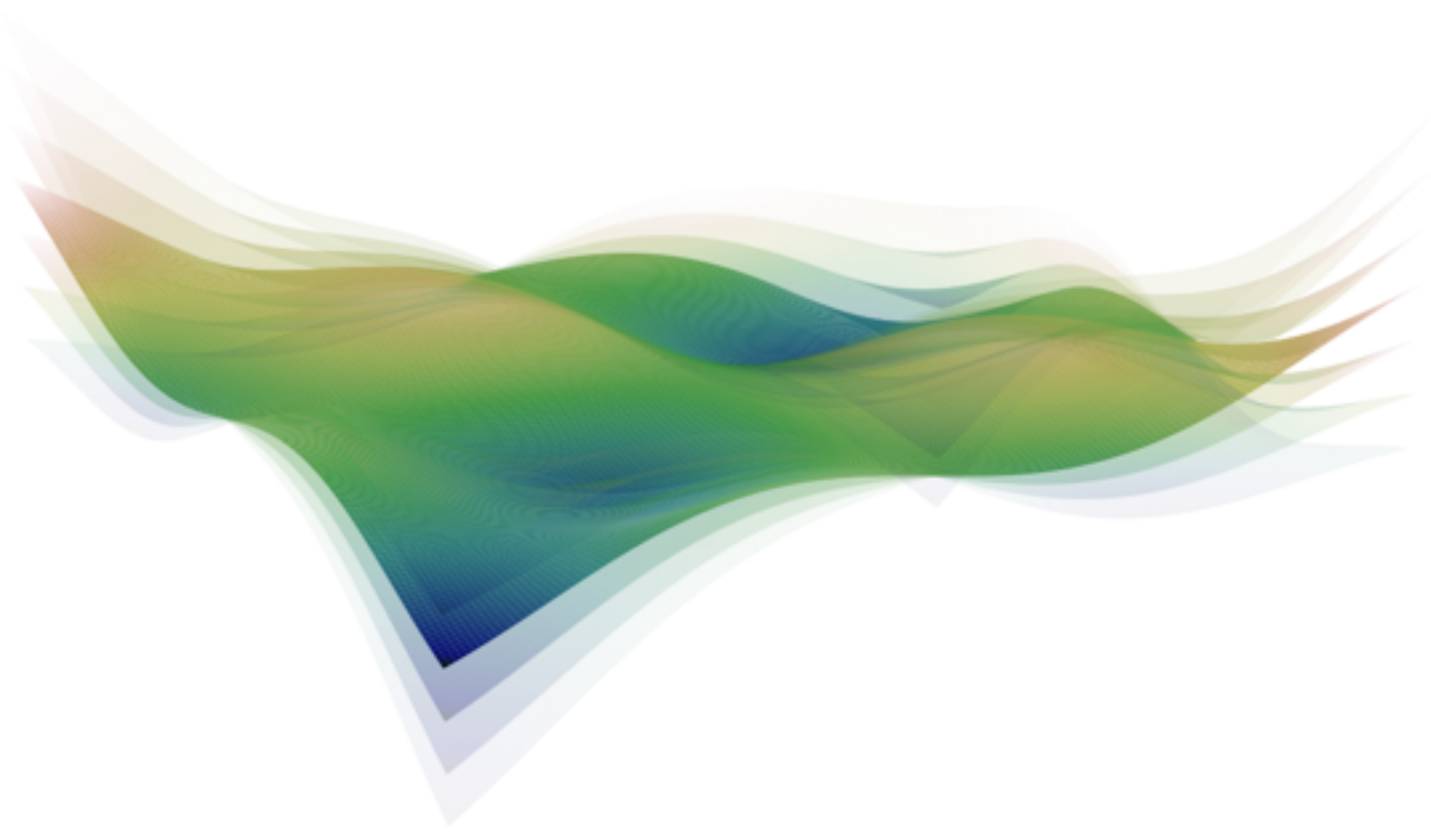
Sobol Tensor Trains for Global Sensitivity Analysis

Rafael Ballester-Ripoll, Enrique G. Paredes, Renato Pajarola



SIAM Mini-symposium: “Low-rank Tensors and High-dimensional Problems”

10th July 2018

University of Zurich[UZH]

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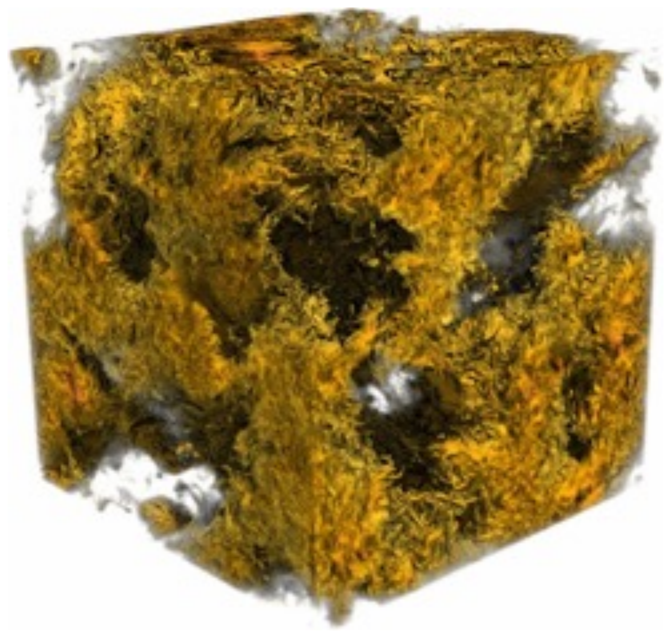
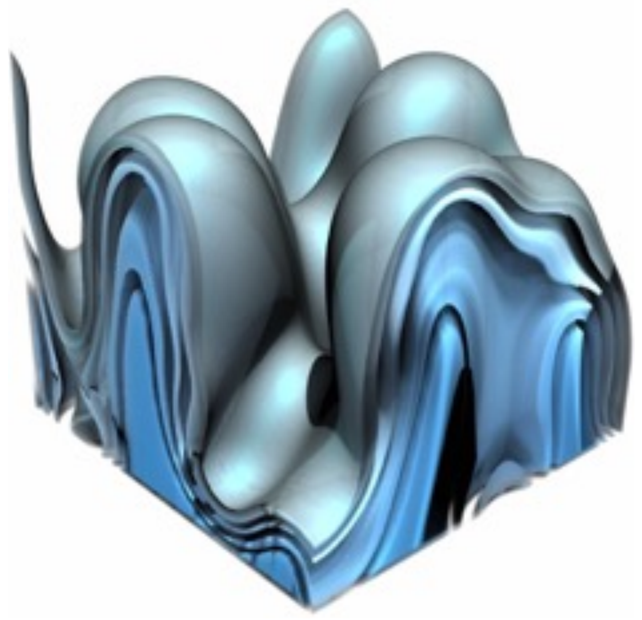
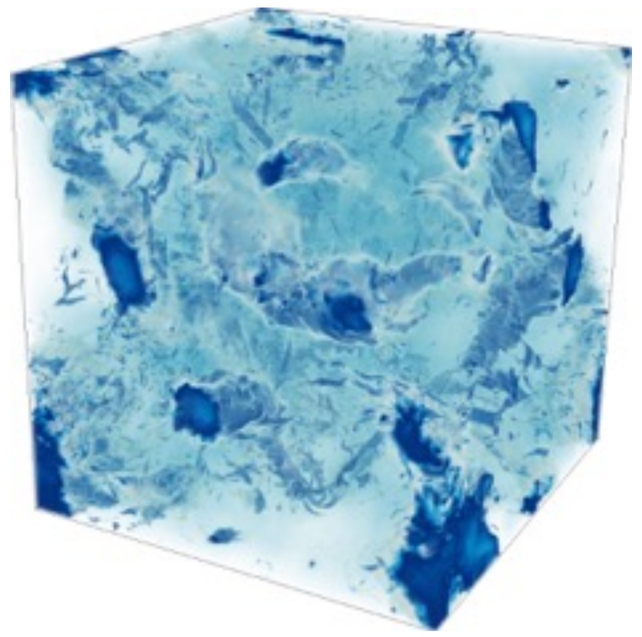
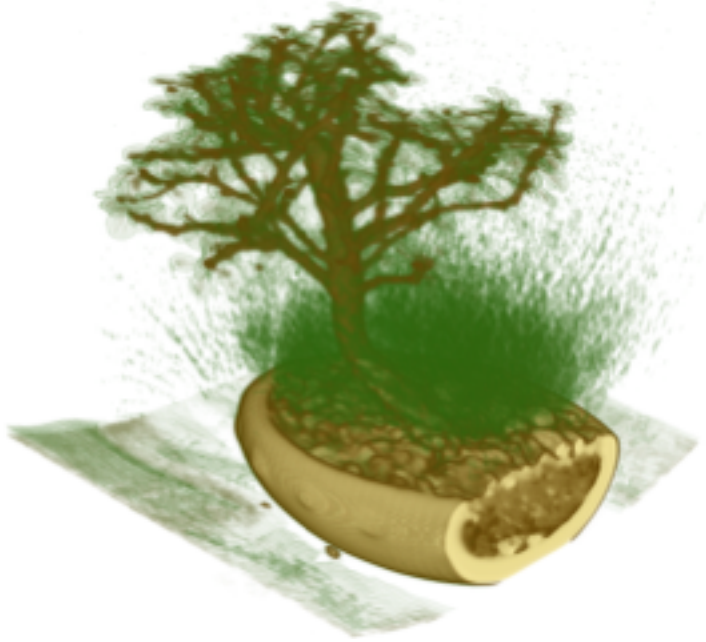
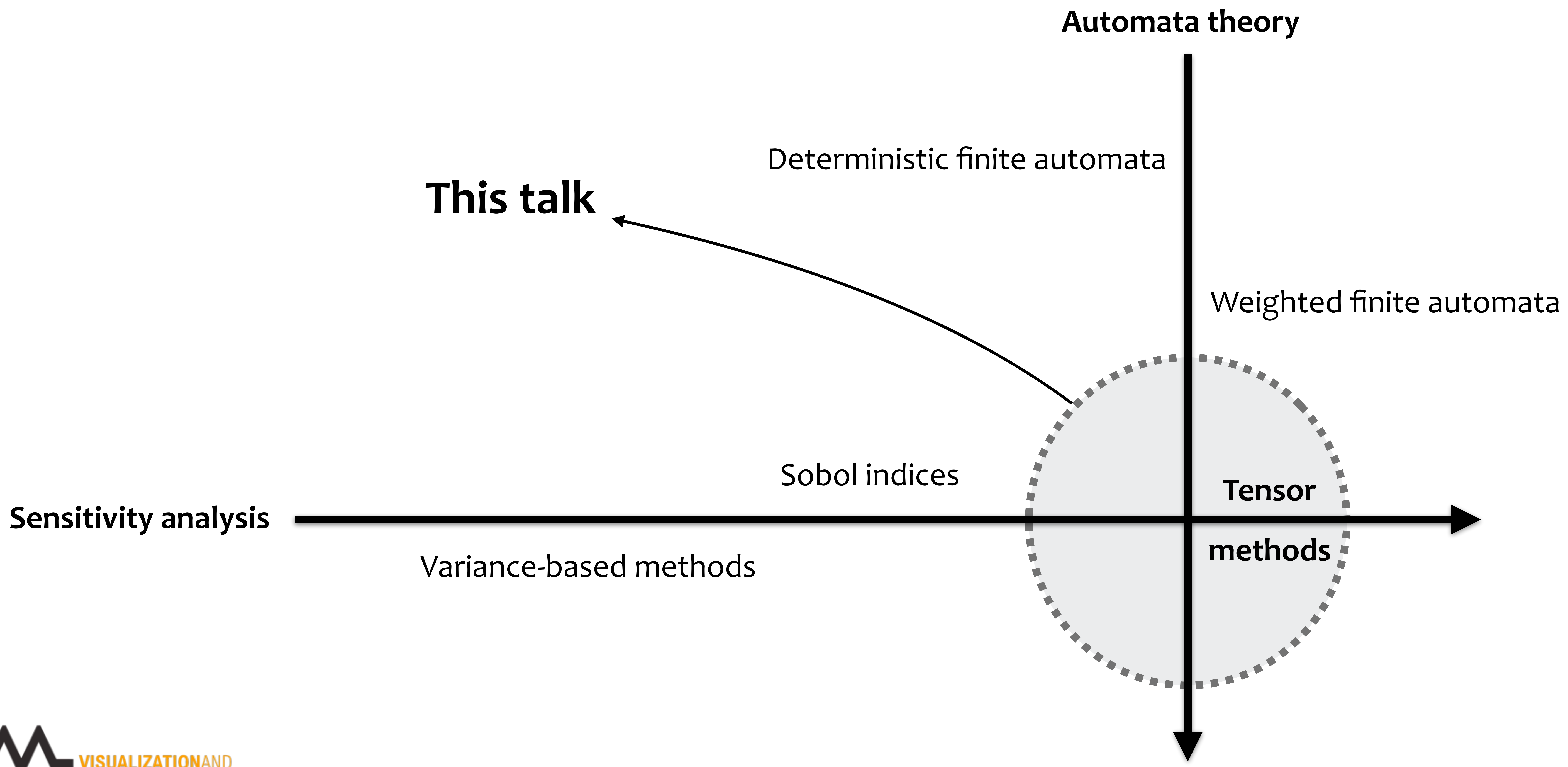
Background

- Initial research: tensors for **volume compression** and **rendering**

- Later:
  - **Surrogate modeling**
  - **High-dimensional learning**
  - **Sensitivity analysis**

