Uncertainty quantification by random measures and fields

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Abstract

We present a general framework for uncertainty quantification that is a mosaic of interconnected models. We define global first and second order structural and correlative sensitivity analyses for random counting measures acting on risk functionals of input-output maps. These are the ANOVA decomposition of the intensity measure and the decomposition of the random measure variance, each into subspaces. Orthogonal random measures furnish sensitivity distributions. We show that the random counting measure may be used to construct positive random fields, which admit decompositions of covariance and sensitivity indices and may be used to represent interacting particle systems. The first and second order global sensitivity analyses conveyed through random counting measures elucidate and integrate different notions of uncertainty quantification, and the global sensitivity analysis of random fields conveys the proportionate functional contributions to covariance. This framework complements others when used in conjunction with for instance algorithmic uncertainty and model selection uncertainty frameworks.

1 Introduction

Uncertainty quantification (UQ) is a fundamental area. There are multiple notions of UQ in various applications. Perhaps the most common notion is propagation of input uncertainty through a model in uncertainty propagation (UP), such as in global sensitivity analysis based on decomposition of variance. Another is uncertainty of estimators, a second-order analysis based on decomposition of variance. Another is focusing on entropy, instead of variance. Another is model uncertainty, such as that of Bayesian model averaging.

We shall assume the reader has access to some independency of input-output random variables \((X, Y) = \{(X_i, Y_i)\}\) taking values in measurable space \((E \times F, \mathcal{E} \otimes \mathcal{F})\) with distribution \(\nu \times Q\), where \(\nu\) is a probability measure on \((E, \mathcal{E})\) and \(Q\) is a transition probability kernel from \((E, \mathcal{E})\) into \((F, \mathcal{F})\). Oftentimes \(Q\) is deterministic and specified through function \(g : E \mapsto F\) as \(Q(x, \cdot) = \delta_{g(x)}(\cdot)\). For example, \(g\) could be a regressor or a classifier or some other function.

Here we let \(\mathcal{E}_+\) denote the collection of positive \(\mathcal{E}\)-measurable functions. Suppose we have some risk function \(f \in \mathcal{E}_+\) that is a function of \(g\). The statistics of \(f\) are readily computed as

\[
\mathbb{E} f = \nu f \\
\text{Var} f = \nu f^2 - (\nu f)^2
\]

Many times, one estimates these statistics using \(n\) samples using the empirical distribution

\[
F_n(A) = \frac{1}{n} \sum_{i=1}^{n} 1_A(X_i) \quad \text{for} \quad A \in \mathcal{E}
\]

in view of the fact that

\[
\lim_{n \to \infty} F_n f = \nu f \quad \text{for} \quad f \in \mathcal{E}_+
\]
almost surely. Further for \( f \in \mathcal{E}_+ \) we have

\[
\mathbb{E} F_n f = \nu f \\
\text{Var} F_n f = \frac{1}{n} \text{Var} f
\]

and for \( f, g \in \mathcal{E}_+ \) we have

\[
\text{Cov}(F_n f, F_n g) = \frac{1}{n} (\nu(fg) - \nu f \nu g)
\]

If \( f \) and \( g \) are disjoint, then the covariance simplifies to \( \text{Cov}(F_n f, F_n g) = -\frac{1}{n} \nu f \nu g \). The empirical distribution has negative covariance for disjoint functions and so its uncertainties are correlated. The Monte Carlo estimator of the expected value with respect to the empirical distribution is called the bootstrap estimator [Efron and Tibshirani, 1993]. As we shall see later in the article, the correlation destroys the probabilistic interpretation of the normalized variances.

Another area of focus is on \( g \). In most settings, \( E \) is finite with dimension \( n \). For regression, a common tool is global sensitivity analysis to understand the propagation of input uncertainty. This conducts a functional analysis of variance (ANOVA) analysis which conveys a decomposition of variance into subspaces. Functional HDMR has other remarkable properties, such as in many practical settings low-order expansions well approximate \( g \) and the fact that the expansion is exact and finite.

