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Task-Agnostic Amortized Inference of Gaussian Process Hyperparameters

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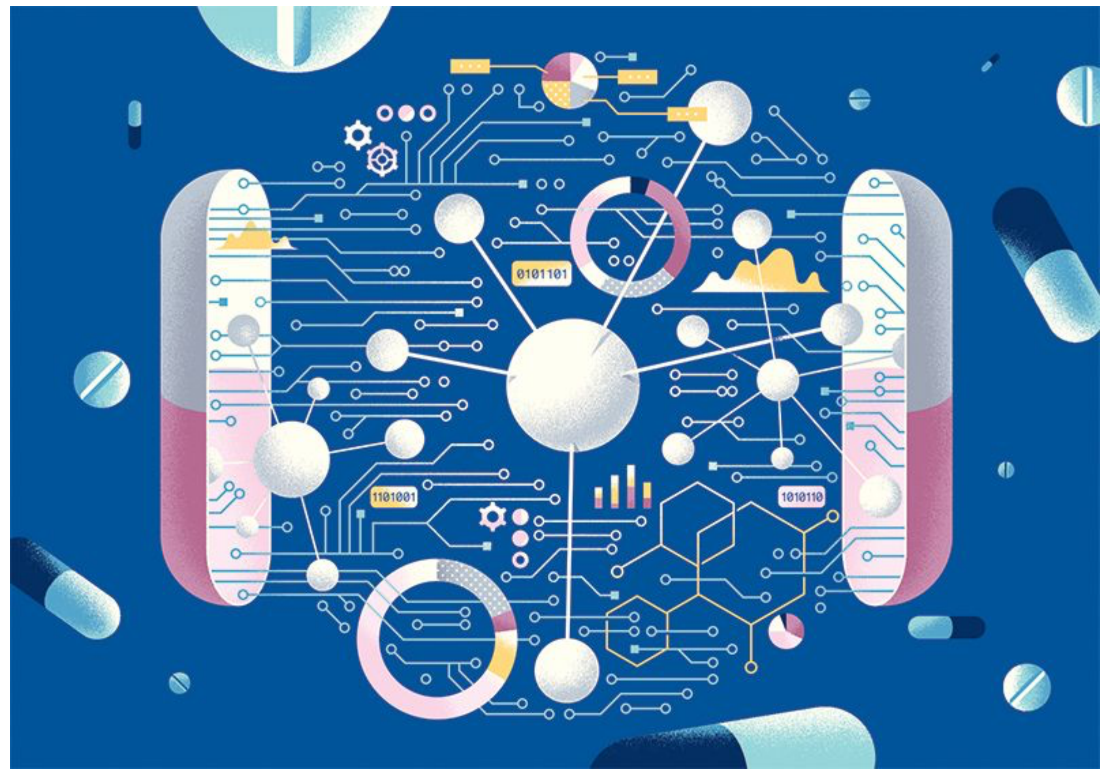
Joint work with Xingyuan Sun, Peter J. Ramadge, Ryan P. Adams

TL;DR: A single neural net is able to perform comparably well on unseen GP tasks, while being ~100 times faster than conventional procedures

PRINCETON
LABORATORY FOR INTELLIGENT PROBABILISTIC SYSTEMS

Gaussian processes

- GPs are **flexible** priors for modeling functions with **tractable** inference



BayesOpt for drug discovery

BayesOpt for hyperparameter tuning of DNN

Planning and control

Model selection problem in GPs

- GP prediction performance depends critically on its **kernel function** accurately **reflecting the structure of the problem**
- But finding a good kernel function is:
  - **Tricky**: figuring out what kernel function to use, Squared Exponential or Matérn? Periodicity?
  - **Costly**: searching for good kernel hyperparameters, usually through costly marginal likelihood maximization (**$O(n^3)$** per iteration)

Motivation

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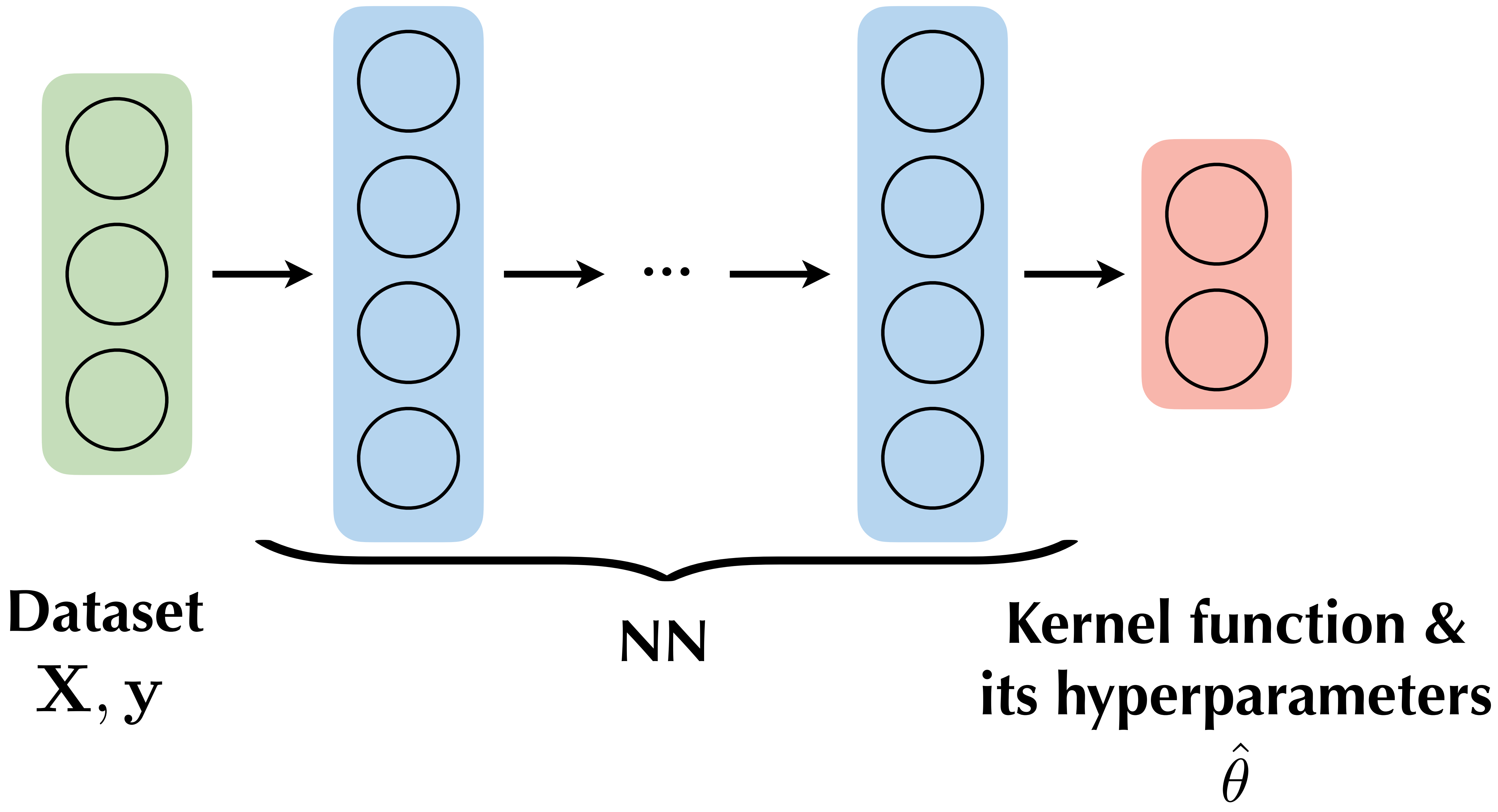
- Idea: can we **amortize** this expensive model selection procedure with direct estimate from a neural network?
    - Inspiration from amortized variational inference literature (e.g. VAE)



