f(b) = \langle f, k(\cdot, b) \rangle_{\mathcal{H}}}_{\text{reproducing property}}.$$



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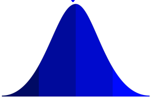

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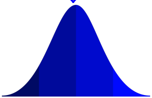

$$\xrightarrow{\text{spec.}} k(a,b) = \langle k(\cdot,a), k(\cdot,b) \rangle_{\mathcal{H}}. \quad \boxed{\mathcal{H}_k = \overline{\left\{\sum_{i=1}^n \alpha_i k(\cdot,x_i)\right\}}}.$$

Kernel: continued

- Def-1 (feature space):

$$k(a,b) = \langle \varphi(a), \varphi(b) \rangle_{\mathcal{H}}.$$

- Def-2 (reproducing kernel, constructive):

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- All these definitions are equivalent, $k \overset{1:1}{\leftrightarrow} \mathcal{H}_k$.

In this talk

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$$k_p(\mathbf{x},\mathbf{y}) = (\langle \mathbf{x},\mathbf{y}\rangle + \gamma)^p\text{: NO!}, \quad k_G(\mathbf{x},\mathbf{y}) = e^{-\gamma\|\mathbf{x}-\mathbf{y}\|_2^2}\text{: YES!},$$

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Bochner theorem $\Rightarrow$

$$k(\mathbf{x},\mathbf{y}) = \int_{\mathbb{R}^d} \cos\left(\boldsymbol{\omega}^T(\mathbf{x}-\mathbf{y})\right) \mathrm{d}\Lambda(\boldsymbol{\omega}).$$

Cost: function values ← curve fitting

Given sample $\{(\mathbf{x}_n, y_n)\}_{n\in[N]} \subset \mathbb{R}^d \times \mathbb{R}$, kernel k on $\mathbb{R}^d$.

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1. Kernel ridge regression ($\lambda > 0$):

$$\min_{f\in\mathcal{H}_k} C(f) := \frac{1}{N}\sum_{n\in[N]} [f(\mathbf{x}_n) - y_n]^2 + \lambda \|f\|_{\mathcal{H}_k}^2 .$$

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2. Classification with hinge loss ($y_n \in \{\pm 1\}$):

$$\min_{f\in\mathcal{H}_k} C(f) := \frac{1}{N}\sum_{n\in[N]} \max(1 - y_n f(\mathbf{x}_n), 0) + \lambda \|f\|^2_{\mathcal{H}_k}.$$

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Optimization over function spaces.

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- $\Rightarrow$ finite-dimensional optimization problem:

$\min_{f \in \mathcal{H}_k}$ switched to $\min_{\mathbf{a} \in \mathbb{R}^N}$.

Cost: function values & derivatives ← curve & slope fitting

1. Hermite learning with gradient data:

$$\min_{f\in\mathcal{H}_k} C(f) := \frac{1}{N}\sum_{n\in[N]}\left(\left[f(\mathbf{x}_n)-y_n\right]^2+\left\|f'(\mathbf{x}_n)-\mathbf{y}'_n\right\|_2^2\right)+\lambda\left\|f\right\|_{\mathcal{H}_k}^2.$$

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2. Nonlinear variable selection:

$$\min_{f\in\mathcal{H}_k} C(f) := \frac{1}{N}\sum_{n\in[N]}[f(\mathbf{x}_n) - y_n]^2 + \sum_{j\in[d]}\left\|\partial_j f\right\|,$$

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Cost: function values & derivatives – continued

A bit more generally:

$$\min_{f \in \mathcal{H}_k} C\left(\left\{\partial^{\mathbf{p}} f(\mathbf{x}_n)\right\}_{\substack{n \in [N] \\ \mathbf{p} \in D_n}}, \|f\|_{\mathcal{H}_k}^2\right) \quad \partial^{\mathbf{p}} f(\mathbf{x}_n) := \frac{\partial^{p_1 + \ldots + p_d} f(\mathbf{x}_n)}{\partial_{x_1}^{p_1} \cdots \partial_{x_d}^{p_d}}.$$

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Examples: semi-supervised learning with gradient information [Zhou, 2008], nonlinear variable selection [Rosasco et al., 2010, Rosasco et al., 2013], learning of piecewise-smooth functions [Lauer et al., 2012], multi-task gradient learning [Ying et al., 2012], structure optimization in parameter-varying ARX processes [Duijkers et al., 2014], density estimation with infinite-dimensional exponential families [Sriperumbudur et al., 2017], Bayesian inference (adaptive samplers) [Strathmann et al., 2015].