In this article we introduce a counting distribution \( \kappa \), which in conjunction with \( \nu \times Q \), forms a random counting measure. This framework integrates random measure and mean measure uncertainty quantification for risk functionals of the form \( f = (g - \mathbb{E} g)^2 \in \mathcal{E}_+ \). We introduce a positive measurable mapping \( k \) that, in conjunction with the random counting measure \((\kappa, \nu \times Q)\), forms a random field \((\kappa, \nu \times Q, k)\). Each aspect has a foundational theorem. As a ‘case-control’ analysis, we compare the binomial process \( nF_n \) (control) to the mixed binomial process (case) \( N \) with \( \kappa \) having positive variance throughout the article. Each analysis furnishes an ANOVA. The relations among these models are shown below in Figure 1.

Importantly, despite the generality of the RM-MM-RF-ANOVA UQ framework, the presentation here is not of a complete system—in this article we do not consider algorithmic uncertainty neither do we consider uncertainty of model selection, such as Bayesian model averaging; nor do we consider real-valued fields, as our random fields are necessarily positive being derived from (driven by) random counting measures. We believe the RM-MM-RF-ANOVA is coherent and complements other frameworks such as those mentioned but not contained.

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**Figure 1:** Relations among mathematical models (green = random variables, measures, and fields, distributions, and positive functions; blue = general and positive valued test functions; purple = sensitivities)
In Section 2.1 we give the formal backdrop in terms of the mixed binomial process, which generalizes the binomial process (bootstrap estimator). In Section 2.2 we give a brief description of functional ANOVA (high dimensional model representation) and global sensitivity analysis. In Section 3 we give ANOVA decompositions of the mean (intensity measure) and variance of the random counting measure into subspaces. In Section 3.5 we discuss related work. In Section 4 we apply this framework to risk functionals. In Section 5 we discuss random fields built from random measures and their ANOVA decompositions. In Section 7 we perform UQ comparing analysis and interpretation across different counting distributions and mean measures. In Section 8 we end with discussion and conclusions. In the appendices, we provide additional examples. In Table 1, we show the examples, their locations in this article, and the principal ANOVA analyses conducted for the examples.

| Example Name | Section | Law \( \nu \) | Dimension \( n \) | MM | RM | RF |
|--------------|---------|----------------|---------------|----|----|----|
| Elementary symmetric polynomial | 7.1 | \( \nu : \text{mean} \neq 0, \text{Bernoulli} \) | \( \mathbb{N}_{>0}, 100, 1 \) | ● | ● |    |
| Ishigami function | 7.2 | Uniform\([−\pi, \pi]^3\) | 3 | ● | ● |    |
| Gaussian process regressor | 7.3 | general, Ishigami | any, 3 | ● | ● |    |
| \( m \)-class classifier | 7.4 | general | any | ● | ● | ● |
| Interacting particle systems | 7.5 | general, Wiener | \( \infty \) | ● |    | ● |
| Adaptive randomized controlled trials | 7.6 | general | any | ● |    | ● |
| Symmetric polynomial with correlation | C.1 | Gaussian | 2 | ● |    | ● |
| Graph property | C.2 | Erdős-Renyi | \( \mathbb{N}_{>0}, 10 \) | ● | ● |    |
| Ising model | C.3 | nearest-neighbor Ising | any |    | ● |    |

Table 1: Article examples of RM-MM-RF ANOVAs (RM = random measure; MM = mean measure; RF = random field)

2 Background

In this section we give the mathematical backdrop of the article. In Section 2.1 we discuss the mixed binomial process, whereas in Section 2.2 we describe global sensitivity analysis as conveyed through functional ANOVA or high dimensional model representation (HDMR).

2.1 Mixed binomial process

Let \((E, \mathcal{E})\) be a measure space and let \( \nu \) be a probability measure on it. Let \( X = \{X_i\} \) be an independency (collection) of (iid) \( E \) valued random variables with law \( \nu \). Let \( K \sim \kappa \) be a \( \mathbb{N}_{\geq 0} \)-valued random variable independent of \( X \) with mean \( c > 0 \) and variance \( \delta^2 \geq 0 \). The mixed binomial process is identified to the pair of deterministic probability measures \( N = (\kappa, \nu) \) on \((E, \mathcal{E})\) through stone throwing construction (Cinlar, 2011; Bastian and Rempala, 2020; Kallenberg, 2017) (STC) as

\[
N(A) = N I_A = E N(dx)I_A(x) = \sum_{i=1}^{K} I_A(X_i) \quad \text{for} \quad A \in \mathcal{E}
\]  

where \( I_A \) is a set function. We denote \( \mathcal{E}_+ \) the set of non-negative \( \mathcal{E} \)-measurable functions. \( N \) is said to be orthogonal if \( c = \delta^2 \); for disjoint \( f, g \in \mathcal{E}_+ \) we have \( \text{Var}(Nf + Ng) = \text{Var}Nf + \text{Var}Ng \).