Amortized Type II Maximum Likelihood:

$$\hat{\theta} \approx \arg\max_{\theta} \; \log p(\mathbf{y}|\mathbf{X}, \theta)$$

How to parametrize the space of kernel functions?

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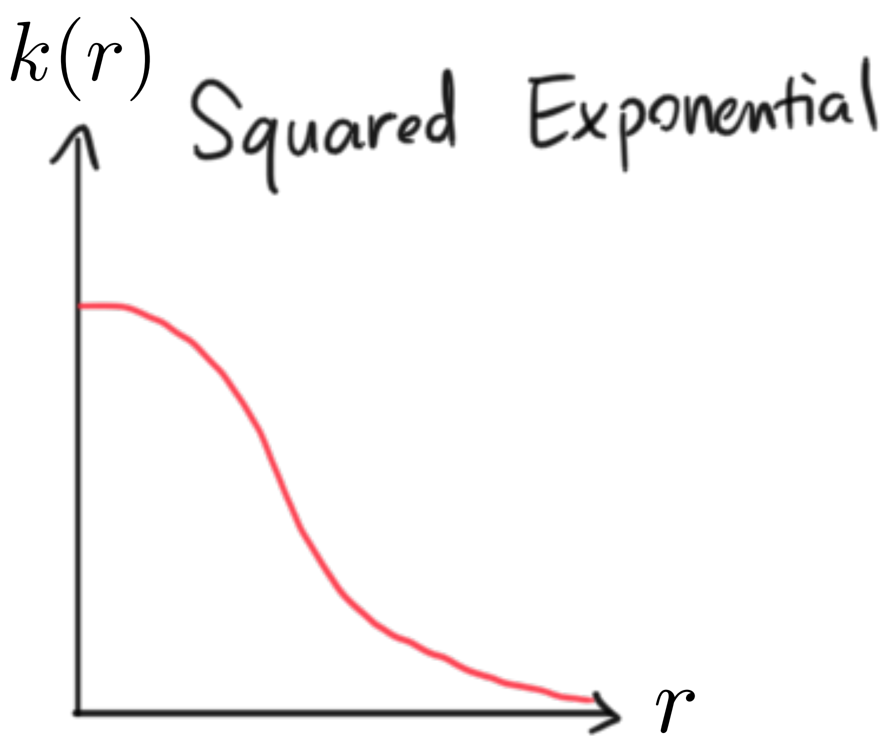
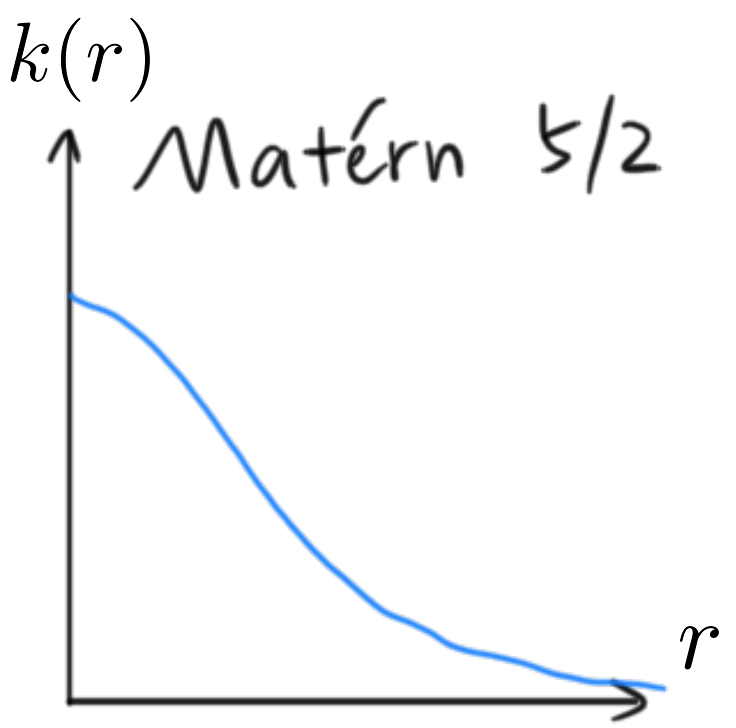


