Coalitional Decompositions of Quantities of Interest

Generalized Möbius Inversion and the Input/Model-Centric Paradigms

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Paving the way towards solutions for general QoI decomposition with dependent inputs.

What is a coalitional decomposition ?

Definition *(Coalitional decomposition of a quantity of interest).*

Let $X = (X_1, \dots, X_d)^\top$ *be random inputs, and let* $G(X)$ *be a random output.*

Let $\mathrm{QoI}(G(X))$ *be a quantity of interest (QoI) on the ouput.*

Let $D = \{1, \dots, d\}$*, and let* $\mathcal{P}(D)$ *denote the set of subsets of* D *(power-set).*

If $\mathrm{QoI}(G(X))$ *can be written as:*

$$\mathrm{QoI}(G(X)) = \sum_{A \in \mathcal{P}(D)} \psi(A)$$

then the right-hand side of the equality is called a coalitional decomposition of $\mathrm{QoI}(G(X))$*.*

Two ways to define coalitional decompositions: an **input-centric** approach and a **model-centric** approach.

Let's take an example with the variance decomposition.

Model-centric : Sobol' indices

Let $X_1, \dots, X_d$ be **mutually independent** inputs. Let $G(X)$ be real-valued random variable such that $\mathbb{V}\left(G(X)\right) < \infty$.

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From Hoeffding (1948), one has that:

$$\mathbb{L}^2(P_X) = \bigoplus_{A \in \mathcal{P}(D)} \overline{V_A}, \quad \text{and} \quad G(X) = \sum_{A \in \mathcal{P}(D)} G_A(X_A)$$

where the summands are **pairwise orthogonal**.

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where the summands are **pairwise orthogonal**.

Moreover, for any $A \in \mathcal{P}(D)$ (Da Veiga et al. 2021):

$$\mathbb{V}(\mathbb{E}[G(X) \mid X_A]) = \sum_{B \in \mathcal{P}(A)} \mathbb{V}(G_A(X_A))$$

which implies that (Sobol' 1990), $\forall A \in \mathcal{P}(D)$:

$$\mathbb{V}(G_A(X_A)) = \sum_{B \in \mathcal{P}(A)} (-1)^{|A|-|B|} \mathbb{V}(\mathbb{E}[G(X) \mid X_B]) = \mathbb{V}(G(X)) \times S_A,$$

and in particular ($A = D$),

$$\mathbb{V}(G(X)) = \sum_{A \in \mathcal{P}(D)} \mathbb{V}(G_A(X_A))$$

Input-centric : Cooperative games for variance-based GSA

Now suppose that $X_1, \dots X_d$ are **not mutually independent**, and $\mathbb{V}\left(G(X)\right) < \infty$.

By analogy between Cooperative Game Theory and GSA, Owen (2014) proposed to view **dependent inputs** as **players**, whose value is chosen to be:

$$v(A) = \mathbb{V}\left(\mathbb{E}\left[G(X) \mid X_A\right]\right).$$

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The Harsanyi (1963) dividends of this game are, $\forall A \in \mathcal{P}\left(D\right)$:

$$\psi(A) = \sum_{B \in \mathcal{P}(A)} (-1)^{|A|-|B|} \mathbb{V}\left(\mathbb{E}\left[G(X) \mid X_B\right]\right),$$

and it implies that (Bilbao 2000), $\forall A \in \mathcal{P}\left(D\right)$:

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Input-centric and Model-centric approaches for variance decomposition

(Traditional) Model-centric approach

$X_1, \ldots, X_d$ **mutually independent.**

Decompose $G(X)$ into orthogonal $G_A(X_A)$.