We point out that the STC of the mixed binomial process is also known as a proper point process. Similar ideas are of randomly-stopped sums. Our interpretation and treatment here is from the random counting measure perspective. For \( f \in \mathcal{E}_+ \) we have mean and variance of the random variable \( Nf \)

\[
\mathbb{E}Nf = cvf
\]

\[
\text{Var}Nf = cvf^2 + (\delta^2 - c)(vf)^2
\]
The mean $c\nu$ is also known as the \textit{intensity measure} of $N$. For arbitrary $f, g \in \mathcal{E}_+$, we have \textit{covariance}

$$\text{Cov}(Nf, Ng) = cv(fg) + (\delta^2 - c)\nu f \nu g \quad (4)$$

For disjoint partition $A, \cdots, B$ of $E$, we have joint probability

$$\mathbb{P}(N(A) = i, \ldots, N(B) = j) = \mathbb{P}(N(A) = i, \ldots, N(B) = j|K = k)\mathbb{P}(K = k)$$

$$= \frac{k!}{i! \cdots j!} \nu^i(A) \cdots \nu^j(B)\mathbb{P}(K = k).$$

Recall that the law of $N$ is uniquely determined by the \textit{Laplace functional} $L$ from $\mathcal{E}_+$ into $[0, 1]$

$$L(f) = \mathbb{E}e^{-Nf} = \mathbb{E}e^{-\int_{E} N(dx)f(x)} = \psi(\nu e^{-f}) \quad \text{for} \quad f \in \mathcal{E}_+ \quad (5)$$

where $\psi$ is the \textit{probability generating function} (pgf) of $K$. The Laplace functional encodes all the information of $N$: its distribution, moments, etc. The \textit{moments} of $Nf$ (if they exist) can be attained from the Laplace functional

$$\mathbb{E}(Nf)^n = (-1)^n \lim_{q \downarrow 0} \frac{\partial^n}{\partial q^n} L(qf) \quad \text{for} \quad n \in \mathbb{N}_{>0}$$

\begin{table}[h]
\centering
\begin{tabular}{|c|l|}
\hline
Symbol & Definition \\
\hline
$\mathbb{N}_{\geq 0}$ & the set of the natural numbers \{0, 1, \ldots\} \\
$\mathbb{R}$ & the set of the real numbers \((-\infty, \infty)\) \\
$\mathbb{R}_+$ & the set of the non-negative real numbers \([0, \infty)\) \\
$(E, \mathcal{E})$ & measurable space \\
$\nu$ & probability measure on $(E, \mathcal{E})$ \\
$X$ & independency of random variables \{X_i\} with law $\nu$ taking values in $(E, \mathcal{E})$ \\
$(F, \mathcal{F})$ & measurable space \\
$(E \times F, \mathcal{E} \otimes \mathcal{F})$ & measurable product space \\
$Q$ & transitional probability kernel from $(E, \mathcal{E})$ into $(F, \mathcal{F})$ \\
$\mu = \nu \times Q$ & probability measure $\mu(dx, dy) = \nu(dx)Q(x, dy)$ on $(E \times F, \mathcal{E} \otimes \mathcal{F})$ \\
$Y$ & independency of random variables \{Y_i\} with law $Q(X_i, \cdot)$ taking values in $(F, \mathcal{F})$ \\
$(X, Y)$ & independency of random variables \{(X_i, Y_i)\} with law $\nu \times Q$ taking values in $(E \times F, \mathcal{E} \otimes \mathcal{F})$ \\
$K$ & $\mathbb{N}_{\geq 0}$-valued random variable \\
$\psi$ & probability generating function of $K$ \\
$N = (\kappa, \nu)$ & random counting measure on $(E, \mathcal{E})$ \\
$L$ & Laplace functional of $N$ \\
$Nf$ & random variable in $(\mathbb{R}_+, \mathcal{B}_+)$ \\
$F$ & Laplace transform of $Nf$ \\
$\eta$ & distribution of $Nf$ \\
$\eta_n$ & distribution of $Nf$ attained by maximum entropy with $n$ evaluations of $F$ \\
$\text{PT}(c, \delta^2)$ & Poisson-type (PT) distribution with mean $c > 0$ and variance $\delta^2 > 0$ with family members binomial, Poisson, and negative binomial \\
$M = (K, \nu \times Q)$ & random counting measure on $(E \times F, \mathcal{E} \otimes \mathcal{F})$ \\
$\mathcal{E}_+$ & the collection of positive $\mathcal{E}$-measurable functions \\
$\delta_c$ & Dirac measure sitting at $c \in \mathbb{N}_{\geq 0}$ \\
$L^2(E, \mathcal{E}, \nu)$ & space of square-integrable functions \\
k & positive $\mathcal{E} \otimes \mathcal{F}$ measurable function \\
$G = (\kappa, \nu, k)$ & positive random field on $(F, \mathcal{F})$ formed by $N = (\kappa, \nu)$ and $k$ \\
$U$ & mean of random field \\
$C$ & covariance of random field \\
\hline
\end{tabular}
\caption{Symbols and definitions}
\end{table}
Then by Fubini’s theorem,