kern_type = 0, lengthscale = 2



kern_type = 1, lengthscale = 3

Compositional kernel modeling

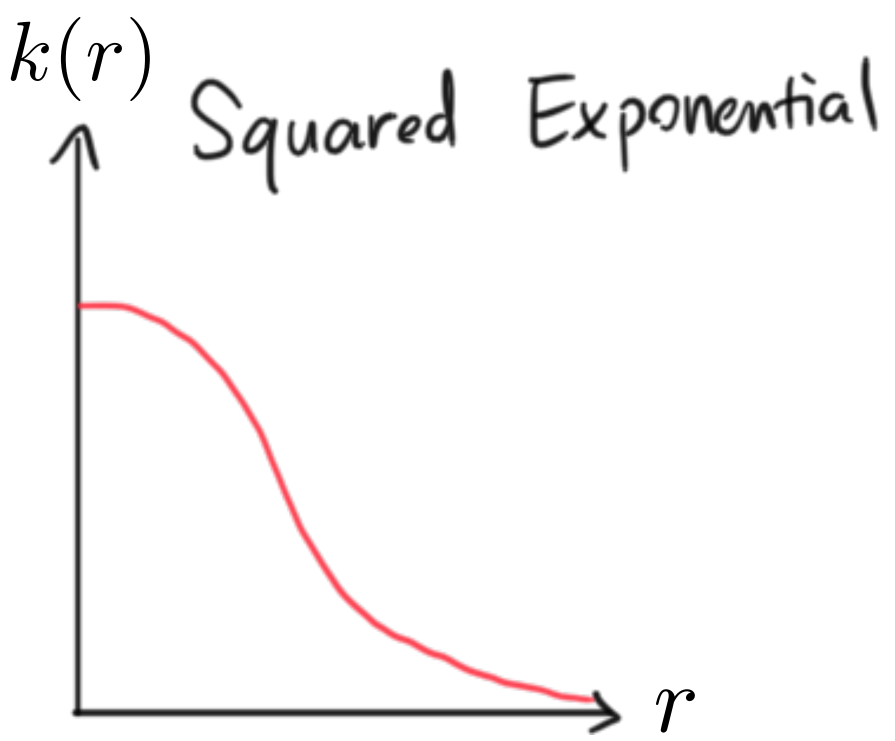
Use composition rules to build more complicated ones

- $k_0 + k_1 + \ldots$
- $k_0 * k_1 * \ldots$

A **very hard** learning problem!

1. a mix of discrete and continuous variables
2. intercorrelated variables: such as kern_type and lengthscale in this case

How to parametrize the space of kernel functions?



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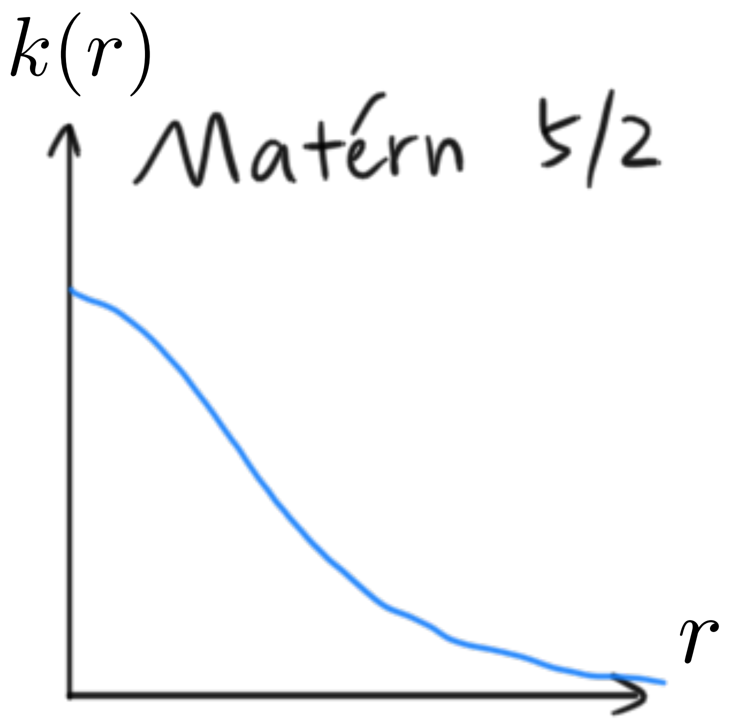

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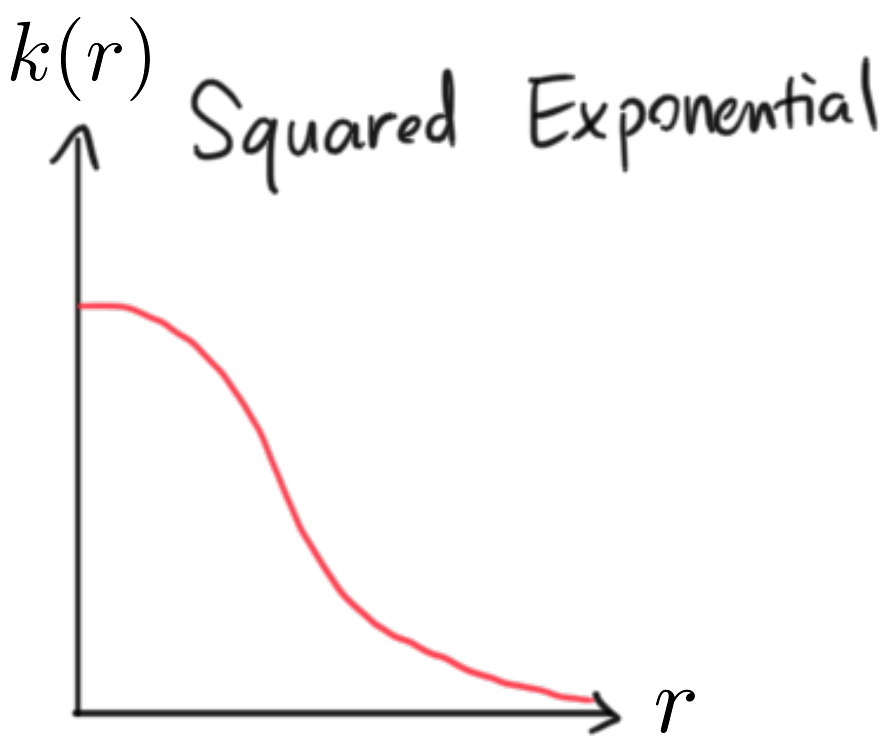

