Random Feature Expansions for Deep Gaussian Processes

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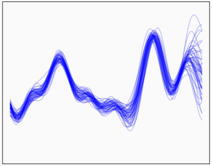
Deep Gaussian Processes

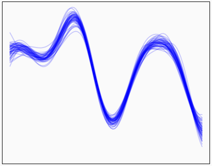
- Deep probabilistic models
- Composition of functions

$$\mathrm{f}(\mathrm{x}) = \left(\mathrm{h}^{(N_{\mathrm{h}}-1)}\left(\boldsymbol{\theta}^{(N_{\mathrm{h}}-1)}\right) \circ \ldots \circ \mathrm{h}^{(0)}\left(\boldsymbol{\theta}^{(0)}\right)\right)(\mathrm{x})$$

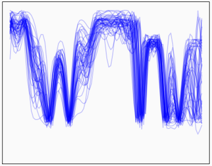
$\mathrm{h}^{(0)}(\mathrm{x})$



$\mathrm{h}^{(1)}(\mathrm{x})$



$\mathrm{h}^{(1)}\left(\mathrm{h}^{(0)}(\mathrm{x})\right)$



- Inference requires calculating the marginal likelihood:

$$
\begin{aligned}
p(Y|X,\boldsymbol{\theta}) \quad = \quad & \int p\left(Y|F^{(N_\mathrm{h})},\boldsymbol{\theta}^{(N_\mathrm{h})}\right) \times \\
& p\left(F^{(N_\mathrm{h})}|F^{(N_\mathrm{h}-1)},\boldsymbol{\theta}^{(N_\mathrm{h}-1)}\right) \times \ldots \times \\
& p\left(F^{(1)}|X,\boldsymbol{\theta}^{(0)}\right) dF^{(N_\mathrm{h})} \ldots dF^{(1)}
\end{aligned}
$$

- **Very challenging!**

Related Work

- Variational DGP (Damianou and Lawrence, 2013)
- Sequential Inference for DGPs (Wang et al., 2016)
- DGP with Expectation Propagation (Bui et al., 2016)
- Variational Auto-Encoded DGP (Dai et al., 2017)
- Dropout as a Bayesian Approximation (Gal and Gahramani, 2016)
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Motivation

Can we develop better DGP models using their connection to DNNs?

1. Faster learning without compromising performance
2. Scalable to very large datasets
3. Extendable to a moderate number of layers

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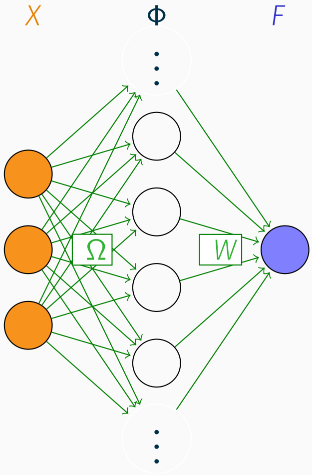
DGP Architecture

DGPs with Random Features

- GPs are single-layered Neural Nets with an infinite number of hidden units



- Weight-space view of a GP

$$F = \Phi W$$

- The priors over the weights are

$$p\left(W_{\cdot i}\right) = \mathcal{N}\left(\mathbf{0}, \mathrm{I}\right)$$

Random Feature Expansion of Kernels

- The **RBF kernel**
- The first order **Arc-Cosine kernel**

Random Feature Expansion of Kernels

- The **RBF kernel** can be approximated using **trigonometric functions**

$$\Phi_{\text{RBF}} = \sqrt{\frac{\sigma^2}{N_{\mathrm{RF}}}} \left[\cos\left(F\Omega\right), \sin\left(F\Omega\right)\right] \quad \text{with} \quad p\left(\Omega_{\cdot j} \middle| \boldsymbol{\theta}\right) = \mathcal{N}\left(\mathbf{0}, \Lambda^{-1}\right)$$

allowing for scaling factors σ^2 and $\Lambda = \mathrm{diag}(l_1^2, \ldots, l_d^2)$

