Online Supplement for "Multiple-target Robust Design with Multiple Functional Outputs"

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Appendix A: Experimental Design and Outputs of the Simulator

The SLHD used as experiment design for the stent computer experiment is given in Table A1.

Table A1: 50-run SLHD for the stent computer experiment

Run	d	x_1	x_2	x_3	x_4
1	0.57125	0.985	0	-0.026	-0.026
2	0.66875	0.965	0	0.01	0.034
3	0.75875	0.955	0	0.082	0.046
4	0.71375	0.925	0	0.09	-0.046
5	0.55625	0.905	0	-0.062	0.058
6	0.50375	0.885	0	0.066	-0.058
7	0.83375	0.875	0	-0.034	-0.034
8	0.80375	0.855	0	-0.082	0.086
9	0.72875	0.825	0	0.03	0.094
10	0.86375	0.805	0	0.094	-0.018
11	0.59375	0.795	0	-0.01	-0.082
12	0.69875	0.775	0	-0.09	0.018
13	0.57875	0.745	0	-0.002	0.022
14	0.63125	0.735	0	-0.098	-0.066
15	0.77375	0.705	0	0.014	-0.09
16	0.82625	0.695	0	0.026	0.006
17	0.53375	0.675	0	0.054	0.082
18	0.51875	0.655	0	-0.042	-0.042
19	0.64625	0.625	0	-0.054	0.066
20	0.69125	0.605	0	0.042	0.074
21	0.65375	0.585	0	-0.05	-0.098
22	0.84875	0.575	0	-0.074	0.038
23	0.78875	0.545	0	0.07	-0.07
24	0.60875	0.535	0	0.046	-0.01
25	0.74375	0.515	0	-0.018	-0.002
26	0.54125	0.995	1	0.022	0.062
27	0.81875	0.975	1	-0.006	0.078
28	0.68375	0.945	1	0.018	-0.086
29	0.73625	0.935	1	-0.058	0.03
30	0.79625	0.915	1	0.034	-0.022
31	0.63875	0.895	1	-0.07	-0.094
32	0.54875	0.865	1	-0.094	-0.014
33	0.60125	0.845	1	0.074	0.054
34	0.85625	0.835	1	0.058	0.07
35	0.61625	0.815	1	0.05	-0.03
36	0.70625	0.785	1	-0.014	0.002
37	0.76625	0.765	1	-0.066	-0.078
38	0.84125	0.755	1	-0.03	0.05
39	0.56375	0.725	1	-0.022	0.098
40	0.72125	0.715	1	0.078	0.014
41	0.67625	0.685	1	0.086	-0.074
42	0.51125	0.665	1	0.038	-0.062
43	0.66125	0.645	1	0.002	-0.05
44	0.62375	0.635	1	-0.078	-0.006
45	0.87125	0.615	1	-0.038	-0.038
46	0.81125	0.595	1	0.006	0.09
47	0.58625	0.565	1	0.098	0.042
48	0.75125	0.555	1	-0.086	-0.054
49	0.78125	0.525	1	0.062	0.01
50	0.52625	0.505	1	-0.046	0.026

The functional outputs of the stent simulator, central radial displacement $D_{central}(t,x)$ and distal radial displacement $D_{distal}(t,x)$, obtained in the 50-run SLHD experiment are plotted in Figure A1.