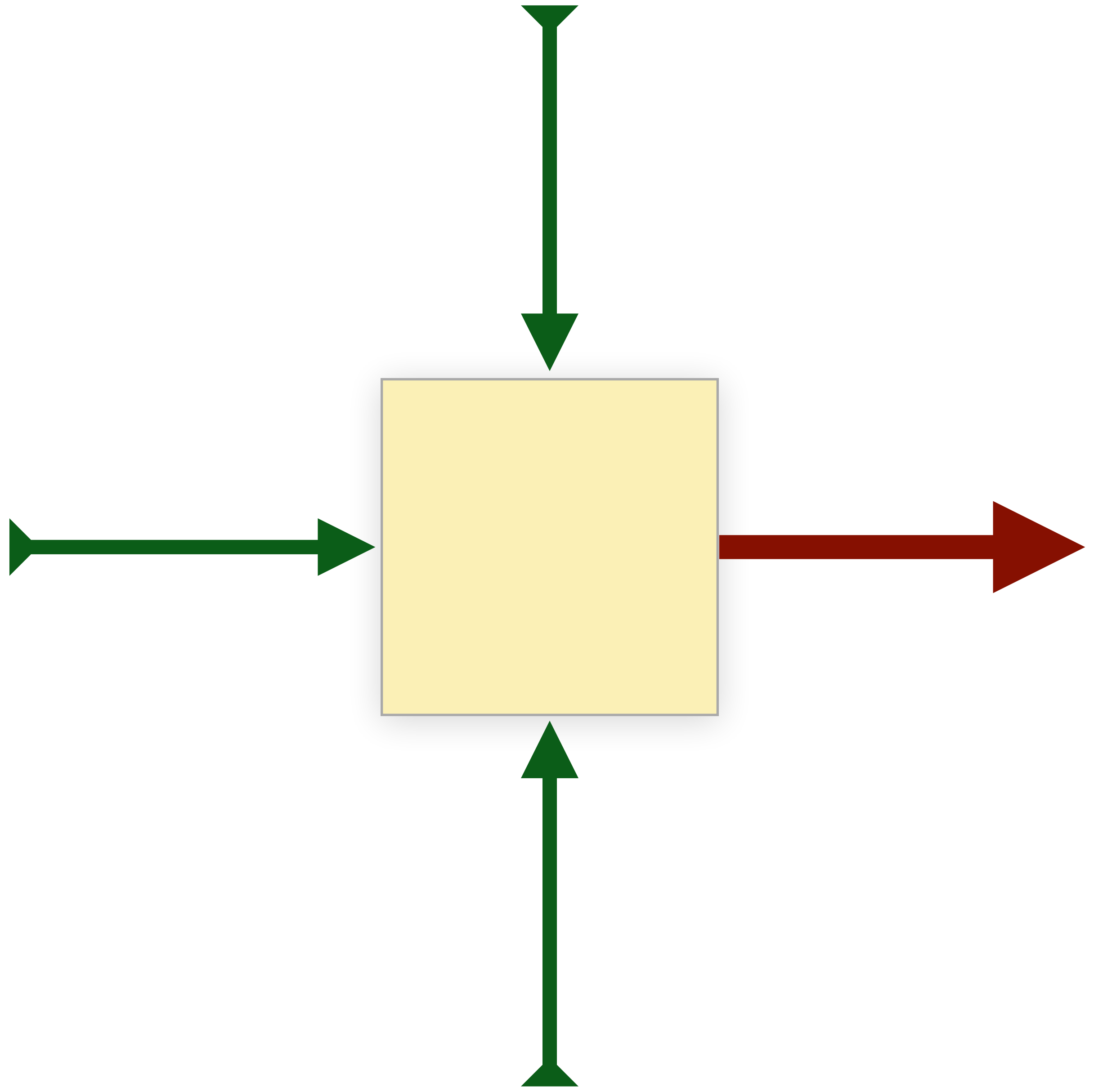
Background



Automata theory
Deterministic finite automata
This talk
Weighted finite automata
Sobol indices
Tensor methods
Sensitivity analysis
Variance-based methods

Sobol’s Method for
Global Sensitivity Analysis

Sensitivity Analysis



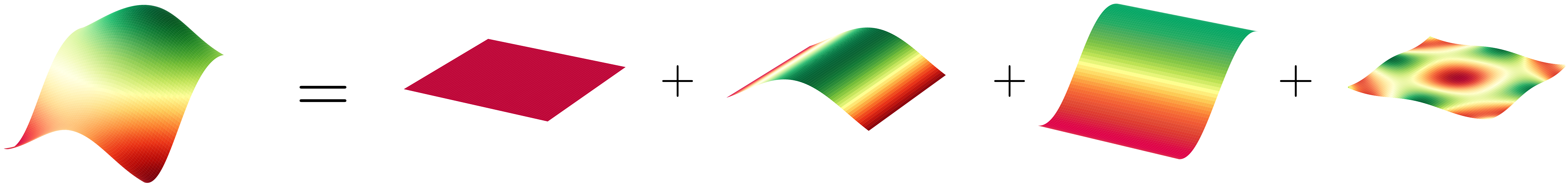
inputs $\longrightarrow$ **output(s)**

$$f : (x_0, \ldots, x_{N-1}) \mapsto \mathbb{R}^M$$

- Influence of each variable?
- Influence of groups of variables?

ANOVA Decomposition

- **Partition** $f(x_0, \ldots, x_{N-1})$ into 2^N subfunctions: **[Hoeffding '48]**
  - A **constant**
  - **One-variable** functions
  - **Two-variable** functions, etc.



$$f(\boldsymbol{x}) = \sum_{\boldsymbol{\alpha} \subseteq \{1,\ldots,N\}} f_{\boldsymbol{\alpha}}(\boldsymbol{x}_{\boldsymbol{\alpha}})$$

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ANOVA Decomposition

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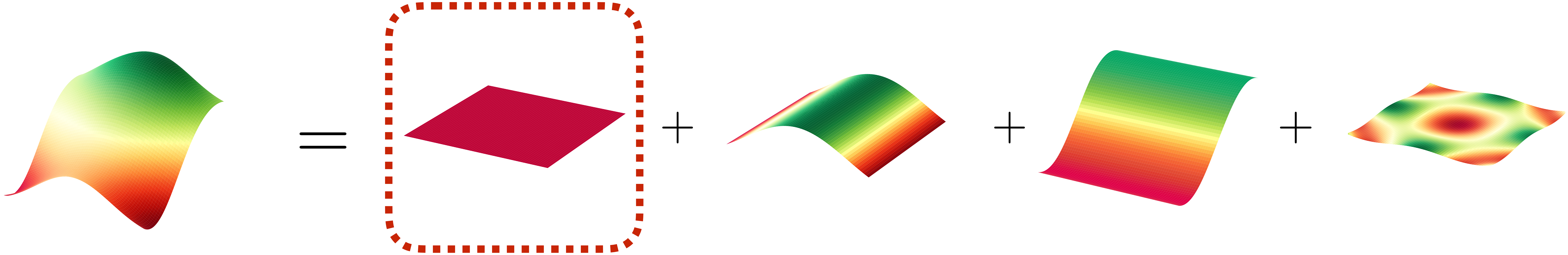

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ANOVA Decomposition

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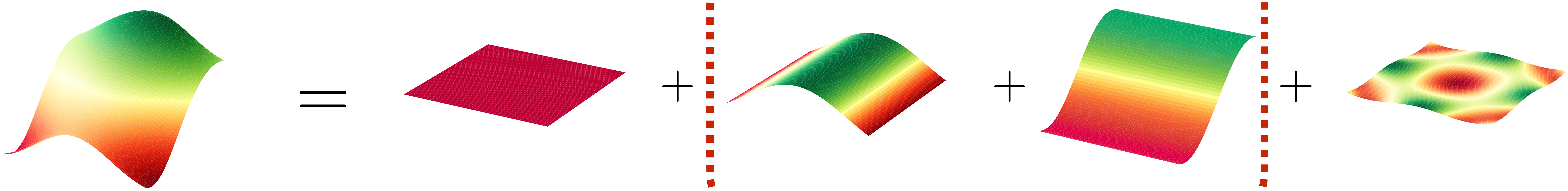

$$f(\boldsymbol{x}) = \sum_{\boldsymbol{\alpha} \subseteq \{1,\ldots,N\}} f_{\boldsymbol{\alpha}}(\boldsymbol{x}_{\boldsymbol{\alpha}})$$

ANOVA Decomposition

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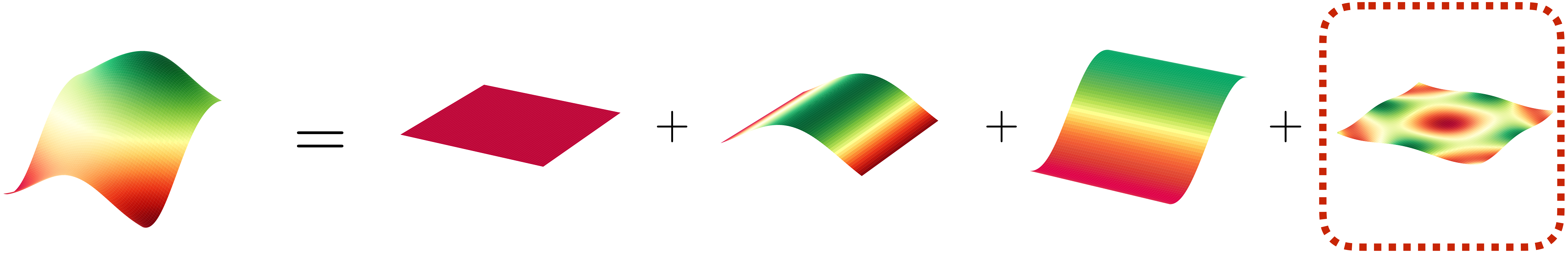

$$f(\boldsymbol{x}) = \sum_{\boldsymbol{\alpha}\subseteq\{1,\ldots,N\}} f_{\boldsymbol{\alpha}}(\boldsymbol{x}_{\boldsymbol{\alpha}})$$

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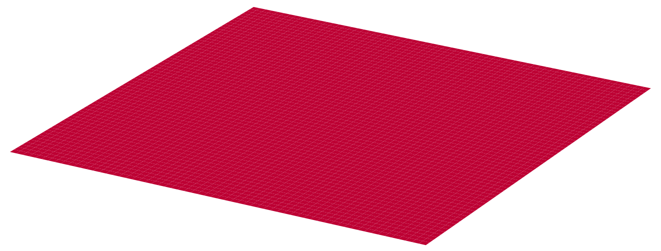
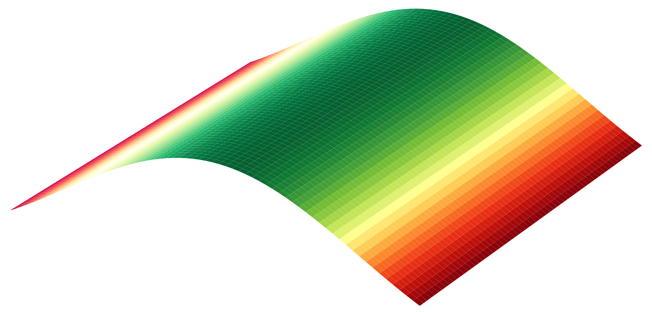
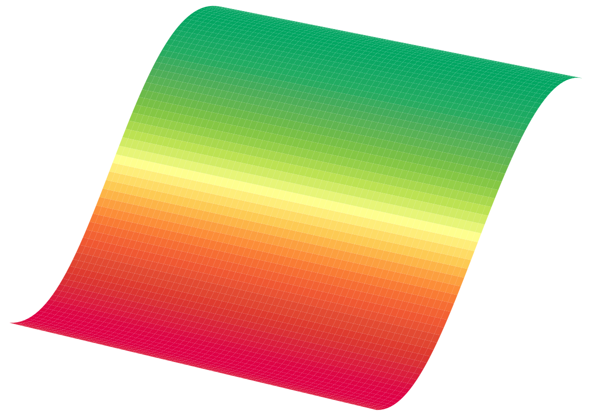
Construction

- $f_\emptyset = \mathbb{E}[f]$

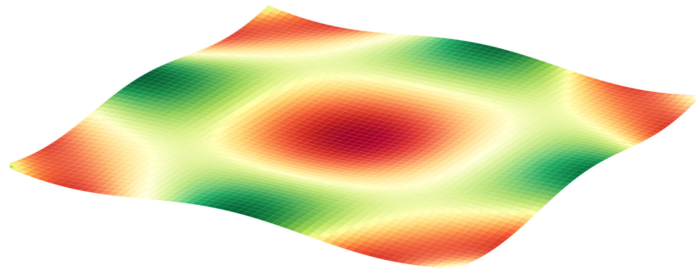


- $f_n(x_n) = \mathbb{E}[f(\ldots, x_n, \ldots)] - \mathbb{E}[f]$





- $f_{n,m}(x_n, x_m) = \mathbb{E}[f(\ldots, x_n, \ldots, x_m, \ldots)] - \mathbb{E}[f(\ldots, x_n. \ldots)] - \mathbb{E}[f(\ldots, x_m, \ldots)] + \mathbb{E}[f]$



- Etc.

