Sensitivity Analysis and Emulation for Functional Data using Bayesian Adaptive Splines - Supplementary Material

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1 Simulation Details

We obtain the Sobol' decomposition of the function

$$f(\mathbf{x}) = 10\sin(2\pi x_1 x_2) + 20\left(x_3 - \frac{1}{2}\right)^2 + 10x_4 + 5x_5 \tag{1}$$

using the the approach where we treat x_1 as another input (augmentation approach) and where we get other sensitivity indices as a function of x_1 (functional approach).

1.1 Augmentation Approach

The overall mean is given by

$$\begin{aligned} f_0 &= \int_0^1 \dots \int_0^1 f(\mathbf{x})d\mathbf{x} \\ &= \underbrace{\int_0^1\int_0^1 10\sin(2\pi x_1 x_2)dx_1dx_2}_{a_1} + \underbrace{\int_0^1 20\left(x_3 - \frac{1}{2}\right)^2 dx_3}_{a_2=5/3} + \underbrace{\int_0^1 10x_4dx_4}_{a_3=5} + \underbrace{\int_0^1 5x_5dx_5}_{a_4=5/2} \end{aligned}$$

where

$$
\begin{aligned}
a_1 &= \int_0^1 \frac{10\sin^2(\pi x)}{\pi x} dx \\
&= \frac{5}{\pi}\left[\log(2\pi) + \gamma - Ci(2\pi)\right] \\
Ci(x) &= \gamma + \log(x) + \sum_{k=1}^{\infty} \frac{(-x^2)^k}{2k(2k)!} \\
\Rightarrow a_1 &= -\frac{5}{\pi}\sum_{k=1}^{\infty} \frac{(-4\pi^2)^k}{2k(2k)!}
\end{aligned}
$$

The main effects are given by

$$
\begin{aligned}
f_1(x_1) &= \int_0^1 10\sin(2\pi x_1 x_2) dx_2 + a_2 + a_3 + a_4 - f_0 \\
&= \frac{10\sin^2(\pi x_1)}{\pi x_1} - a_1 \\
f_2(x_2) &= \frac{10\sin^2(\pi x_2)}{\pi x_2} - a_1 \\
f_3(x_3) &= 20\left(x_3 - \frac{1}{2}\right)^2 - a_2 \\
f_4(x_4) &= 10x_4 - a_3 \\
f_5(x_5) &= 5x_5 - a_4
\end{aligned}
$$

and the interaction effect is given by

$$
f_{12}(x_1, x_2) = 10\sin(2\pi x_1 x_2) - \frac{10\sin^2(\pi x_1)}{\pi x_1} - \frac{10\sin^2(\pi x_2)}{\pi x_2} + a_1.
$$

Then the overall variance is given by

$$
\begin{aligned}
Var(f(\mathbf{x})) &= \int_0^1 \dots \int_0^1 f^2(\mathbf{x}) d\mathbf{x} \\
&= \int_0^1 \dots \int_0^1 \underbrace{100\sin^2(2\pi x_1 x_2)}_{50-25Si(4\pi)/2\pi} + \underbrace{400\left(x_3 - \frac{1}{2}\right)^4}_{5} + \underbrace{100x_4^2}_{100/3} + \underbrace{25x_5^2}_{25/3} \\
&+ \underbrace{400\sin(2\pi x_1 x_2)\left(x_3 - \frac{1}{2}\right)^2}_{2a_1a_2} + \underbrace{200x_4\sin(2\pi x_1 x_2)}_{2a_1a_3} + \underbrace{100x_5\sin(2\pi x_1 x_2)}_{2a_1a_4} \\
&+ \underbrace{400x_4\left(x_3 - \frac{1}{2}\right)^2}_{2a_2a_3} + \underbrace{200x_5\left(x_3 - \frac{1}{2}\right)^2}_{2a_2a_4} + \underbrace{100x_4x_5}_{2a_3a_4} d\mathbf{x} - f_0^2 \\
&= 50 - 25Si(4\pi)/2\pi + 5 + 125/3 + 2(a_1a_2 + a_1a_3 + a_1a_4 + a_2a_3 + a_2a_4 + a_3a_4) - f_0^2
\end{aligned}
$$

where the underbraces give the quantity after integration and

$$
Si(x) = \int_0^x \frac{\sin t}{t} dt = \sum_{k=1}^{\infty} (-1)^{k-1} \frac{x^{2k-1}}{(2k-1)(2k-1)!}.
$$

