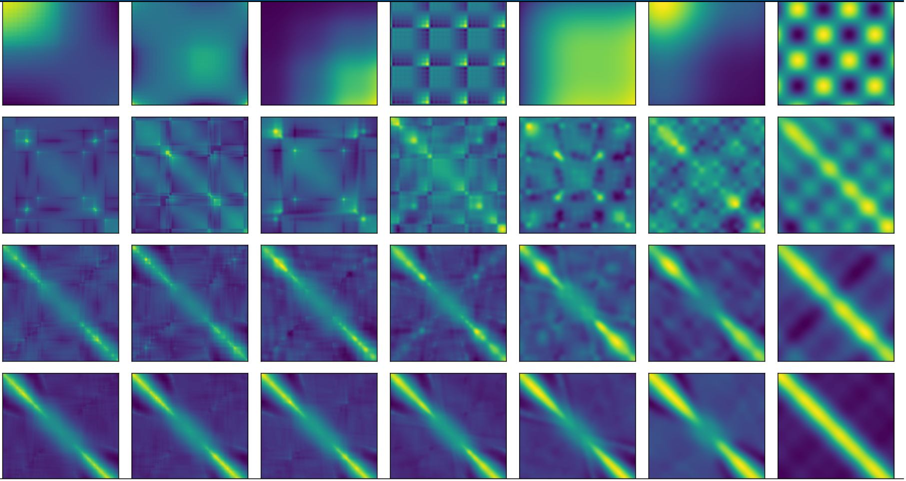
Random Fourier Series Features

Defense “Expert Lab on Robot Learning”



Motivation

Outline

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Methodology

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Conclusion

Deep Learning and Neural Networks

- (Deep) neural networks dominate AI

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  - extremely expressive
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Deep Learning and Neural Networks

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  - lack uncertainty estimation
- Lead to the development of *Bayesian* neural networks

Deep Learning and Neural Networks

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- (Deep) neural networks dominate AI
  - extremely expressive
  - great predictive power
  - lack uncertainty estimation
- Lead to the development of *Bayesian* neural networks
  - intractable exact inference
  - complicated training
  - ...

Gaussian Processes (GPs)

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- but performance highly depends on the kernel choice…
  - tackled by kernel learning

Gaussian Processes (GPs)

- GPs are still the go-to model for reliable uncertainty quantification
- but performance highly depends on the kernel choice…
  - tackled by kernel learning
- exact inference complexity is cubic w.r.t. number of data points
  - prohibits online use of GPs

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Random Fourier Features

$$\boldsymbol{z}_\omega(\boldsymbol{x}) = \begin{bmatrix} \cos(\langle \omega | \boldsymbol{x} \rangle) \\ \sin(\langle \omega | \boldsymbol{x} \rangle) \end{bmatrix}$$

- resort to “classical” Bayesian regression
- explicit posterior over the weights

Random Fourier Features

$$\boldsymbol{z}_\omega(\boldsymbol{x}) = \begin{bmatrix} \cos(\langle \omega | \boldsymbol{x} \rangle) \\ \sin(\langle \omega | \boldsymbol{x} \rangle) \end{bmatrix}$$

- resort to “classical” Bayesian regression
- explicit posterior over the weights
- approximate every stationary kernel $k(\cdot)$:

$$k(\boldsymbol{x} - \boldsymbol{y}) = \mathbb{E}_{\omega \sim p(\cdot)} \left[\langle \boldsymbol{z}_\omega(\boldsymbol{x}) | \boldsymbol{z}_\omega(\boldsymbol{y}) \rangle \right] \approx \frac{1}{N} \sum_{i=1}^{N} \langle \boldsymbol{z}_{\omega_i}(\boldsymbol{x}) | \boldsymbol{z}_{\omega_i}(\boldsymbol{y}) \rangle , \quad \omega_i \sim p(\cdot)$$

Random Fourier Features

Approximating the Squared Exponential

For the SE kernel: tractable Fourier transform

Random Fourier Features

Approximating the Squared Exponential

For the SE kernel: tractable Fourier transform

$$k_{\mathrm{SE}}(\boldsymbol{x} - \boldsymbol{y}) = \exp\left\{ -\langle \boldsymbol{x} - \boldsymbol{y} | \boldsymbol{x} - \boldsymbol{y} \rangle / 2 \right\}$$

$$p(\omega) = \left(\mathcal{F} k_{\mathrm{SE}}\right)(\omega) = \mathcal{N}(\omega \mid \mathbf{0}, \mathbf{I})$$