Recursive definition

$$f_{\boldsymbol{\alpha}} = \mathbb{E}\left[f(x_{\boldsymbol{\alpha}}) - \sum_{\boldsymbol{\beta} \subsetneq \boldsymbol{\alpha}} f_{\boldsymbol{\beta}}(x_{\boldsymbol{\beta}}) \right]$$

Sobol's Method

[Sobol' 90]

Variance Components

$$S_{\boldsymbol{\alpha}} := \mathrm{Var}[f_{\boldsymbol{\alpha}}]/\mathrm{Var}[f]$$

Closed Indices

$$S^C_{\boldsymbol{\alpha}} := \sum_{\boldsymbol{\beta}|\boldsymbol{\alpha}\supseteq\boldsymbol{\beta}} S_{\boldsymbol{\beta}}$$

Total Indices

$$S^T_{\boldsymbol{\alpha}} := \sum_{\boldsymbol{\beta}|\boldsymbol{\alpha}\cap\boldsymbol{\beta}\neq\emptyset} S_{\boldsymbol{\beta}}$$

Superset Indices

$$S^S_{\boldsymbol{\alpha}} := \sum_{\boldsymbol{\beta}|\boldsymbol{\alpha}\subseteq\boldsymbol{\beta}} S_{\boldsymbol{\beta}}$$

- Each index measures **effects** of a **group of variables**

Curse of Dimensionality

- Each index: N-**dimensional integral**
- N dimensions $\rightarrow$ $\mathbf{2^N}$ **indices** of each type
- Much research since the 1990s
  - Monte Carlo integration
  - Quasi random sequences (Sobol, Saltelli)
- Still quite slow

Metamodeling

Tensor metamodeling

Tensor Metamodeling

- **Black box functions**
  - Simulations
  - Analytical models
  - Engineering systems

- **Tensor decompositions**
  - CP
  - Tucker
  - TT, QTT
  - Spectral, functional TT
  - Exponential machines

- **Processing**
  - Integration
  - Sensitivity analysis
  - Visualization

[Grasedyck et al. '13] **[Vervliet et al. '14]** **[Rai '14]**

[Dolgov et al. '14] **[Novikov et al. '16]** **[Bigoni et al. '16]** **[Gorodetsky & Jakeman '18]**

Here: we will assume

$$f(x_0, \ldots, x_{N-1}) \approx \mathcal{T}[i_0, \ldots, i_{N-1}]$$

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Tensors for Sobol's Method

- Main burden: **computing variances**
- *Easy* with tensors: $\sum(\mathcal{T}^2) = \langle \mathcal{T}, \mathcal{T} \rangle$
- Dot products have polynomial cost on the rank
  - E.g. $O(R^3)$: quite good
- Used to **extract Sobol indices** from various low-rank formats

[Dolgov et al. '14] **[Rai '14]** **[Bigoni et al. '16]** **[Konakli & Sudret '16]**

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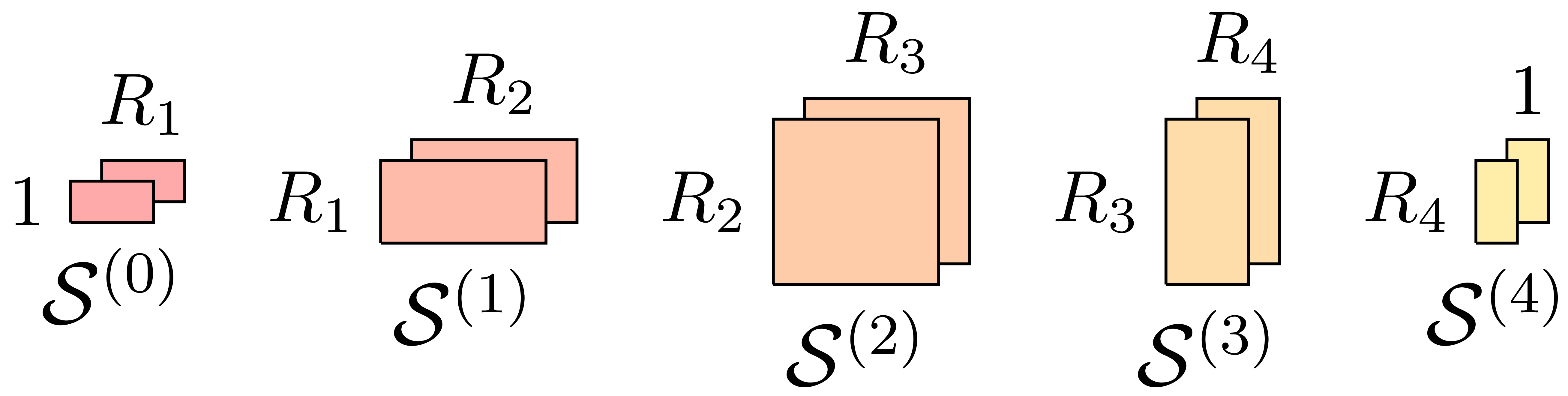
Sobol Tensor Trains

Sobol Tensor Trains

Sobol TT

$$\mathcal{S} = [[\mathcal{S}^{(0)}, \dots, \mathcal{S}^{(N-1)}]]$$

- Our alternative idea **[Ballester-Ripoll et al. '17]**
- Gather *all* indices in **one tensor train**



- Read an index = decompress one tensor entry
- Moves all the effort to the **preprocessing**

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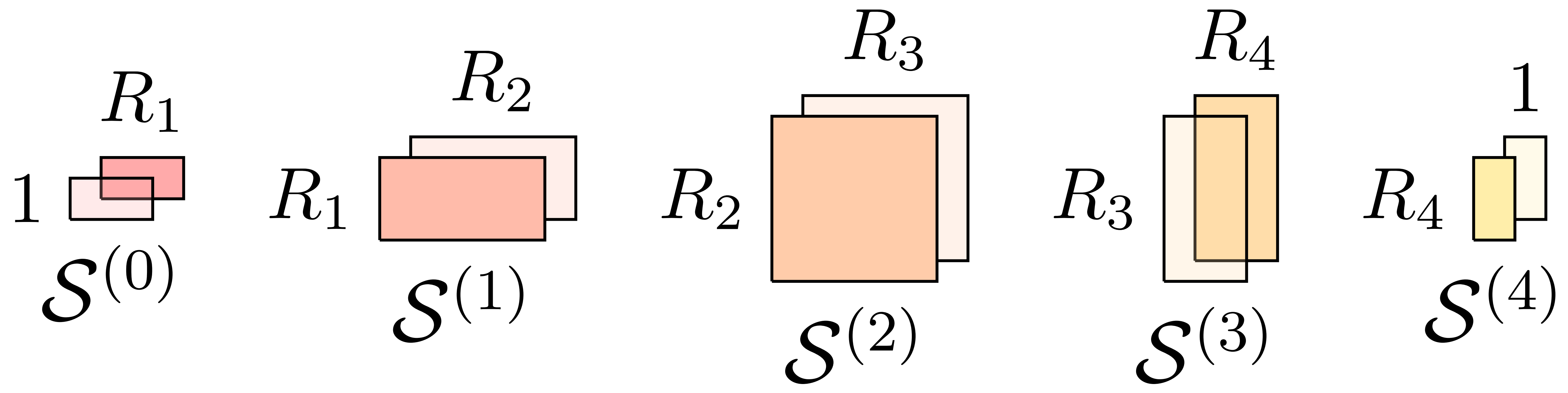
Sobol Tensor Trains

- Indexing example
  - Read variance component for variables $\{x_0, x_3\}$

$$S_{0,3} \approx \mathcal{S}_{0,3} = \mathcal{S}^{(0)}[1] \cdot \mathcal{S}^{(1)}[0] \cdot \mathcal{S}^{(2)}[0] \cdot \mathcal{S}^{(3)}[1] \cdot \mathcal{S}^{(4)}[0]$$



Recipe: Sobol Tensor

- A $4 \times 4 \times 4$ tensor $\mathcal{T} = [[\mathcal{T}^{(0)}, \mathcal{T}^{(1)}, \mathcal{T}^{(2)}]]$:

$$\left\lfloor \begin{array}{c} \mathcal{T}^{(0)}[3] \\ \mathcal{T}^{(0)}[2] \\ \mathcal{T}^{(0)}[1] \\ \mathcal{T}^{(0)}[0] \end{array} \right\rfloor \cdot \left\lfloor \begin{array}{c} \mathcal{T}^{(1)}[3] \\ \mathcal{T}^{(1)}[2] \\ \mathcal{T}^{(1)}[1] \\ \mathcal{T}^{(1)}[0] \end{array} \right\rfloor \cdot \left\lfloor \begin{array}{c} \mathcal{T}^{(2)}[3] \\ \mathcal{T}^{(2)}[2] \\ \mathcal{T}^{(2)}[1] \\ \mathcal{T}^{(2)}[0] \end{array} \right\rfloor$$

Recipe: Sobol Tensor

- Element $\mathcal{T}[2,3,0]$:

$$\begin{bmatrix} \mathcal{T}^{(0)}[3] \\ \boldsymbol{\mathcal{T}^{(0)}[2]} \\ \mathcal{T}^{(0)}[1] \\ \mathcal{T}^{(0)}[0] \end{bmatrix} \cdot \begin{bmatrix} \boldsymbol{\mathcal{T}^{(1)}[3]} \\ \mathcal{T}^{(1)}[2] \\ \mathcal{T}^{(1)}[1] \\ \mathcal{T}^{(1)}[0] \end{bmatrix} \begin{bmatrix} \mathcal{T}^{(2)}[3] \\ \mathcal{T}^{(2)}[2] \\ \mathcal{T}^{(2)}[1] \\ \boldsymbol{\mathcal{T}^{(2)}[0]} \end{bmatrix}$$

Recipe: Sobol Tensor

- Modified tensor $\mathcal{T}_*$, has size $5 \times 5 \times 5$:

$$\begin{bmatrix} \mathcal{T}^{(0)}[3] - \mathbb{E}[\mathcal{T}^{(0)}] \\ \mathcal{T}^{(0)}[2] - \mathbb{E}[\mathcal{T}^{(0)}] \\ \mathcal{T}^{(0)}[1] - \mathbb{E}[\mathcal{T}^{(0)}] \\ \mathcal{T}^{(0)}[0] - \mathbb{E}[\mathcal{T}^{(0)}] \\ \mathbb{E}[\mathcal{T}^{(0)}] \end{bmatrix} \cdot \begin{bmatrix} \mathcal{T}^{(1)}[3] - \mathbb{E}[\mathcal{T}^{(1)}] \\ \mathcal{T}^{(1)}[2] - \mathbb{E}[\mathcal{T}^{(1)}] \\ \mathcal{T}^{(1)}[1] - \mathbb{E}[\mathcal{T}^{(1)}] \\ \mathcal{T}^{(1)}[0] - \mathbb{E}[\mathcal{T}^{(1)}] \\ \mathbb{E}[\mathcal{T}^{(1)}] \end{bmatrix} \cdot \begin{bmatrix} \mathcal{T}^{(2)}[3] - \mathbb{E}[\mathcal{T}^{(2)}] \\ \mathcal{T}^{(2)}[2] - \mathbb{E}[\mathcal{T}^{(2)}] \\ \mathcal{T}^{(2)}[1] - \mathbb{E}[\mathcal{T}^{(2)}] \\ \mathcal{T}^{(2)}[0] - \mathbb{E}[\mathcal{T}^{(2)}] \\ \mathbb{E}[\mathcal{T}^{(2)}] \end{bmatrix}$$

$\mathcal{T}_*$ encodes all 2^N ANOVA terms $f_{\boldsymbol{\alpha}}$

Recipe: Sobol Tensor

- Example: global mean $f_\emptyset$

$$\underbrace{\begin{bmatrix} \mathcal{T}^{(0)}[3] - \mathbb{E}[\mathcal{T}^{(0)}] \\ \mathcal{T}^{(0)}[2] - \mathbb{E}[\mathcal{T}^{(0)}] \\ \mathcal{T}^{(0)}[1] - \mathbb{E}[\mathcal{T}^{(0)}] \\ \mathcal{T}^{(0)}[0] - \mathbb{E}[\mathcal{T}^{(0)}] \end{bmatrix}}_{\mathbb{E}[\mathcal{T}^{(0)}]} \cdot \underbrace{\begin{bmatrix} \mathcal{T}^{(1)}[3] - \mathbb{E}[\mathcal{T}^{(1)}] \\ \mathcal{T}^{(1)}[2] - \mathbb{E}[\mathcal{T}^{(1)}] \\ \mathcal{T}^{(1)}[1] - \mathbb{E}[\mathcal{T}^{(1)}] \\ \mathcal{T}^{(1)}[0] - \mathbb{E}[\mathcal{T}^{(1)}] \end{bmatrix}}_{\mathbb{E}[\mathcal{T}^{(1)}]} \cdot \underbrace{\begin{bmatrix} \mathcal{T}^{(2)}[3] - \mathbb{E}[\mathcal{T}^{(2)}] \\ \mathcal{T}^{(2)}[2] - \mathbb{E}[\mathcal{T}^{(2)}] \\ \mathcal{T}^{(2)}[1] - \mathbb{E}[\mathcal{T}^{(2)}] \\ \mathcal{T}^{(2)}[0] - \mathbb{E}[\mathcal{T}^{(2)}] \end{bmatrix}}_{\mathbb{E}[\mathcal{T}^{(2)}]}$$

$$\mathbb{E}[\mathcal{T}^{(0)}] \cdot \mathbb{E}[\mathcal{T}^{(1)}] \cdot \mathbb{E}[\mathcal{T}^{(2)}] = \mathbb{E}[\mathcal{T}] = f_\emptyset$$

Recipe: Sobol Tensor

- Example: global mean $f_\emptyset$

$$\left\lfloor \begin{matrix} \mathcal{T}^{(0)}[3] - \mathbb{E}[\mathcal{T}^{(0)}] \\ \mathcal{T}^{(0)}[2] - \mathbb{E}[\mathcal{T}^{(0)}] \\ \mathcal{T}^{(0)}[1] - \mathbb{E}[\mathcal{T}^{(0)}] \\ \mathcal{T}^{(0)}[0] - \mathbb{E}[\mathcal{T}^{(0)}] \\ \boldsymbol{\mathbb{E}[\mathcal{T}^{(0)}]} \end{matrix} \right\rfloor \cdot \left\lfloor \begin{matrix} \mathcal{T}^{(1)}[3] - \mathbb{E}[\mathcal{T}^{(1)}] \\ \mathcal{T}^{(1)}[2] - \mathbb{E}[\mathcal{T}^{(1)}] \\ \mathcal{T}^{(1)}[1] - \mathbb{E}[\mathcal{T}^{(1)}] \\ \mathcal{T}^{(1)}[0] - \mathbb{E}[\mathcal{T}^{(1)}] \\ \boldsymbol{\mathbb{E}[\mathcal{T}^{(1)}]} \end{matrix} \right\rfloor \cdot \left\lfloor \begin{matrix} \mathcal{T}^{(2)}[3] - \mathbb{E}[\mathcal{T}^{(2)}] \\ \mathcal{T}^{(2)}[2] - \mathbb{E}[\mathcal{T}^{(2)}] \\ \mathcal{T}^{(2)}[1] - \mathbb{E}[\mathcal{T}^{(2)}] \\ \mathcal{T}^{(2)}[0] - \mathbb{E}[\mathcal{T}^{(2)}] \\ \boldsymbol{\mathbb{E}[\mathcal{T}^{(2)}]} \end{matrix} \right\rfloor$$

$$\mathbb{E}[\mathcal{T}^{(0)}] \cdot \mathbb{E}[\mathcal{T}^{(1)}] \cdot \mathbb{E}[\mathcal{T}^{(2)}] = \boxed{\mathbb{E}[\mathcal{T}]} = f_\emptyset$$