Random Feature Expansion of Kernels

- The first order **Arc-Cosine kernel** can be approximated using **Rectified Linear Units (ReLU)**

$$\Phi_{\mathrm{ARC}} = \sqrt{\frac{2\sigma^2}{N_{\mathrm{RF}}}} \max\left(\mathbf{0}, F\Omega\right) \qquad \text{with} \qquad p\left(\Omega_{\cdot j} \middle| \boldsymbol{\theta}\right) = \mathcal{N}\left(\mathbf{0}, \Lambda^{-1}\right)$$

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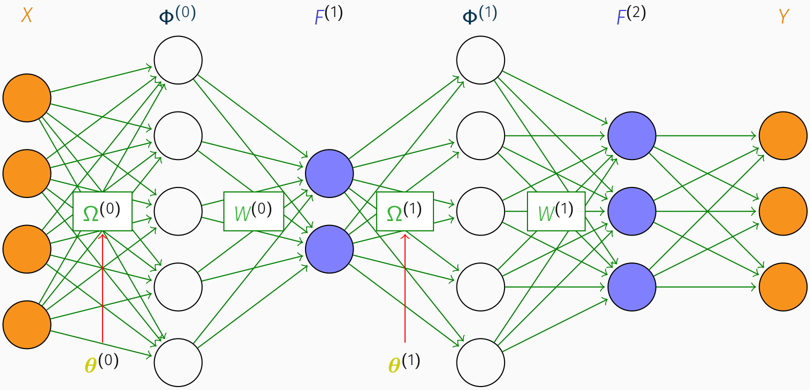
DGPs with RFs become DNNs



Approximating the Marginal Likelihood

DGPs with RFs - Stochastic Variational Inference

- Define $\Psi = \left(\Omega^{(0)}, \dots, \Omega^{(L)}, W^{(0)}, \dots, W^{(L)}\right)$
- Evidence lower bound

$$\log\left[p(Y|\boldsymbol{\theta})\right] \geq \mathbb{E}_{q(\Psi)}\left(\log\left[p\left(Y|\Psi\right)\right]\right) - \mathrm{D_{KL}}\left[q(\Psi)\|p\left(\Psi|\boldsymbol{\theta}\right)\right]$$

where $q(\Psi)$ approximates $p(\Psi|Y, \boldsymbol{\theta})$

- $\mathrm{D_{KL}}$ computable analytically if q and p are Gaussian!

DGPs with RFs - Stochastic variational inference

- Assume factorized likelihood:

$$p(Y|X, \Psi, \theta) = \prod_{\mathrm{k}} p(\mathbf{y}_{\mathrm{k}}|\mathbf{x}_{\mathrm{k}}, \Psi, \theta)$$

- Stochastic **unbiased** estimate of the expectation term
  - **Mini-batch**

$$\mathbb{E}_{q(\Psi)}\left(\log\left[p(Y|X, \Psi, \theta)\right]\right) \approx \frac{n}{m} \sum_{\mathrm{k} \in \mathcal{I}_m} \mathbb{E}_{q(\Psi)}\left(\log[p(y_{\mathrm{k}}|\mathbf{x}_{\mathrm{k}}, \tilde{\Psi}, \theta)]\right)$$

  - **Monte Carlo**

$$\mathbb{E}_{q(\Psi)}\left(\log\left[p(y_{\mathrm{k}}|x_{\mathrm{k}}, \Psi, \theta)\right]\right) \approx \frac{1}{N_{\mathrm{MC}}} \sum_{r=1}^{N_{\mathrm{MC}}} \log[p(y_{\mathrm{k}}|x_{\mathrm{k}}, \tilde{\Psi}_r, \theta)]$$

with $\tilde{\Psi}_r \sim q(\Psi)$

DGPs with RFs - Stochastic variational inference

- Factorized approximate posterior

$$q(\Psi) = \prod_{ijl} q\left(\Omega_{ij}^{(l)}\right) \prod_{ijl} q\left(W_{ij}^{(l)}\right)$$

where

$$q\left(\Omega_{ij}^{(l)}\right) = \mathcal{N}\left(\mu_{ij}^{(l)}, (\sigma^2)_{ij}^{(l)}\right) \quad \text{and} \quad q\left(W_{ij}^{(l)}\right) = \mathcal{N}\left(m_{ij}^{(l)}, (s^2)_{ij}^{(l)}\right)$$