Random Fourier Features
Approximating the Squared Exponential

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For the SE kernel: tractable Fourier transform

$$k_{\mathrm{SE}}(\boldsymbol{x}-\boldsymbol{y}) = \exp\left\{ -\langle \boldsymbol{x}-\boldsymbol{y} | \boldsymbol{x}-\boldsymbol{y} \rangle / \, 2 \right\}$$

$$p(\omega) = \left(\mathcal{F} k_{\mathrm{SE}}\right)(\omega) = \mathcal{N}(\omega \mid \mathbf{0}, \mathbf{I})$$

$$\begin{aligned}
\mathbb{E}\left[\langle \boldsymbol{z}_\omega(\boldsymbol{x}) | \boldsymbol{z}_\omega(\boldsymbol{y}) \rangle\right] &= \mathbb{E}\left[\left\langle \begin{bmatrix} \cos(\langle \omega | \boldsymbol{x} \rangle) \\ \sin(\langle \omega | \boldsymbol{x} \rangle) \end{bmatrix} \middle| \begin{bmatrix} \cos(\langle \omega | \boldsymbol{y} \rangle) \\ \sin(\langle \omega | \boldsymbol{y} \rangle) \end{bmatrix} \right\rangle\right] \\
&= \mathbb{E}\left[\cos(\langle \omega | \boldsymbol{x} \rangle) \cos(\langle \omega | \boldsymbol{y} \rangle) + \sin(\langle \omega | \boldsymbol{x} \rangle) \sin(\langle \omega | \boldsymbol{y} \rangle)\right] \\
&= \mathbb{E}\left[\cos(\langle \omega | \boldsymbol{x}-\boldsymbol{y} \rangle)\right] = \mathrm{Re}\left(\mathbb{E}\left[\exp\{i \langle \omega | \boldsymbol{x}-\boldsymbol{y} \rangle\}\right]\right) \\
&= \mathrm{Re}\left(\left(\mathcal{F}^{-1} p\right)(\boldsymbol{x}-\boldsymbol{y})\right) = \mathrm{Re}\left(k_{\mathrm{SE}}(\boldsymbol{x}-\boldsymbol{y})\right) = k_{\mathrm{SE}}(\boldsymbol{x}-\boldsymbol{y})
\end{aligned}$$

Random Fourier Features

Approximating the Squared Exponential

For the SE kernel: tractable Fourier transform

$$k_{\mathrm{SE}}(\boldsymbol{x}-\boldsymbol{y}) = \exp\big\{-\langle \boldsymbol{x}-\boldsymbol{y} | \boldsymbol{x}-\boldsymbol{y}\rangle / 2\big\}$$

$$p(\omega) = \big(\mathcal{F}k_{\mathrm{SE}}\big)(\omega) = \mathcal{N}(\omega \,|\, \mathbf{0}, \mathbf{I})$$

$$\begin{aligned}
\mathbb{E}\big[\langle \boldsymbol{z}_\omega(\boldsymbol{x}) | \boldsymbol{z}_\omega(\boldsymbol{y})\rangle\big] &= \mathbb{E}\left[\left\langle \begin{bmatrix}\cos(\langle\omega|\boldsymbol{x}\rangle) \\ \sin(\langle\omega|\boldsymbol{x}\rangle)\end{bmatrix} \middle| \begin{bmatrix}\cos(\langle\omega|\boldsymbol{y}\rangle) \\ \sin(\langle\omega|\boldsymbol{y}\rangle)\end{bmatrix} \right\rangle\right] \\
&= \mathbb{E}\big[\cos(\langle\omega|\boldsymbol{x}\rangle)\cos(\langle\omega|\boldsymbol{y}\rangle) + \sin(\langle\omega|\boldsymbol{x}\rangle)\sin(\langle\omega|\boldsymbol{y}\rangle)\big] \\
&= \mathbb{E}\big[\cos(\langle\omega|\boldsymbol{x}-\boldsymbol{y}\rangle)\big] = \mathrm{Re}\Big(\mathbb{E}\big[\exp\{i\,\langle\omega|\boldsymbol{x}-\boldsymbol{y}\rangle\}\big]\Big) \\
&= \mathrm{Re}\Big(\big(\mathcal{F}^{-1}p\big)(\boldsymbol{x}-\boldsymbol{y})\Big) = \mathrm{Re}\big(k_{\mathrm{SE}}(\boldsymbol{x}-\boldsymbol{y})\big) = k_{\mathrm{SE}}(\boldsymbol{x}-\boldsymbol{y})
\end{aligned}$$

- SE kernel is extremely smooth (Stein, 1999)