Recipe: Sobol Tensor

- Example: global mean $f_\emptyset$

$$\underbrace{\begin{bmatrix} \mathcal{T}^{(0)}[3] - \mathbb{E}[\mathcal{T}^{(0)}] \\ \mathcal{T}^{(0)}[2] - \mathbb{E}[\mathcal{T}^{(0)}] \\ \mathcal{T}^{(0)}[1] - \mathbb{E}[\mathcal{T}^{(0)}] \\ \mathcal{T}^{(0)}[0] - \mathbb{E}[\mathcal{T}^{(0)}] \end{bmatrix}}_{\mathbb{E}[\boldsymbol{\mathcal{T}}^{(\mathbf{0})}]} \cdot \underbrace{\begin{bmatrix} \mathcal{T}^{(1)}[3] - \mathbb{E}[\mathcal{T}^{(1)}] \\ \mathcal{T}^{(1)}[2] - \mathbb{E}[\mathcal{T}^{(1)}] \\ \mathcal{T}^{(1)}[1] - \mathbb{E}[\mathcal{T}^{(1)}] \\ \mathcal{T}^{(1)}[0] - \mathbb{E}[\mathcal{T}^{(1)}] \end{bmatrix}}_{\mathbb{E}[\boldsymbol{\mathcal{T}}^{(\mathbf{1})}]} \cdot \underbrace{\begin{bmatrix} \mathcal{T}^{(2)}[3] - \mathbb{E}[\mathcal{T}^{(2)}] \\ \mathcal{T}^{(2)}[2] - \mathbb{E}[\mathcal{T}^{(2)}] \\ \mathcal{T}^{(2)}[1] - \mathbb{E}[\mathcal{T}^{(2)}] \\ \mathcal{T}^{(2)}[0] - \mathbb{E}[\mathcal{T}^{(2)}] \end{bmatrix}}_{\mathbb{E}[\boldsymbol{\mathcal{T}}^{(\mathbf{2})}]}$$

$$\mathbb{E}[\mathcal{T}^{(0)}] \cdot \mathbb{E}[\mathcal{T}^{(1)}] \cdot \mathbb{E}[\mathcal{T}^{(2)}] = \mathbb{E}[\mathcal{T}] = f_\emptyset$$

Recipe: Sobol Tensor

- Example: $f_2(3)$

$$
\begin{bmatrix}
\mathcal{T}^{(0)}[3] - \mathbb{E}[\mathcal{T}^{(0)}] \\
\mathcal{T}^{(0)}[2] - \mathbb{E}[\mathcal{T}^{(0)}] \\
\mathcal{T}^{(0)}[1] - \mathbb{E}[\mathcal{T}^{(0)}] \\
\mathcal{T}^{(0)}[0] - \mathbb{E}[\mathcal{T}^{(0)}] \\
\boldsymbol{\mathbb{E}[\mathcal{T}^{(0)}]}
\end{bmatrix}
\cdot
\begin{bmatrix}
\mathcal{T}^{(1)}[3] - \mathbb{E}[\mathcal{T}^{(1)}] \\
\mathcal{T}^{(1)}[2] - \mathbb{E}[\mathcal{T}^{(1)}] \\
\mathcal{T}^{(1)}[1] - \mathbb{E}[\mathcal{T}^{(1)}] \\
\mathcal{T}^{(1)}[0] - \mathbb{E}[\mathcal{T}^{(1)}] \\
\boldsymbol{\mathbb{E}[\mathcal{T}^{(1)}]}
\end{bmatrix}
\cdot
\begin{bmatrix}
\boldsymbol{\mathcal{T}^{(2)}[3] - \mathbb{E}[\mathcal{T}^{(2)}]} \\
\mathcal{T}^{(2)}[2] - \mathbb{E}[\mathcal{T}^{(2)}] \\
\mathcal{T}^{(2)}[1] - \mathbb{E}[\mathcal{T}^{(2)}] \\
\mathcal{T}^{(2)}[0] - \mathbb{E}[\mathcal{T}^{(2)}] \\
\mathbb{E}[\mathcal{T}^{(2)}]
\end{bmatrix}
$$

$$
\begin{aligned}
&\mathbb{E}[\mathcal{T}^{(0)}] \cdot \mathbb{E}[\mathcal{T}^{(1)}] \cdot \mathcal{T}^{(2)}[3] - \mathbb{E}[\mathcal{T}^{(0)}] \cdot \mathbb{E}[\mathcal{T}^{(1)}] \cdot \mathbb{E}[\mathcal{T}^{(2)}] \\
&= \mathbb{E}[f(\cdot, \cdot, 3)] - \mathbb{E}[f] = f_2(3)
\end{aligned}
$$

Recipe: Sobol Tensor

- Example: $f_2(3)$

$$\begin{bmatrix} \mathcal{T}^{(0)}[3] - \mathbb{E}[\mathcal{T}^{(0)}] \\ \mathcal{T}^{(0)}[2] - \mathbb{E}[\mathcal{T}^{(0)}] \\ \mathcal{T}^{(0)}[1] - \mathbb{E}[\mathcal{T}^{(0)}] \\ \mathcal{T}^{(0)}[0] - \mathbb{E}[\mathcal{T}^{(0)}] \\ \boxed{\mathbb{E}[\mathcal{T}^{(0)}]} \end{bmatrix} \cdot \begin{bmatrix} \mathcal{T}^{(1)}[3] - \mathbb{E}[\mathcal{T}^{(1)}] \\ \mathcal{T}^{(1)}[2] - \mathbb{E}[\mathcal{T}^{(1)}] \\ \mathcal{T}^{(1)}[1] - \mathbb{E}[\mathcal{T}^{(1)}] \\ \mathcal{T}^{(1)}[0] - \mathbb{E}[\mathcal{T}^{(1)}] \\ \boxed{\mathbb{E}[\mathcal{T}^{(1)}]} \end{bmatrix} \cdot \begin{bmatrix} \boxed{\mathcal{T}^{(2)}[3]} - \mathbb{E}[\mathcal{T}^{(2)}] \\ \mathcal{T}^{(2)}[2] - \mathbb{E}[\mathcal{T}^{(2)}] \\ \mathcal{T}^{(2)}[1] - \mathbb{E}[\mathcal{T}^{(2)}] \\ \mathcal{T}^{(2)}[0] - \mathbb{E}[\mathcal{T}^{(2)}] \\ \mathbb{E}[\mathcal{T}^{(2)}] \end{bmatrix}$$

$$\boxed{\mathbb{E}[\mathcal{T}^{(0)}] \cdot \mathbb{E}[\mathcal{T}^{(1)}] \cdot \mathcal{T}^{(2)}[3]} - \mathbb{E}[\mathcal{T}^{(0)}] \cdot \mathbb{E}[\mathcal{T}^{(1)}] \cdot \mathbb{E}[\mathcal{T}^{(2)}]$$
$$= \mathbb{E}[f(\cdot, \cdot, 3)] - \mathbb{E}[f] = f_2(3)$$

Recipe: Sobol Tensor

- Example: $f_2(3)$

$$\begin{bmatrix} \mathcal{T}^{(0)}[3] - \mathbb{E}[\mathcal{T}^{(0)}] \\ \mathcal{T}^{(0)}[2] - \mathbb{E}[\mathcal{T}^{(0)}] \\ \mathcal{T}^{(0)}[1] - \mathbb{E}[\mathcal{T}^{(0)}] \\ \mathcal{T}^{(0)}[0] - \mathbb{E}[\mathcal{T}^{(0)}] \\ \boxed{\mathbb{E}[\mathcal{T}^{(0)}]} \end{bmatrix} \cdot \begin{bmatrix} \mathcal{T}^{(1)}[3] - \mathbb{E}[\mathcal{T}^{(1)}] \\ \mathcal{T}^{(1)}[2] - \mathbb{E}[\mathcal{T}^{(1)}] \\ \mathcal{T}^{(1)}[1] - \mathbb{E}[\mathcal{T}^{(1)}] \\ \mathcal{T}^{(1)}[0] - \mathbb{E}[\mathcal{T}^{(1)}] \\ \boxed{\mathbb{E}[\mathcal{T}^{(1)}]} \end{bmatrix} \cdot \begin{bmatrix} \boldsymbol{\mathcal{T}^{(2)}[3]} - \boxed{\mathbb{E}[\mathcal{T}^{(2)}]} \\ \mathcal{T}^{(2)}[2] - \mathbb{E}[\mathcal{T}^{(2)}] \\ \mathcal{T}^{(2)}[1] - \mathbb{E}[\mathcal{T}^{(2)}] \\ \mathcal{T}^{(2)}[0] - \mathbb{E}[\mathcal{T}^{(2)}] \\ \mathbb{E}[\mathcal{T}^{(2)}] \end{bmatrix}$$

$$\mathbb{E}[\mathcal{T}^{(0)}] \cdot \mathbb{E}[\mathcal{T}^{(1)}] \cdot \mathcal{T}^{(2)}[3] - \boxed{\mathbb{E}[\mathcal{T}^{(0)}] \cdot \mathbb{E}[\mathcal{T}^{(1)}] \cdot \mathbb{E}[\mathcal{T}^{(2)}]}$$
$$= \mathbb{E}[f(\cdot, \cdot, 3)] - \mathbb{E}[f] = f_2(3)$$

Recipe: Sobol Tensor

- Example: $f_2(3)$

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\begin{bmatrix}
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\mathcal{T}^{(2)}[1]-\mathbb{E}[\mathcal{T}^{(2)}] \\
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\mathbb{E}[\mathcal{T}^{(2)}]
\end{bmatrix}
$$

$$
\begin{aligned}
&\mathbb{E}[\mathcal{T}^{(0)}]\cdot\mathbb{E}[\mathcal{T}^{(1)}]\cdot\mathcal{T}^{(2)}[3]-\mathbb{E}[\mathcal{T}^{(0)}]\cdot\mathbb{E}[\mathcal{T}^{(1)}]\cdot\mathbb{E}[\mathcal{T}^{(2)}] \\
&= \mathbb{E}[f(\cdot,\cdot,3)]-\mathbb{E}[f] = f_2(3)
\end{aligned}
$$

Recipe: Sobol Tensor

- Example: $f_2(3)$

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\begin{bmatrix}
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\mathcal{T}^{(0)}[2] - \mathbb{E}[\mathcal{T}^{(0)}] \\
\mathcal{T}^{(0)}[1] - \mathbb{E}[\mathcal{T}^{(0)}] \\
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\boldsymbol{\mathbb{E}[\mathcal{T}^{(0)}]}
\end{bmatrix}
\cdot
\begin{bmatrix}
\mathcal{T}^{(1)}[3] - \mathbb{E}[\mathcal{T}^{(1)}] \\
\mathcal{T}^{(1)}[2] - \mathbb{E}[\mathcal{T}^{(1)}] \\
\mathcal{T}^{(1)}[1] - \mathbb{E}[\mathcal{T}^{(1)}] \\
\mathcal{T}^{(1)}[0] - \mathbb{E}[\mathcal{T}^{(1)}] \\
\boldsymbol{\mathbb{E}[\mathcal{T}^{(1)}]}
\end{bmatrix}
\cdot
\begin{bmatrix}
\boldsymbol{\mathcal{T}^{(2)}[3] - \mathbb{E}[\mathcal{T}^{(2)}]} \\
\mathcal{T}^{(2)}[2] - \mathbb{E}[\mathcal{T}^{(2)}] \\
\mathcal{T}^{(2)}[1] - \mathbb{E}[\mathcal{T}^{(2)}] \\
\mathcal{T}^{(2)}[0] - \mathbb{E}[\mathcal{T}^{(2)}] \\
\mathbb{E}[\mathcal{T}^{(2)}]
\end{bmatrix}
$$

$$
\begin{aligned}
&\mathbb{E}[\mathcal{T}^{(0)}] \cdot \mathbb{E}[\mathcal{T}^{(1)}] \cdot \mathcal{T}^{(2)}[3] - \mathbb{E}[\mathcal{T}^{(0)}] \cdot \mathbb{E}[\mathcal{T}^{(1)}] \cdot \mathbb{E}[\mathcal{T}^{(2)}] \\
&= \mathbb{E}[f(\cdot, \cdot, 3)] - \mathbb{E}[f] = f_2(3)
\end{aligned}
$$