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- Reparameterization trick

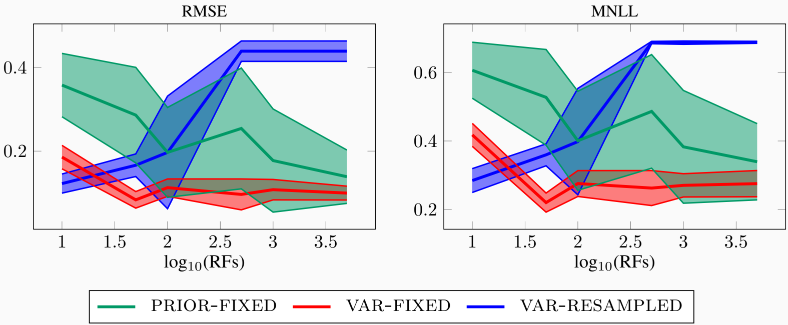
$$\left(\tilde{W}_r^{(l)}\right)_{ij} = \left(s^2\right)_{ij}^{(l)} \epsilon_{rij}^{(l)} + m_{ij}^{(l)}$$

with $\epsilon_{rij}^{(l)} \sim \mathcal{N}(0, 1)$

Optimization Strategies for Ω

- Random features can be **fixed**
  - PRIOR-FIXED

  or treated **variationally**
  - VAR-FIXED (with fixed randomness)
  - VAR-RESAMPLED (resampled at each iteration)

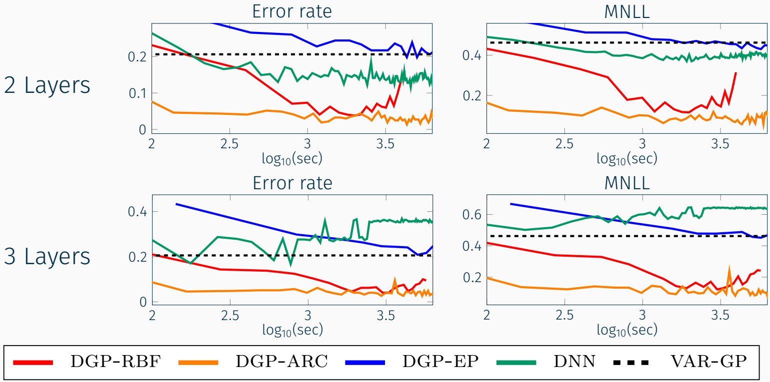


Evaluation

Model Comparison - Binary Classification

EEG Dataset

(n = 14979, d = 14)

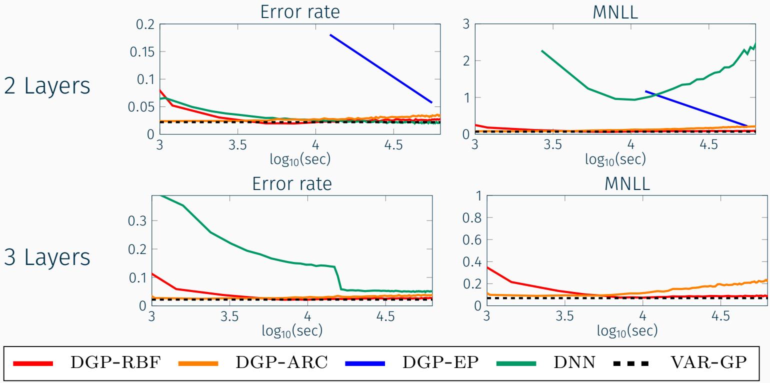


- Consistently outperforms competing techniques both in terms of **speed** and **predictive performance**