One then has $\forall A \in \mathcal{P}(D)$:

$$\mathbb{V}\left(\mathbb{E}\left[G(X) \mid X_A\right]\right) = \sum_{A \in \mathcal{P}(D)} \mathbb{V}\left(G_A(X_A)\right).$$

which implies that:

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Input-centric approach

$X_1, \ldots, X_d$ **not necessarily mutually independent.**

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If the inputs are **actually mutually independent**:

- $\psi(A) = \mathbb{V}\left(G_A(X_A)\right)$ and both approaches are equivalent.
- The **input-centric** approach **did not require the $G_A(X_A)$ to be pairwise orthogonal**.

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It is due to a **generalization of the Möbius inversion formula** to **locally finite partially ordered sets** (Rota 1964).

One of the **cornerstones** of the field of **combinatorics** (Kung, Rota, and Hung Yan 2012).

The (very general) result of Rota admits a particular form when **dealing with power-sets**.

It can be understood as a generalization of the **inclusion-exclusion principle**.

Möbius inversion on power-sets

Corollary *(Möbius inversion on power-sets (Rota 1964; Kung, Rota, and Hung Yan 2012)).*

Let $D = \{1, \ldots, d\}$*, and any two set functions:*

$$f : \mathcal{P}(D) \to \mathbb{A}, \quad g : \mathcal{P}(D) \to \mathbb{A},$$

where $\mathbb{A}$ *is an* ***abelian group****. Then the following equivalence holds:*

$$f(A) = \sum_{B \in \mathcal{P}(A)} g(B), \quad \forall A \in \mathcal{P}(D) \quad \Longleftrightarrow \quad g(A) = \sum_{B \mathcal{P}(A)} (-1)^{|A|-|B|} f(B), \quad \forall A \in \mathcal{P}(D).$$

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Three remarks:

- **Left to right:** traditional **model-centric approach**.
- **Right to left:** **Input-centric approach**.
- The set functions f and g can be valued in an **abelian group**, and not necessarily $\mathbb{R}$: **we can generalize input-centric decompositions to a broad range of QoIs.**

Examples of abelian groups: $\mathbb{R}$, $\mathbb{R}^d$, spaces of matrices, polynomials, vector spaces...

Möbius inversion mechanism

The Möbius inversion is a **mechanical process**.

Variance decomposition: Let's compute $\sum_{A\in\mathcal{P}(D)} \sum_{B\in\mathcal{P}(A)} (-1)^{|A|-|B|} \mathbb{V}\left(\mathbb{E}\left[G(X) \mid X_B\right]\right)$ with $d = 3$.

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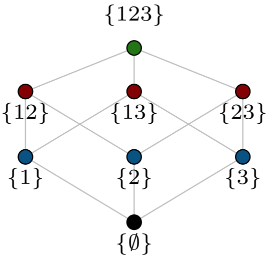

Powerset of $\{1, 2, 3\}$

Let $\mathbb{V}_A = \mathbb{V}\left(\mathbb{E}\left[G(X) \mid X_A\right]\right)$.

A							
123	$\mathbb{V}(G(X))$	- $\mathbb{V}_{12}$	- $\mathbb{V}_{23}$	- $\mathbb{V}_{13}$	$+\mathbb{V}_1$	$+\mathbb{V}_2$	$+\mathbb{V}_3$
12		+ $\mathbb{V}_{12}$			-$\mathbb{V}_1$	-$\mathbb{V}_2$	
23			+ $\mathbb{V}_{23}$			-$\mathbb{V}_2$	-$\mathbb{V}_3$
13				+ $\mathbb{V}_{13}$	-$\mathbb{V}_1$		-$\mathbb{V}_3$
1					$+\mathbb{V}_1$		
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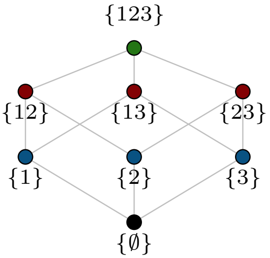

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Sum	$\mathbb{V}(G(X))$	+0	+0	+0	+0	+0	+0

This is just a fancy way to write $\mathrm{QoI}(G(X)) = \mathrm{QoI}(G(X)) + 0.$

Meaningfulness

Many coalitional decompositions built using Möbius inversion formula **are not meaningful**.