\[ F(\alpha) = \mathbb{E}e^{-\alpha Nf} = \mathbb{E}e^{-N(\alpha f)} = L(\alpha f) \quad \text{for} \quad \alpha \in \mathbb{R}_+ \]

We can replace \( \nu \) with \( \nu \times Q \) in all expressions for the random measure \( M = (\kappa, \nu \times Q) \) on \((E \times F, \mathcal{E} \otimes \mathcal{F})\).

To illustrate some of the expressive power of the mixed binomial process, in Section 2.1.1 we give canonical examples of how the mixed binomial process may be used to construct fundamental random quantities: additive (completely random) measures (and by specialization, compound random variables), the gamma distribution, the Wiener process and by extension the Gaussian distribution, de-noising of mean-squared-error, and cluster processes. We give short and simple proofs. These are listed below in Table 3.

| Object | Location |
|--------|----------|
| Additive (completely random) random measure | Proposition 1 |
| Compound Poisson distribution | Remark 2 |
| Gamma distribution | Proposition 2 |
| Wiener process | Proposition 3 |
| Gaussian distribution | Remark 3 |
| Mean-squared-error with Gaussian noise | Proposition 4 |
| Cluster process | Proposition 5 |

Table 3: Mixed binomial process examples

2.1.1 Examples

In all examples but the last two, we take \( \kappa = \text{Poisson}(c) \). First we construct additive (completely random) measures.

**Proposition 1** (Additive random measures). Let \( N = (\kappa, \nu) \) be a Poisson random measure on \((E \times \mathbb{R}_+, \mathcal{E} \otimes \mathcal{B}_{\mathbb{R}_+})\). Then

\[ L(A) = \int_{A \times \mathbb{R}_+} N(dx, dz) \quad \text{for} \quad A \in \mathcal{E} \]

defines an additive random measure \( L \) on \((E, \mathcal{E})\), where \( L(A), \cdots, L(B) \) are independent for all choices of finitely many disjoint \( A, \cdots, B \) in \( \mathcal{E} \). The law of \( L(A) \) is defined through the Laplace transform for \( A \in \mathcal{E} \) as

\[ \mathbb{E}e^{-\alpha L(A)} = \exp -c \int_{A \times \mathbb{R}_+} \nu(dx, dz)(1 - e^{-\alpha z}) \quad \text{for} \quad \alpha \in \mathbb{R}_+ \]

