

Orlicz Random Fourier Features

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Notations



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

Objective: examples

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

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

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

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

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

Objective: examples

Given $\{(\mathbf{x}_n, y_n, \mathbf{y}'_n)\}_{n \in [N]} \subset \mathbb{R}^d \times \mathbb{R} \times \mathbb{R}^d$ samples, k kernel on \mathbb{R}^d , \mathcal{H}_k RKHS.

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- ③ Hermite learning with **gradient** data:

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

Objective function

A bit more generally:

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

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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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Optimization over **function spaces**.

Representer theorem, reproducing property

- Function values [$f(\mathbf{x}_n)$]:

$$f(\cdot) = \sum_{n \in [N]} a_n k(\cdot, \mathbf{x}_n), \quad a_n \in \mathbb{R}.$$

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$$f(\cdot) = \sum_{\substack{n \in [N] \\ \mathbf{p} \in D_n}} a_{n,\mathbf{p}} \partial^{\mathbf{p}, \mathbf{0}} k(\cdot, \mathbf{x}_n) \quad a_{n,\mathbf{p}} \in \mathbb{R}.$$

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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_a : can still be computationally heavy.

RFF [Rahimi and Recht, 2007, Rahimi and Recht, 2008]:

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

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- Explicit low-dimensional feature approximation (Λ_M):

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

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

Goodness of RFFs – related work

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

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

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

Goodness of RFFs – related 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 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 work

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

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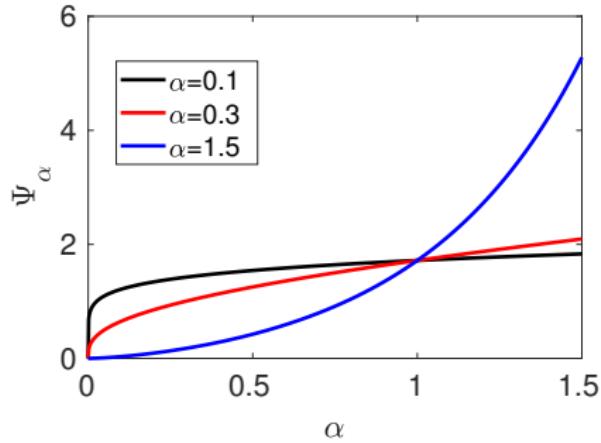
Our question

- Avoid the Bernstein condition.
- With (essentially) $f_\Lambda(\omega) \propto e^{-|\omega|^\alpha}$: guarantees for $\frac{\alpha}{n} \leq 1$.

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

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

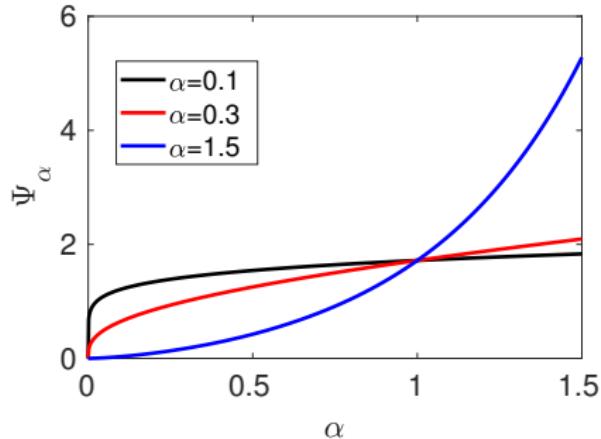
- Let $\Psi_\alpha : x \in \mathbb{R}^{\geq 0} \mapsto e^{x^\alpha} - 1 \in \mathbb{R}^{\geq 0}$.