For instance:

$$\textcolor{red}{v(A)} = \begin{cases} \mathbb{V}\left(G(X)\right) & \text{if } A = D, \\ c_A & \text{for any } c_A \in \mathbb{A} \text{ otherwise.} \end{cases}$$

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Definition *(Gradual coalitional decomposition (I. et al. 2023)).*

Let $X = (X_1, \dots, X_d)^\top$ be random inputs, and let $\mathcal{Q}\text{o}\mathcal{I}(G(X))$ be an $\mathbb{A}$-valued QoI on G.

For any $A \in \mathcal{P}(D)$, let $f_A(X_A)$ be a $\sigma(X_A)$-measurable ***representation*** *of $G(X)$. If the coalitional decomposition can be written as:*

$$\mathcal{Q}\text{o}\mathcal{I}(G(X)) = \sum_{A \in \mathcal{P}(D)} \sum_{B \in \mathcal{P}(A)} (-1)^{|A|-|B|} \mathcal{Q}\text{o}\mathcal{I}(f_A(X_A))$$

it is said to be ***gradual****.*

Recipe

To build an **input-centric** **gradual coalitional QoI decomposition**:

- Choose **candidates** $f_A(X_A)$ to **represent** $G(X)$ as a function of X_A.
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But, how can these decompositions be interpreted ?

Interpretation

The interpretation of each:

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For the **variance decomposition**:

- If the inputs are **mutually independent**, and we choose $f_A(X_A) = \mathbb{E}\left[G(X) \mid X_A\right]$, we saw that **both approaches are equivalent**:

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  and hence the $\psi(A)$ can be interpreted as **pure interaction effects.**
- If the inputs are **not mutually independent**, $\mathbb{V}\left(\mathbb{E}\left[G(X) \mid X_A\right]\right)$ and $\psi(A)$ **can vary according to the dependence structure**, and hence **cannot quantify pure interaction**.

Illustration: Linear model with interaction and gaussian inputs

$$G(X) = X_1 + X_2 X_3, \quad X = \begin{pmatrix} X_1 \\ X_2 \\ X_3 \end{pmatrix} \sim \mathcal{N}\left(\begin{pmatrix} 0 \\ 0 \\ 0 \end{pmatrix}, \begin{pmatrix} 1 & 0 & \rho \\ 0 & 1 & 0 \\ \rho & 0 & 1 \end{pmatrix} \right) \tag{1}$$

Let, $\forall A \subseteq \{1, 2, 3\}$:

$$\psi(A) = \frac{1}{\mathbb{V}(G(X))} \sum_{B \in \mathcal{P}(A)} (-1)^{|A|-|B|} \mathbb{V}\left(\mathbb{E}\left[G(X) \mid X_A\right]\right)$$

Independent case ($\rho = 0$)
(The $\psi(A)$ are equal to the Sobol′ indices)

$S_1 = 0.5 \quad S_2 = 0, \quad S_3 = 0,$

$S_{12} = 0, \quad S_{13} = 0, \quad S_{23} = 0.5,$

$S_{123} = 0$

Correlated case ($\rho \neq 0$)

$\psi(1) = 0.5 \quad \psi(2) = 0, \quad \psi(3) = \rho^2/2,$

$\psi(12) = \rho^2/2, \quad \psi(13) = -\rho^2/2, \quad \psi(23) = 0.5,$

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$$\psi(1) = 0.5 \quad \psi(2) = 0, \quad \psi(3) = \rho^2/2,$$
$$\psi(12) = \rho^2/2, \quad \psi(13) = -\rho^2/2, \quad \psi(23) = 0.5,$$
$$\psi(123) = -\rho^2/2$$

In both cases $\sum_{A \in \mathcal{P}(D)} \psi(A) = 1$, but in **the correlated case**, we **cannot precisely characterize** what $\psi(A)$ quantifies.