Recipe: Sobol Tensor

- Example: $f_{0,2}(3,1)$

$$\begin{bmatrix} \boldsymbol{\mathcal{T}^{(0)}[3] - \mathbb{E}[\mathcal{T}^{(0)}]} \\ \mathcal{T}^{(0)}[2] - \mathbb{E}[\mathcal{T}^{(0)}] \\ \mathcal{T}^{(0)}[1] - \mathbb{E}[\mathcal{T}^{(0)}] \\ \mathcal{T}^{(0)}[0] - \mathbb{E}[\mathcal{T}^{(0)}] \\ \mathbb{E}[\mathcal{T}^{(0)}] \end{bmatrix} \cdot \begin{bmatrix} \mathcal{T}^{(1)}[3] - \mathbb{E}[\mathcal{T}^{(1)}] \\ \mathcal{T}^{(1)}[2] - \mathbb{E}[\mathcal{T}^{(1)}] \\ \mathcal{T}^{(1)}[1] - \mathbb{E}[\mathcal{T}^{(1)}] \\ \mathcal{T}^{(1)}[0] - \mathbb{E}[\mathcal{T}^{(1)}] \\ \boldsymbol{\mathbb{E}[\mathcal{T}^{(1)}]} \end{bmatrix} \cdot \begin{bmatrix} \mathcal{T}^{(2)}[3] - \mathbb{E}[\mathcal{T}^{(2)}] \\ \mathcal{T}^{(2)}[2] - \mathbb{E}[\mathcal{T}^{(2)}] \\ \boldsymbol{\mathcal{T}^{(2)}[1] - \mathbb{E}[\mathcal{T}^{(2)}]} \\ \mathcal{T}^{(2)}[0] - \mathbb{E}[\mathcal{T}^{(2)}] \\ \mathbb{E}[\mathcal{T}^{(2)}] \end{bmatrix}$$

$$\mathcal{T}^{(0)} \cdot \mathbb{E}[\mathcal{T}^{(1)}] \cdot \mathcal{T}^{(2)}[1] - \mathcal{T}^{(0)}[3] \cdot \mathbb{E}[\mathcal{T}^{(1)}] \cdot \mathbb{E}[\mathcal{T}^{(2)}] -$$

$$-\mathbb{E}[\mathcal{T}^{(0)}] \cdot \mathbb{E}[\mathcal{T}^{(1)}] \cdot \mathcal{T}^{(2)}[1] + \mathbb{E}[\mathcal{T}^{(0)}] \cdot \mathbb{E}[\mathcal{T}^{(1)}] \cdot \mathbb{E}[\mathcal{T}^{(2)}]$$

$$= \mathbb{E}[f(3,\cdot,1)] - \mathbb{E}[f(3,\cdot,\cdot)] - \mathbb{E}[f(\cdot,\cdot,1)] + \mathbb{E}[f] = f_{0,2}(3,1)$$

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Recipe: Sobol Tensor

- Example: $f_{0,2}(3,1)$

$$\begin{bmatrix} \mathcal{T}^{(0)}[3] - \mathbb{E}[\mathcal{T}^{(0)}] \\ \mathcal{T}^{(0)}[2] - \mathbb{E}[\mathcal{T}^{(0)}] \\ \mathcal{T}^{(0)}[1] - \mathbb{E}[\mathcal{T}^{(0)}] \\ \mathcal{T}^{(0)}[0] - \mathbb{E}[\mathcal{T}^{(0)}] \\ \mathbb{E}[\mathcal{T}^{(0)}] \end{bmatrix} \cdot \begin{bmatrix} \mathcal{T}^{(1)}[3] - \mathbb{E}[\mathcal{T}^{(1)}] \\ \mathcal{T}^{(1)}[2] - \mathbb{E}[\mathcal{T}^{(1)}] \\ \mathcal{T}^{(1)}[1] - \mathbb{E}[\mathcal{T}^{(1)}] \\ \mathcal{T}^{(1)}[0] - \mathbb{E}[\mathcal{T}^{(1)}] \\ \mathbb{E}[\mathcal{T}^{(1)}] \end{bmatrix} \cdot \begin{bmatrix} \mathcal{T}^{(2)}[3] - \mathbb{E}[\mathcal{T}^{(2)}] \\ \mathcal{T}^{(2)}[2] - \mathbb{E}[\mathcal{T}^{(2)}] \\ \mathcal{T}^{(2)}[1] - \mathbb{E}[\mathcal{T}^{(2)}] \\ \mathcal{T}^{(2)}[0] - \mathbb{E}[\mathcal{T}^{(2)}] \\ \mathbb{E}[\mathcal{T}^{(2)}] \end{bmatrix}$$

$$\mathcal{T}^{(0)}[3] \cdot \mathbb{E}[\mathcal{T}^{(1)}] \cdot \mathcal{T}^{(2)}[1] - \mathcal{T}^{(0)}[3] \cdot \mathbb{E}[\mathcal{T}^{(1)}] \cdot \mathbb{E}[\mathcal{T}^{(2)}] -$$
$$- \mathbb{E}[\mathcal{T}^{(0)}] \cdot \mathbb{E}[\mathcal{T}^{(1)}] \cdot \mathcal{T}^{(2)}[1] + \mathbb{E}[\mathcal{T}^{(0)}] \cdot \mathbb{E}[\mathcal{T}^{(1)}] \cdot \mathbb{E}[\mathcal{T}^{(2)}]$$
$$= \mathbb{E}[f(3,\cdot,1)] - \mathbb{E}[f(3,\cdot,\cdot)] - \mathbb{E}[f(\cdot,\cdot,1)] + \mathbb{E}[f] = f_{0,2}(3,1)$$

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Recipe: Sobol Tensor

- Example: $f_{0,2}(3,1)$

$$\begin{bmatrix} \mathcal{T}^{(0)}[3]-\mathbb{E}[\mathcal{T}^{(0)}] \\ \mathcal{T}^{(0)}[2]-\mathbb{E}[\mathcal{T}^{(0)}] \\ \mathcal{T}^{(0)}[1]-\mathbb{E}[\mathcal{T}^{(0)}] \\ \mathcal{T}^{(0)}[0]-\mathbb{E}[\mathcal{T}^{(0)}] \\ \mathbb{E}[\mathcal{T}^{(0)}] \end{bmatrix} \cdot \begin{bmatrix} \mathcal{T}^{(1)}[3]-\mathbb{E}[\mathcal{T}^{(1)}] \\ \mathcal{T}^{(1)}[2]-\mathbb{E}[\mathcal{T}^{(1)}] \\ \mathcal{T}^{(1)}[1]-\mathbb{E}[\mathcal{T}^{(1)}] \\ \mathcal{T}^{(1)}[0]-\mathbb{E}[\mathcal{T}^{(1)}] \\ \mathbb{E}[\mathcal{T}^{(1)}] \end{bmatrix} \cdot \begin{bmatrix} \mathcal{T}^{(2)}[3]-\mathbb{E}[\mathcal{T}^{(2)}] \\ \mathcal{T}^{(2)}[2]-\mathbb{E}[\mathcal{T}^{(2)}] \\ \mathcal{T}^{(2)}[1]-\mathbb{E}[\mathcal{T}^{(2)}] \\ \mathcal{T}^{(2)}[0]-\mathbb{E}[\mathcal{T}^{(2)}] \\ \mathbb{E}[\mathcal{T}^{(2)}] \end{bmatrix}$$

$$\mathcal{T}^{(0)}[3]\cdot\mathbb{E}[\mathcal{T}^{(1)}]\cdot\mathcal{T}^{(2)}[1] - \mathcal{T}^{(0)}[3]\cdot\mathbb{E}[\mathcal{T}^{(1)}]\cdot\mathbb{E}[\mathcal{T}^{(2)}] -$$
$$-\mathbb{E}[\mathcal{T}^{(0)}]\cdot\mathbb{E}[\mathcal{T}^{(1)}]\cdot\mathcal{T}^{(2)}[1] + \mathbb{E}[\mathcal{T}^{(0)}]\cdot\mathbb{E}[\mathcal{T}^{(1)}]\cdot\mathbb{E}[\mathcal{T}^{(2)}]$$
$$= \mathbb{E}[f(3,\cdot,1)] - \mathbb{E}[f(3,\cdot,\cdot)] - \mathbb{E}[f(\cdot,\cdot,1)] + \mathbb{E}[f] = f_{0,2}(3,1)$$

Recipe: Sobol Tensor

- Example: $f_{0,2}(3,1)$

$$\begin{bmatrix} \boldsymbol{\mathcal{T}^{(0)}[3] - \mathbb{E}[\mathcal{T}^{(0)}]} \\ \mathcal{T}^{(0)}[2] - \mathbb{E}[\mathcal{T}^{(0)}] \\ \mathcal{T}^{(0)}[1] - \mathbb{E}[\mathcal{T}^{(0)}] \\ \mathcal{T}^{(0)}[0] - \mathbb{E}[\mathcal{T}^{(0)}] \\ \mathbb{E}[\mathcal{T}^{(0)}] \end{bmatrix} \cdot \begin{bmatrix} \mathcal{T}^{(1)}[3] - \mathbb{E}[\mathcal{T}^{(1)}] \\ \mathcal{T}^{(1)}[2] - \mathbb{E}[\mathcal{T}^{(1)}] \\ \mathcal{T}^{(1)}[1] - \mathbb{E}[\mathcal{T}^{(1)}] \\ \mathcal{T}^{(1)}[0] - \mathbb{E}[\mathcal{T}^{(1)}] \\ \boldsymbol{\mathbb{E}[\mathcal{T}^{(1)}]} \end{bmatrix} \cdot \begin{bmatrix} \mathcal{T}^{(2)}[3] - \mathbb{E}[\mathcal{T}^{(2)}] \\ \mathcal{T}^{(2)}[2] - \mathbb{E}[\mathcal{T}^{(2)}] \\ \boldsymbol{\mathcal{T}^{(2)}[1] - \mathbb{E}[\mathcal{T}^{(2)}]} \\ \mathcal{T}^{(2)}[0] - \mathbb{E}[\mathcal{T}^{(2)}] \\ \mathbb{E}[\mathcal{T}^{(2)}] \end{bmatrix}$$

$$\mathcal{T}^{(0)}[3] \cdot \mathbb{E}[\mathcal{T}^{(1)}] \cdot \mathcal{T}^{(2)}[1] - \mathcal{T}^{(0)}[3] \cdot \mathbb{E}[\mathcal{T}^{(1)}] \cdot \mathbb{E}[\mathcal{T}^{(2)}] -$$

$$- \mathbb{E}[\mathcal{T}^{(0)}] \cdot \mathbb{E}[\mathcal{T}^{(1)}] \cdot \mathcal{T}^{(2)}[1] + \mathbb{E}[\mathcal{T}^{(0)}] \cdot \mathbb{E}[\mathcal{T}^{(1)}] \cdot \mathbb{E}[\mathcal{T}^{(2)}]$$

$$= \mathbb{E}[f(3,\cdot,1)] - \mathbb{E}[f(3,\cdot,\cdot)] - \mathbb{E}[f(\cdot,\cdot,1)] + \mathbb{E}[f] = f_{0,2}(3,1)$$

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Recipe: Sobol Tensor

- Example: $f_{0,2}(3,1)$

$$
\begin{bmatrix}
\boldsymbol{\mathcal{T}^{(0)}[3] - \mathbb{E}[\mathcal{T}^{(0)}]} \\
\mathcal{T}^{(0)}[2] - \mathbb{E}[\mathcal{T}^{(0)}] \\
\mathcal{T}^{(0)}[1] - \mathbb{E}[\mathcal{T}^{(0)}] \\
\mathcal{T}^{(0)}[0] - \mathbb{E}[\mathcal{T}^{(0)}] \\
\mathbb{E}[\mathcal{T}^{(0)}]
\end{bmatrix}
\cdot
\begin{bmatrix}
\mathcal{T}^{(1)}[3] - \mathbb{E}[\mathcal{T}^{(1)}] \\
\mathcal{T}^{(1)}[2] - \mathbb{E}[\mathcal{T}^{(1)}] \\
\mathcal{T}^{(1)}[1] - \mathbb{E}[\mathcal{T}^{(1)}] \\
\mathcal{T}^{(1)}[0] - \mathbb{E}[\mathcal{T}^{(1)}] \\
\boldsymbol{\mathbb{E}[\mathcal{T}^{(1)}]}
\end{bmatrix}
\cdot
\begin{bmatrix}
\mathcal{T}^{(2)}[3] - \mathbb{E}[\mathcal{T}^{(2)}] \\
\mathcal{T}^{(2)}[2] - \mathbb{E}[\mathcal{T}^{(2)}] \\
\boldsymbol{\mathcal{T}^{(2)}[1] - \mathbb{E}[\mathcal{T}^{(2)}]} \\
\mathcal{T}^{(2)}[0] - \mathbb{E}[\mathcal{T}^{(2)}] \\
\mathbb{E}[\mathcal{T}^{(2)}]
\end{bmatrix}
$$

$$
\begin{aligned}
&\mathcal{T}^{(0)}[3] \cdot \mathbb{E}[\mathcal{T}^{(1)}] \cdot \mathcal{T}^{(2)}[1] - \mathcal{T}^{(0)}[3] \cdot \mathbb{E}[\mathcal{T}^{(1)}] \cdot \mathbb{E}[\mathcal{T}^{(2)}] - \\
&- \mathbb{E}[\mathcal{T}^{(0)}] \cdot \mathbb{E}[\mathcal{T}^{(1)}] \cdot \mathcal{T}^{(2)}[1] + \mathbb{E}[\mathcal{T}^{(0)}] \cdot \mathbb{E}[\mathcal{T}^{(1)}] \cdot \mathbb{E}[\mathcal{T}^{(2)}] \\
&= \mathbb{E}[f(3,\cdot,1)] - \mathbb{E}[f(3,\cdot,\cdot)] - \mathbb{E}[f(\cdot,\cdot,1)] + \mathbb{E}[f] = f_{0,2}(3,1)
\end{aligned}
$$