**Proof.** By Fubini’s theorem, \( L \) is a random measure. \( L(A) \) is determined from the trace of \( N \) on \( A \times \mathbb{R}_+ \). The independence follows from the splitting property of Poisson, so \( L \) is additive. The Laplace transform follows from the Laplace functional, noting that \( \alpha L(A) = Nf \) for \( f(x, z) = \alpha z I_A(x) \). Then we have

\[ \nu e^{-f} = \int_{E \times \mathbb{R}_+} \nu(dx, dz)e^{-z I_A(x)} = \int_{A \times \mathbb{R}_+} \nu(dx, dz)e^{-\alpha z} + \int_{A^c \times \mathbb{R}_+} \nu(dx, dz) \]

so that

\[ \nu e^{-f} - 1 = \nu(e^{-f} - 1) = \int_{A \times \mathbb{R}_+} \nu(dx, dz)(e^{-\alpha z} - 1) \]

\[ \mathbb{E}e^{-\beta L(A)} = \exp -c \int_{A \times \mathbb{N}_\geq 0} \nu(dx, dz)(1 - e^{\alpha z}) \quad \text{for} \quad \alpha \in [0, 1], \quad \beta = -\log(\alpha), \alpha \in [0, 1] \]

**Remark 1** (Integer-valued). Suppose Poisson \( N = (\kappa, \nu) \) is on \((E \times \mathbb{N}_0, \mathcal{E} \otimes 2^{\mathbb{N}_0})\). We define \( \beta L(A) = Nf \) for \( f(x, z) = \beta z I_A(x) \) where \( \beta = -\log(\alpha), \alpha \in [0, 1] \). Then

\[ \mathbb{E}e^{-\beta L(A)} = \exp -c \int_{A \times \mathbb{N}_0} \nu(dx, dz)(1 - e^{\alpha z}) \quad \text{for} \quad \alpha \in [0, 1], \quad \beta = -\log(\alpha) \in \mathbb{R}_+ \]
These results allow us to define the compound Poisson random measure.

**Remark 2 (Compound Poisson).** Let \( N \) be Poisson and consider \( \nu(dx, dz) = \mu(dx)\eta(dz) \). Then \( F(\alpha) = \int_{R_{+}} \eta(dz)e^{-\alpha z} \) is the Laplace transform of \( \eta \) and

\[
\int_{A \times R_{+}} \nu(dx, dz)(1 - e^{-\alpha z}) = \mu(A)(1 - F(\alpha))
\]

so the Laplace transform of \( L(A) \) is given by

\[
\mathbb{E}e^{-\alpha L(A)} = \exp \mu(A)(1 - F(\alpha)) \quad \text{for} \quad \alpha \in R_{+}
\]

which is the compound Poisson distribution with mean \( \mu(A) \) and independent marking distribution \( \eta \) with Laplace transform \( F \). \( L \) is additive. Similarly, for \( \eta \) on \( (N_{\geq 0}, 2^{\mathbb{N}_{\geq 0}}) \), we have

\[
\mathbb{E}e^{-\beta L(A)} = \exp \mu(A)(1 - \phi(\alpha)) \quad \text{for} \quad \alpha \in [0, 1], \quad \beta = -\log(\alpha)
\]

where \( \phi(\alpha) = \sum_{z \in N_{\geq 0}} \eta(z)\alpha^z \) is the probability generating function of \( \eta \).

Next we construct the gamma distribution.

**Proposition 2 (Gamma distribution).** Let \( N = (\kappa, \nu) \) be a Poisson random measure on \([0, t] \times (0, 1], B_{[0, t]} \otimes B_{(0, 1]} \) formed by independency \((X, Y)\). Let \( \nu = \text{Uniform}(0, t] \times \text{Uniform}(0, 1] \) and put \( f(x, y) = \frac{1}{x}e^{-x} \log 1/y \) for \( \lambda \in (0, \infty) \) fixed. Then the random variable \( Nf \) formed as

\[
Nf = \sum_{i}^{\infty} \frac{1}{\lambda}e^{-X_i} \log 1/Y_i
\]

has Laplace transform

\[
F(\alpha) = L(\alpha f) = \mathbb{E}e^{-Nxf} = \left( \frac{\lambda + e^{-\alpha}}{\lambda + \alpha} \right)^{d} \xrightarrow{c,t \to \infty} \left( \frac{\lambda}{\lambda + \alpha} \right)^{d} \quad \text{for} \quad \alpha \in R_{+}
\]

where the limit is the Laplace transform of a gamma random variable with shape parameter \( d \) and rate parameter \( \lambda \), that is

\[
\lim_{c,t \to \infty} Nf = Z \sim \text{Gamma}(d, \lambda)
\]