Model Comparison - Multiclass Classification

MNIST Dataset

$(n = 60000, d = 784)$



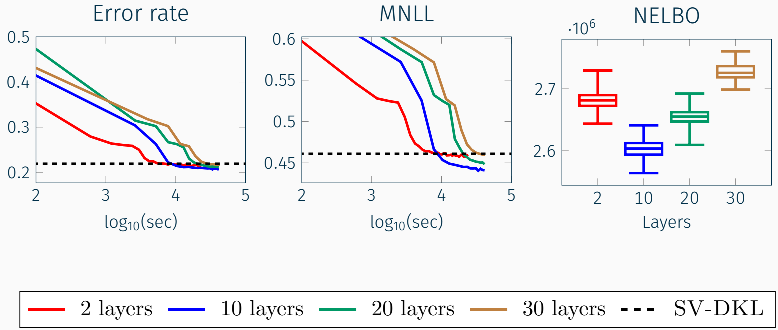
- Model performance remains resilient compared to other techniques

Scalability to Large Datasets

- Over 99% accuracy on variant of MNIST with 8.1 million images!

Dataset	Accuracy		MNLL	
	RBF	ARC	RBF	ARC
MNIST8M	99.14%	99.04%	0.0454	0.0465
AIRLINE	78.55%	72.76%	0.4583	0.5335

Performance of Deeper Models - Airline Dataset



- Model converges to an optimal state for every configuration
- NELBO confirmed to be a suitable criteria for model selection
- Includes feed-forward of inputs to each layer

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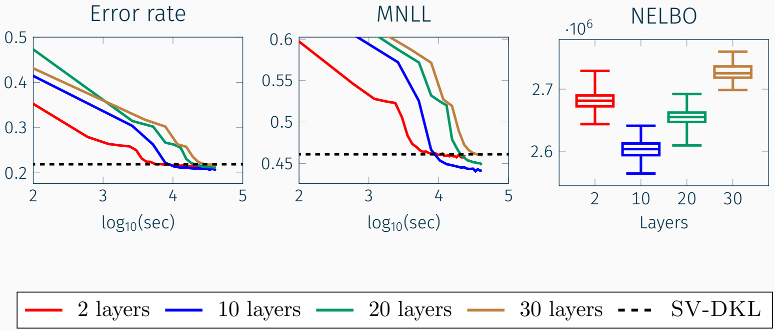

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  - A complete evaluation of DGPs inspired by DNNs
  - Scalable and practical DGP inference without requiring Cholesky
  - A study of various options for optimizing random features
  - Distributed implementation using Parameter-Server framework

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- Contributions
  - A complete evaluation of DGPs inspired by DNNs
  - Scalable and practical DGP inference without requiring Cholesky
  - A study of various options for optimizing random features
  - Distributed implementation using Parameter-Server framework
- Ongoing work
  - Fastfood kernel and orthogonal random features
  - Convolutional GP layers for complex image datasets
  - Hybrid synchronous/asynchronous distributed approach

Code in TensorFlow:

`github.com/mauriziofilippone/deep_gp_random_features`

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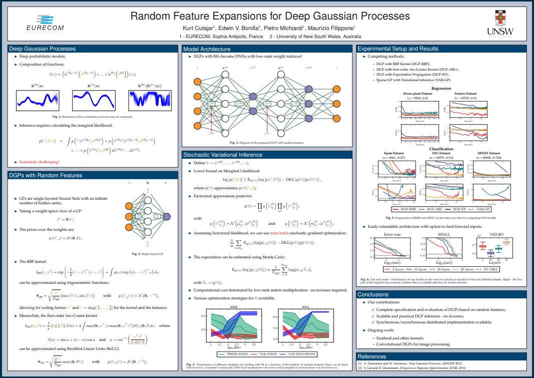

Poster #126

Thank you!