of identical grids, this reduces to $k_0 = 1$ and $k_{\max} = \lceil L_{\alpha,\text{ref}} \rceil$ and $\widetilde{\text{psd}}_\beta$ is only evaluated for integer wavenumbers, i.e. there is no need for interpolation.

B ANOVA

Boqiang; 02/2017

B.1 The Classic ANOVA theory

Definition B.1 *Let $V^{(d)}$ denote the Hilbert space of all functions $f : [0,1]^d \to \mathbb{R}$, and $\mathscr{D}, \mathbf{u}$ denote the coordinate index set, $\mathscr{D} := \{1, \ldots, d\}$, and its subset, $\mathbf{u} \subseteq \mathscr{D}$, respectively. The projection $P_{\mathbf{u}} : V^{(d)} \to V^{|\mathbf{u}|}$ is defined by*

$$P_{\mathbf{u}} f(\mathbf{X}_{\mathbf{u}}) := \int_{[0,1]^{d-|\mathbf{u}|}} f(\mathbf{X}) d\mathbf{X}_{\mathscr{D}\backslash\mathbf{u}}, \tag{6}$$

where $\mathbf{X} := [x_1, \ldots, x_d]^T \in [0,1]^d, \mathbf{X}_{\mathbf{u}} := [x_{j_1}, \ldots, x_{j_{|\mathbf{u}|}}]^T \in [0,1]^{|\mathbf{u}|}, j_k \in \mathbf{u}$, and $d\mathbf{X}_{\mathscr{D}\backslash\mathbf{u}} := \prod_{j \notin \mathbf{u}, j \in \mathscr{D}} dx_j, |\mathscr{D}\backslash\mathbf{u}| = d - |\mathbf{u}|$. When $\mathbf{u} = \varnothing$, the constant projection can be obtained, $P_\varnothing f(\mathbf{X}_\varnothing) := \int_{[0,1]^d} f(\mathbf{X}) d\mathbf{X} \in \mathbb{R}$; when $\mathbf{u} = \mathscr{D}$, the projection is the function itself $P_{\mathscr{D}} f(\mathbf{X}_{\mathscr{D}}) = f(\mathbf{X})$.

Definition B.2 *The ANOVA decomposition of a given multivariate function $f : [0,1]^d \to \mathbb{R}$ is defined by*

$$f(\mathbf{X}) := \sum_{\mathbf{u} \subseteq \mathscr{D}} f_{\mathbf{u}}(\mathbf{X}_{\mathbf{u}}), \tag{7}$$

where each decomposed component $f_{\mathbf{u}}(\mathbf{X}_{\mathbf{u}})$ can be recursively formulated by

$$f_{\mathbf{u}}(\mathbf{X}_{\mathbf{u}}) := P_{\mathbf{u}} f(\mathbf{X}_{\mathbf{u}}) - \sum_{\mathbf{v} \subset \mathbf{u}} f_{\mathbf{v}}(\mathbf{X}_{\mathbf{v}}), \tag{8}$$

or straightforwardly formulated by

$$f_{\mathbf{u}}(\mathbf{X}_{\mathbf{u}}) := \sum_{\mathbf{v} \subseteq \mathbf{u}} (-1)^{|\mathbf{u}|-|\mathbf{v}|} P_{\mathbf{v}} f(\mathbf{X}_{\mathbf{v}}). \tag{9}$$

In total, there are 2^d integrated terms and decomposed ANOVA terms if $\mathbf{u} = \varnothing$ and $\mathbf{u} = \mathscr{D}$ are counted.

Proposition B.3 *The ANOVA decomposition implies two remarkable properties: the zero-mean and the orthogonality.*

(i) each decomposed ANOVA component $f_{\mathbf{u}}(\mathbf{X}_{\mathbf{u}}), \mathbf{u} \subseteq \mathscr{D}, \mathbf{u} \neq \varnothing$ has the zero-mean average, $\int_{[0,1]} f_{\mathbf{u}}(\mathbf{X}_{\mathbf{u}}) dx_j = 0, j \in \mathbf{u}$.

(ii) every two decomposed ANOVA components $f_{\mathbf{u}}(\mathbf{X}_{\mathbf{u}})$ and $f_{\mathbf{v}}(\mathbf{X}_{\mathbf{v}})$ are orthogonal to each other, $\int_{[0,1]^d} f_{\mathbf{u}}(\mathbf{X}_{\mathbf{u}}) f_{\mathbf{v}}(\mathbf{X}_{\mathbf{v}}) d\mathbf{X} = 0, \mathbf{u}, \mathbf{v} \subseteq \mathscr{D}, \mathbf{u} \neq \mathbf{v}$.