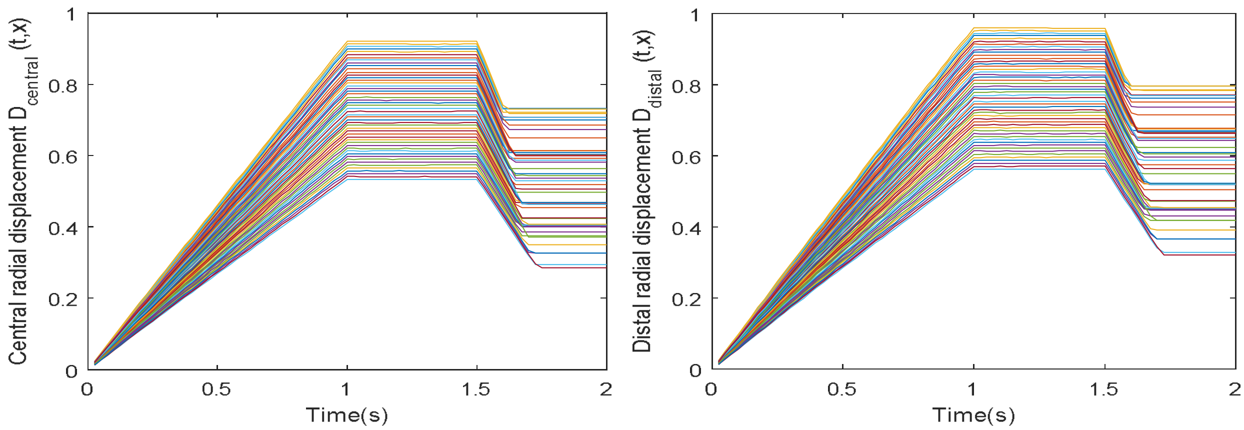

Figure A1 Plot of functional outputs $D_{central}(t,x)$ and $D_{distal}(t,x)$ observed in the experiment

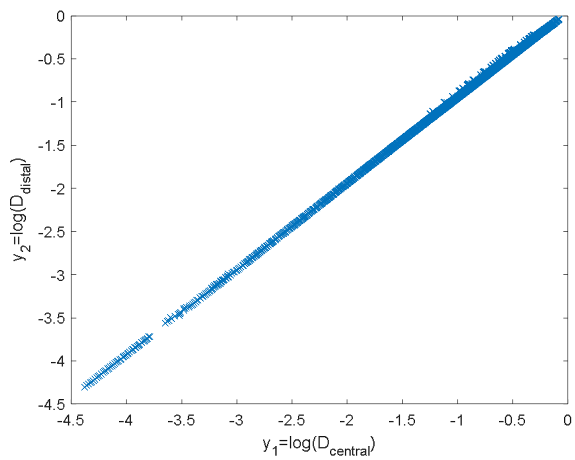

Figure A2 Plot of $y_2(t_i, x_{(j)}) = \log[D_{distal}(t_i, x_{(j)})]$ versus $y_1(t_i, x_{(j)}) = \log[D_{central}(t_i, x_{(j)})]$

Appendix B: Derivation of the Posterior Mean and Covariance Functions, and Maximum Integrated Likelihood Estimators of Parameters of the SMFOGP Emulator

Let $\mathbb{R}_{m,n}$ denote the set of real $m \times n$ matrices. The following properties of Kronecker product matrix algebra operations are needed (see Laub (2005)):

$(A \otimes B)(C \otimes D) = (AC \otimes BD)$, if matrix products AC and BD can be formed. (B1)

$\det(A \otimes B) = \det(A)^m \det(B)^n, A \in \mathbb{R}_{n,n}, B \in \mathbb{R}_{m,m}$ (B2)

$(B^T \otimes A)\ \mathrm{vec}(X) = \mathrm{vec}(AXB)$, $\mathrm{vec}(X)$ is the vectorization of matrix X (B3)

$(A \otimes B)^T = A^T \otimes B^T$ (B4)

$(A \otimes B)^{-1} = A^{-1} \otimes B^{-1}$ (B5)

By standard multivariate normal distribution theory, the conditional posterior distribution of Y is:

$$(Y(t,x),Y(t',x'))|Z,\beta,\Sigma,\theta \sim N_{2p}\left((m(t,x),m(t',x')),\begin{pmatrix} c(t,x,t,x) & c(t,x,t',x') \\ c(t',x',t,x) & c(t',x',t',x') \end{pmatrix}\right),$$