Random Fourier *Series* Features

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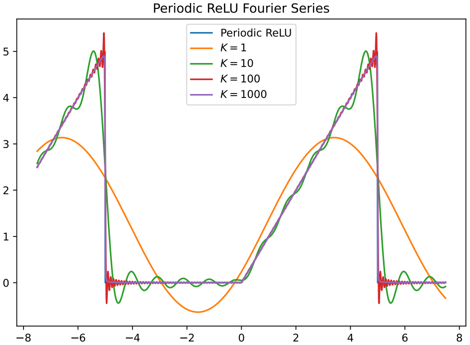
We extend random Fourier features:

$$\boldsymbol{z}_\omega(\boldsymbol{x}) = \begin{bmatrix} \cos(\langle \omega | \boldsymbol{x} \rangle) \\ \sin(\langle \omega | \boldsymbol{x} \rangle) \end{bmatrix} \longrightarrow \begin{aligned} \boldsymbol{z}_\omega(\boldsymbol{x}) &= \sum_{k=1}^{K} \boldsymbol{z}_\omega^{(k)}(\boldsymbol{x}), \\ \boldsymbol{z}_\omega^{(k)}(\boldsymbol{x}) &= \begin{bmatrix} a_k \cos\left(\pi \widetilde{T}^{-1} k \left\langle \omega | \boldsymbol{\Lambda}^{-1} | \boldsymbol{x} \right\rangle\right) \\ b_k \sin\left(\pi \widetilde{T}^{-1} k \left\langle \omega | \boldsymbol{\Lambda}^{-1} | \boldsymbol{x} \right\rangle\right) \end{bmatrix} \end{aligned}$$

- similar to the sine-cosine formulation of Fourier series

Fourier Series
Sine-Cosine Formulation

$$\widehat{f}_K(x) = \frac{a_0}{2} + \sum_{k=1}^{K} a_k \cos\left(\pi \widetilde{T}^{-1} k x\right) + b_k \sin\left(\pi \widetilde{T}^{-1} k x\right)$$



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Hypothesis

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Central Hypothesis

Random Fourier series features outperform random Fourier features.

Evaluation

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- Datasets:
  - Synthetic Data (Cosine, Heaviside, Heavi-Cosine, Gap-Cosine)
  - UCI (Boston, Concrete, Power, Yacht, Energy, Kin8nm, Naval, Protein, Wine)
  - Cartpole

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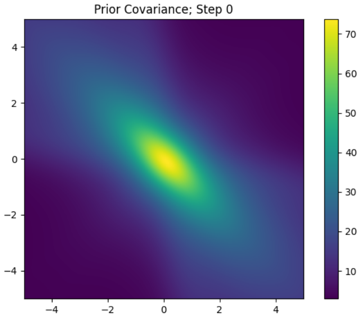
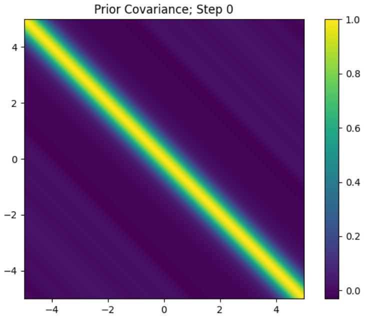
  - UCI (Boston, Concrete, Power, Yacht, Energy, Kin8nm, Naval, Protein, Wine)
  - Cartpole
- Different RFSF Initializations:
  - Random
  - ReLU
  - Single Harmonic (SH)

How the Kernel Learns

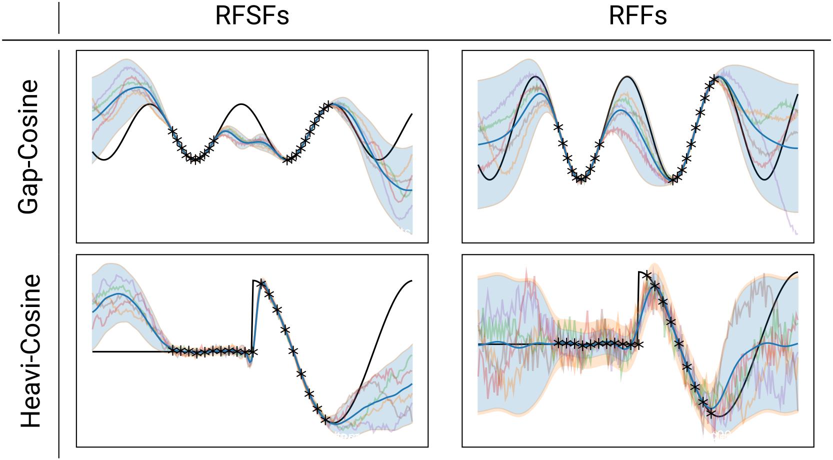


RFSF on Gap-Cosine



RFFs on Gap-Cosine

Results on the Synthetic Data



Quantified Results

Synthetic Data Sets and Cartpole

	Model		Data Set				
			Cosine	Heaviside	Heavi-Cosine	Gap-Cosine	Cartpole
Log-Lik.	*RFSF*	*Random*	***2.43***	*0.11*	*-1.66*	*1.27*	*-9.88 ± 1.86*
		ReLU	*2.34*	***0.80***	*-0.90*	*1.50*	*-12.30 ± 2.31*
		SH	*2.37*	***0.21***	*-1.23*	*1.52*	*-9.73 ± 2.10*
	GP	SE	**2.44**	0.73	**0.77**	**2.58**	**-3.21 ± 1.64**
		RFF	**2.44**	0.73	**0.78**	**2.59**	-7.38 ± 1.94