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Finite-dimensional optimization problem $\left[\partial^{\mathbf{p},\mathbf{q}} k(\mathbf{x},\mathbf{y}) := \frac{\partial^{\sum_{i=1}^{d}(p_i+q_i)} k(\mathbf{x},\mathbf{y})}{\partial_{x_1}^{p_1} \cdots \partial_{x_d}^{p_d} \partial_{y_1}^{q_1} \cdots \partial_{y_d}^{q_d}}\right]$:

$$\min_{\mathbf{a}} C\left(\left\{\sum_{\substack{m \in [N] \\ \mathbf{q} \in D_m}} a_{m,\mathbf{q}} \partial^{\mathbf{p},\mathbf{q}} k(\mathbf{x}_n, \mathbf{x}_m)\right\}_{\substack{n \in [N] \\ \mathbf{p} \in D_n}}, \sum_{\substack{n,m \in [N] \\ \mathbf{p} \in D_n \\ \mathbf{q} \in D_m}} a_{n,\mathbf{p}} a_{m,\mathbf{q}} \partial^{\mathbf{p},\mathbf{q}} k(\mathbf{x}_n, \mathbf{x}_m)\right).$$

Random Fourier feature (RFF) trick

$\min_{\mathbf{a}}$: can still be computionally heavy.

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- Recall:

$$k(\mathbf{x}, \mathbf{y}) = \int_{\mathbb{R}^d} \cos\left(\boldsymbol{\omega}^T(\mathbf{x} - \mathbf{y})\right) \mathrm{d}\Lambda(\boldsymbol{\omega}), \quad f(\mathbf{x}) = \langle f, k(\cdot, \mathbf{x})\rangle_{\mathcal{H}_k}.$$

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- Explicit low-dimensional feature approximation (Λ_M):

$$k(\mathbf{x}, \mathbf{x}') \approx \left\langle \varphi(\mathbf{x}), \varphi(\mathbf{x}') \right\rangle_{\mathbb{R}^{2M}}, \qquad \hat{f}_{\mathbf{w}}(\mathbf{x}) = \langle \mathbf{w}, \varphi(\mathbf{x})\rangle_{\mathbb{R}^{2M}}.$$

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- Estimate $\mathbf{w}$ by leveraging fast linear primal solvers.

RFF trick: a few applications

Differential privacy preserving [Chaudhuri et al., 2011], fast function-to-function regression [Oliva et al., 2015], learning message operators in expectation propagation [Jitkrittum et al., 2015], causal discovery [Lopez-Paz et al., 2015, Strobl et al., 2019], independence testing [Zhang et al., 2017], prediction and filtering in dynamical systems [Downey et al., 2017], convolution neural networks [Cui et al., 2017], bandit optimization [Li et al., 2018], estimation of Gaussian mixture models [Keriven et al., 2018].

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10-year test-of-time award (NIPS-2017).

Goodness of RFFs – related & optimal work

- Kernel values [Rahimi and Recht, 2007, Sutherland and Schneider, 2015]

$$\left\|k - \widehat{k}\right\|_{L^\infty(S_M)} = \mathcal{O}_p\left(|S_M|\sqrt{\frac{\log M}{M}}\right)$$

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$$\left\|k - \hat{k}\right\|_{L^\infty(S_M)} = \mathcal{O}_{a.s.}\left(\sqrt{\frac{\log |S_M|}{M}}\right).$$

Goodness of RFFs – related & optimal work

- Kernel ridge regression [Rudi and Rosasco, 2017, Li et al., 2019]:
  - $\mathcal{O}\left(\frac{1}{\sqrt{N}}\right)$ generalization with $M = o(N) = \mathcal{O}\left(\sqrt{N}\log N\right)$ / less RFFs.