where $m(t,x) = f(x)\beta^T + r^T R^{-1}(Z - F_m\beta^T), c(t,x,t',x') = \Sigma(R_1(t,t')R_2(x,x') - r^T R^{-1} r')$, with $r = R_X^*(x) \otimes R_\tau^*(t)$, $r' = R_X^*(x') \otimes R_\tau^*(t')$, $R_X^*(x) = \left[R_2\left(x_{(1)},x\right),\dots,R_2\left(x_{(n)},x\right)\right]^T$, $R_\tau^*(t) = [R_1(t_1,t),\dots,R_1(t_m,t)]^T$, $R = R_X \otimes R_\tau$, $R_X = \left[R_2\left(x_{(i)},x_{(j)}\right)\right]$, $R_\tau = \left[R_1\left(t_i,t_j\right)\right]$, $F_m = F \otimes 1_m$ is the regression model matrix, and Z is the $mn \times p$ data matrix. The formulas for m and c can be derived by applying (B1), (B3), (B4), and (B5) to simplify the standard conditional mean and covariance matrix formulas for the multivariate normal distribution (Santner et al. (2003), page 211). Further applying (B1), (B4) and (B5) to simplify the expressions, we obtain:

$$m(t,x) = f(x)\beta^T + [(R_X^{*T}(x)R_X^{-1}) \otimes (R_\tau^{*T}(t)R_\tau^{-1})](Z - (F \otimes 1_m)\beta^T),$$

$$c(t,x,t',x') = \Sigma\left[R_1(t,t')R_2(x,x') - (R_X^{*T}(x)R_X^{-1}R_X^*(x'))\left(R_\tau^{*T}(t)R_\tau^{-1}R_\tau^*(t')\right)\right].$$

Note that $m(t,x)$ is dependent on β while $c(t,x,t',x')$ is independent of β. Thus, $(Y(t,x),Y(t',x'))|Z,\Sigma,\theta$ has the same distribution as $\left(\mathcal{M}(t,x),\mathcal{M}(t',x')\right) + \mathcal{E}$, where $\mathcal{E} \sim N_{2p}\left(0_{2p},\begin{pmatrix} c(t,x,t,x) & c(t,x,t',x') \\ c(t',x',t,x) & c(t',x',t',x') \end{pmatrix}\right)$, 0_{2p} is a $1 \times 2p$ vector of 0's, $\left(\mathcal{M}(t,x),\mathcal{M}(t',x')\right)$ is $\left(m(t,x),m(t',x')\right)$ with distribution induced by $\beta|(Z,\Sigma,\theta)$, and $\left(\mathcal{M}(t,x),\mathcal{M}(t',x')\right)$ and $\mathcal{E}$ are independent. Given the non-informative prior distribution $p(\beta) \propto 1$, it can be shown that

$$\beta^T|(Z,\Sigma,\theta) \sim N_{q,p}\left(\hat{\beta}^T,\left({F_m}^T R^{-1} F_m\right)^{-1},\Sigma\right), \quad \text{(B6)}$$

where $\hat{\beta}^T = \left({F_m}^T R^{-1} F_m\right)^{-1}\left({F_m}^T R^{-1} Z\right) = (F^T R_X^{-1} F)^{-1}(1_m^T R_\tau^{-1} 1_m)^{-1}\left((F^T R_X^{-1}) \otimes (1_m^T R_\tau^{-1})\right)Z$.

Using these facts and applying (B1), (B4) and (B5), we find that

$$\left(Y(t,x),Y(t',x')\right)|Z,\Sigma,\theta \sim N_{2p}\left(\left(M(t,x),M(t',x')\right),\begin{pmatrix} C(t,x,t,x) & C(t,x,t',x') \\ C(t',x',t,x) & C(t',x',t',x') \end{pmatrix}\right), \quad \text{(B7)}$$

where the posterior mean function M is

$$M(t,x) = E(Y|Z,\Sigma,\theta) = f(x)\hat{\beta}^T + [(R_X^{*T}(x)R_X^{-1}) \otimes (R_\tau^{*T}(t)R_\tau^{-1})]\big(Z - (F \otimes 1_m)\hat{\beta}^T\big)$$

and the posterior covariance function is

$$C(t,x,t',x') = \mathrm{cov}(Y(t,x),Y(t',x')|Z,\Sigma,\theta) = c(t,x,t',x')$$

$$+\Sigma\left[\big(f(x) - r^T R^{-1} F_m\big)\big({F_m}^T R^{-1} F_m\big)^{-1}\big(f(x') - r'^T R^{-1} F_m\big)^T\right]. \tag{B8}$$

This follows from the fact that $\mathcal{M}(t,x)^T = \left[I_p \otimes \big(f(x) - r^T R^{-1} F_m\big)\right]\mathrm{vec}(\beta^T) + Z^T R^{-1} r$ and $\mathrm{cov}[\mathrm{vec}(\beta^T)|Z,\Sigma,\theta] = \Sigma \otimes \big({F_m}^T R^{-1} F_m\big)^{-1}$. Note that (B8) can be expanded as in (4.5).