Quantified Results

UCI Data Sets

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	Model		Data Set Boston	Concrete	Power	Yacht
Log-Lik.	*RFSF*	*Random*	*−2.40 ± 0.05*	***−2.94 ± 0.05***	*−2.78 ± 0.01*	*−0.80 ± 0.02*
		ReLU	*−2.39 ± 0.05*	***−2.93 ± 0.04***	*−2.80 ± 0.01*	*−0.86 ± 0.02*
		SH	*−2.44 ± 0.06*	***−2.94 ± 0.05***	*−2.78 ± 0.01*	*−0.83 ± 0.02*
	GP	SE	**−2.38 ± 0.05**	**−2.98 ± 0.06**	−2.82 ± 0.01	−0.80 ± 0.02
		RFF	−2.40 ± 0.06	**−3.01 ± 0.05**	−2.84 ± 0.01	−0.80 ± 0.02
	GBLL[1]	Leaky ReLU	−2.90 ± 0.05	−3.09 ± 0.03	−2.77 ± 0.01	−1.67 ± 0.11
		Tanh	−3.06 ± 0.03	−3.21 ± 0.03	−2.83 ± 0.01	−0.70 ± 0.10
	Ensemble[1]	Leaky ReLU	−2.48 ± 0.09	**−3.04 ± 0.08**	**−2.70 ± 0.01**	−0.35 ± 0.07
		Tanh	−2.48 ± 0.08	**−3.03 ± 0.07**	**−2.72 ± 0.01**	**−0.03 ± 0.05**
	MAP[1]	Leaky ReLU	−2.60 ± 0.07	−3.04 ± 0.04	−2.77 ± 0.01	−5.14 ± 1.62
		Tanh	−2.59 ± 0.06	−3.11 ± 0.04	−2.76 ± 0.01	−1.77 ± 0.53

[1] Results taken from Watson et al. (2021), "Latent Derivative Bayesian Last Layer Networks."

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Conclusion

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Central Hypothesis

Random Fourier series features outperform random Fourier features.

- we compared to RFFs, SE, and BNN methods
- advantage of RFSFs is not consistent
- no performance gain
- also true for the SH initialization

Future Work

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- theoretical analysis what RFSFs approximate
- better understanding of the half-period initialization

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Methodology

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Hyper-Parameter Optimization

- Hyper-Parameters
  - $\boldsymbol{a}_{1:K}$ (sine coefficients)
  - $\boldsymbol{b}_{1:K}$ (cosine coefficients)
  - $\boldsymbol{\Lambda}$ (length-scales)
  - $\widetilde{T}$ (half-period)
  - σ_n^2 (aleatoric noise variance)
- maximization of the marginal log-likelihood
- using the empirical Bayes approximation

$$\boldsymbol{z}_\omega(\boldsymbol{x}) = \sum_{k=1}^{K} \boldsymbol{z}_\omega^{(k)}(\boldsymbol{x}),$$

$$\boldsymbol{z}_\omega^{(k)}(\boldsymbol{x}) = \begin{bmatrix} a_k \cos\left(\pi \widetilde{T}^{-1} k \left\langle \omega \middle| \boldsymbol{\Lambda}^{-1} \middle| \boldsymbol{x} \right\rangle\right) \\ b_k \sin\left(\pi \widetilde{T}^{-1} k \left\langle \omega \middle| \boldsymbol{\Lambda}^{-1} \middle| \boldsymbol{x} \right\rangle\right) \end{bmatrix}$$

Evaluation

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UCI Data Sets; Cont.

		Model	Energy	Kin8nm	Naval	Protein	Wine
			Data Set				
Log-Lik.	*RFSF*	*Random*	***-0.70 ± 0.02***	*0.68 ± 0.05*	*-78.19 ± 69.72*	*-2.94 ± 0.03*	*-0.11 ± 0.07*
		ReLU	*-0.74 ± 0.02*	***0.97 ± 0.03***	*-172.57 ± 104.83*	*-629.05 ± 384.60*	*-0.11 ± 0.06*
		SH	*-0.74 ± 0.02*	*0.52 ± 0.07*	*-62.69 ± 55.40*	*-2.96 ± 0.03*	***0.01 ± 0.06***
	GP	SE	**-0.68 ± 0.02**	-0.22 ± 0.24	**6.91 ± 0.15**	**-2.89 ± 0.00**	-0.84 ± 0.05
		RFF	**-0.69 ± 0.02**	0.75 ± 0.04	-1941.56 ± 248.64	-2.90 ± 0.00	-0.89 ± 0.04