**Proof.** The result follows from noting that

\[
\mu e^{-\alpha f} = \frac{1}{t} \log \left( \frac{\lambda + e^{-\alpha}}{\lambda + \alpha} \right) + 1
\]

and that the uniform random variable \( U \sim \text{Uniform}(0, 1] \) random variable forms an exponential random variable \( W \sim \text{Exponential}(\lambda) \) as \( W = \frac{1}{\lambda} \log 1/U \).

This shows that the gamma distribution can be interpreted as the limit of a Poisson random measure involving uniform random variables. This idea also shows up in our next example, where we construct the Wiener process.

**Proposition 3 (Wiener process).** Let \( N = (\kappa, \nu) \) be a Poisson random measure on \([0, T], B_{[0,T]} \) with \( \nu = \text{Uniform}[0, T] \). Define

\[
N_t = \frac{N([0, t]) - tc/T}{\sqrt{c/T}} \quad \text{for} \quad t \in [0, T]
\]

Then

(i) \( N_t \) is a Lévy process

(ii) \( N_t \) has limit

\[
\lim_{c \to \infty} N_t \overset{D}{=} W_t \quad \text{for} \quad t \in [0, T]
\]

where \( W_t \) is the Wiener process

(iii) \( N_t \) has mean, variance, and covariance

\[
\mathbb{E}N_t = 0
\]

\[
\text{Var}N_t = t
\]

\[
\text{Cov}(N_s, N_t) = s \wedge t
\]
The characteristic function of $N$

**Remark 3** (Gaussian random variables)

Then we have that

By the splitting property of Poisson, $N((t, t+u])$ is independent of $N((0, t])$ and hence $N_{t+u} - N_t$ is independent of $N_t$. (c) Moreover, $N((t, t+u] \sim \text{Poisson}(cu/T)$ has the same distribution as $N((0, u])$ for all $t \in \mathbb{R}_+$, so $N_{t+u} - N_t$ has the same distribution as $N_u$. By (a), (b), (c), $N_t$ is a Lévy process.

(2) Because $N_t$ is a Lévy process, so is $W_t$. The law of $W_t$ is therefore specified through the characteristic function. Hence it suffices to show the claimed limit through characteristic functions. The characteristic function of $aN([0, t]) = \frac{\sqrt{c/T}}{\sqrt{c/T}} N([0, t])$ is

$$
\varphi_{aN([0,t])}(r) = \sum_{k \geq 0} e^{irka}(ct/T)^k e^{-ct/T} / k! = \exp \left( \frac{ct}{T}(e^{-ra} - 1) = \varphi_{N([0,t])}(ar) \right) \text{ for } r \in \mathbb{R}
$$

The characteristic function of $N_t$ is given by

$$
\varphi_{N_t}(r) = \varphi_{aN([0,t])}(r)\varphi_{\delta_{-\sqrt{cT}}}(r) = \exp \left( \frac{ct}{T}(e^{-r/\sqrt{cT}} - 1) - i\frac{t}{\sqrt{cT}} \right) \text{ for } r \in \mathbb{R}
$$

Then we have that

$$
\lim_{c \to \infty} \varphi_{N_t}(r) = e^{-r^2 t/2} = \varphi_{W_t}(r) \text{ for } r \in \mathbb{R}
$$

which is the characteristic function of a Lévy process where $W_t$ is a Gaussian random variable with mean zero and variance $t$, i.e. the Wiener process.

(3) The mean, variance, and covariance follow from rescaling of the Poisson random measure by the factor $1/\sqrt{c/T}$, where $\mathbb{E}N([0, t]) = ct/T$ and $\text{Cov}(N_s, N_t) = \frac{T}{c} \mathbb{E}[(0, s] \cap [0, t]) = s \land t$.

\[\square\]

**Proposition 4** allows us to construct generic one-dimensional Gaussian random variables.

**Remark 3** (Gaussian random variables). By Proposition 4 the Poisson distribution may be used to construct Gaussian random variables $Z$: For $c \in (0, \infty)$, take $X \sim \text{Poisson}(c\sigma^2)$ and put $N = \mu + (K - c\sigma^2)/\sqrt{c}$. Then $\lim_{c \to \infty} N \overset{D}{=} Z \sim \text{Gaussian}(\mu, \sigma^2)$.