The estimates of θ and Σ are obtained by maximizing the integrated likelihood, i.e., the likelihood after integrating out β . Based on Equation (2.5) in Paulo (2005), we obtain the log integrated likelihood

$L = -\frac{1}{2}\ln|\Sigma \otimes R_X \otimes R_\tau| - \frac{1}{2}\ln\left|\big(I_p \otimes F \otimes 1_m\big)^T (\Sigma \otimes R_X \otimes R_\tau)^{-1}\big(I_p \otimes F \otimes 1_m\big)\right| -$

$\frac{1}{2}\mathrm{vec}\big(Z - F_m\hat{\beta}^T\big)^T(\Sigma^{-1} \otimes R_X^{-1} \otimes R_\tau^{-1})\mathrm{vec}\big(Z - F_m\hat{\beta}^T\big)$

$= -\frac{mp}{2}\ln|R_X| - \frac{np}{2}\ln|R_\tau| - \frac{mn-q}{2}\ln|\Sigma| - \frac{p}{2}\ln\left|F^T R_X^{-1} F\right| - \frac{pq}{2}\ln\left|{1_m}^T R_\tau^{-1} 1_m\right| - \frac{1}{2}\mathrm{trace}\Big[\Sigma^{-1}\big(Z -$

$F_m\hat{\beta}^T\big)^T(R_X^{-1} \otimes R_\tau^{-1})\big(Z - F_m\hat{\beta}^T\big)\Big]. \tag{B9}$

Maximizing (B9) for fixed θ, we have the MILE of Σ given by

$$\hat{\Sigma} = \frac{1}{mn-q}\big(Z - (F \otimes 1_m)\hat{\beta}^T\big)^T(R_X^{-1} \otimes R_\tau^{-1})\big(Z - (F \otimes 1_m)\hat{\beta}^T\big). \tag{B10}$$

By setting $\Sigma = \hat{\Sigma}$ in (B9), we see that the MILE of θ minimizes (4.8).

Appendix C: Proofs of Proposition 1, Proposition 2, and Corollary 1

Proof of Proposition 1: By (4.4),

$$M(\tau,x) = \begin{pmatrix} f(x)\hat{\beta}^T \\ \vdots \\ f(x)\hat{\beta}^T \end{pmatrix} + \begin{pmatrix} (R_X^{*T}(x)R_X^{-1}) \otimes (R_\tau^{*T}(t_1)R_\tau^{-1}) \\ \vdots \\ (R_X^{*T}(x)R_X^{-1}) \otimes (R_\tau^{*T}(t_m)R_\tau^{-1}) \end{pmatrix}\big(Z - (F \otimes 1_m)\hat{\beta}^T\big)$$

$= 1_m f(x)\hat{\beta}^T + [(R_X^{*T}(x)R_X^{-1}) \otimes (R_\tau R_\tau^{-1})]\big(Z - (F \otimes 1_m)\hat{\beta}^T\big)$

$= 1_m f(x)\hat{\beta}^T + [(R_X^{*T}(x)R_X^{-1}) \otimes I]\Big(\big(\mathrm{vec}(Z^1),\dots,\mathrm{vec}(Z^p)\big) - F\Big(\big(\hat{\beta}^1\big)^T,\dots,\big(\hat{\beta}^p\big)^T\Big) \otimes 1_m\Big)$

$= 1_m f(x)\hat{\beta}^T + [(R_X^{*T}(x)R_X^{-1}) \otimes I]\Big(\mathrm{vec}\big(Z^1 - 1_m\hat{\beta}^1 F^T\big),\dots,\mathrm{vec}\big(Z^p - 1_m\hat{\beta}^p F^T\big)\Big)$