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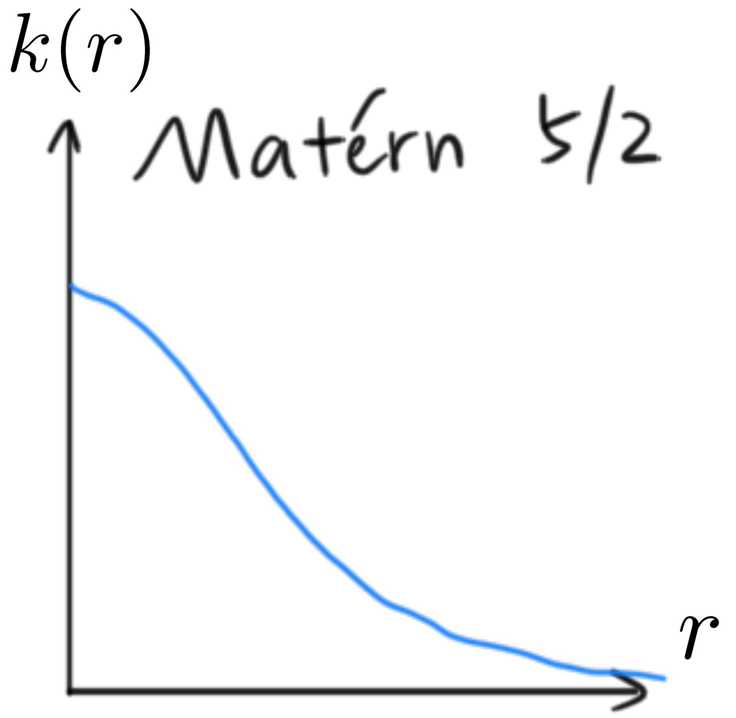
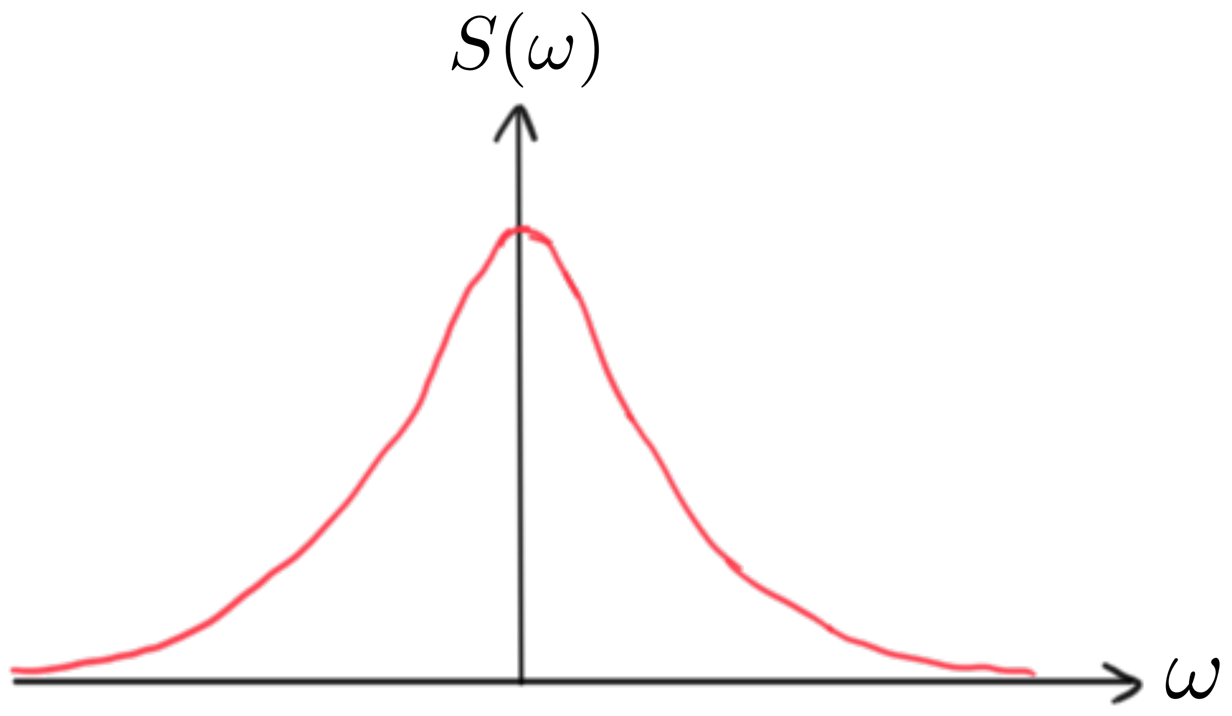