Another idea is experimental uncertainty. We give a proposition that shows how to attain the denoised meansquared-error when the contaminating noise is independent additive Gaussian.

**Proposition 4** (Denoising). Let $(X, Y)$ an independency distributed according to $\nu \times Q$ on $(\mathbb{R} \times \mathbb{R}, \mathcal{E} \otimes \mathcal{B}_\mathbb{R})$, and let $Z$ be independent Gaussian($0, \sigma^2$) noise on $(\mathbb{R}, \mathcal{B}_\mathbb{R})$, where $\sigma^2 \in \mathbb{R}_+$. The triple $(X, Y, Z)$ forms a random measure $N = (\kappa, \mu = \nu \times Q \times \xi)$ on $(\mathbb{R} \times \mathbb{R}, \mathcal{E} \otimes \mathcal{B}_\mathbb{R} \otimes \mathcal{B}_\mathbb{R})$. Consider $f(x, y, z) = (g(x) + z - y)^2$ where $g \in L^2(E, \mathcal{E}, \nu)$ and define $h(x, y) = (g(x) - y)^2$. Then the random variable $Nf$ formed as

$$
Nf = \sum_{i=1}^K (g(X_i) + Z_i - Y_i)^2
$$

has mean and variance

$$
\mathbb{E}Nf = c(\sigma^2 + (\nu \times Q)h)
$$

$$
\text{Var}Nf = c \left( (3\sigma^4 + (\nu \times Q)(6\sigma^2 h + h^2)) + (\delta^2 - c)(\sigma^2 + (\nu \times Q)h)^2 \right)
$$

and Laplace transform

$$
F(\alpha) = \psi(\mu e^{-\alpha f}) = \psi(F_f(\alpha)) \text{ for } \alpha \in \mathbb{R}_+
$$

where $F_f$ is the Laplace transform of $f$ given by

$$
F_f(\alpha) = \frac{1}{\sqrt{1 + 2\sigma^2 \alpha}} (\nu \times Q) e^{-\alpha h/(1 + 2\sigma^2 \alpha)} = \frac{1}{\sqrt{1 + 2\sigma^2 \alpha}} F_h \left( \frac{\alpha}{1 + 2\sigma^2 \alpha} \right) \text{ for } \alpha \in \mathbb{R}_+
$$

and $F_h$ is the Laplace transform of $h$ given by

$$
F_h(\alpha) = (\nu \times Q) e^{-\alpha h} \text{ for } \alpha \in \mathbb{R}_+
$$
Proof. The result follows from

\[
\mu_f = \sigma^2 + (\nu \times Q)h \\
\mu f^2 = 3\sigma^4 + (\nu \times Q) (6\sigma^2 h + h^2)
\]

and

\[
\xi e^{-\alpha f} = \frac{1}{\sqrt{1 + 2\sigma^2\alpha}} e^{-\alpha h/(1+2\sigma^2\alpha)}
\]

so that

\[
\mu e^{-\alpha f} = (\nu \times Q)(\xi e^{-\alpha f}) = \frac{1}{\sqrt{1 + 2\sigma^2\alpha}} (\nu \times Q)e^{-\tilde{\alpha} h} = \frac{1}{\sqrt{1 + 2\sigma^2\alpha}} F_h(\tilde{\alpha})
\]

where \(\tilde{\alpha} = \alpha/(1 + 2\sigma^2\alpha) \in [0, \frac{1}{2\sigma^2}]\) and \(F_h(\alpha) = (\nu \times Q)e^{-\alpha h}\) is the Laplace transform of \(h\).

**Remark 4 (Chi-square).** Consider the set-up of Proposition 4. Take \(\kappa = \text{Dirac}(c)\) for \(c \in \mathbb{N}_{>0}\) assume that \(\sigma^2 = 1\) and \(h = 0\). Then

\[
F(\alpha) = \frac{1}{(1 + 2\alpha)^{c/2}}
\]

is the Laplace transform of a Chi-square distribution with \(c\) degrees of freedom.