Recipe: Sobol Tensor

- Example: $f_{0,2}(3,1)$

$$
\begin{bmatrix} \boldsymbol{\mathcal{T}^{(0)}[3]-\mathbb{E}[\mathcal{T}^{(0)}]} \\ \mathcal{T}^{(0)}[2]-\mathbb{E}[\mathcal{T}^{(0)}] \\ \mathcal{T}^{(0)}[1]-\mathbb{E}[\mathcal{T}^{(0)}] \\ \mathcal{T}^{(0)}[0]-\mathbb{E}[\mathcal{T}^{(0)}] \\ \mathbb{E}[\mathcal{T}^{(0)}] \end{bmatrix} \cdot \begin{bmatrix} \mathcal{T}^{(1)}[3]-\mathbb{E}[\mathcal{T}^{(1)}] \\ \mathcal{T}^{(1)}[2]-\mathbb{E}[\mathcal{T}^{(1)}] \\ \mathcal{T}^{(1)}[1]-\mathbb{E}[\mathcal{T}^{(1)}] \\ \mathcal{T}^{(1)}[0]-\mathbb{E}[\mathcal{T}^{(1)}] \\ \boldsymbol{\mathbb{E}[\mathcal{T}^{(1)}]} \end{bmatrix} \cdot \begin{bmatrix} \mathcal{T}^{(2)}[3]-\mathbb{E}[\mathcal{T}^{(2)}] \\ \mathcal{T}^{(2)}[2]-\mathbb{E}[\mathcal{T}^{(2)}] \\ \boldsymbol{\mathcal{T}^{(2)}[1]-\mathbb{E}[\mathcal{T}^{(2)}]} \\ \mathcal{T}^{(2)}[0]-\mathbb{E}[\mathcal{T}^{(2)}] \\ \mathbb{E}[\mathcal{T}^{(2)}] \end{bmatrix}
$$

$$
\begin{aligned}
&\mathcal{T}^{(0)}[3]\cdot\mathbb{E}[\mathcal{T}^{(1)}]\cdot\mathcal{T}^{(2)}[1]-\mathcal{T}^{(0)}[3]\cdot\mathbb{E}[\mathcal{T}^{(1)}]\cdot\mathbb{E}[\mathcal{T}^{(2)}]- \\
&-\mathbb{E}[\mathcal{T}^{(0)}]\cdot\mathbb{E}[\mathcal{T}^{(1)}]\cdot\mathcal{T}^{(2)}[1]+\mathbb{E}[\mathcal{T}^{(0)}]\cdot\mathbb{E}[\mathcal{T}^{(1)}]\cdot\mathbb{E}[\mathcal{T}^{(2)}] \\
&=\mathbb{E}[f(3,\cdot,1)]-\mathbb{E}[f(3,\cdot,\cdot)]-\mathbb{E}[f(\cdot,\cdot,1)]+\mathbb{E}[f]=f_{0,2}(3,1)
\end{aligned}
$$

Recipe: Sobol Tensor

- Example: $f_{0,2}(3,1)$

$$\begin{bmatrix} \boldsymbol{\mathcal{T}^{(0)}[3]-\mathbb{E}[\mathcal{T}^{(0)}]} \\ \mathcal{T}^{(0)}[2]-\mathbb{E}[\mathcal{T}^{(0)}] \\ \mathcal{T}^{(0)}[1]-\mathbb{E}[\mathcal{T}^{(0)}] \\ \mathcal{T}^{(0)}[0]-\mathbb{E}[\mathcal{T}^{(0)}] \\ \mathbb{E}[\mathcal{T}^{(0)}] \end{bmatrix} \cdot \begin{bmatrix} \mathcal{T}^{(1)}[3]-\mathbb{E}[\mathcal{T}^{(1)}] \\ \mathcal{T}^{(1)}[2]-\mathbb{E}[\mathcal{T}^{(1)}] \\ \mathcal{T}^{(1)}[1]-\mathbb{E}[\mathcal{T}^{(1)}] \\ \mathcal{T}^{(1)}[0]-\mathbb{E}[\mathcal{T}^{(1)}] \\ \boldsymbol{\mathbb{E}[\mathcal{T}^{(1)}]} \end{bmatrix} \cdot \begin{bmatrix} \mathcal{T}^{(2)}[3]-\mathbb{E}[\mathcal{T}^{(2)}] \\ \mathcal{T}^{(2)}[2]-\mathbb{E}[\mathcal{T}^{(2)}] \\ \boldsymbol{\mathcal{T}^{(2)}[1]-\mathbb{E}[\mathcal{T}^{(2)}]} \\ \mathcal{T}^{(2)}[0]-\mathbb{E}[\mathcal{T}^{(2)}] \\ \mathbb{E}[\mathcal{T}^{(2)}] \end{bmatrix}$$

$$\mathcal{T}^{(0)}[3]\cdot\mathbb{E}[\mathcal{T}^{(1)}]\cdot\mathcal{T}^{(2)}[1]-\mathcal{T}^{(0)}[3]\cdot\mathbb{E}[\mathcal{T}^{(1)}]\cdot\mathbb{E}[\mathcal{T}^{(2)}]-$$

$$-\mathbb{E}[\mathcal{T}^{(0)}]\cdot\mathbb{E}[\mathcal{T}^{(1)}]\cdot\mathcal{T}^{(2)}[1]+\mathbb{E}[\mathcal{T}^{(0)}]\cdot\mathbb{E}[\mathcal{T}^{(1)}]\cdot\mathbb{E}[\mathcal{T}^{(2)}]$$

$$=\mathbb{E}[f(3,\cdot,1)]-\mathbb{E}[f(3,\cdot,\cdot)]-\mathbb{E}[f(\cdot,\cdot,1)]+\mathbb{E}[f]=f_{0,2}(3,1)$$

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Recipe: Sobol Tensor

- Element-wise square $\mathcal{T}_*^2$: Kronecker product of each slice by itself

$$\begin{bmatrix} (\mathcal{T}^{(0)}[3]-\mathbb{E}[\mathcal{T}^{(0)}])^2 \\ (\mathcal{T}^{(0)}[2]-\mathbb{E}[\mathcal{T}^{(0)}])^2 \\ (\mathcal{T}^{(0)}[1]-\mathbb{E}[\mathcal{T}^{(0)}])^2 \\ (\mathcal{T}^{(0)}[0]-\mathbb{E}[\mathcal{T}^{(0)}])^2 \\ \mathbb{E}[\mathcal{T}^{(0)}]^2 \end{bmatrix} \cdot \begin{bmatrix} (\mathcal{T}^{(1)}[3]-\mathbb{E}[\mathcal{T}^{(1)}])^2 \\ (\mathcal{T}^{(1)}[2]-\mathbb{E}[\mathcal{T}^{(1)}])^2 \\ (\mathcal{T}^{(1)}[1]-\mathbb{E}[\mathcal{T}^{(1)}])^2 \\ (\mathcal{T}^{(1)}[0]-\mathbb{E}[\mathcal{T}^{(1)}])^2 \\ \mathbb{E}[\mathcal{T}^{(1)}]^2 \end{bmatrix} \cdot \begin{bmatrix} (\mathcal{T}^{(2)}[3]-\mathbb{E}[\mathcal{T}^{(2)}])^2 \\ (\mathcal{T}^{(2)}[2]-\mathbb{E}[\mathcal{T}^{(2)}])^2 \\ (\mathcal{T}^{(2)}[1]-\mathbb{E}[\mathcal{T}^{(2)}])^2 \\ (\mathcal{T}^{(2)}[0]-\mathbb{E}[\mathcal{T}^{(2)}])^2 \\ \mathbb{E}[\mathcal{T}^{(2)}]^2 \end{bmatrix}$$

Notation: $\text{slice}^2 \equiv \text{slice} \otimes \text{slice}$

Recipe: Sobol Tensor

- Average slices of $\mathcal{T}_*^2$

$$\begin{bmatrix} (\mathcal{T}^{(0)}[3] - \mathbb{E}[\mathcal{T}^{(0)}])^2 \\ (\mathcal{T}^{(0)}[2] - \mathbb{E}[\mathcal{T}^{(0)}])^2 \\ (\mathcal{T}^{(0)}[1] - \mathbb{E}[\mathcal{T}^{(0)}])^2 \\ (\mathcal{T}^{(0)}[0] - \mathbb{E}[\mathcal{T}^{(0)}])^2 \\ \mathbb{E}[\mathcal{T}^{(0)}]^2 \end{bmatrix} \cdot \begin{bmatrix} (\mathcal{T}^{(1)}[3] - \mathbb{E}[\mathcal{T}^{(1)}])^2 \\ (\mathcal{T}^{(1)}[2] - \mathbb{E}[\mathcal{T}^{(1)}])^2 \\ (\mathcal{T}^{(1)}[1] - \mathbb{E}[\mathcal{T}^{(1)}])^2 \\ (\mathcal{T}^{(1)}[0] - \mathbb{E}[\mathcal{T}^{(1)}])^2 \\ \mathbb{E}[\mathcal{T}^{(1)}]^2 \end{bmatrix} \cdot \begin{bmatrix} (\mathcal{T}^{(2)}[3] - \mathbb{E}[\mathcal{T}^{(2)}])^2 \\ (\mathcal{T}^{(2)}[2] - \mathbb{E}[\mathcal{T}^{(2)}])^2 \\ (\mathcal{T}^{(2)}[1] - \mathbb{E}[\mathcal{T}^{(2)}])^2 \\ (\mathcal{T}^{(2)}[0] - \mathbb{E}[\mathcal{T}^{(2)}])^2 \\ \mathbb{E}[\mathcal{T}^{(2)}]^2 \end{bmatrix}$$

Recipe: Sobol Tensor

- Average slices of $\mathcal{T}_*^2$

$$\left[\frac{\begin{matrix}(\mathcal{T}^{(0)}[3]-\mathbb{E}[\mathcal{T}^{(0)}])^2\\(\mathcal{T}^{(0)}[2]-\mathbb{E}[\mathcal{T}^{(0)}])^2\\(\mathcal{T}^{(0)}[1]-\mathbb{E}[\mathcal{T}^{(0)}])^2\\(\mathcal{T}^{(0)}[0]-\mathbb{E}[\mathcal{T}^{(0)}])^2\end{matrix}}{\mathbb{E}[\mathcal{T}^{(0)}]^2}\right]\cdot\left[\frac{\begin{matrix}(\mathcal{T}^{(1)}[3]-\mathbb{E}[\mathcal{T}^{(1)}])^2\\(\mathcal{T}^{(1)}[2]-\mathbb{E}[\mathcal{T}^{(1)}])^2\\(\mathcal{T}^{(1)}[1]-\mathbb{E}[\mathcal{T}^{(1)}])^2\\(\mathcal{T}^{(1)}[0]-\mathbb{E}[\mathcal{T}^{(1)}])^2\end{matrix}}{\mathbb{E}[\mathcal{T}^{(1)}]^2}\right]\cdot\left[\frac{\begin{matrix}(\mathcal{T}^{(2)}[3]-\mathbb{E}[\mathcal{T}^{(2)}])^2\\(\mathcal{T}^{(2)}[2]-\mathbb{E}[\mathcal{T}^{(2)}])^2\\(\mathcal{T}^{(2)}[1]-\mathbb{E}[\mathcal{T}^{(2)}])^2\\(\mathcal{T}^{(2)}[0]-\mathbb{E}[\mathcal{T}^{(2)}])^2\end{matrix}}{\mathbb{E}[\mathcal{T}^{(2)}]^2}\right]$$

$$\Downarrow$$

$$\left[\frac{\mathbb{E}[(\mathcal{T}^{(0)}-\mathbb{E}[\mathcal{T}^{(0)}])^2]}{\mathbb{E}[\mathcal{T}^{(0)}]^2}\right]\cdot\left[\frac{\mathbb{E}[(\mathcal{T}^{(1)}-\mathbb{E}[\mathcal{T}^{(1)}])^2]}{\mathbb{E}[\mathcal{T}^{(1)}]^2}\right]\cdot\left[\frac{\mathbb{E}[(\mathcal{T}^{(2)}-\mathbb{E}[\mathcal{T}^{(2)}])^2]}{\mathbb{E}[\mathcal{T}^{(2)}]^2}\right]$$

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Recipe: Sobol Tensor

Sobol Tensor $\mathcal{S}$

normalize by $\mathrm{Var}[\mathcal{T}]$

$$\left\lfloor \frac{\mathbb{E}[(\mathcal{T}^{(0)} - \mathbb{E}[\mathcal{T}^{(0)}])^2]}{\mathbb{E}[\mathcal{T}^{(0)}]^2} \right\rfloor \cdot \left\lfloor \frac{\mathbb{E}[(\mathcal{T}^{(1)} - \mathbb{E}[\mathcal{T}^{(1)}])^2]}{\mathbb{E}[\mathcal{T}^{(1)}]^2} \right\rfloor \cdot \left\lfloor \frac{\mathbb{E}[(\mathcal{T}^{(2)} - \mathbb{E}[\mathcal{T}^{(2)}])^2]}{\mathbb{E}[\mathcal{T}^{(2)}]^2} \right\rfloor$$

