# Shaping the Neural Linear Model

Max Guo

Data to Actionable Knowledge Lab
Summer Program for Undergraduates in Data Science (SPUDS)
Harvard University

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# Research Overview

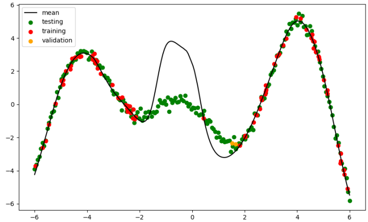
**Problems:**

- Deep neural networks do not provide predictive uncertainties.
- Probabilistic inference via Gaussian Processes (GPs) is computationally expensive and requires complicated tuning to perform well on some types of data.
- Combining Bayesian inference with neural networks via a model known as the *Neural Linear Model* (NLM) may suffer from overfitting to the data and tuning issues.

**My Research:**

- Develop and analyze variations of the NLM that can combine the strengths of the traditional NLM and fixed-kernel GPs.

# Lack of Predictive Uncertainty in Neural Networks



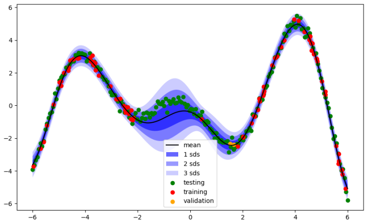




Figure: Feedforward Neural Network vs. Gaussian Process with RBF Kernel

# Neural Linear Model (NLM)

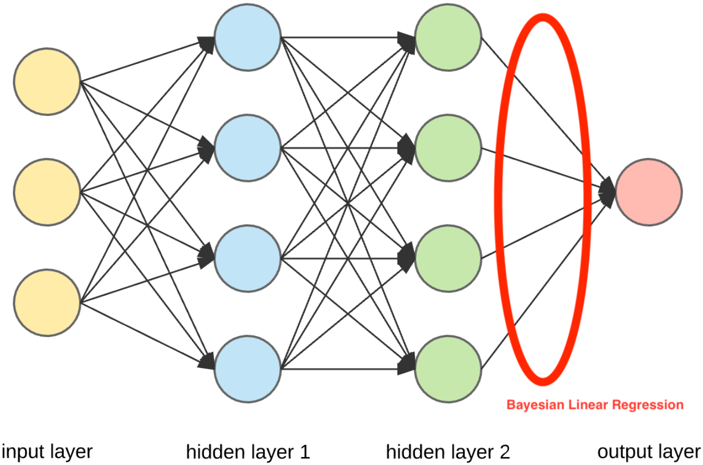



Figure: Neural Linear Model, Visual

# Predictive Uncertainty in NLMs

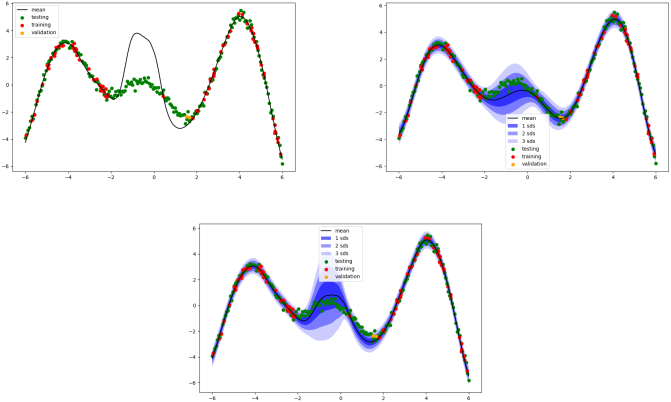



Figure: Top: Feedforward Neural Network (Left) GP (Right)
Bottom: NLM

# Problems with NLMs

- NLMs also suffer from problems:
  - NLMs require much hyperparameter tuning
  - NLMs may not express desirable uncertainties in areas of data sparsity.

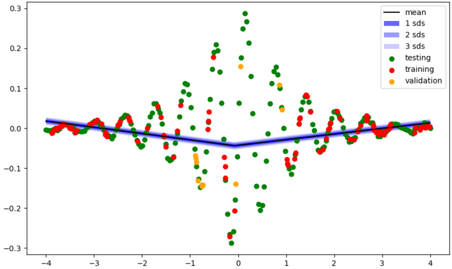



Figure: Trained NLM does not fit data at all.

# Problems with GPs

- Besides computational issues, fixed-kernel GPs do not adapt well to varying data attributes across the input space (e.g. smoothness).

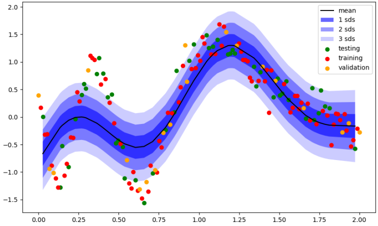



Figure: Fixed-kernel GP does not capture all of the function.

