



Highlights from NeurIPS 2019

Vancouver, Canada

Function-Space Distributions over Kernels

Gregory W. Benton^{*1} Wesley J. Maddox^{*2} Jayson P. Salkey^{*1}
Júlio Albinati^{‡3} Andrew Gordon Wilson^{1,2}

¹Courant Institute of Mathematical Sciences, New York University

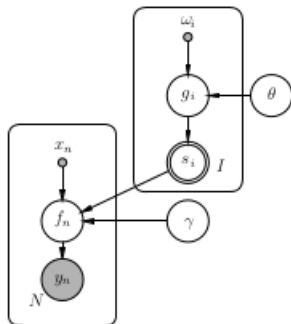
²Center for Data Science, New York University

³Microsoft

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¹Gregory Benton et al. “Function-Space Distributions over Kernels”. In: *Advances in Neural Information Processing Systems*. 2019, pp. 14939–14950.

Spectral Representation



Bochner's Theorem: Can represent a (positive definite) kernel as

$$k(\tau) = \int_{\mathbb{R}} e^{2\pi i \omega \tau} S(\omega) d\omega,$$

with $\tau = |x - x'|$, the distance between any two inputs, and some positive finite function $S(\omega)$. Only need to learn the (unnormalized) spectral density $S(\omega)$ to learn $k(\tau)$.

Model Specification

{Hyperprior}

$$p(\phi) = p(\theta, \gamma)$$

{Latent GP}

$$g(\omega) | \theta \sim \mathcal{GP}(\mu(\omega; \theta), k_g(\omega, \omega'; \theta))$$

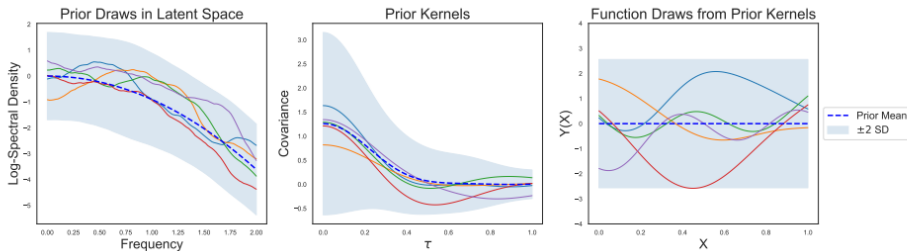
{Spectral Density}

$$S(\omega) = \exp\{g(\omega)\}$$

{Data GP}

$$f(x_n) | S(\omega), \gamma \sim \mathcal{GP}(\gamma_0, k(\tau; S(\omega))).$$

Forward sampling



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Updating Hyper-Parameters: Considering the model specification in Eq. 4, we can define a loss as a function of $\phi = \{\theta, \gamma\}$ for an observation of the density, $\tilde{g}(\omega)$, and data observations $y(x)$. This loss corresponds to the entropy, marginal log-likelihood of the latent GP with fixed data GP, and the marginal log-likelihood of the data GP.

$$\mathcal{L}(\phi) = -(\log p(\phi) + \log p(\tilde{g}(\omega)|\theta, \omega) + \log p(y(x)|\tilde{g}(\omega), \gamma, x)). \quad (7)$$

Updating Latent Gaussian Process: With fixed hyper-parameters ϕ , the posterior of the latent GP is

$$p(g(\omega)|\phi, x, y(x), f(x)) \propto \mathcal{N}(\mu(\omega; \theta), k_g(\omega; \theta))p(f(x)|g(\omega), \gamma). \quad (9)$$

Prediction: The predictive distribution for any test input x^* is given by

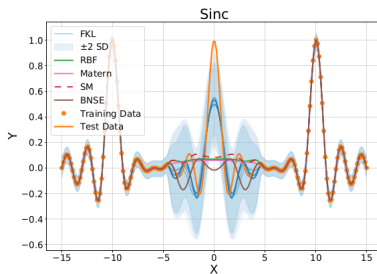
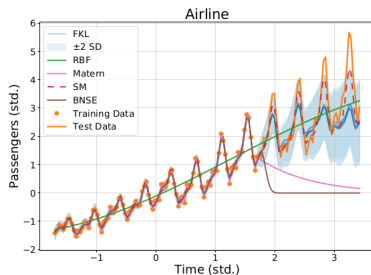
$$p(f^*|x^*, x, y, \phi) = \int p(f^*|x^*, x, y, \phi, k)p(k|x^*, x, y, \phi)dk$$

$$p(f^*|x^*, x, y, \phi) \approx \frac{1}{J} \sum_{j=1}^J p(f^*|x^*, x, y, \phi, k_j), \quad k_j \sim p(k|x^*, x, y, \phi).$$

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Extrapolation and Interpolation



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1. Matthew D Hoffman and Yian Ma. "Langevin Dynamics as Nonparametric Variational Inference". In: *2nd Symposium on Advances in Approximate Bayesian Inference* (2019) "Best Industry paper"
2. Yoshua Bengio Keynote on "Going from System 1 to System 2 Deep learning"
3. NeurIPS Summaries (on Medium):

What we learned from NeurIPS 2019 data



Neural Information Processing Systems Conference Following

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