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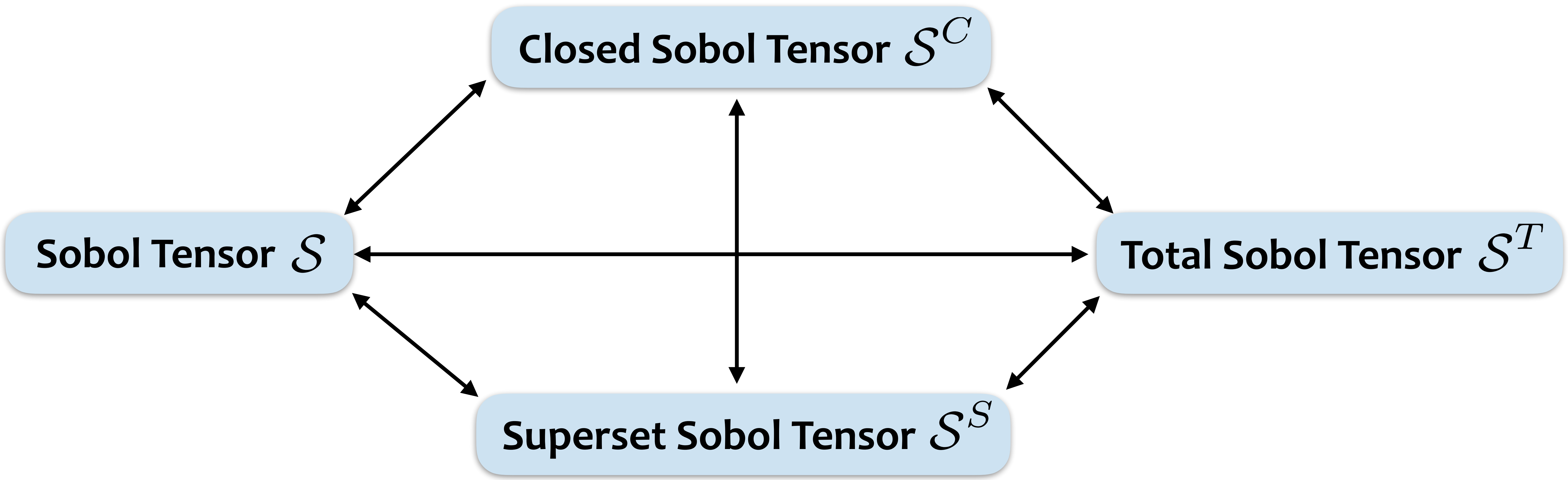
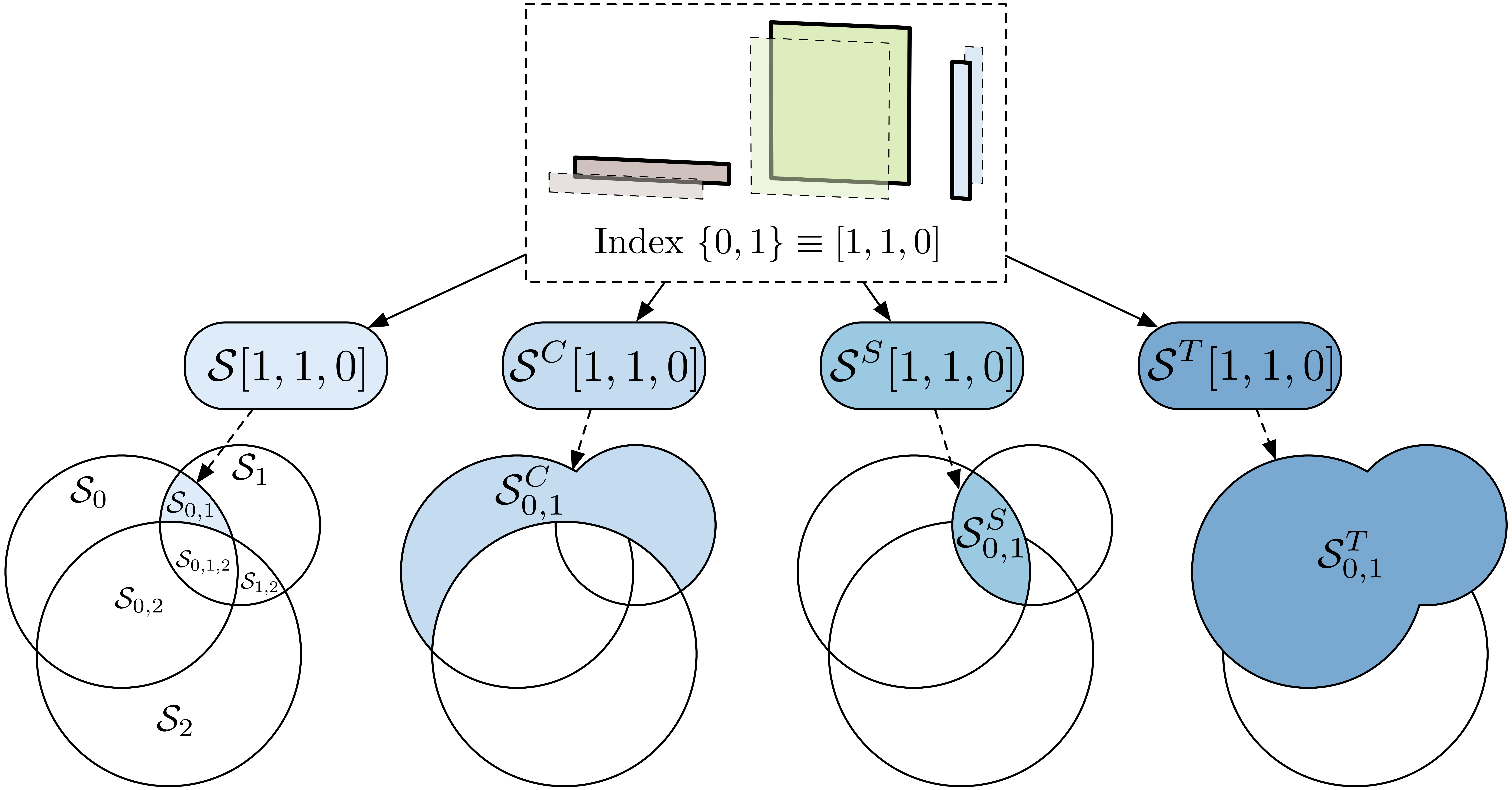
Related Tensors

- $\mathcal{S}$ only gives variance components
- How to get other indices?



Indexing Example



Recipe: Closed Sobol Tensor

- Example: getting $\mathcal{S}^C$ from $\mathcal{S}$

Memo: Closed Indices

$$S^C_{\boldsymbol{\alpha}} := \sum_{\boldsymbol{\beta} | \boldsymbol{\alpha} \supseteq \boldsymbol{\beta}} S_{\boldsymbol{\beta}}$$

$$\mathcal{S} = \begin{bmatrix} \mathcal{S}^{(0)}[1] \\ \mathcal{S}^{(0)}[0] \end{bmatrix} \cdot \begin{bmatrix} \mathcal{S}^{(1)}[1] \\ \mathcal{S}^{(1)}[0] \end{bmatrix} \cdot \begin{bmatrix} \mathcal{S}^{(2)}[1] \\ \mathcal{S}^{(2)}[0] \end{bmatrix}$$

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Recipe: Closed Sobol Tensor

- Example: getting $\mathcal{S}^C$ from $\mathcal{S}$

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Recipe: Closed Sobol Tensor

- Example: getting $\mathcal{S}^C$ from $\mathcal{S}$

Memo: Closed Indices

$$S^C_{\boldsymbol{\alpha}} := \sum_{\boldsymbol{\beta} | \boldsymbol{\alpha} \supseteq \boldsymbol{\beta}} S_{\boldsymbol{\beta}}$$

$$\mathcal{S} = \begin{bmatrix} \mathcal{S}^{(0)}[1] \\ \mathcal{S}^{(0)}[0] \end{bmatrix} \cdot \begin{bmatrix} \mathcal{S}^{(1)}[1] \\ \mathcal{S}^{(1)}[0] \end{bmatrix} \cdot \begin{bmatrix} \mathcal{S}^{(2)}[1] \\ \mathcal{S}^{(2)}[0] \end{bmatrix}$$

$$\downarrow$$

$$\mathcal{S}^C = \begin{bmatrix} \mathcal{S}^{(0)}[0] + \mathcal{S}^{(0)}[1] \\ \mathcal{S}^{(0)}[0] \end{bmatrix} \cdot \begin{bmatrix} \mathcal{S}^{(1)}[0] + \mathcal{S}^{(1)}[1] \\ \mathcal{S}^{(1)}[0] \end{bmatrix} \cdot \begin{bmatrix} \mathcal{S}^{(2)}[0] + \mathcal{S}^{(2)}[1] \\ \mathcal{S}^{(2)}[0] \end{bmatrix}$$

Tensor Train Automata

Main Ideas

- Tensor contraction ≡ weighting & counting
  - Graph coloring problems: **[Penrose '71]**
  - Weighted tree automata: **[Rabusseau '16]**
  - Matrix product algorithms: **[Crosswhite & Bacon '08]**
  - A survey: **[Biamonte & Bergholm '17]**
  - Our take: **[Ballester-Ripoll et al. '18]**

Main Ideas

- Tensor contraction ≡ weighting & counting
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Quantum physics community

Main Ideas

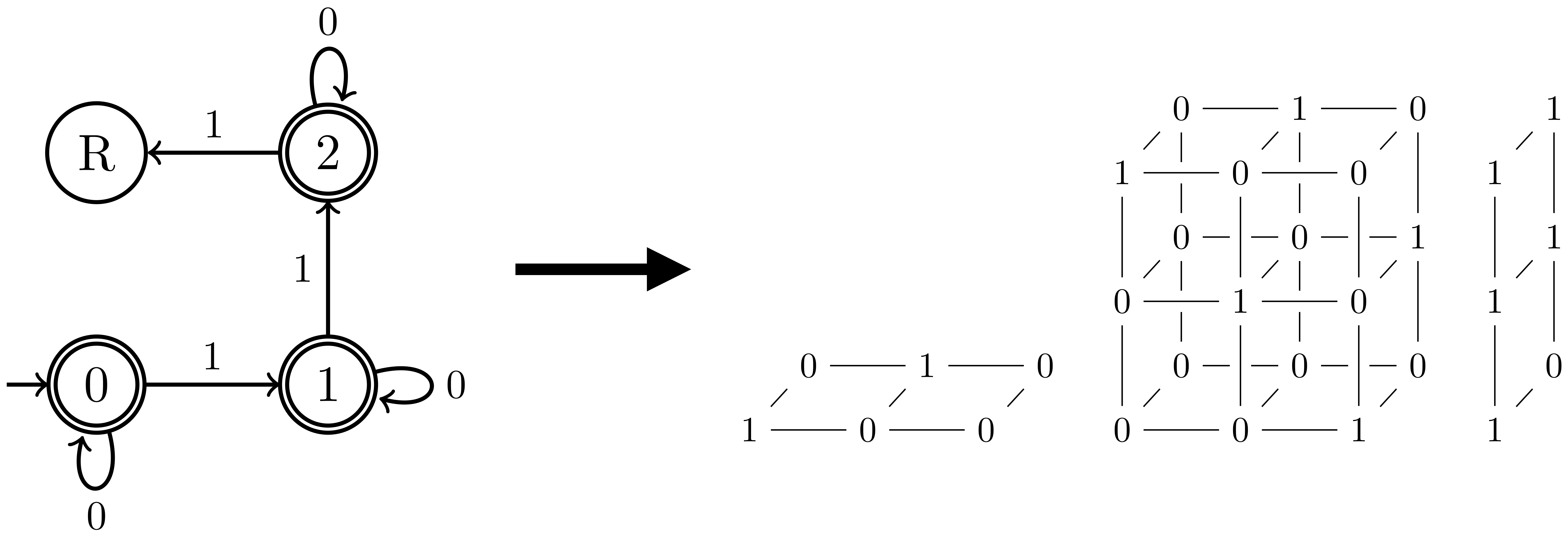
Deterministic Finite Automaton $\mathbf{A} \sim$ Tensor Train $\mathcal{T}$

- Assume N symbols are read → $\mathcal{T}$ has dimension N
- Input string → tensor entry
  - E.g. '001101' → $\mathcal{A}[0, 0, 1, 1, 0, 1]$
- String s is accepted $\Leftrightarrow \mathcal{A}[s] = 1$
- String s is rejected $\Leftrightarrow \mathcal{A}[s] = 0$
- # states → tensor ranks
- Transition matrices → TT core slices

Example: Hamming Mask

$\mathcal{M}^{\leq k}$: **accept s if and only if s has $\leq k$ ones**

- Example: $N = 3$ symbols, $k = 2$



Some Important Masks

Presence

$$\mathcal{P}^n_{\boldsymbol{\alpha}} = 1 \Leftrightarrow n \in \boldsymbol{\alpha}$$

Hamming

$$\mathcal{M}^{\leq k}_{\boldsymbol{\alpha}} = 1 \Leftrightarrow \|\boldsymbol{\alpha}\|_1 \leq k$$

$$\mathcal{M}^{k}_{\boldsymbol{\alpha}} = 1 \Leftrightarrow \|\boldsymbol{\alpha}\|_1 = k$$

Absence

$$\mathcal{A}^n_{\boldsymbol{\alpha}} = 1 \Leftrightarrow n \notin \boldsymbol{\alpha}$$

Length

$\mathcal{L}^k_{\boldsymbol{\alpha}} = 1 \Leftrightarrow$ first/last '1' in $\boldsymbol{\alpha}$ are k symbols apart

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Mask Algebra

- NOT operator: $1 - \mathcal{A}$
- AND operator: $\mathcal{A}_1 \circ \mathcal{A}_2$
- OR operator: $\mathcal{A}_1 + \mathcal{A}_2 - \mathcal{A}_1 \circ \mathcal{A}_2$
- XOR operator: $\mathcal{A}_1 + \mathcal{A}_2 - 2(\mathcal{A}_1 \circ \mathcal{A}_2)$

Recommended: **recompress** afterwards (*TT-round*)

- Is a mask $\mathcal{A}$ satisfiable? It is iff $\sum \mathcal{A} > 0$

To apply a mask $\mathcal{A}$ to a tensor $\mathcal{T}$: $\mathcal{A} \circ \mathcal{T}$

Sensitivity Analysis Tasks

- **Task:** *"How well can we approximate the model using variable triplets only?"*
- **Answer:** $\langle \mathcal{M}^3, \mathcal{S}^C \rangle$

- **Task:** *"Find 5 variables that can be frozen with the least impact."*
- **Answer:** $\arg\max\{\mathcal{M}^5 \circ (1 - \mathcal{S}^T)\}$

TT global optimization

[Mikhalev & Oseledets '14]
[Oferkin et al. '15]
etc.

