

A Appendix

Our posited structural equation for INR (Y) is a linear regression of the parents of Y in Figure 6. In the statistical uncertainty quantification community, one technique for parameter calibration when the computer model is misspecified is to jointly estimate model parameters with an explicit discrepancy function that captures model inadequacy (Kennedy and O’Hagan, 2001). The discrepancy function has a Gaussian process prior. The parameters to estimate are the linear regression parameters β , the observation noise scale σ , the RBF kernel output scale γ , and the kernel lengthscales ℓ .

We placed the following priors on parameters:

$$\begin{aligned}\gamma &\sim \text{Half}\mathcal{N}(1) \\ \sigma &\sim \text{Half}\mathcal{N}(1) \\ \ell &\sim \text{Gamma}(4, 4) \\ \beta_0 &\sim \mathcal{N}(0, 1) \\ \beta_1, \beta_2^{(1,2,3,5)}, \beta_3^{(1)} &\sim \mathcal{N}(1, 0.1) \\ \beta_2^{(4)}, \beta_3^{(2)} &\sim \mathcal{N}(-1, 0.1) \\ \beta_4 &\sim \mathcal{N}(0, 0.1)\end{aligned}$$

We used the PyMC3 FITC sparse GP approximation implementation with 20 inducing points initialized with k-means.