Example B.4 *Considering a given 2D+time data denoted as* $f(\mathbf{X}) := f(x,y,t) \in \mathbb{R}, \mathbf{X} := (x,y,t)^T \in [0,1]^3$*, the corresponding ANOVA decomposition can be calculated in two steps:*

Step 1: the integration

$$
\begin{aligned}
P_{\{x,y\}} f(x,y) &:= \int_{[0,1]} f(x,y,t)dt, \\
P_{\{x,t\}} f(x,t) &:= \int_{[0,1]} f(x,y,t)dy, \\
P_{\{y,t\}} f(y,t) &:= \int_{[0,1]} f(x,y,t)dx, \\
P_{\{x\}} f(x) &:= \int_{[0,1]^2} f(x,y,t)dydt, \\
P_{\{y\}} f(y) &:= \int_{[0,1]^2} f(x,y,t)dxdt, \\
P_{\{t\}} f(t) &:= \int_{[0,1]^2} f(x,y,t)dxdy, \\
P_{\varnothing} f(\mathbf{X}_{\varnothing}) &:= \int_{[0,1]^3} f(x,y,t)dxdydt.
\end{aligned}
$$

Step 2: the decomposition

$$
\begin{aligned}
f_{\varnothing}(\mathbf{X}_{\varnothing}) &:= P_{\varnothing} f(\mathbf{X}_{\varnothing}), \\
f_{\{x\}}(x) &:= P_{\{x\}} f(x) - f_{\varnothing}(\mathbf{X}_{\varnothing}) = P_{\{x\}} f(x) - P_{\varnothing} f(\mathbf{X}_{\varnothing}), \\
f_{\{y\}}(y) &:= P_{\{y\}} f(y) - f_{\varnothing}(\mathbf{X}_{\varnothing}) = P_{\{y\}} f(y) - P_{\varnothing} f(\mathbf{X}_{\varnothing}), \\
f_{\{t\}}(t) &:= P_{\{t\}} f(t) - f_{\varnothing}(\mathbf{X}_{\varnothing}) = P_{\{t\}} f(t) - P_{\varnothing} f(\mathbf{X}_{\varnothing}), \\
f_{\{x,y\}}(x,y) &:= P_{\{x,y\}} f(x,y) - f_{\{x\}}(x) - f_{\{y\}}(y) - f_{\varnothing}(\mathbf{X}_{\varnothing}) \\
&= P_{\{x,y\}} f(x,y) - P_{\{x\}} f(x) - P_{\{y\}} f(y) + P_{\varnothing} f(\mathbf{X}_{\varnothing}), \\
f_{\{x,t\}}(x,t) &:= P_{\{x,t\}} f(x,t) - f_{\{x\}}(x) - f_{\{t\}}(t) - f_{\varnothing}(\mathbf{X}_{\varnothing}) \\
&= P_{\{x,t\}} f(x,t) - P_{\{x\}} f(x) - P_{\{t\}} f(t) + P_{\varnothing} f(\mathbf{X}_{\varnothing}), \\
f_{\{y,t\}}(y,t) &:= P_{\{y,t\}} f(y,t) - f_{\{y\}}(y) - f_{\{t\}}(t) - f_{\varnothing}(\mathbf{X}_{\varnothing}) \\
&= P_{\{y,t\}} f(y,t) - P_{\{y\}} f(y) - P_{\{t\}} f(t) + P_{\varnothing} f(\mathbf{X}_{\varnothing}), \\
f_{\{x,y,t\}}(x,y,t) &:= f(x,y,t) - f_{\{x,y\}}(x,y) - f_{\{x,t\}}(x,t) - f_{\{y,t\}}(y,t) - f_{\{x\}}(x) - f_{\{y\}}(y) - f_{\{t\}}(t) - f_{\varnothing}(\mathbf{X}_{\varnothing}) \\
&= f(x,y,t) - P_{\{x,y\}} f(x,y) - P_{\{x,t\}} f(x,t) - P_{\{y,t\}} f(y,t) + P_{\{x\}} f(x) + P_{\{y\}} f(y) + P_{\{t\}} f(t) - P_{\varnothing} f(\mathbf{X}_{\varnothing})
\end{aligned}
$$

Definition B.5 *If the multivariate function* $f : [0,1]^d \to \mathbb{R}$ *is square integrable, the total variance of* $f(\mathbf{X})$ *and the variance of each decomposed ANOVA component can be defined by*

$$
\begin{aligned}
D &:= \int_{[0,1]^d} (f(\mathbf{X}) - P_{\varnothing} f(\mathbf{X}_{\varnothing}))^2 d\mathbf{X} = \int_{[0,1]^d} f^2(\mathbf{X}) d\mathbf{X} - (P_{\varnothing} f(\mathbf{X}_{\varnothing}))^2, && (10) \\
D_{\mathbf{u}} &:= \int_{[0,1]^{|\mathbf{u}|}} f_{\mathbf{u}}^2(\mathbf{X}_{\mathbf{u}}) d\mathbf{X}_{\mathbf{u}}. && (11)
\end{aligned}
$$