Shapley effects with dependent inputs

Hence, **the precise interpretation of**

$$\psi(A) = \frac{1}{\mathbb{V}\left(G(X)\right)} \sum_{B \in \mathcal{P}(A)} (-1)^{|A|-|B|} \mathbb{V}\left(\mathbb{E}\left[G(X) \mid X_A\right]\right)$$

is still an open question : it clearly is a **mixture of interaction and dependence effects**.

But **which mixture** ?

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The **Shapley effects** for an input $i \in D$ can be written as (Harsanyi 1963):

$$\mathrm{Sh}_i = \sum_{A \in \mathcal{P}(D), i \in A} \frac{\psi(A)}{|A|}.$$

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which is an **egalitarian aggregation of a (not so clear) mixture of interaction and dependence effects**.

Choosing $v(A) = \mathbb{V}\left(\mathbb{E}\left[G(X) \mid X_A\right]\right)$, leads to an uncharacterized quantification.

Conclusions

Coalitional decompositions of QoIs:

- We saw two approaches: **Input-centric** and **Model-centric**.
- Defining **input-centric** **gradual** QoI decomposition **reduces to the choice of a representant** $f_A(X_A)$.
- The **input-centric** approach **bypasses the need** for **input independence** and, in the case of $\mathbb{L}^2$, an **orthogonal functional decomposition**.
- The interpretation of these decompositions **vary w.r.t. the dependence structure and the choice of representant**.

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Cooperative games based GSA indices:

- Allocations are aggregations of **input-centric** coalitional QoI decompositions, driven by the choice of value function $v(A)$.
- The Shapley effects (for dependent inputs) are an **egalitarian redistribution** of the gradual QoI decomposition with $v(A) = \mathbb{V}\left(\mathbb{E}\left[G(X) \mid X_A\right]\right)$.
- **At this time, we cannot characterize exactly what they quantify**.

Perspectives

But...

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For **(not necessarily mutually independent)** inputs $X = (X_1, \ldots, X_d)^\top$, is it possible de **find representants** $f_A(X_A)$ such that each term

$$\psi(A) = \sum_{B \in \mathcal{P}(A)} (-1)^{|A|-|B|} \mathbb{V}\left(f_A(X_A)\right)$$

of the **input-centric gradual variance decomposition**

$$\mathbb{V}\left(G(X)\right) = \sum_{A \in \mathcal{P}(D)} \psi(A)$$

quantifies pure interaction ?

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Our intuition:

- **Model-centric** approach to find the representants $f_A(X_A)$.
- **Input-centric** approach to define a gradual variance decomposition using these representants.

Perspective

In the case of models in $\mathbb{L}^2$, the **model-centric** approach would amount to show that:

$$\mathbb{L}^2(P_X) = \bigoplus_{A \in \mathcal{P}(D)} \overline{V_A},$$

hold whenever the inputs are **not necessarily mutually independant**, where the $\overline{V_A}$ are **not necessarily pairwise orthogonal.**

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If so, the **projections** of $G(X)$ onto each $\overline{V_A}$ could allow to define **promising representants**.

For fixed marginals and a fixed model, there would be **one set of representants** for **a particular dependence structure.**

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For fixed marginals and a fixed model, there would be **one set of representants** for **a particular dependence structure.**

What would be the properties of gradual variance decompositions with this choice of representants ?

We don't know yet... But we're working on it :)

Coalitional decompositions of parameters of interest

For a more in-depth (and more general) study of the **relationship** between **Möbius inversion** and **coalitional decompositions** of QoIs, check-out our **pre-print** (HAL/arXiv):

On the coalitional decomposition of parameters of interest

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Bilbao, J. M. 2000. *Cooperative Games on Combinatorial Structures* [in en]. Edited by W. Leinfellner and G. Eberlein. Vol. 26. Theory and Decision Library. Boston, MA: Springer US. ISBN: 978-1-4613-6976-9 978-1-4615-4393-0. https://doi.org/10.1007/978-1-4615-4393-0. http://link.springer.com/10.1007/978-1-4615-4393-0.