Goodness of RFFs – related & optimal work

- Kernel PCA [Sriperumbudur and Sterge, 2018, Ullah et al., 2018], classification with 0-1 loss [Gilbert et al., 2018]: $M = o(N)$ RFFs, spectrum decay.

Goodness of RFFs – related & optimal work

- Kernel derivatives [Szabó and Sriperumbudur, 2019]: same bound as for kernel values (unbounded empirical processes, Bernstein condition).

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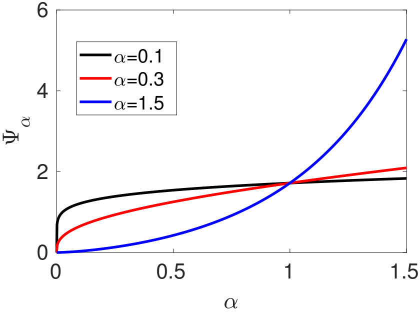
Our question

- Avoid the Bernstein condition.
- With (essentially) $f_\Lambda(\omega) \propto e^{-|\omega|^\alpha}$: guarantees for $\alpha \leq n$.

α-exponential Orlicz norm $(\alpha > 0)$

With $f_\Lambda(\omega) \propto e^{-|\omega|^\alpha}$ in mind,

- Let $\Psi_\alpha : x \in \mathbb{R}^{\geq 0} \mapsto e^{x^\alpha} - 1 \in \mathbb{R}^{\geq 0}$.



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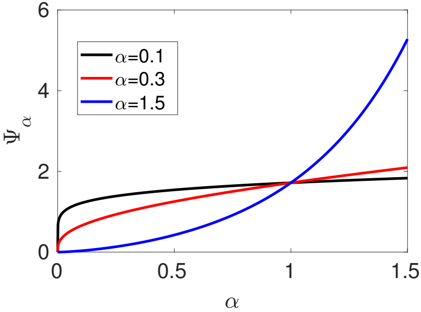

- $L_{\Psi_\alpha} := \left\{\Lambda : \|\Lambda\|_{\Psi_\alpha} := \inf\left\{c > 0 : \mathbb{E}_{\boldsymbol{\omega}\sim\Lambda}\Psi_\alpha\left(\frac{\|\boldsymbol{\omega}\|_2}{c}\right) \leq 1\right\} < +\infty\right\}$.

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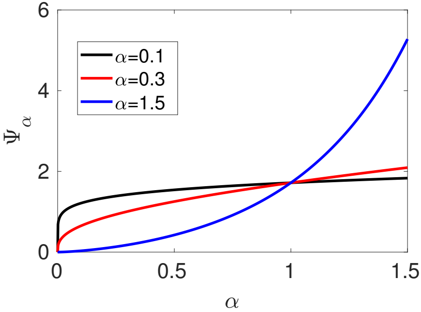
- Let $\Psi_\alpha : x \in \mathbb{R}^{\geq 0} \mapsto e^{x^\alpha} - 1 \in \mathbb{R}^{\geq 0}$.



- $L_{\Psi_\alpha} := \left\{\Lambda : \|\Lambda\|_{\Psi_\alpha} := \inf\left\{c > 0 : \mathbb{E}_{\boldsymbol{\omega}\sim\Lambda}\Psi_\alpha\left(\frac{\|\boldsymbol{\omega}\|_2}{c}\right) \leq 1\right\} < +\infty\right\}$.
- $\Lambda \in L_{\Psi_2}$: sub-Gaussian, $\Lambda \in L_{\Psi_1}$: sub-exponential.

- Intuition:
  - $f_\Lambda(\omega) \propto e^{-|\omega|^\alpha} \Rightarrow \Lambda \in L_{\Psi_\alpha}$ (polynomial decorations: ✓).

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then $\Lambda \in L_{\Psi_\alpha}$ with $\alpha = \min_{i \in [d]} \alpha_i$.