The global sensitivity index (GSI) of the corresponding variables indexed by the coordinate index subset $\mathbf{u} \subseteq \mathscr{D}, \mathbf{u} \neq \varnothing$*, is defined by*

$$
S_{\mathbf{u}} := \frac{D_{\mathbf{u}}}{D}. \qquad (12)
$$

Based on the above definition, one can easily derive following two equalities:

$$\sum_{\mathbf{u}\subseteq\mathscr{D},\mathbf{u}\neq\varnothing} D_{\mathbf{u}} = D, \tag{13}$$

$$\sum_{\mathbf{u}\subseteq\mathscr{D},\mathbf{u}\neq\varnothing} S_{\mathbf{u}} = 1. \tag{14}$$

Definition B.6 *The given multivariate function $f : [0,1]^d \to \mathbb{R}$ can be arbitrarily approximated by*

$$\tilde{f}(\mathbf{X}) := \sum_{\substack{\mathbf{u}_k\subseteq\mathscr{D} \\ k\in\mathbf{k},|\mathbf{k}|\leq 2^d}} f_{\mathbf{u}_k}(\mathbf{X}_{\mathbf{u}_k}), \tag{15}$$

where the index subset $\mathbf{k} \subseteq \mathbf{K}, \mathbf{K} := \{1,\dots,2^d\}$. The corresponding approximation error can be measured by means of the ℓ_2 norm:

$$\delta(f,\tilde{f}) := \frac{1}{D}\int_{[0,1]^d} (f(\mathbf{X}) - \tilde{f}(\mathbf{X}))^2 d\mathbf{X}. \tag{16}$$

Based on the above definition of the ANOVA decomposition with its zero-mean average and orthogonality properties, one can easily prove the following theorem:

Theorem B.7 *If the given multivariate function $f : [0,1]^d \to \mathbb{R}$ can be approximated by Eq.Eq. (15), then the approximation error is*

$$\delta(f,\tilde{f}) := 1 - \sum_{\substack{\mathbf{u}_k\subseteq\mathscr{D} \\ k\in\mathbf{k},|\mathbf{k}|\leq 2^d}} S_{\mathbf{u}_k} = \sum_{\substack{\mathbf{u}_k\subseteq\mathscr{D} \\ k\in\mathbf{K}\setminus\mathbf{k},|\mathbf{k}|\leq 2^d}} S_{\mathbf{u}_k}, \tag{17}$$

Remark B.8 *In definition B.6, the decomposed ANOVA components $f_{\mathbf{u}_k}(\mathbf{X}_{\mathbf{u}_k})$, which were used to approximate the given function $f(\mathbf{X})$, can be arbitrarily selected. However, in particular cases, the selection should be under some proper rule. For instance, if the dimension number d is very large or goes to infinity, it is impossible to calculate or estimate all 2^d integrated terms (in Eq.Eq. (6)) such that all 2^d decomposed ANOVA components (in Eq.Eq. (7)) can be obtained. One possible solution is to approximate the function in a progressive approach. Let the subset $\mathbf{u}_{l,n}$ denote the coordinate index subset containing l indices in the n-th enumerated case, where the cardinality index $l = |\mathbf{u}|$, and the enumerator index $n \in \mathbf{n}, \mathbf{n} := \{1,\cdots,\binom{l}{d}\}$. In fact, one can derive $2^d = \sum_{l=0}^{d}\binom{l}{d}$. Now, the approximation can be realized by adding all calculated $f_{\mathbf{u}_{l,n}}(\mathbf{X}_{\mathbf{u}_{l,n}})$ where l is set from 0 to some threshold $L, L < d$, that can be determined based on the available computation resources.*

Now, we can modify the definition B.6 and the theorem B.7 based on the above mentioned movitation on very high dimentional problem.

Definition B.9 *The given multivariate function* $f : [0,1]^d \to \mathbb{R}$ *can be progressively approximated by*

$$\tilde{f}(\mathbf{X}) := \sum_{l=0}^{L} \sum_{n=1}^{\binom{l}{d}} f_{\mathbf{u}_{l,n}}(\mathbf{X}_{\mathbf{u}_{l,n}}), \tag{18}$$

where $l := |\mathbf{u}|$, *and* $L < d$.

