Functional Emulation of Temperature Profiles in Spatial Domain

Yiming Yang

Supervisor: Prof. Serge Guillas

Department of Statistical Science, University College London

1. Motivation

- The need to fit smooth physical profiles widely ranges in physics and engineering research.
- High-resolution simulation is unaffordable in computation, statistical emulators or surrogates are necessary for further tasks like model calibration and uncertainty qualification.
- Functional representation for spatial data performs better in capturing the inherent smoothness and variation than discretisation.

2. Methods: Outer Product Emulator

The high-resolution physical simulation will output high-dimensional data over some discretised spatial domains. For example, the wave heights in a part of the ocean and temperature fields over a heating system. Such high-dimensionality brings serious challenges in building statistical emulators. Traditional emulators either struggle with scalability or accuracy.

For balancing these two factors, the Outer Product Emulator (OPE) is introduced. The OPE creates one emulator for all the simulation outputs over the whole domain and simplifies the representation of fitted functions by products of component functions. In general, the OPE has the form:

$$f_i(r) = \sum_{j=1}^{v} \beta_j g_j(r, s_i) + \epsilon(r, s_i)$$

where $f_i(r)$ is the ith simulator output with input r, the g_j are the regressor functions, the β_j are unknown coefficients and ϵ is the residual assumed to be a Gaussian Process (GP) such that $\epsilon \sim GP(0, \kappa_\lambda(\cdot))$.

Two main characteristics distinguish the OPE from conventional multivariate emulator. The first is that the covariance function of the residuals is separated into inputs r and outputs s, that is, $\kappa_\lambda(r, s, r', s') = \kappa_\lambda^r(r, r') \times \kappa_\lambda^s(s, s')$. The second is that the regressor functions g_j are given by products $g_j(r, s) = g_j^r(r) \otimes g_j^s(s)$ where $\otimes$ is the outer product symbol.

3. Example: 2-D model of Anisotropic Heat Transport

The model for time evolution of the temperature field T is thermal diffusion, which in a plasma after Braginskii parametrization gives:

$$\frac{3}{2} N \frac{\partial T}{\partial t} = \nabla \cdot (k_{\|} \mathbf{b}[\mathbf{b} \nabla T] + k_{\perp}(\nabla T - \mathbf{b}[\mathbf{b} \nabla T])$$

where b indicates the magnetic field and $k_{\|}, k_{\perp}$ are the thermal conductivities with respect to the direction parallel or perpendicular along the b. The homogenous Dirichlet boundary conditions are set on the left, top, and right boundaries of the spatial domain.

In this example, we are interested in emulating the relationship between direction θ of $\mathbf{b}$ and the temperature profile T_x on the bottom boundary at steady state by OPE such that:

$$f_{OPE} : \theta \to T_x,\ \theta \in [0, \frac{\pi}{2}],\ T_x \in C[0,1]$$

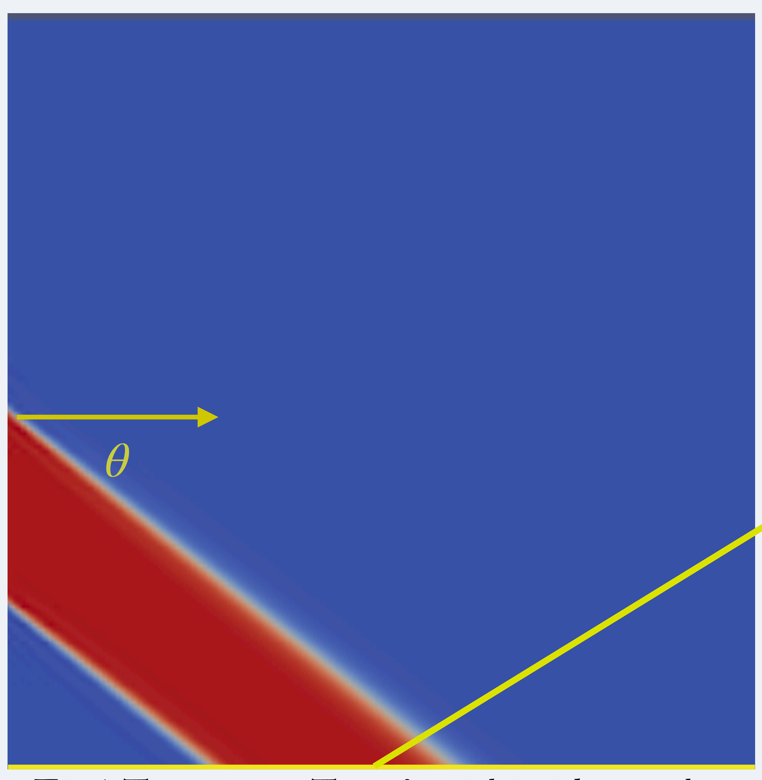

Fig.1 Temperature Transfer with incident angle θ

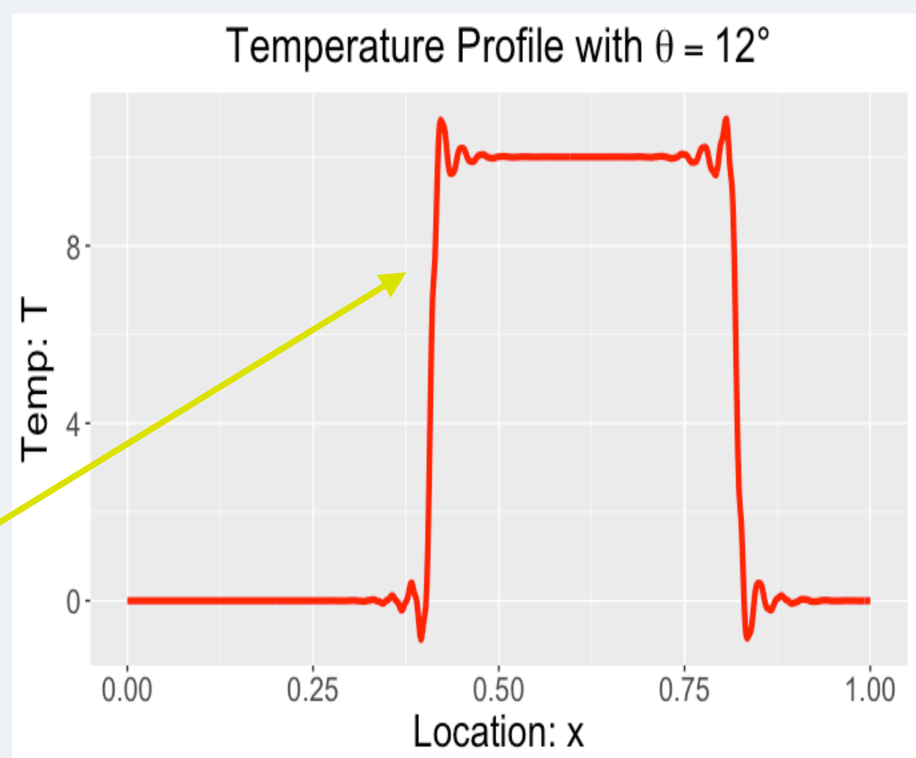

Fig.2 Temperature Profile on bottom boundaries given θ

We conducted the OPE with the following settings:

- Input Regressor: $g_j^r(\theta) = \{1,\ 6\theta - 1,\ 6\theta^2 - 6\}$ which is the Legendre Polynomials up to the second order.
- Output Regressor: $g^s(x) = \{h_j(x)\}_{j=0}^{3}$ where $h_j(x)$ is the j_{th} Haar Wavelets functions. We choose Haar Wavelets based on the shape of temperature profile shown in Fig. 2.
- Covariance Kernel: $k(x, \theta, x', \theta') = \exp(-(\frac{|\theta - \theta'|}{\lambda_r})^{\frac{3}{2}}) \times \exp(-(\frac{|x - x'|}{\lambda_s})^{\frac{3}{2}})$ which is widely used power exponential kernel.