Da Veiga, S., F. Gamboa, B. Iooss, and C. Prieur. 2021. *Basics and Trends in Sensitivity Analysis: Theory and Practice in R* [in en]. Philadelphia, PA: Society for Industrial / Applied Mathematics, January. ISBN: 978-1-61197-668-7 978-1-61197-669-4. https://doi.org/10.1137/1.9781611976694. https://epubs.siam.org/doi/book/10.1137/1.9781611976694.

Gamboa, F., A. Janon, T. Klein, and A. Lagnoux. 2013. "Sensitivity indices for multivariate outputs." *Comptes Rendus Mathematique* 351 (7): 307–310. ISSN: 1631-073X. https://doi.org/10.1016/j.crma.2013.04.016.

Harsanyi, J. C. 1963. "A Simplified Bargaining Model for the n-Person Cooperative Game." Publisher: [Economics Department of the University of Pennsylvania, Wiley, Institute of Social and Economic Research, Osaka University], *International Economic Review* 4 (2): 194–220. ISSN: 0020-6598. https://doi.org/10.2307/2525487. https://www.jstor.org/stable/2525487.

Herin, M., M. I., V. Chabridon, and B. Iooss. 2022. *Proportional marginal effects for global sensitivity analysis* [in en], October. https://hal.science/hal-03825935.

Hoeffding, W. 1948. "A Class of Statistics with Asymptotically Normal Distribution." Publisher: Institute of Mathematical Statistics, *The Annals of Mathematical Statistics* 19, no. 3 (September): 293–325. ISSN: 0003-4851, 2168-8990. https://doi.org/10.1214/aoms/1177730196. https://projecteuclid.org/journals/annals-of-mathematical-statistics/volume-19/issue-3/A-Class-of-Statistics-with-Asymptotically-Normal-Distribution/10.1214/aoms/1177730196.full.

I., M., N. Bousquet, F. Gamboa, B. Iooss, and J. Loubes. 2023. *On the coalitional decomposition of parameters of interest* [in en], January. Accessed April 2, 2023. https://hal.science/hal-03927476.

Kung, J. P. S., G-C. Rota, and C. Hung Yan. 2012. *Combinatorics: the Rota way.* OCLC: 1226672593. New York: Cambridge University Press. ISBN: 978-0-511-80389-5.

Owen, Art B. 2014. "Sobol' Indices and Shapley Value" [in en]. *SIAM/ASA Journal on Uncertainty Quantification* 2, no. 1 (January): 245–251. ISSN: 2166-2525. https://doi.org/10.1137/130936233. http://epubs.siam.org/doi/10.1137/130936233.

Rota, G-C. 1964. "On the foundations of combinatorial theory I. Theory of Möbius Functions." *Zeitschrift für Wahrscheinlichkeitstheorie und Verwandte Gebiete* 2 (4): 340–368. ISSN: 1432-2064. https://doi.org/10.1007/BF00531932.

Sobol', I M. 1990. "On sensitivity estimation for nonlinear mathematical models" [in Russian]. *Mathematical Modelling and Computational Experiments* 2 (1): 112–118.

Thank you for your attention!

Any questions?

Cooperative game theory

In a nutshell, cooperative game theory can be summarized as **“the art of cutting a cake”**.

Given a **set of players** $D = \{1, \dots, d\}$, who produces a **quantity** $v(D)$, how can one allocate shares of $v(D)$ among the d players ?

The **“cake cutting process”** is often described through **axioms** (i.e., desired properties), and results in an **allocation**.