Theorem B.10 *If the given multivariate function* $f : [0,1]^d \to \mathbb{R}$ *can be approximated by Eq.Eq. (18), then the approximation error is*

$$\delta(f, \tilde{f}) := 1 - \sum_{l=0}^{L} \sum_{n=1}^{\binom{l}{d}} S_{\mathbf{u}_{l,n}} = \sum_{l=L+1}^{d} \sum_{n=1}^{\binom{l}{d}} S_{\mathbf{u}_{l,n}}, \tag{19}$$

B.2 The subspace ANOVA decomposition

Now, we consider a special ANOVA decomposition of the multivariate function $f(\mathbf{X}), f : [0,1]^d \to \mathbb{R}, \mathbf{X} := [x_1, \ldots, x_d]^T$, where partial variables in $\mathbf{X}$ will be fixed during the whole decomposition. Let $\mathscr{D} := \{1, \ldots, d\}$ represents the full indices set of all dimensional coordinates, its two independent subsets are $\mathscr{U}, \mathscr{W}$, where $\mathscr{U} \cup \mathscr{W} = \mathscr{D}, \mathscr{U} \cap \mathscr{W} = \varnothing$, and $\mathscr{W} \neq \varnothing$. Now the variable vector $\mathbf{X}$ can be represented as $\mathbf{X} = A[\mathbf{Y}, \mathbf{Z}]^T$. Here, A is the corresponding perturbation matrix. Y represents the free variables that can be integrated in the ANOVA decomposition, within which the corresponding coordinate indices are in the subset $\mathscr{U}, \mathbf{Y} := [x_{j_1}, \ldots, x_{j_{|\mathscr{U}|}}]^T, j_k \in \mathscr{U}$. Similarily, $\mathbf{Z}$ represents the fixed variables that cannot be integrated in the ANOVA decomposition, within which the corresponding coordinate indices are in the subset $\mathscr{W}, \mathbf{Z} := [x_{j_1}, \ldots, x_{j_{|\mathscr{W}|}}]^T, j_k \in \mathscr{W}$.

Definition B.11 *Let* $V^{(d)}$ *denote the Hilbert space of all functions* $f : [0,1]^d \to \mathbb{R}$, $\mathscr{D}, \mathscr{U}, \mathscr{W}$ *denote the coordinate index set,* $\mathscr{D} := \{1, \ldots, d\}$, *and its two independent subset,* $\mathscr{U} \subseteq \mathscr{D}, \mathscr{W} \subseteq \mathscr{D}$, *and following set relationships exist,* $\mathscr{U} \cup \mathscr{W} = \mathscr{D}, \mathscr{U} \cap \mathscr{W} = \varnothing, \mathscr{W} \neq \varnothing$. *The projection* $P_{\mathbf{u}} : V^{(d)} \to V^{|\mathbf{u}|+|\mathscr{W}|}$ *is defined by*

$$P_{\mathbf{u}} f(\mathbf{X}_{\mathbf{u},\mathscr{W}}) := \int_{[0,1]^{|\mathscr{U}|-|\mathbf{u}|}} f(\mathbf{X}) d\mathbf{X}_{\mathscr{U} \setminus \mathbf{u}}, \tag{20}$$

where $\mathbf{X} := [x_1, \ldots, x_d]^T \in [0,1]^d, \mathbf{X}_{\mathbf{u},\mathscr{W}} := [x_{j_1}, \ldots, x_{j_{|\mathbf{u}|+|\mathscr{W}|}}]^T \in [0,1]^{|\mathbf{u}|+|\mathscr{W}|}, j_k \in \mathbf{u} \cup \mathscr{W}$, *and* $d\mathbf{X}_{\mathscr{U} \setminus \mathbf{u}} := \prod_{j \notin \mathbf{u}, j \in \mathscr{U}} dx_j$.

When $\mathbf{u} = \varnothing$, *the projected function is the* $|\mathscr{W}|$*-D multivariate function,* $P_{\varnothing} f(\mathbf{X}_{\varnothing,\mathscr{W}}) := \int_{[0,1]^{|\mathscr{U}|}} f(\mathbf{X}) d\mathbf{X}_{\mathscr{U}} \in \mathbb{R}^{|\mathscr{W}|}$, *where* $\mathbf{X}_{\varnothing,\mathscr{W}} = \mathbf{X}_{\mathscr{W}} := [x_{j_1}, \ldots, x_{j_{|\mathscr{W}|}}]^T, j_k \in \mathscr{W}$, *and* $d\mathbf{X}_{\mathscr{U}} := \prod_{j \in \mathscr{U}} dx_j$; *when* $\mathbf{u} = \mathscr{U}$, *the projection is the function itself* $P_{\mathscr{U}} f(\mathbf{X}_{\mathscr{U},\mathscr{W}}) = f(\mathbf{X})$.

In fact, the subspace ANOVA decomposition considers the decomposition