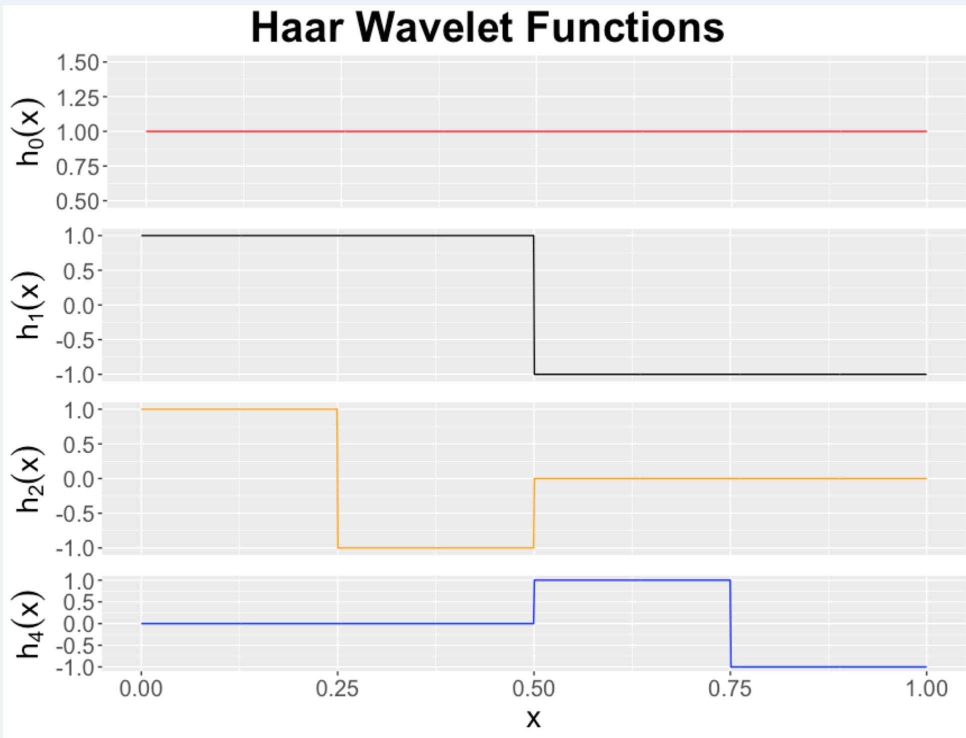

Fig.3 First 4 Haar wavelet Functions

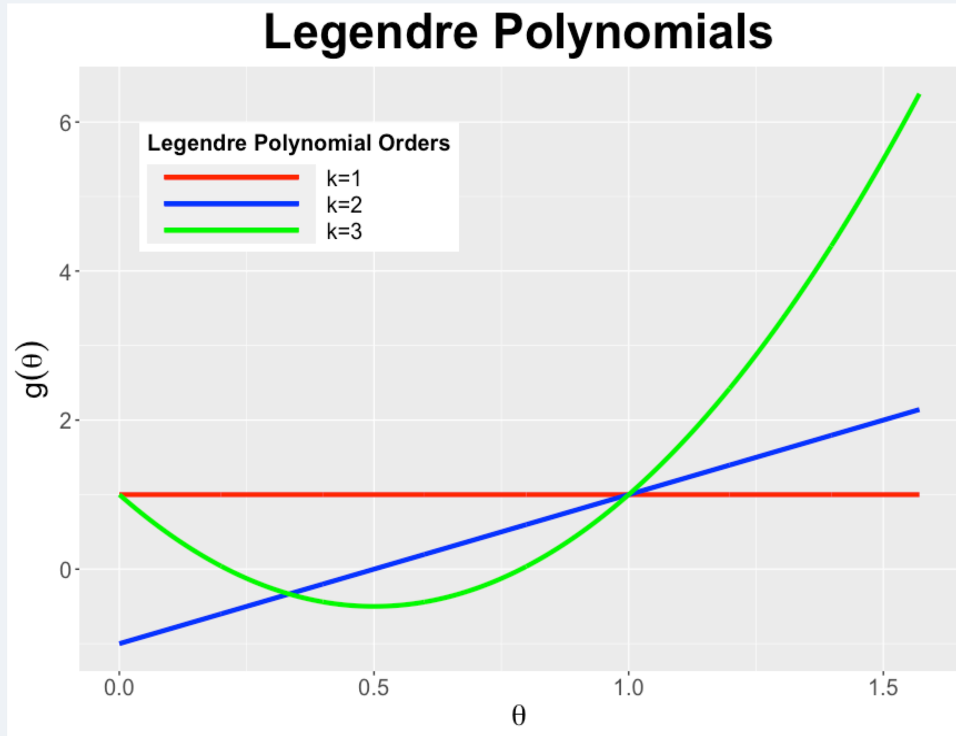

Fig.4 Legendre Polynomials up to second order

4. Results

Model evaluations are available for 40 different θs which are evenly chosen to cover the input parameter space. For each evaluation, There are 641 discretised values.

We implement the OPE in two settings:

- **Emulation for Simulation output**: In this case, We use all the 641 discretised values to fit the OPE for emulating the computational model.
- **Emulation for Experimental observation**: We uniformly sampled 80 values from the 641 discretised values added with random noise for fitting a profile by observed experimental data.