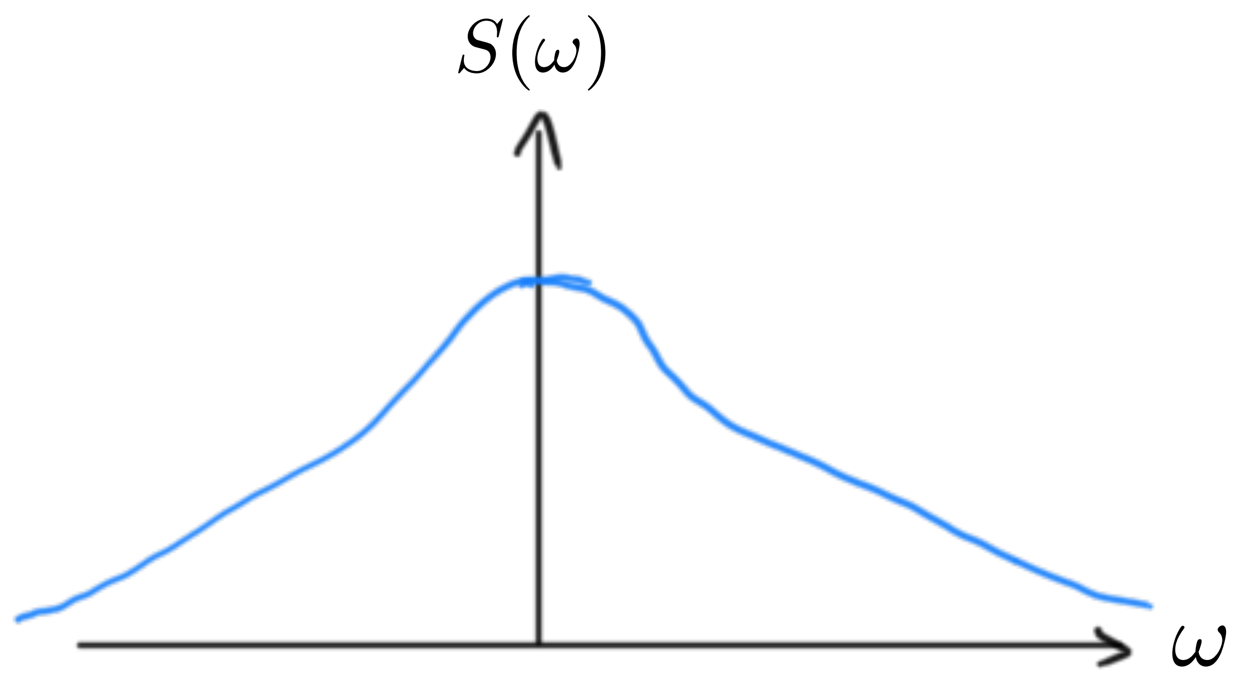
kern_type = 1, lengthscale = 3

Bochner's Theorem

$$k(r) \Leftrightarrow S(\omega)$$

$$S(\omega) = \int k(r) e^{-2\pi i \omega r} dr$$





Compositional kernel modeling

Spectral density modeling

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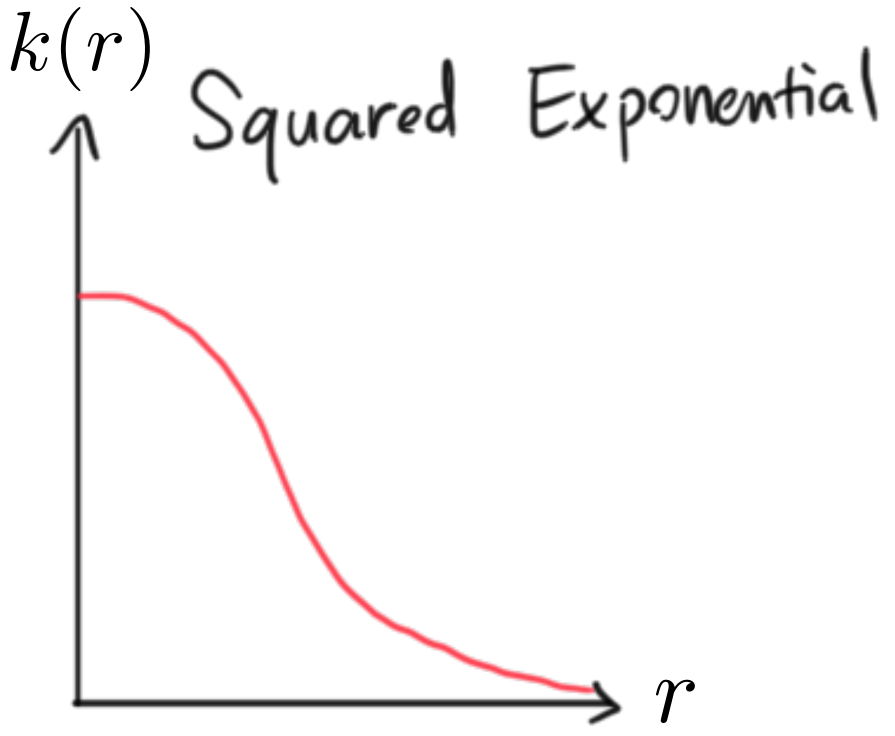

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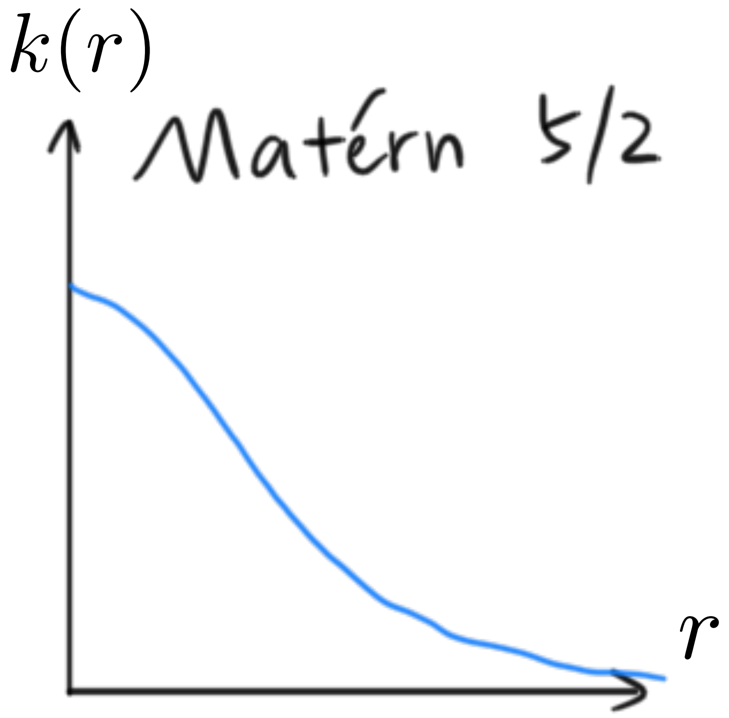