- **Task:** *"Find the most important triplet that includes x_1 or x_3, but not x_4"*
- **Answer:** $\arg\max\{\mathcal{S} \wedge \mathcal{M}^3 \wedge (\mathcal{P}^1 \vee \mathcal{P}^3) \wedge \mathcal{A}^4\}$

Advanced Metrics

Mean Dimension

[Caflisch et al. ’97]

Dimension Distribution

[Owen ‘03]

Effective Dimensions

- Superposition sense
- Truncation sense **[Caflisch et al. ’97]**
- Successive sense **[L’Ecuyer & Lemieux ’00]**

Shapley Values

[Owen ‘14]

TT automata can do all

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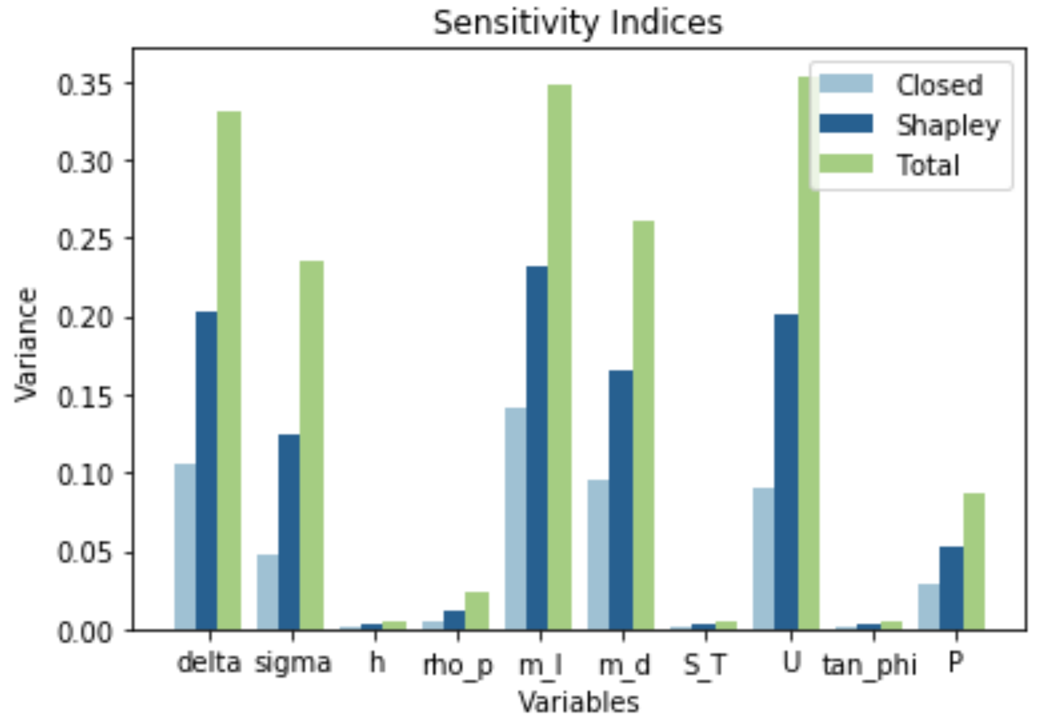
A Case of Study

- **Fire-spread rate in the Mediterranean shrublands** [Song et al. '16]
  - 10 variables
  - Non-uniform marginal distributions
  - High-order interactions

```
rmax = sigma**1.5 / (495 + 0.0594 * sigma**1.5)
bop = 3.348 * sigma**(-0.8189)
A = 133 * sigma**(-0.7913)
thestar = (301.4 - 305.87 * (ml - md) + 2260 * md) / (2260 * ml)
theta = np.minimum(1, np.maximum(thestar, 0))
muM = np.exp(-7.3 * P * md - (7.3 * theta + 2.13) * (1 - P) * ml)
muS = np.minimum(0.174 * S**(-0.19), 1)
C = 7.47 * np.exp(-0.133 * sigma**0.55)
B = 0.02526 * sigma**0.54
E = 0.715 * np.exp(-3.59 * 10**(-4) * sigma)
wn = w0 * (1 - S)
rhob = w0 / delta
eps = np.exp(-138 / sigma)
Qig = (401.41 + md * 2565.87) * 0.4536 / 1.060
beta = rhob / rho
r = rmax * (beta / bop)**A * np.exp(A * (1 - beta / bop))
xi = ((192 + 0.2595 * sigma)**(-1) * np.exp((0.792 + 0.681 * sigma**0.5) * (beta + 0.1)))
phiW = C * U**B * (beta / bop)**(-E)
phiS = 5.275 * beta**(-0.3) * tanphi**2
IR = r * wn * h * muM * muS
R = IR * xi * (1 + phiW + phiS) / (rhob * eps * Qig)
return R * 30.48 / 60
```

A Case of Study

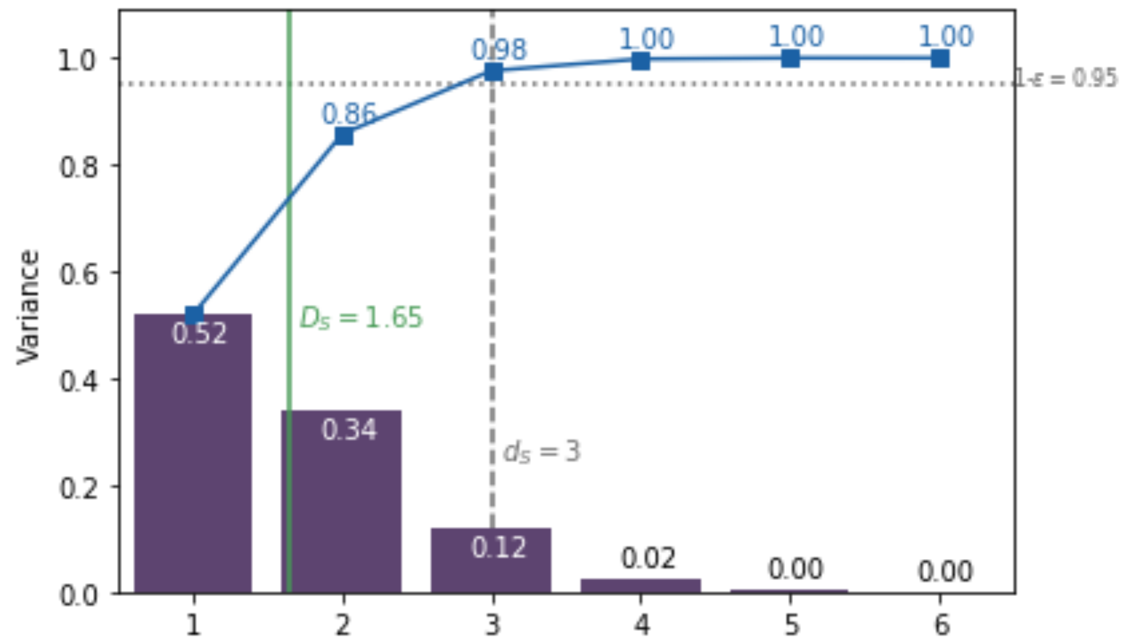
- Using our Python package “**ttrecipes**” (github.com/rballester/ttrecipes)
- Metamodeling phase:
  - ~ 3M samples (*cross-approximation* routine from `ttpy` library)
  - ~10 seconds
  - Maximal rank = 42
  - Relative error $\sim 1.3 \cdot 10^{-4}$
- Analysis phase:
  - ~1 second
  - Maximal rank: 21
  - Relative error $\sim 2.8 \cdot 10^{-5}$



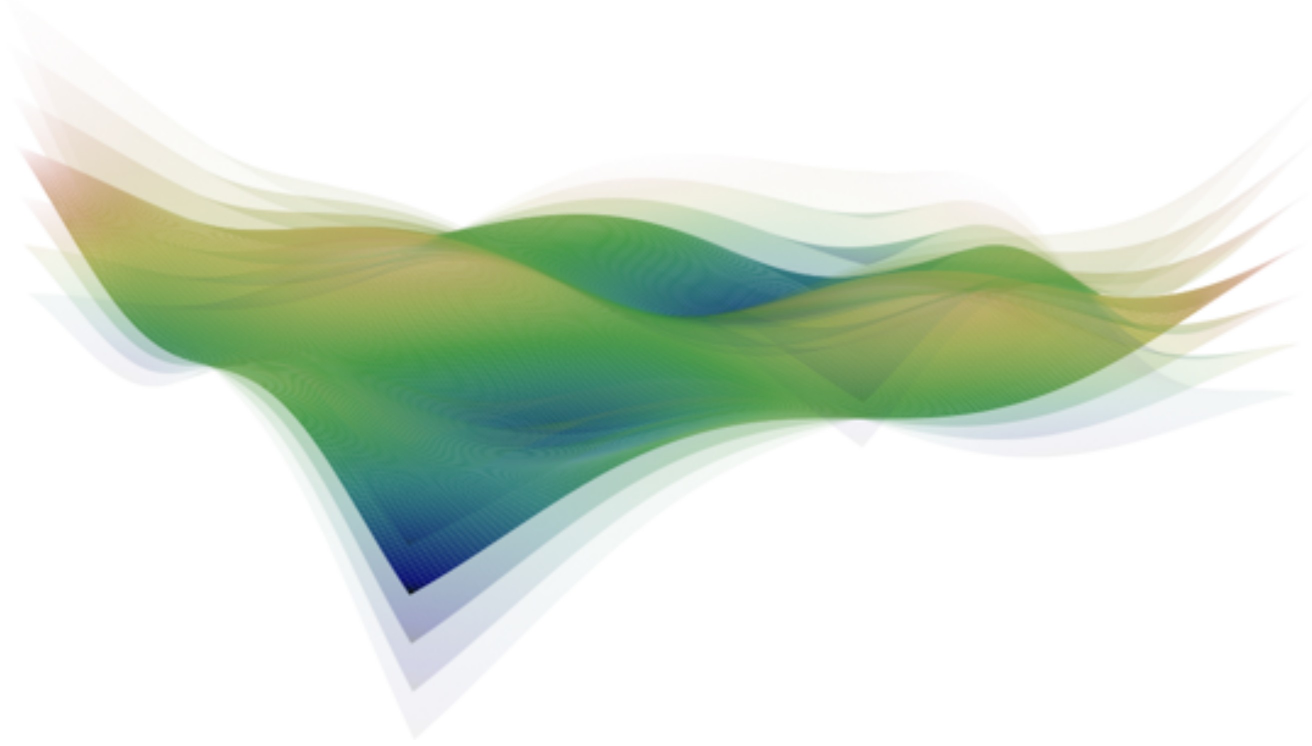
Dimension Metric	Value	Rel. Variance	Variables
Mean dimension	1.648475		
Effective (superposition)	3.000000	0.976255	
Effective (successive)	8.000000	0.964790	
Effective (truncation)	6.000000	0.961562	delta, sigma, m_l, m_d, U, P

Variable	Var. components	Total	Shapley	Banzhaf-Coleman
delta	0.105950	0.331275	0.203047	0.195286
sigma	0.047720	0.234205	0.124683	0.116566
h	0.001229	0.005179	0.002837	0.002655
rho_p	0.004507	0.023303	0.012106	0.011211
m_l	0.142140	0.345899	0.230826	0.224247
m_d	0.095279	0.259603	0.165685	0.159828
S_T	0.001069	0.004507	0.002469	0.002310
U	0.090246	0.353033	0.201571	0.191561
tan_phi	0.002080	0.005788	0.003737	0.003638
P	0.029142	0.085682	0.053041	0.050867

Order	Rel. Variance	Cumul. Variance
1	0.519362	0.519362
2	0.338528	0.857890
3	0.118365	0.976255
4	0.021838	0.998092
5	0.001835	0.999927
6	0.000072	0.999999
7	0.000001	1.000000
8	0.000000	1.000000
9	0.000000	1.000000
10	0.000000	1.000000



Thank You!



Papers: *"Sobol Tensor Trains for Global Sensitivity Analysis"* (arXiv 1712.00233)

"Tensor Algorithms for Advanced Sensitivity Metrics" (arXiv 1712.01633, to appear in SIAM JUQ)

Code: *https://www.github.com/rballester/ttrecipes*

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https://www.uzh.ch

References

Sensitivity Analysis

- [**Hoeffding '48**]: "A class of statistics with asymptotically normal distributions"
- [**Sobol '90**]: "Sensitivity Estimates for Nonlinear Mathematical Models"
- [**Caflisch et al. '97**]: "Valuation of Mortgage-backed Securities Using Brownian Bridges to Reduce Effective Dimension"
- [**L'Ecuyer & Lemieux '00**]: "Variance Reduction Via Lattice Rules"
- [**Owen '03**]: "The Dimension Distribution and Quadrature Test Functions"
- [**Owen '14**]: "Sobol' Indices and Shapley Value"
- [**Song '16**]: "Shapley Effects for Global Sensitivity Analysis: Theory and Computation"

Tensors

- [**Penrose '71**]: "Applications of Negative Dimensional Tensors"
- [**Crosswhite & Bacon '08**]: "Finite Automata for Caching in Matrix Product Algorithms"
- [**Grasedyck et al. '13**]: "A Literature Survey of Low-rank Tensor Approximation Techniques"
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- [**Konakli & Sudret '16**]: "Global Sensitivity Analysis Using Low-rank Tensor Approximations"
- [**Bigoni et al. '16**]: "Spectral Tensor-Train Decomposition"
- [**Biamonte & Bergholm '17**]: "Quantum Tensor Networks in a Nutshell"
- [**Gorodetsky & Jakeman '18**]: "Gradient-based Optimization for Regression in the Functional Tensor-Train Format"

Backup Slide: Superset Sobol Tensor

- Example: getting $\mathcal{S}^S$ from $\mathcal{S}$

Memo: Superset Indices

$$S^S_{\boldsymbol{\alpha}} := \sum_{\boldsymbol{\beta} | \boldsymbol{\alpha} \subseteq \boldsymbol{\beta}} S_{\boldsymbol{\beta}}$$

$$\mathcal{S} = \begin{bmatrix} \mathcal{S}^{(0)}[1] \\ \mathcal{S}^{(0)}[0] \end{bmatrix} \cdot \begin{bmatrix} \mathcal{S}^{(1)}[1] \\ \mathcal{S}^{(1)}[0] \end{bmatrix} \cdot \begin{bmatrix} \mathcal{S}^{(2)}[1] \\ \mathcal{S}^{(2)}[0] \end{bmatrix}$$

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$$\Downarrow$$

$$\mathcal{S}^S = \begin{bmatrix} \mathcal{S}^{(0)}[1] \\ \mathcal{S}^{(0)}[0] + \mathcal{S}^{(0)}[1] \end{bmatrix} \cdot \begin{bmatrix} \mathcal{S}^{(1)}[1] \\ \mathcal{S}^{(1)}[0] + \mathcal{S}^{(1)}[1] \end{bmatrix} \cdot \begin{bmatrix} \mathcal{S}^{(2)}[1] \\ \mathcal{S}^{(2)}[0] + \mathcal{S}^{(2)}[1] \end{bmatrix}$$