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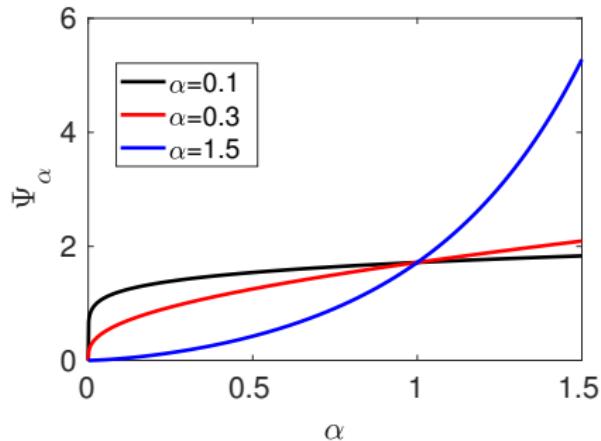


- $L_{\Psi_\alpha} := \left\{ \Lambda : \|\Lambda\|_{\Psi_\alpha} := \inf \left\{ c > 0 : \mathbb{E}_{\omega \sim \Lambda} \Psi_\alpha \left(\frac{\|\omega\|_2}{c} \right) \leq 1 \right\} < +\infty \right\}$.

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- $\Lambda \in L_{\Psi_2}$: 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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- $k(\mathbf{x}, \mathbf{y}) = \prod_{i \in [d]} k_i(x_i, y_i)$, i.e. $\Lambda = \otimes_{i \in [d]} \Lambda_i$,

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

Kernel examples with α -exponential Orlicz spectrum - 3

Spectrum	$f_\Lambda(\omega)$	α
Rayleigh (S)	$\frac{ \omega }{2\sigma^2} e^{-\frac{\omega^2}{2\sigma^2}}$	2
Maxwell-Boltzmann (S)	$\frac{1}{\sqrt{2\pi}} \frac{\omega^2 e^{-\frac{\omega^2}{2a^2}}}{a^3}$	2
chi (S)	$\frac{1}{2^{\frac{s}{2}} \Gamma(\frac{s}{2})} \omega ^{s-1} e^{-\frac{\omega^2}{2}}$	2
exponential-logarithmic (S)	$-\frac{1}{2 \log(p)} \frac{\beta(1-p)e^{-\beta \omega }}{1-(1-p)e^{-\beta \omega }}$	1
Weibull-logarithmic (S)	$-\frac{1}{2 \log(p)} \frac{\alpha\beta(1-p) \omega ^{\alpha-1}e^{-\beta \omega ^\alpha}}{1-(1-p)e^{-\beta \omega ^\alpha}}$	α
Gamma/Gompertz (S)	$\frac{bse^{b \omega }\beta^s}{2(\beta-1+e^{b \omega })^{s+1}}$	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	$\frac{\alpha\delta K_1(\alpha\sqrt{\delta^2+\omega^2})}{\pi\sqrt{\delta^2+\omega^2}} e^{\delta\alpha}$	1
hyperbolic	$\frac{1}{2\delta K_1(\delta\alpha)} e^{-\alpha\sqrt{\delta^2+\omega^2}}$	1
generalized hyperbolic	$\frac{(\alpha/\delta)^\lambda}{\sqrt{2\pi}K_\lambda(\delta\gamma)} \frac{K_{\lambda-\frac{1}{2}}(\alpha\sqrt{\delta^2+\omega^2})}{\left(\frac{\sqrt{\delta^2+\omega^2}}{\alpha}\right)^{\frac{1}{2}-\lambda}}$	1

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

Kernel name	$k(x, y)$	Spectrum
Gaussian	$e^{-\frac{\sigma^2(x-y)^2}{2}}$	Gaussian
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
-	$\text{sech}(x - y)$	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.

Assume:

- k : continuous, bounded, shift-invariant kernel on \mathbb{R}^d .
- $\Lambda \in L_{\Psi_\alpha}$ ($\alpha > 0$).
- Let $\mathbf{p}, \mathbf{q} \in \mathbb{N}^d$, $[\mathbf{p}; \mathbf{q}] \neq \mathbf{0}$, $n := \sum_{i \in [d]} (p_i + q_i)$, $\frac{\alpha}{n} \leq 1$.

Our result (finite-sample guarantee \Rightarrow asymptotics)

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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

Acks: This research benefited from the support of the Chair Stress Test, RISK Management and Financial Steering, led by the French Ecole polytechnique and its Foundation and sponsored by BNP Paribas.

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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