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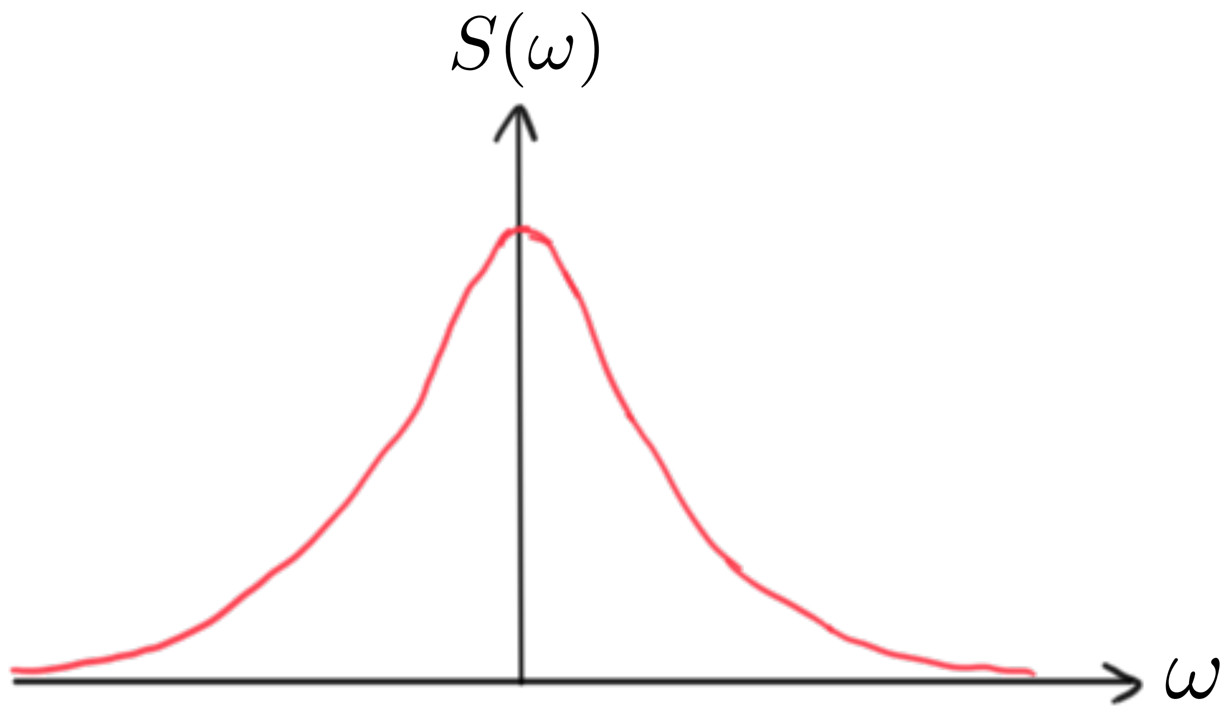
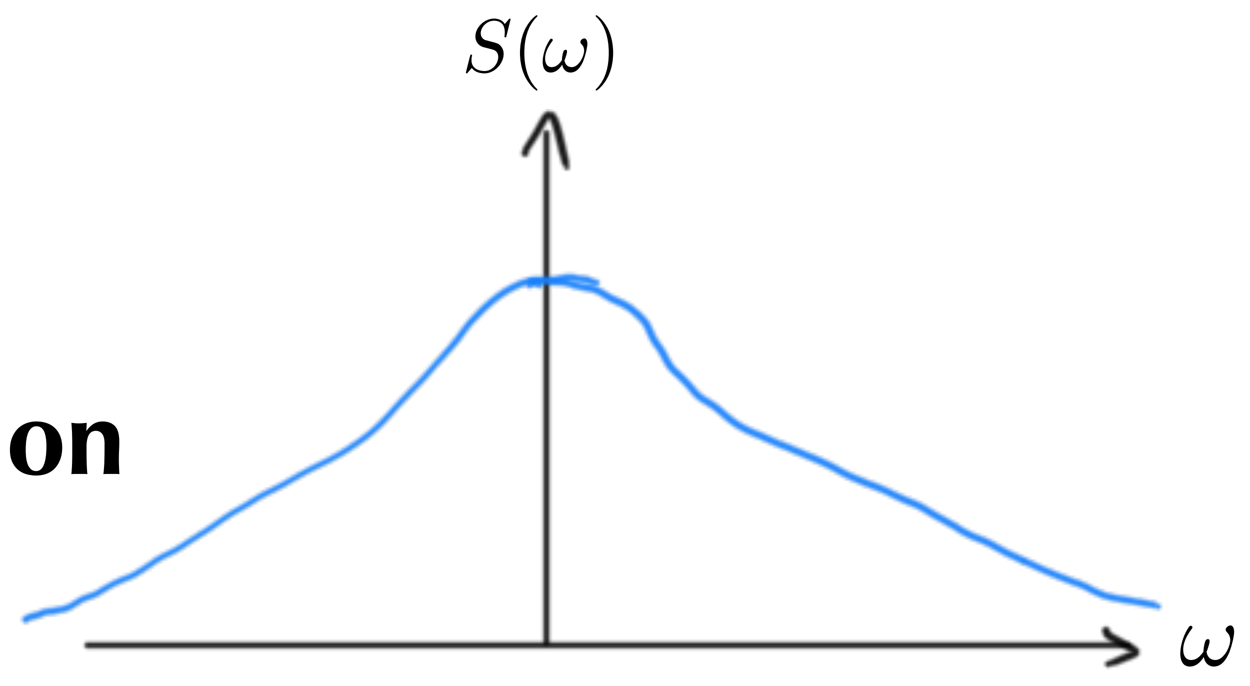
For any stationary kernel function