$= 1_m f(x)\hat{\beta}^T + \left[\left(Z^1 - 1_m\hat{\beta}^1 F^T\right)R_X^{-1}R_X^*(x), \dots, \left(Z^p - 1_m\hat{\beta}^p F^T\right)R_X^{-1}R_X^*(x)\right].$

Proof of Proposition 2: By (4.5), the cross covariance between $\left(Y_1(t_i,x),\dots,Y_p(t_i,x)\right)^T$ and $\left(Y_1(t_j,x'),\dots,Y_p(t_j,x')\right)^T$ is given by

$C(t_i,x,t_j,x') = \Sigma\left[R_1(t_i,t_j)R_2(x,x') - \left(R_X^{*T}(x)R_X^{-1}R_X^*(x')\right)\left(R_\tau^{*T}(t_i)R_\tau^{-1}R_\tau^*(t_j)\right)\right]$

$+ \Sigma e(x,t_i)\ (F^T R_X^{-1}F)^{-1}(1_m^T R_\tau^{-1}1_m)^{-1}e(x',t_j)^T$

$= \Sigma\left[R_1(t_i,t_j)R_2(x,x') - \left(R_X^{*T}(x)R_X^{-1}R_X^*(x')\right)R_1(t_i,t_j)\right]$

$+ \Sigma[f(x) - (R_x^{*T}(x)R_X^{-1}F)]\ (F^T R_X^{-1}F)^{-1}(1_m^T R_\tau^{-1}1_m)^{-1}[f(x') - (R_x^{*T}(x')R_X^{-1}F)]^T,$

where we have used the fact that $R_\tau^{*T}(t_i)R_\tau^{-1}$ is a row vector with a one in the ith position and zeros elsewhere to simplify $e(x,t_i) = f(x) - (R_X^{*T}(x)R_X^{-1}F)(R_\tau^{*T}(t_i)R_\tau^{-1}1_m)$. Thus, $C_\tau(x,x')$ is given by

$C_\tau(x,x') = \Sigma\otimes\left[R_\tau R_2(x,x') - R_\tau\left(R_X^{*T}(x)R_X^{-1}R_X^*(x')\right)\right]$

$+[\Sigma\otimes(1_m 1_m^T)][f(x) - (R_x^{*T}(x)R_X^{-1}F)]\ (F^T R_X^{-1}F)^{-1}(1_m^T R_\tau^{-1}1_m)^{-1}[f(x') - (R_x^{*T}(x')R_X^{-1}F)]^T$

$= (\Sigma\otimes R_\tau)[R_2(x,x') - R_X^{*T}(x)R_X^{-1}R_X^*(x')] + [\Sigma\otimes(1_m 1_m^T)](1_m^T R_\tau^{-1}1_m)^{-1}[f(x) -$

$(R_x^{*T}(x)R_X^{-1}F)]\ (F^T R_X^{-1}F)^{-1}[f(x') - (R_x^{*T}(x')R_X^{-1}F)]^T.$

Proof of Corollary 1: This follows from Proposition 2, where we have used the facts that $R_1(t,t) = R_2(x,x) = 1$ for any t, and $1 - R_X^{*T}(x)R_X^{-1}R_X^*(x)$ and $(1_m^T R_\tau^{-1}1_m)^{-1}[f(x) - (R_x^{*T}(x)R_X^{-1}F)]\ (F^T R_X^{-1}F)^{-1}[f(x) - (R_x^{*T}(x)R_X^{-1}F)]^T$ are scalar quantities that do not depend on t_i.

References

1. Laub, A. J. (2005). *Matrix analysis for scientists and engineers* (Vol. 91). Philadelphia: Siam.

2. Paulo, R. (2005). Default priors for Gaussian processes. *The Annals of Statistics*, **33**(2), 556-582.

3. Santner, T. J., Williams, B. J., and Notz, W. I. (2003). *The design and analysis of computer experiments*. New York: Springer Science & Business Media.