Kernel examples with α-exp. Orlicz spectrum: $d=1$

Spectrum	$f_\Lambda(\omega)$	α
Gaussian	$\frac{1}{\sqrt{2\pi}\sigma}e^{-\frac{\omega^2}{2\sigma^2}}$	2
Laplace	$\frac{\sigma}{2}e^{-\sigma\|\omega\|}$	1
generalized Gaussian	$\frac{\alpha}{2\beta\Gamma\left(\frac{1}{\alpha}\right)}e^{-\frac{\|\omega\|}{\beta}^{\alpha}}$	α
variance Gamma	$\frac{\sigma^{2b}\|\omega\|^{b-\frac{1}{2}}K_{b-\frac{1}{2}}(\sigma\|\omega\|)}{\sqrt{\pi}\Gamma(b)(2\sigma)^{b-\frac{1}{2}}}$	1
Weibull (S)	$\frac{s}{2\lambda}\left(\frac{\|\omega\|}{\lambda}\right)^{s-1}e^{-\left(\frac{\|\omega\|}{\lambda}\right)^s}$	s
exponentiated exponential (S)	$\frac{\alpha}{2\lambda}\left(1-e^{-\frac{\|\omega\|}{\lambda}}\right)^{\alpha-1}e^{-\frac{\|\omega\|}{\lambda}}$	1

$I_a(z)=\sum_{n\in\mathbb{N}}\frac{1}{n!\Gamma(n+a+1)}\left(\frac{z}{2}\right)^{2n+a}$, $K_a(z)=\frac{\pi}{2}\frac{I_{-a}(z)-I_a(z)}{\sin(a\pi)}$ for $z\in\mathbb{R}$ and non-integer a; when a is an integer the limit is taken.

Kernel examples with α-exponential Orlicz spectrum - 2

Spectrum	$f_\Lambda(\omega)$	α
exponentiated Weibull (S)	$\frac{\alpha s}{2\lambda}\left(\frac{\lvert\omega\rvert}{\lambda}\right)^{s-1}\left[1-e^{-\left(\frac{\lvert\omega\rvert}{\lambda}\right)^s}\right]^{\alpha-1}\times$ $\times e^{-\left(\frac{\lvert\omega\rvert}{\lambda}\right)^s}$	s
Nakagami (S)	$\frac{m^m}{\Gamma(m)\Omega^m}\lvert\omega\rvert^{2m-1}e^{-\frac{m\omega^2}{\Omega}}$	2
chi-squared (S)	$\frac{1}{2^{\frac{s}{2}+1}\Gamma\left(\frac{s}{2}\right)}\lvert\omega\rvert^{\frac{s}{2}-1}e^{-\frac{\lvert\omega\rvert}{2}}$	1
Erlang (S)	$\frac{\lambda^s\lvert\omega\rvert^{s-1}e^{-\lambda\lvert\omega\rvert}}{2(s-1)!}$	1
Gamma (S)	$\frac{1}{2\Gamma(s)\theta^s}\lvert\omega\rvert^{s-1}e^{-\frac{\lvert\omega\rvert}{\theta}}$	1
generalized Gamma (S)	$\frac{p/a^D}{2\Gamma\left(\frac{D}{p}\right)}\lvert\omega\rvert^{D-1}e^{-\left(\frac{\lvert\omega\rvert}{a}\right)^p}$	p

Kernel examples with α-exponential Orlicz spectrum - 3

Spectrum	$f_\Lambda(\omega)$	α
Rayleigh (S)	$\frac{\lvert\omega\rvert}{2\sigma^2}e^{-\frac{\omega^2}{2\sigma^2}}$	2
Maxwell-Boltzmann (S)	$\frac{1}{\sqrt{2\pi}}\frac{\omega^2 e^{-\frac{\omega^2}{2a^2}}}{a^3}$	2
chi (S)	$\frac{1}{2^{\frac{s}{2}}\Gamma\left(\frac{s}{2}\right)}\lvert\omega\rvert^{s-1}e^{-\frac{\omega^2}{2}}$	2
exponential-logarithmic (S)	$-\frac{1}{2\log(p)}\frac{\beta(1-p)e^{-\beta\lvert\omega\rvert}}{1-(1-p)e^{-\beta\lvert\omega\rvert}}$	1
Weibull-logarithmic (S)	$-\frac{1}{2\log(p)}\frac{\alpha\beta(1-p)\lvert\omega\rvert^{\alpha-1}e^{-\beta\lvert\omega\rvert^\alpha}}{1-(1-p)e^{-\beta\lvert\omega\rvert^\alpha}}$	α
Gamma/Gompertz (S)	$\frac{bse^{b\lvert\omega\rvert}\beta^s}{2\left(\beta-1+e^{b\lvert\omega\rvert}\right)^{s+1}}$	bs