Compositional kernel modeling

Spectral density modeling

Amortized hyperparameter inference for Gaussian processes (AHGP)

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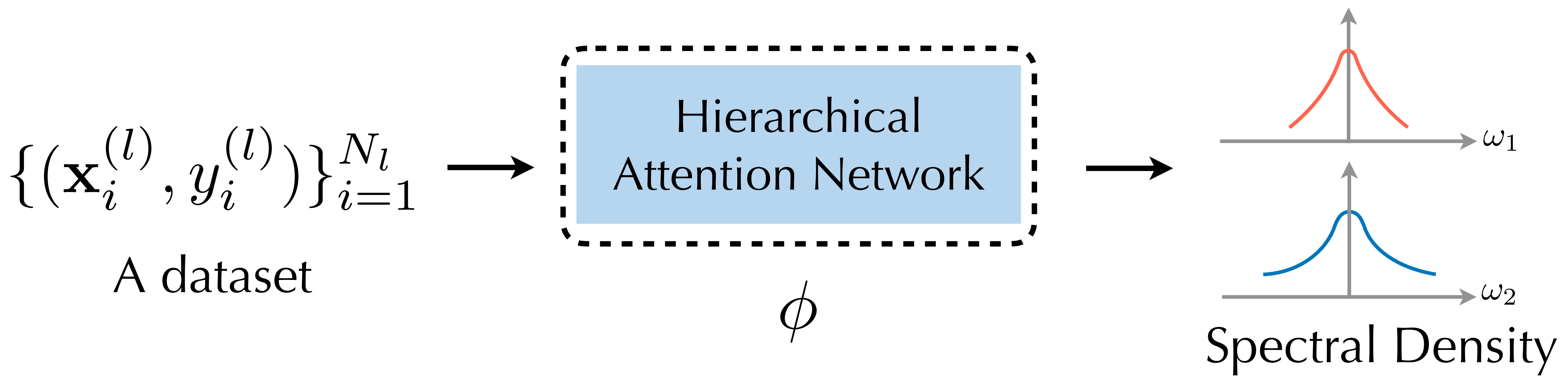
$\{(\mathbf{x}_i^{(l)}, y_i^{(l)})\}_{i=1}^{N_l}$

A dataset

Amortized hyperparameter inference for Gaussian processes (AHGP)

$$\underbrace{\{(\mathbf{x}_i^{(l)}, y_i^{(l)})\}_{i=1}^{N_l}}_{\text{A dataset}} \longrightarrow \underbrace{\boxed{\text{Hierarchical Attention Network}}}_{\phi}$$

Amortized hyperparameter inference for Gaussian processes (AHGP)



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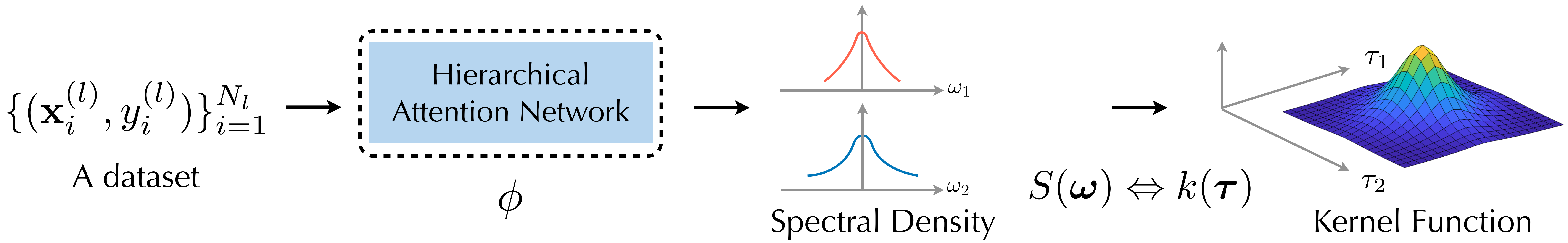

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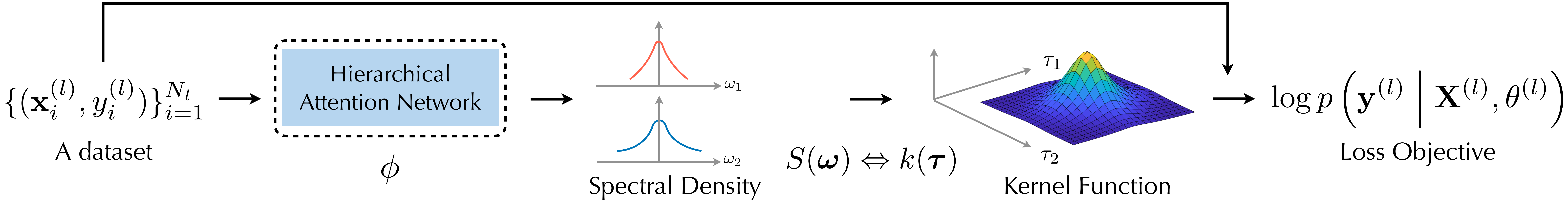

