Appendix D: Relationships between Fourier Coefficients over the Auxiliary Variable *s* and Fourier Coefficients in the θ-space

Note that this derivation is based on Cukier et al. (1978). However, the original proof in Cukier et al. (1978) only examined the relationship between Fourier coefficients over the auxiliary variable s and Fourier coefficients in the θ-space for frequencies which are harmonics of assigned fundamental frequency of model parameters (i.e., $k = r_i^{(s)}\omega_i$). In this derivation, we generalize the relationship for all frequencies (i.e., $k = \sum_i r_i^{(s)}\omega_i$), so that we are able to calculate higher-order sensitivity indices in the sampling scheme based on auxiliary variable *s*.

Based on eq.(25), the Fourier coefficient at frequency $k = \sum_i r_i^{(s)}\omega_i = \vec{r}\cdot\vec{\omega}^T$ [where $\vec{r} = (r_1^{(s)},...,r_j^{(s)},...r_n^{(s)})$ and $\vec{\omega} = (\omega_1,...,\omega_n)$] over the auxiliary variable *s* can be calculated as follows,

$$C^{(s)}{}_{(\vec{r}\cdot\vec{\omega}^T)} = E_s(g(G(\varphi(\omega_1 s)),...,G(\varphi(\omega_n s)))e^{-\mathbf{i}(\sum_i r_i^{(s)}\omega_i)s})$$

Following Cukier et al. (1978), replace the multiple Fourier transformation of $g(G(\theta_1),...,G(\theta_n))$ in eq. (12) into above equation, we have

$$\begin{aligned} C^{(s)}{}_{(\vec{r}\cdot\vec{\omega}^T)} &= E_s\{\left[\sum_{r_1^{(\theta)},...,r_n^{(\theta)}=-\infty}^{+\infty} C^{(\theta)}{}_{r_1^{(\theta)}..r_n^{(\theta)}} e^{\mathbf{i}(r_1^{(\theta)}\omega_1+\cdots+r_n^{(\theta)}\omega_n)s}\right] e^{-\mathbf{i}(\sum_i r_i^{(s)}\omega_i)s}\} \\ &= \sum_{r_1^{(\theta)},...,r_n^{(\theta)}=-\infty}^{+\infty} E_s\left[C^{(\theta)}{}_{r_1^{(\theta)}..r_n^{(\theta)}} e^{\mathbf{i}(r_1^{(\theta)}\omega_1+\cdots+r_n^{(\theta)}\omega_n)s} e^{-\mathbf{i}(\sum_i r_i^{(s)}\omega_i)s}\right] \\ &= \sum_{r_1^{(\theta)},...,r_n^{(\theta)}=-\infty}^{+\infty} E_s\left[C^{(\theta)}{}_{r_1^{(\theta)}..r_n^{(\theta)}} e^{\mathbf{i}[(r_1^{(\theta)}\omega_1+\cdots+r_n^{(\theta)}\omega_n)-(\sum_i r_i^{(s)}\omega_i)]s}\right]. \end{aligned}$$

If $\left[(r_1^{(\theta)}\omega_1 + \cdots + r_n^{(\theta)}\omega_n) - (\sum_i r_i^{(s)}\omega_i)\right] = 0$, we have

$$E_s\left[C^{(\theta)}{}_{r_1^{(\theta)}..r_n^{(\theta)}} e^{\mathbf{i}[(r_1^{(\theta)}\omega_1+\cdots+r_n^{(\theta)}\omega_n)-(\sum_i r_i^{(s)}\omega_i)]s}\right] = C^{(\theta)}{}_{r_1^{(\theta)}..r_n^{(\theta)}}.$$

If $\left[(r_1^{(\theta)}\omega_1+\cdots+r_n^{(\theta)}\omega_n)-(\sum_i r_i^{(s)}\omega_i)\right]\neq 0$, we have

$$
\begin{aligned}
&E_s\left[C^{(\theta)}{}_{r_1^{(\theta)}..r_n^{(\theta)}}e^{\mathbf{i}[(r_1^{(\theta)}\omega_1+\cdots+r_n^{(\theta)}\omega_n)-(\sum_i r_i^{(s)}\omega_i)]s}\right]\\
&=C^{(\theta)}{}_{r_1^{(\theta)}..r_n^{(\theta)}}E_s\left[e^{\mathbf{i}[(r_1^{(\theta)}\omega_1+\cdots+r_n^{(\theta)}\omega_n)-(\sum_i r_i^{(s)}\omega_i)]s}\right]\\
&=0.
\end{aligned}
$$

Finally, Fourier coefficient at frequency $k=\vec{r}\cdot\vec{\omega}^T$ over the auxiliary variable *s* can be approximated by the Fourier coefficients in the θ-space as follows,

$$C^{(s)}{}_{(\vec{r}\cdot\vec{\omega}^T)}=C^{(\theta)}{}_{\vec{r}}+\sum_{\vec{r}\,'}C^{(\theta)}{}_{\vec{r}\,'} \qquad \text{(D1)}$$

where $\vec{r}\,'$ is a vector different from $\vec{r}$ (i.e., $\vec{r}\neq\vec{r}\,'$) with $\vec{r}\cdot\vec{\omega}^T=\vec{r}\,'\cdot\vec{\omega}^T$. If a frequency set $\{\omega_1,...,\omega_n\}$ is strictly free of interferences as defined in eq. (21), then

$$\vec{r}\cdot\vec{\omega}^T\neq\vec{r}\,'\cdot\vec{\omega}^T\text{, for } 1\leq|r_i|\leq M \text{ and } 0\leq|r_j\,'|\leq M.$$

Thus, for $\vec{r}\,'=(r_1\,',...,r_j\,',...r_n\,')$ in eq. (D1), there is at least one $r_j\,'>M$, for $j=1,...,n$. Since the higher order harmonics is negligible (i.e., $C^{(\theta)}{}_{\vec{r}\,'}\approx 0$ for any of $r_j\,'>M$), we can approximate $C^{(s)}{}_{(\vec{r}\cdot\vec{\omega}^T)}$ using $C^{(\theta)}{}_{\vec{r}}$. Namely,

$$C^{(s)}{}_{(\vec{r}\cdot\vec{\omega}^T)}\approx C^{(\theta)}{}_{\vec{r}} \qquad \text{(D2)}$$

for a frequency set $\{\omega_1,...,\omega_n\}$ strictly free of interferences to an order of *M.*

References

Cukier, R. I., H. B. Levine, and K. E. Shuler. 1978. Nonlinear sensitivity analysis of multiparameter model systems. Journal of Computational Physics 26:1-42.