Kernel examples with α-exponential Orlicz spectrum - 4

Spectrum	$f_\Lambda(\omega)$	α
hyperbolic secant	$\frac{1}{2}\operatorname{sech}\left(\frac{\pi}{2}\omega\right)$	1
logistic	$\frac{e^{-\frac{\omega}{s}}}{s\left[1+e^{-\frac{\omega}{s}}\right]^2} = \frac{1}{4s}\operatorname{sech}^2\left(\frac{\omega}{2s}\right)$	1
normal-inverse Gaussian	$\frac{\alpha\delta K_1\left(\alpha\sqrt{\delta^2+\omega^2}\right)}{\pi\sqrt{\delta^2+\omega^2}}e^{\delta\alpha}$	1
hyperbolic	$\frac{1}{2\delta K_1(\delta\alpha)}e^{-\alpha\sqrt{\delta^2+\omega^2}}$	1
generalized hyperbolic	$\frac{(\alpha/\delta)^\lambda}{\sqrt{2\pi}K_\lambda(\delta\gamma)}\frac{K_{\lambda-\frac{1}{2}}\left(\alpha\sqrt{\delta^2+\omega^2}\right)}{\left(\frac{\sqrt{\delta^2+\omega^2}}{\alpha}\right)^{\frac{1}{2}-\lambda}}$	1

$$\operatorname{sech}(x) = \frac{1}{\cosh(x)} = \frac{2}{e^x+e^{-x}}.$$

Spectrum $\mapsto$ kernel examples $(b > \frac{1}{2},\ s > 0)$

Kernel name	$k(x,y)$	Spectrum
Gaussian	$e^{-\frac{\sigma^2(x-y)^2}{2}}$	Gaussian
Cauchy / inverse quadric	$\frac{\sigma^2}{\sigma^2+(x-y)^2}$	Laplace
inverse multiquadric	$\left[\frac{\sigma^2}{\sigma^2+(x-y)^2}\right]^b$	variance Gamma
–	$\operatorname{sech}(x-y)$	hyperbolic secant
–	$\frac{\pi s(x-y)}{\sinh(\pi s(x-y))}$	logistic

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+Analytical kernel values: generalized Gaussian, Weibull (S), chi-squared (S), Erlang (S), Gamma (S), Rayleigh (S), chi (S), Weibull-logarithmic (S), Gamma/Gompertz (S), normal-inverse Gaussian, hyperbolic, generalized hyperbolic.

Our result (finite-sample guarantee $\Rightarrow$ asymptotics)

Assume:

- k: continuous, bounded, shift-invariant kernel on $\mathbb{R}^d$.
- $\Lambda \in L_{\Psi_\alpha}$ $(\alpha > 0)$.
- Let $\mathbf{p}, \mathbf{q} \in \mathbb{N}^d$, $[\mathbf{p}; \mathbf{q}] \neq \mathbf{0}$, $n := \sum_{i \in [d]} (p_i + q_i)$, $\alpha \leq n$.

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Then

$$\left\| \partial^{\mathbf{p},\mathbf{q}} k - \widehat{\partial^{\mathbf{p},\mathbf{q}} k} \right\|_{L^\infty(S_M)} = \mathcal{O}_{a.s.}\left(|S_M| \frac{\log^r(M)}{\sqrt{M}} \right), \quad r = \frac{n}{\alpha}.$$

Summary

- Focus: RFF-based acceleration & high-order derivatives.
- Result:
  - spectrum: α-exponential Orlicz assumption.
  - $n \geq \alpha$-order derivative: ✓
- Preprint: in the oven.

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Stress Test
RISK Management and Financial Steering

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Proof idea

Decomposition into 3 terms:

1. Unbounded part: Talagrand & Hoffman-Jorgensen inequalities.
2. Bounded part: Klein-Rio inequality & Dudley entropy integral bound.
3. Truncation: bound on the incomplete Gamma function.

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