# Research Goal

**Goal**: Create a variation on the NLM to capture strengths of both NLMs and fixed-kernel GPs.

**Goal, Rephrased**: Because NLMs are GPs with data-adaptive kernels, can we create a spectra of models that interpolates between NLMs and GPs?


Figure: Slider between NLM and Fixed-kernel GP

# Proposed Models

I consider three variations on NLMs that can interpolate between a traditional NLM and a fixed-kernel GP:

1. NLMSubset
2. NLMDecoupled
3. NLMRegularize

# NLMSubset and NLMDecoupled

- Train a subset of the bases normally
- Train the other subset to match a fixed-kernel GP on mini-batches of data in terms of the Gram matrix.
- (For NLMSubset) Combine the losses for the loss function:

$$L(\theta) = L_1(\theta_1) + \lambda \cdot L_2(\theta_2)$$

- Number of bases is the sliding parameter.

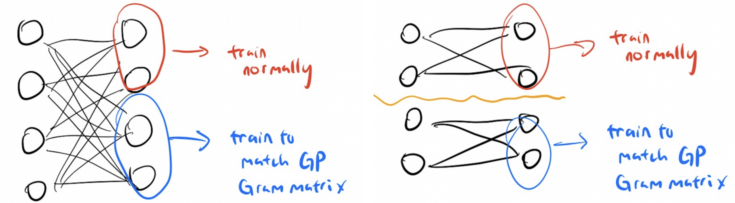



Figure: NLMSubset (left), NLMDecoupled (right)

# NLMRegularize

- Modify the training objective so all of the bases jointly attempt to fit the data and match the GP Gram matrix:

$$L(\theta) = L_1(\theta) + \lambda \cdot L_2(\theta)$$

- Regularizing constant $\lambda$ is the sliding parameter.

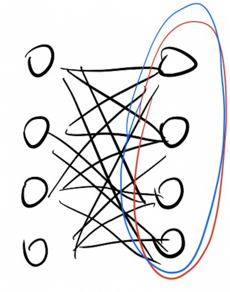


Figure: NLMRegularize

# Preliminary Results

On synthetic 1 dimensional datasets, these methods often give us desirable solutions to the problems that traditional NLMs and GPs present:

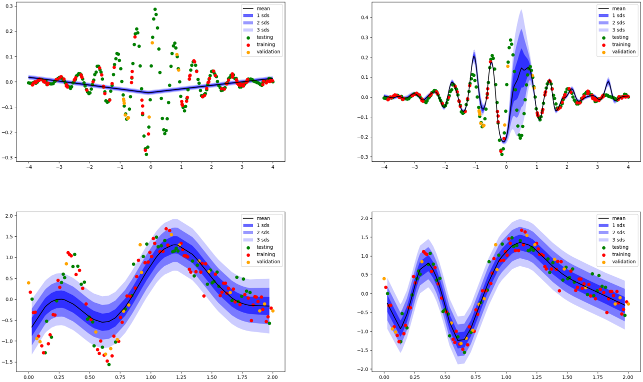
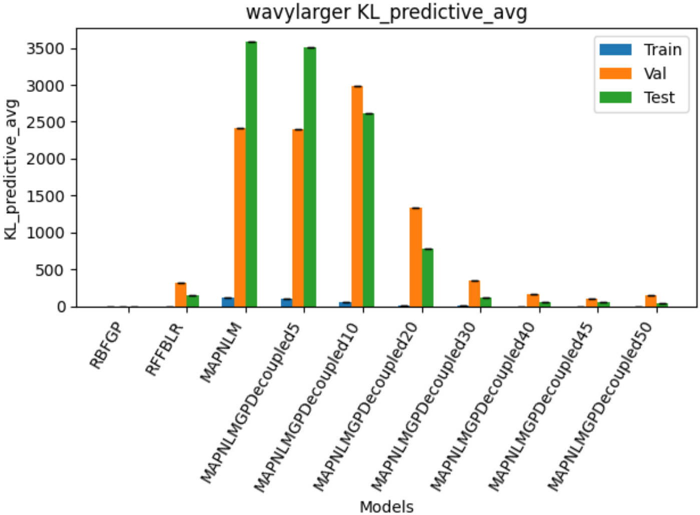



Figure: Wavy (top) and nonstationary (bottom) datasets, where NLMs and GPs fail, respectively (left). NLMRegularize (right) succeeds.

# Preliminary Results

On synthetic 1 dimensional datasets, each of these methods gives us a desired interpolation of models:



# Future Directions

Though the three models are relatively successful in carefully constructed, simple scenarios, more research is required before ascertaining conclusions.

Questions that need to be addressed:

- What distinguishes these three types of models from each other?
- Does the interpolation for these models generalize to higher dimensional, real-world datasets?
- How do these methods compare to kernel-learning in GPs?

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