Supplementary Materials to

Transformation and Additivity in Gaussian Processes by Li-Hsiang Lin and V. Roshan Joseph

In this supplementary material, we provide more details of the example functions and datasets used in Section 5 of "Transformation and Additivity in Gaussian Process". The first five example functions can be found in Surjanovic and Bingham (2019) and the last two datasets are from Qian et al. (2006).

1. The robot arm function describes the end position of a robot arm with 4 segements:
$$y = (u^2 + v^2)^{1/2}, u = \sum_{i=1}^{4} L_i \cos(\sum_{j=1}^{i} \theta_j), \text{ and } v = \sum_{i=1}^{4} L_i \sin(\sum_{j=1}^{i} \theta_j),$$
where the eight inputs are the segements $L_i \in [0, 1]$ and angles $\theta_i \in [0, 2\pi]$ for $i = 1, 2, 3,$ and 4.

2. The OTL circuit function models an output transformerless push-pull circuit:
$$y = \frac{(V_{b1} + 0.74)\beta(R_{c2} + 9)}{\beta(R_{c2} + 9) + R_f} + \frac{11.35R_f}{\beta(R_{c2} + 9) + R_f} + \frac{0.74R_f\beta(R_{c2} + 9)}{\{\beta(R_{c2} + 9) + R_f\}R_{c1}} \text{ and } V_{b1} = \frac{12R_{b2}}{R_{b1} + R_{b2}},$$
where the six inputs with their ranges are $R_{b1} \in [50, 150], R_{b2} \in [25, 70], R_f \in [0.5, 3], R_{c1} \in [1.2, 2.5], R_{c2} \in [0.25, 1.2]$, and $\beta \in [50, 300]$.

3. The piston simulation function describes a piston moving within a cylinder:
$$y = 2\pi\sqrt{\frac{M}{k + S^2 \frac{P_0 V_0}{T_0} \frac{T_a}{V^2}}}, V = \frac{S}{2k}\left(\sqrt{A^2 + 4k\frac{P_0 V_0}{V_0}T_a} - A\right), \text{ and } A = P_0 S + 19.62M - \frac{kV_0}{S},$$
where the ranges of the seven variables are $M \in [30, 60], S \in [0.005, 0.02], V_0 \in [0.002, 0.01], k \in [1000, 5000], P_0 \in [90000, 110000], T_a \in [290, 296]$, and $T_0 \in [340, 360]$.

4. Wing weight function models a light aircraft wing:
$$y = 0.036 S_w^{0.758} W_{fw}^{0.0035} \left(\frac{A}{\cos^2(\Lambda)}\right)^{0.6} q^{0.006} \lambda^{0.04} \left(\frac{100t_c}{\cos(\Lambda)}\right)^{-0.3} (N_z W_{dg})^{0.49} + S_w W_p,$$
where the ten input variables and their usual input ranges are $S_w \in [150, 200], W_{fw} \in [220, 300], A \in [6, 10], \Lambda \in [-10, 10], q \in [16, 45], \lambda \in [0.5, 1], t_c \in [0.08, 0.18], N_z \in [2.5, 6], W_{dg} \in [1700, 2500]$, and $W_p \in [0.025, 0.08]$.

5. The Franke function describes a surface with two peaks of different heights and a smaller dip:

$$\begin{aligned} y &= \frac{3}{4}\exp(-\frac{(9x_1-2)^2}{4} - \frac{(9x_2-2)^2}{4}) + \frac{3}{4}\exp(-\frac{(9x_1+1)^2}{49} - \frac{(9x_2+1)^2}{10}) + \\ & \frac{1}{2}\exp(-\frac{(9x_1-7)^2}{4} - \frac{(9x_2-3)^2}{4}) - \frac{1}{5}\exp(-(9x_1-4)^2 - (9x_2-7)^2), \end{aligned}$$

where the two inputs x_1 and x_2 are in $[0, 1]$.

6. The approximate HE dataset is used to design a heat exchanger to maximize the total rate of a steady state heat transfer. The dataset contains 64 simulations with 4 input variables including the mass flow rate of entry air $\dot{m} \in (.00055, .001)$, the temperature of entry air $T_{\text{in}} \in (270, 303.15)$, the temperature of the heat source $T_{\text{wall}} \in (202.4, 360)$ and the solid material thermal conductivity $k \in (330, 400)$. This dataset also includes 14 runs of simulations as a testing dataset. These datasets are from Qian et al. (2006).

7. The detailed HE dataset is generated with the same goal as the approximate HE dataset but by a more expensive simulation dataset. The dataset contains 22 runs of simulations with the same 4 input variables as the approximate HE dataset.

References

Qian, Z., Seepersad, C. C., Joseph, V. R., Allen, J. K., and Wu, C. J. (2006), "Building Surrogate Models Based on Detailed and Approximate Simulations," *Journal of Mechanical Design*, 128, 668–677.

Surjanovic, S., and Bingham, D. (2019), *Virtual Library of Simulation Experiments: Test Functions and Datasets,* from http://www.sfu.ca/∼ssurjano, Retrieved June 3, 2019.