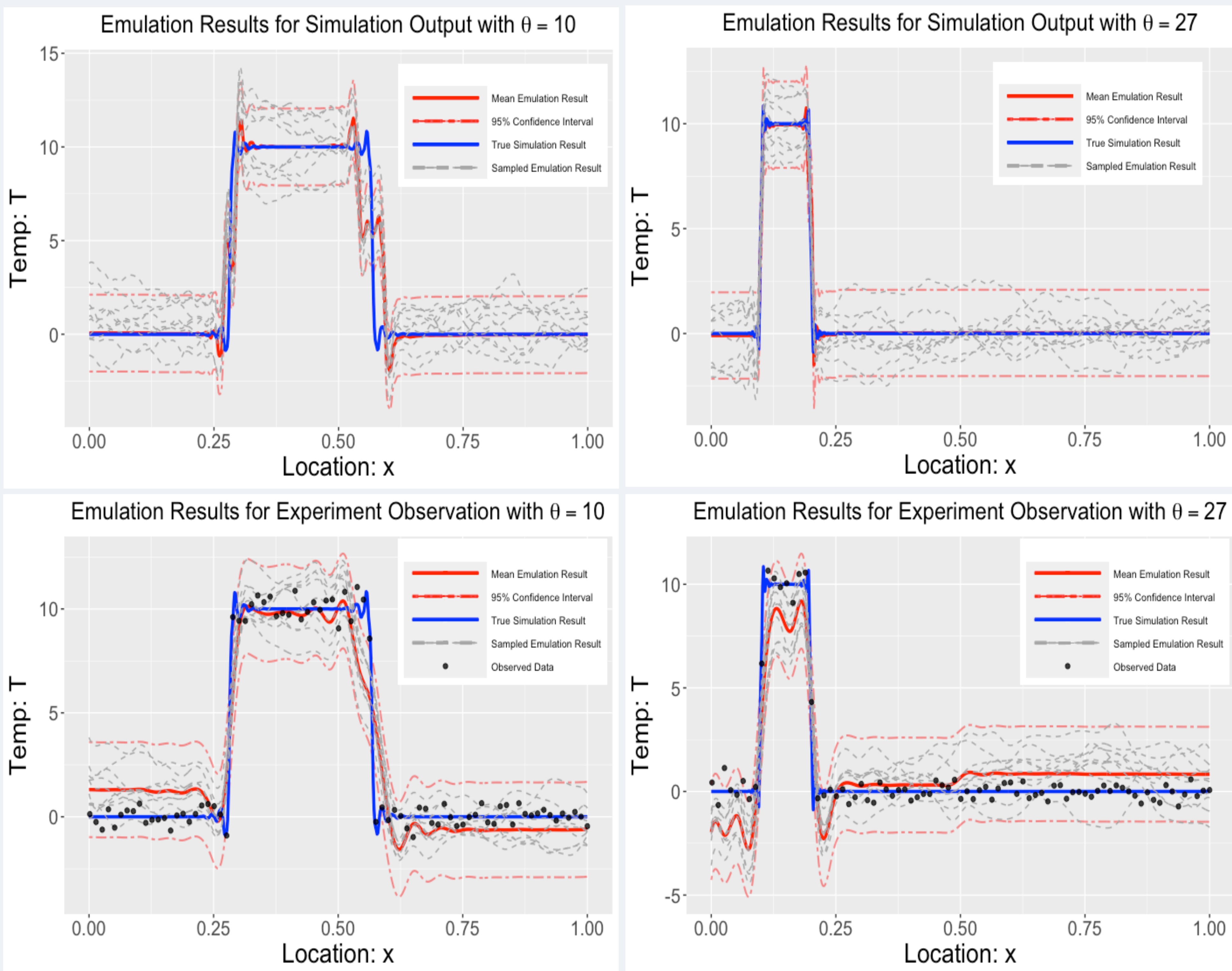

Fig.5 Emulation Results for Simulation outputs and experimental observations with two different θs

5. Findings & Next Steps

- OPE is an efficient statistical emulator for both high-resolution simulation models and actual experiments.
- Use the emulator to conduct the sensitivity analysis over large physical domains to input parameters, with uncertainty propagations.
- Generalise the OPE in the manifold to emulate the functions in some curved domains like tori by designing the covariance kernels and regressors