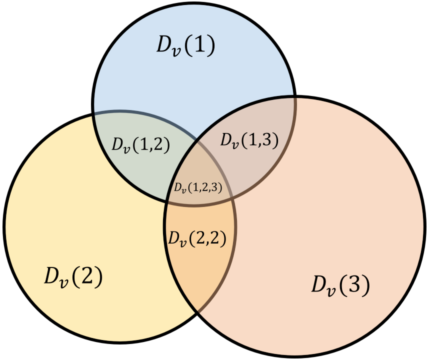
Formally, a cooperative game is denoted (D, v) where D is a **set of players**, and $v : \mathcal{P}(D) \to \mathbb{R}$ is a **value function**, mapping every possible subset of players to a real value.

Interpreting the Shapley values: Harsanyi dividends

Another equivalent enlightening representation of the Shapley values can be done using **Harsanyi dividends** (Harsanyi 1963).

Let (D, v) be a cooperative game, and for any $A \subseteq D$, let the **Harsanyi dividend** of the coalition A be:

$$D_v(A) = \sum_{B \subseteq A} (-1)^{|A|-|B|} v(A).$$



The Harsanyi dividends can be interpreted as the **surplus (or shortfall)** that a coalition generates:

$$D_v(1) = v(1), \quad D_v(2) = v(2),$$

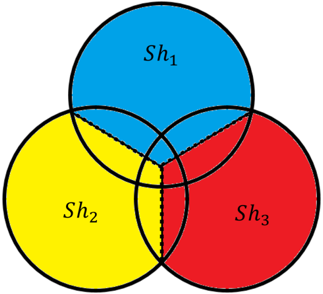
$$D_v(1,2) = v(1,2) - v(1) - v(2).$$

Interpreting the Shapley values: Harsanyi dividends

The Shapley values are then defined as:

$$\mathrm{Sh}_i = \sum_{A \subseteq D : i \in A} \frac{D_v(A)}{|A|},$$

or, in other words, each dividend of a coalition is **equally** redistributed between the players that composes it.



Quick example: Eve and John are two developers, Eve produces 10.000 lines of code, John produces 8.000 lines of code.
However, John really likes to play babyfoot, but Eve is a hard-worker.
When working together, they only produce 10.000 lines of code.
This means that the dividend of their coalition is -8.000.
Is it fair to attribute Eve -4.000 **lines of code, even if she did all the work ?**

Example - Covariance Matrix decomposition

Suppose that $G(X) = (G_1(X), \dots G_k(X))^\top$ is valued in R^k, and that $G(X) \in \mathbb{L}^2(P_X, \mathbb{R}^k)$ (Gamboa et al. 2013).

The QoI is the covariance matrix of the outputs $\mathbb{V}(G(X)) \in \mathbb{R}^{k\times k}$.

Let $\Sigma(A) = \mathbb{V}(\mathbb{E}[G(X) \mid X_A]) \in \mathbb{R}^{k\times k}$ be defined element-wise as:

$$\Sigma_{i,j}(A) = \mathrm{Cov}\left(\mathbb{E}[G_i(X) \mid X_A], \mathbb{E}[G_j(X) \mid X_A]\right).$$

Let, $\forall A \in \mathcal{P}(D)$:

$$\psi(A) = \sum_{B \in \mathcal{P}(A)} (-1)^{|A|-|B|} \Sigma(A) \in \mathbb{R}^{k\times k}.$$

Then, using the Möbius inversion on power-sets, one has the following coalitional decomposition of the output covariance matrix:

$$\mathbb{V}(G(X)) = \sum_{A \in \mathcal{P}(D)} \psi(A).$$

Posets, incidence algebra and Möbius inverse

A *partially ordered set* (poset) is defined as a pair $(\mathcal{S}, \leq)$ where $\mathcal{S}$ is a non-empty set, and $\leq$ is a partial order binary relation on elements of $\mathcal{S}$. A poset $(\mathcal{S}, \leq)$ is said to be *locally finite* if, for any $x, z \in \mathcal{S}$, the sets $\{y \in \mathcal{S} : x \leq y \leq z\}$ (also called *segments* of $\mathcal{S}$) are finite.

