Appendix A: Relationship between Conditional Variances in the Parameter Space and θ-space

Using the search function in eq. (5), for each *N* sampled value of θ_i $\{\theta_i^{(1)},...,\theta_i^{(N)}\}$, we can draw the corresponding sampled values of the parameter $x_i\{x_i^{(1)},...,x_i^{(N)}\}$. Combining all parameters together assuming parameter independence, for *N* random samples

$$\begin{bmatrix} \theta_1^{(1)} & \cdots & \theta_n^{(1)} \\ \vdots & \ddots & \vdots \\ \theta_1^{(N)} & \cdots & \theta_n^{(N)} \end{bmatrix}$$

drawn from the θ-space ($K_\theta{}^n = \{\theta_1,...,\theta_n \,|\, 0 < \theta_i < 2\pi, i = 1,...,n\}$), we can get *N* corresponding random samples for the parameters using the search function of eq. (5)

$$\begin{bmatrix} x_1^{(1)} & \cdots & x_n^{(1)} \\ \vdots & \ddots & \vdots \\ x_1^{(N)} & \cdots & x_n^{(N)} \end{bmatrix},$$

and *N* corresponding random samples of model output $\{y^{(1)},..., y^{(N)}\}$ with

$$y^{(j)} = g(G(\theta_1^{(j)}),...,G(\theta_n^{(j)})) \text{, } j\text{=1,..., } N.$$

Using the *N* samples from the θ-space, we can get an estimate of the m^{th} moment for the model output *y*,

$$\frac{1}{N}\sum_{j=1}^{N}(y^{(j)})^m = \frac{1}{N}\sum_{j=1}^{N} g(x_1^{(j)},...,x_n^{(j)})^m = \frac{1}{N}\sum_{j=1}^{N} g(G(\theta_1^{(j)}),..., G(\theta_n^{(j)}))^m. \qquad \text{(A1)}$$

It is notable that the random samples drawn from the θ-space can ergodically explore the parameter space. Based on the Strong Law of Large Numbers, we have

$$\lim_{N\to\infty}\frac{1}{N}\sum_{j=1}^{N}(y^{(j)})^m = E(y)^m,$$

$$\lim_{N\to\infty}\frac{1}{N}\sum_{j=1}^{N} g(x_1^{(j)},...,x_n^{(j)})^m = E_x(g(x_1^{(j)},...,x_n^{(j)}))^m = \iiint\limits_{x_1,...,x_n} g^m(x_1,...,x_n) f(x_1,...,x_n)dx_1\cdots dx_n, \quad \text{(A2)}$$

$$\lim_{N\to\infty}\frac{1}{N}\sum_{j=1}^{N} g(G(\theta_1^{(j)}),...,G(\theta_n^{(j)}))^m = E_\theta(g(G(\theta_1^{(j)}),...,G(\theta_n^{(j)}))^m = (\frac{1}{2\pi})^n \iiint\limits_{\theta_1,...,\theta_n} g^m(G(\theta_1),...,G(\theta_n))d\theta_1\cdots d\theta_n$$

where $f(x_1,...,x_n)$ is the joint probability density function for the set of parameters.

Thus, based on eq. (A1) and eq. (A2), we have

$$E(y)^m = E_x(g(x_1^{(j)},...,x_n^{(j)}))^m = E_\theta(g(G(\theta_1^{(j)}),...,G(\theta_n^{(j)}))^m. \quad \text{(A3)}$$

Based on eq. (A3), it is clear that

$$V(y) = V^{(x_1,...,x_n)} = V_x(g(x_1^{(j)},...,x_n^{(j)})) = V_\theta(g(G(\theta_1^{(j)}),...,G(\theta_n^{(j)})) \quad \text{(A4)}$$

Eq. (A4) shows that the variance of the model output y can be estimated in the θ-space. For the conditional variances in eq. (6), we first consider the expected value of *y* in the parameter space and θ-space,

$$\begin{aligned} u_x(x_{sub}) &= E_x(y \mid x_{sub}) \\ u_\theta(\theta_{sub}) &= E_\theta(y \mid \theta_{sub}) \end{aligned} \quad \text{(A5)}$$

where x_{sub} is a subset of all parameters $\{x_1,...,x_n\}$ with size less than *n*; and θ_{sub} is a subset of $\{\theta_1,...,\theta_n\}$ corresponding to x_{sub}. For a specific value $\theta_{sub} = \theta_{sub}^{(*)}$, based on eq. (5), we get $x_{sub} = x_{sub}^{(*)}$. It can be shown that

$$E_\theta(y \mid \theta_{sub} = \theta_{sub}^{(*)}) = E_x(y \mid x_{sub} = x_{sub}^{(*)}). \quad \text{(A6)}$$

Proof:

By drawing *N* samples for θ_{-sub} (the set of $\{\theta_1,...,\theta_n\}$ excluding θ_{sub}) and the corresponding sample for x_{-sub} (the set of $\{x_1,...,x_n\}$ excluding x_{sub}) using the search function of eq. (5), the sample mean of $y\,|\,\theta_{sub}=\theta_{sub}{}^{(*)}$ and $y\,|\,x_{sub}=x_{sub}{}^{(*)}$ can be calculated by

$$\frac{1}{N}\sum_{j=1}^{N}(g(\vec{G}(\theta_{-sub}{}^{(j)}),\vec{G}(\theta_{sub}{}^{(*)}))=\frac{1}{N}\sum_{j=1}^{N}(g(x_{-sub}{}^{(j)},x_{sub}{}^{(*)}) \qquad \text{(A7)}$$

where $\theta_{-sub}{}^{(j)}$ is the j^{th} sample for θ_{-sub} and $x_{-sub}{}^{(j)}$ is the corresponding sample for x_{-sub}. The $\vec{G}(\theta_{-sub})$ is a vector version of the search function of eq. (5). For example, if $\theta_{-sub}=\{\theta_i,\theta_j\}$, then $\vec{G}(\theta_{-sub})=\{G(\theta_i),G(\theta_j)\}$. Based on the Strong Law of Large Numbers, we have

$$\begin{gathered}\operatorname*{Lim}_{N\to\infty}\frac{1}{N}\sum_{j=1}^{N}g(\vec{G}(\theta_{-sub}{}^{(j)}),\vec{G}(\theta_{sub}{}^{(*)}))=E_\theta(y\,|\,\theta_{sub}=\theta_{sub}{}^{(*)})\\ \operatorname*{Lim}_{N\to\infty}\frac{1}{N}\sum_{j=1}^{N}g(x_{-sub}{}^{(j)},x_{sub}{}^{(*)})=E_x(y\,|\,x_{sub}=x_{sub}{}^{(*)})\end{gathered}, \qquad \text{(A8)}$$

Based on eq. (A7) and eq. (A8), we prove eq. (A6).

To calculate the variance of $u_\theta(\theta_{sub})$ and $u_x(x_{sub})$, we first look at the expected value of the m^{th} moment of $u_\theta(\theta_{sub})$ and $u_x(x_{sub})$ (i.e., $E[u_x(x_{sub})]^m$ and $E[u_\theta(\theta_{sub})]^m$). $E[u_x(x_{sub})]^m$ and $E[u_\theta(\theta_{sub})]^m$ can be estimated by drawing N random samples for θ_{sub} $\{\theta_{sub}{}^{(1)},...,\theta_{sub}{}^{(N)}\}$ and the corresponding samples for x_{sub} $\{x_{sub}{}^{(1)},...,x_{sub}{}^{(N)}\}$ by the search function in eq. (5). Namely,

$$\begin{aligned}\hat{E}[u_x(x_{sub})]^m&=\frac{1}{N}\sum_{j=1}^{N}(u_x(x_{sub}{}^{(j)}))^m\\ \hat{E}[u_\theta(\theta_{sub})]^m&=\frac{1}{N}\sum_{j=1}^{N}(u_\theta(\theta_{sub}{}^{(j)}))^m.\end{aligned} \qquad \text{(A9)}$$

Based on eq. (A6), the sample averages in eq. (A9) are equal. Namely,

$$\frac{1}{N}\sum_{j=1}^{N}(u_x(x_{sub}{}^{(j)}))^m = \frac{1}{N}\sum_{j=1}^{N}(u_\theta(\theta_{sub}{}^{(j)}))^m. \quad \text{(A10)}$$

Using the Strong Law of Large Numbers, we have

$$\begin{aligned}\lim_{N\to\infty}\frac{1}{N}\sum_{j=1}^{N}(u_x(x_{sub}{}^{(j)}))^m &= E_x(u_x(x_{sub}))^m,\\ \lim_{N\to\infty}\frac{1}{N}\sum_{j=1}^{N}(u_\theta(\theta_{sub}{}^{(j)}))^m &= E_\theta(u_\theta(\theta_{sub}))^m.\end{aligned} \quad \text{(A11)}$$

Using eq. (A10) and (A11), we get

$$E_x(u_x(x_{sub}))^m = E_\theta(u_\theta(\theta_{sub}))^m. \quad \text{(A12)}$$

Based on eq. (A12), it is clear that

$$V^{(x_{sub})} = V_x(E_x(y \mid x_{sub})) = V_\theta(E_\theta(y \mid \theta_{sub})) . \quad \text{(A13)}$$

Eq. (A13) indicates that the conditional variance of the expected value of model output *y* in the parameters space is equal to that in the θ-space.