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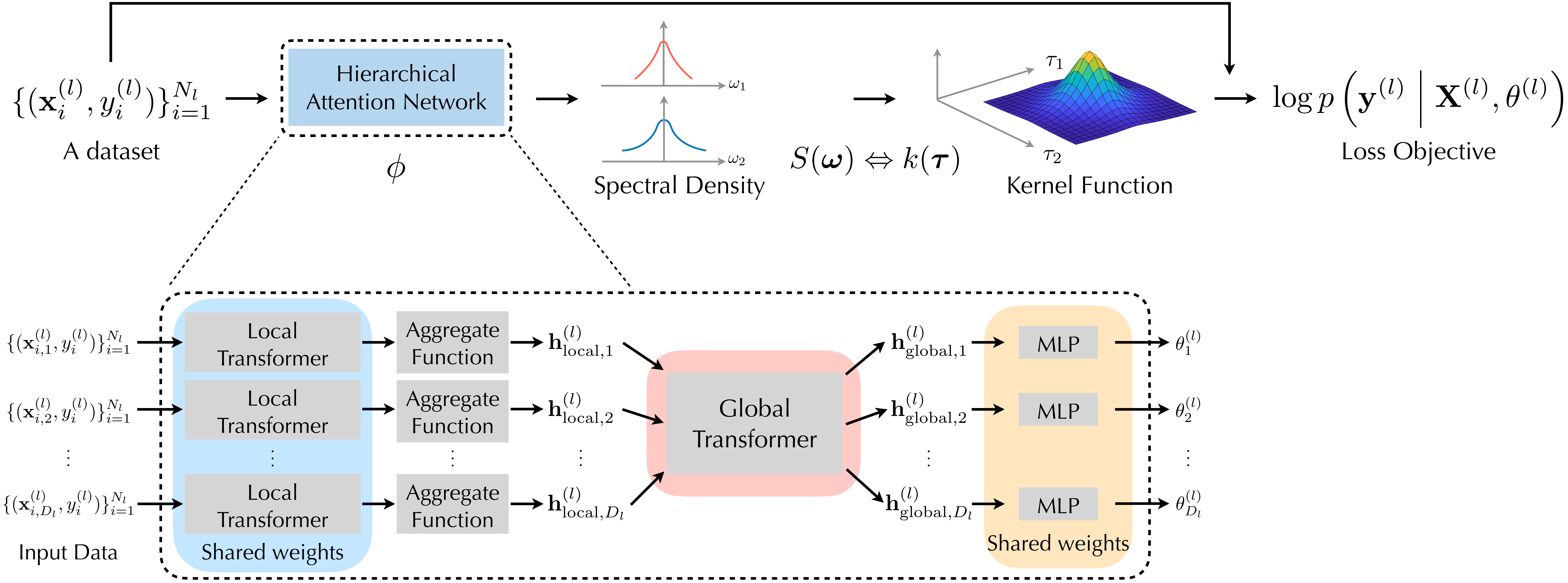

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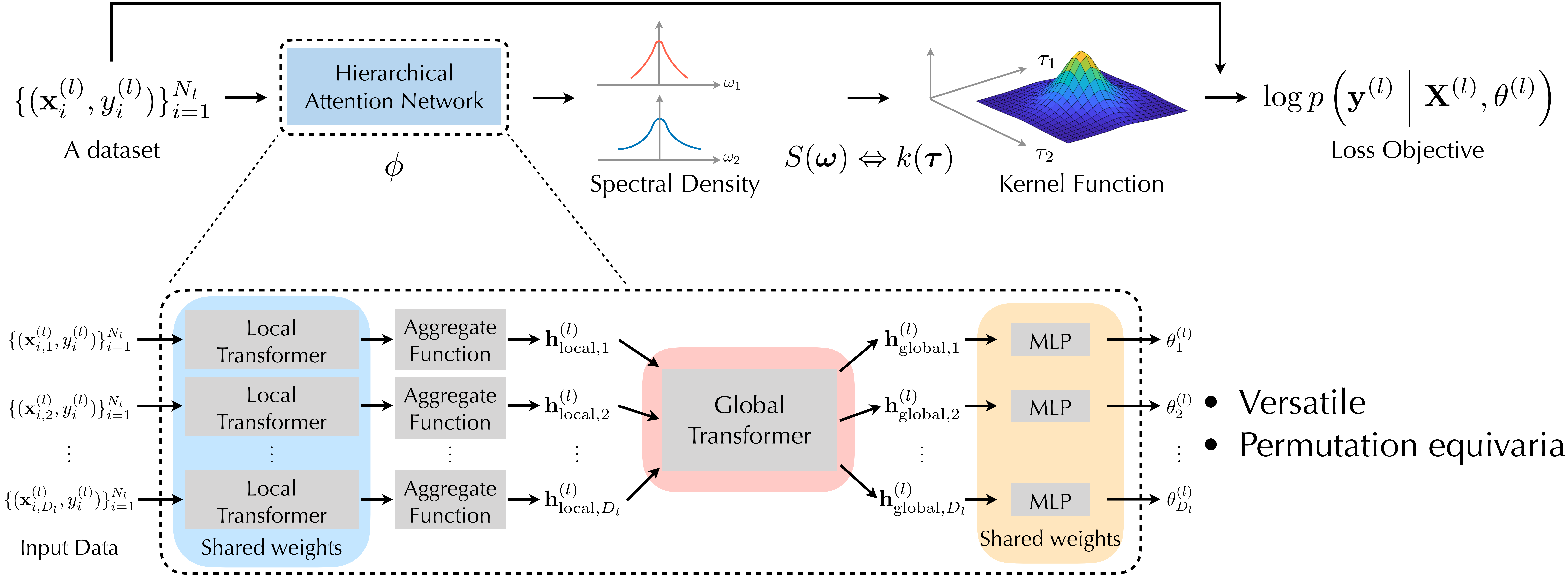

- Versatile
- Permutation equivariant

Experimental results

- Training data: 5k **synthetic** datasets generated from GP priors with stationary kernels
- Training objective: $\mathcal{L}\left(\phi, \left\{\mathcal{D}^{(l)}\right\}_{l=1}^{L}\right) = -\frac{1}{L}\sum_{l=1}^{L}\frac{1}{N_l}\log p\left(\mathbf{y}^{(l)} \,\middle|\, \mathbf{X}^{(l)}, \theta^{(l)}\right)$
- Training method: Adam with fixed learning rate, dropout on self-attention encoders
- Results:
  - **One trained model for all**: a **single** trained neural net is able to produce hyperparameters of comparable quality to MLL-opt methods across different **unseen** real-world benchmarks (regression, BayesOpt, BayesQuadrature)
  - **Super lightweight**: ~100 times faster than MLL-opt
  - Even performs slightly **better** on relatively **smaller** dataset (due to implicit regularization in training)

Interested in AHGP?
Come to our poster session :)

Code: https://github.com/PrincetonLIPS/AHGP

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