The variances for the main effects are given by

$$
\begin{aligned}
Var(f_1(x_1)) &= \int_0^1 f_1^2(x_1) dx_1 \\
&= \int_0^1 \underbrace{\frac{100\sin^4(\pi x_1)}{\pi^2 x_1^2}}_{50/\pi[2Si(2\pi)-Si(4\pi)]} + \underbrace{a_1^2 - 20a_1\frac{\sin^2(\pi x_1)}{\pi x_1}}_{a_1^2-2a_1^2=-a_1^2} dx_1 \\
Var(f_2(x_2)) &= Var(f_1(x_1)) \\
Var(f_3(x_3)) &= \int_0^1 \underbrace{400\left(x_3 - \frac{1}{2}\right)^4}_{5} + \underbrace{a_2^2 - 40a_2\left(x_3 - \frac{1}{2}\right)^2}_{-a_2^2} dx_3 \\
Var(f_4(x_4)) &= \int_0^1 \underbrace{100x_4^2}_{100/3} + \underbrace{a_3^2 - 20a_3x_4}_{-a_3^2} dx_4 \\
Var(f_5(x_5)) &= \int_0^1 \underbrace{25x_5^2}_{25/3} + \underbrace{a_4^2 - 10a_4x_5}_{-a_4^2} dx_5.
\end{aligned}
$$

The variance for the interaction is given by

$$
\begin{aligned}
Var(f_{12}(x_1,x_2)) &= \int_0^1 \int_0^1 f_{12}^2(x_1,x_2)dx_1dx_2 \\
&= \int_0^1 \int_0^1 \underbrace{100\sin^2(2\pi x_1x_2)}_{50-25Si(4\pi)/2\pi} + \underbrace{\frac{100\sin^4(\pi x_1)}{\pi^2 x_1^2} + \frac{100\sin^4(\pi x_2)}{\pi^2 x_2^2} + a_1^2}_{100/\pi[2Si(2\pi)-Si(4\pi)]+a_1^2} \\
& \underbrace{-2\frac{10\sin^2(\pi x_1)}{\pi x_1}10\sin(2\pi x_1x_2) - 2\frac{10\sin^2(\pi x_2)}{\pi x_2}10\sin(2\pi x_1x_2)}_{-200/\pi[2Si(2\pi)-Si(4\pi)]} \\
& + \underbrace{2a_1 10\sin(2\pi x_1x_2)}_{2a_1^2} + \underbrace{2\frac{10\sin^2(\pi x_1)}{\pi x_1}\frac{10\sin^2(\pi x_2)}{\pi x_2}}_{2a_1^2} \\
& \underbrace{-2\frac{10\sin^2(\pi x_1)}{\pi x_1}a_1 - 2\frac{10\sin^2(\pi x_2)}{\pi x_2}a_1}_{-4a_1^2} dx_1dx_2 \\
&= 50 - 25Si(4\pi)/2\pi - 100/\pi[2Si(2\pi) - Si(4\pi)] + a_1^2
\end{aligned}
$$

1.2 Functional Approach

As a function of x_1, the main effects are

$$
\begin{aligned}
f_0(x_1) &= \frac{10\sin^2(\pi x_1)}{\pi x_1} + a_2 + a_3 + a_4 \\
f_2(x_1,x_2) &= 10\sin(2\pi x_1x_2) - \frac{10\sin^2(\pi x_1)}{\pi x_1} \\
f_3(x_1,x_3) &= f_3(x_3) \\
f_4(x_1,x_4) &= f_4(x_4) \\
f_5(x_1,x_5) &= f_5(x_5).
\end{aligned}
$$

Then the variance functions are

$$
\begin{aligned}
D(x_1) &= \int_0^1 \dots \int_0^1 f^2(\mathbf{x}) d\mathbf{x}_{-1} \\
&= 50 - \frac{25\sin(4\pi x_1)}{2\pi x_1} + 5 + 125/3 + 2(a_2 + a_3 + a_4)\frac{10\sin^2(\pi x_1)}{\pi x_1} \\
&+ 2a_2a_3 + 2a_2a_4 + 2a_3a_4 - f_0^2(x_1) \\
D_2(x_1) &= \int_0^1 f_2^2(x_1, x_2) dx_2 \\
&= 50 - 25\sin(4\pi x_1)/(2\pi x_1) - \frac{100\sin^4(\pi x_1)}{\pi^2 x_1^2} \\
D_3(x_1) &= 5 - a_2^2 \\
D_4(x_1) &= 100/3 - a_3^2 \\
D_5(x_1) &= 25/3 - a_4^2.
\end{aligned}
$$