Denote $I_{\mathbb{A}}(\mathcal{S})$ the incidence algebra of a locally finite poset $(\mathcal{S}, \leq)$ over a commutative ring with identity $\mathbb{A}$, i.e., the set of functions $f : \mathcal{S} \times \mathcal{S} \to \mathbb{A}$ such that $f(x, y) = 0$ if $x \nleq y$. $(I_{\mathbb{A}}(\mathcal{S}), +, *)$ forms an $\mathbb{A}$-algebra with the usual pointwise addition $+$ and the usual convolution $*$, i.e., for any $f, g \in I_{\mathbb{A}}(\mathcal{S})$, and any $x, z \in \mathcal{S}$ such that the segment $\{y \in \mathcal{S} : x \leq y \leq z\}$ is non-empty,

$$(f * g)(x, z) = \sum_{x \leq y \leq z} f(x, y) g(y, z).$$

The zeta function $\zeta \in I_{\mathbb{A}}(\mathcal{S})$ is the convolutional identity of the incidence algebra, and is defined as, $\forall x, y \in \mathcal{S}$:

$$\zeta(x, y) = \begin{cases} 1 & \text{if } x = y, \\ 0 & \text{otherwise.} \end{cases}$$

Posets, incidence algebra and Möbius inverse

The Möbius function, denoted $\mu \in I_{\mathbb{A}}(\mathcal{S})$, in the case of locally finite posets $\mathcal{S}$, is defined as the *inverse of the zeta function for the convolution operator* defined on the incidence algebra of $\mathcal{S}$, and can be computed recursively, for any $x, y \in \mathcal{S}$ with $x \leq y$, as

$$\mu(x, y) = \begin{cases} 1 & \text{if } x = y \\ -\sum_{x \leq z < y} \mu(x, z) & \text{otherwise.} \end{cases}$$

Theorem *(Möbius inversion formula on locally finite posets). Let $\mathcal{S}$ be any non-empty set and $(\mathcal{S}, \leq)$ form a locally finite poset, where $\leq$ is a binary relation. Let φ and ψ be functions from $\mathcal{S}$ to $\mathbb{A}$. Then, the following equivalence hold:*

$$\varphi(x) = \sum_{y : y \leq x} \psi(y), \quad \forall x \in \mathcal{S} \quad \iff \quad \psi(x) = \sum_{y : y \leq x} \varphi(y)\mu(y, x), \quad \forall x \in \mathcal{S}.$$

where μ is the Möbius function.

Posets, incidence algebra and Möbius inverse

Definition *(Quantity of interest).* *An $\mathbb{A}$-valued QoI on a model G with random inputs $X \sim P_X$, is an application:*

$$\phi : \mathbb{P}(E) \times \mathcal{M}(E) \to \mathbb{A}$$
$$P \times H \mapsto \phi_P(H).$$

onto G and P_X, i.e., $\phi_{P_X}(G)$.

Lemma *(Möbius decomposition).* *Let $G \in \mathcal{M}$ a model with E-valued random inputs $X \sim P_X \in \mathbb{P}(E)$. Let $\phi_{P_X}(G)$ be a QoI on G. Let $\varphi : \mathcal{P}(D) \to \mathbb{A}$ be a set function such that:*

$$\varphi_D = \phi_{P_X}(G).$$

and $\forall A \in \mathcal{P}(D), \varphi_A$ is well-defined. Then, $\phi_{P_X}(G)$ admits the following coalitional decomposition:

$$\phi_{P_X}(G) = \sum_{A \in \mathcal{P}(D)} \psi_A,$$

where, $\forall A \subseteq D, \quad \psi_A = \sum_{B \subseteq A} (-1)^{|A|-|B|} \varphi_B$.