Proposition 4 shows that mean-squared-error may by de-noised for independent additive Gaussian noise. The interpretation of \(f\) may be either the model containing error, i.e. \(g(x) + z\), or the truth containing noise \(z + y\). The result shows that the Laplace transforms of \(f\) and \(h\) are related for known \(\sigma^2\): knowledge of \(F_f\) provides knowledge of \(F_h\) and vice versa. For Gaussian noise, this conveys a deconvolution of the density of \(Nf\) (observed) to attain the density of \(Mh\) (unobserved), where \(M = (\kappa, \nu \times Q)\) is the random measure on \((E \times \mathbb{R}, \mathcal{E} \otimes \mathcal{B}_\mathbb{R})\).

**Remark 5 (Example).** Consider the set-up of Proposition 4. Consider \(g(x) = x\) on \(E = [0, 1]\) with \(\nu = \text{Uniform}[0, 1]\). Let \(Q(x, \cdot) = \delta_{1/2}(\cdot)\) and take \(\sigma^2 = 1\). Put \(f(x, y, z) = (x + z - y)^2\) and \(h(x, y) = (x - y)^2\). Then

\[
F_f(\alpha) = (\nu \times Q \times \xi)e^{-\alpha f} = \sqrt{\pi} \frac{\alpha}{\alpha} \text{Erf} \left( \frac{\sqrt{\alpha}}{2\sqrt{1+2\alpha}} \right)
\]

and

\[
F_h \left( \frac{\alpha}{1 + 2\alpha} \right) = \sqrt{1 + 2\alpha} F_f(\alpha) = \sqrt{\pi} \frac{\alpha}{\alpha} \text{Erf} \left( \frac{\sqrt{\alpha}}{2} \right)
\]

The laws of \(f\) and \(h\) can be determined by the inverse Laplace transforms, which give

\[
(\mu \circ f^{-1})(dx) = dx \frac{1}{2\sqrt{x}} \left( \text{Erf} \left( \frac{1 + 2\sqrt{x}}{2\sqrt{2}} \right) + \text{Erf} \left( \frac{1 - 2\sqrt{x}}{2\sqrt{2}} \right) \right) \quad \text{for} \quad x \in \mathbb{R}_+
\]

and

\[
(\nu \times Q) \circ h^{-1}(dx) = dx \frac{1}{\sqrt{x}} \quad \text{for} \quad x \in (0, 1/4)
\]

Another common usage of the mixed binomial process is construction of cluster processes. This is a nested mixed binomial process, where the mark-space forms a mixed binomial process. We describe the general case below.
Proposition 5 (Cluster process). Let $N = (\kappa, \nu)$ be a random measure on $(E, \mathcal{E})$ where $\kappa$ has mean $c$ and variance $\delta^2$. Consider transition probability kernel $Q$ from $(E, \mathcal{E})$ into the space of random counting measures $(F, \mathcal{F})$, defined as

$$Q(x, dy) = \mathbb{P}(M_x \in dy)$$

where $M_x = (\xi_x, \zeta_x)$ is a random counting measure on $(E, \mathcal{E})$, $\xi_x$ is a $\mathbb{N}_{\geq 0}$-valued distribution conditioned on $x$ with mean $c_x$ and variance $\delta^2_x$, and $\zeta_x$ is a conditional distribution on $(E, \mathcal{E})$. The random measure $M = (\kappa, \nu \times Q)$ on $(E \times F, \mathcal{E} \otimes \mathcal{F})$ is called a cluster process and is formed as

$$Mf = \sum_{i} f \circ (X_i, M_{X_i}) \quad \text{for} \quad f \in (\mathcal{E} \otimes \mathcal{F})_+$$

Consider $f(x, y) = y(E)$. Then $Mf$ is the total number of points of the cluster process with mean and variance

$$\mathbb{E}Mf = cvc_*$$

$$\mathbb{V}arMf = cv(c_*^2 + \delta_*^2) + (\delta^2 - c)(\nu c_*)^2$$

and Laplace transform

$$F(\alpha) = \psi(\nu \phi_*(\beta)) \quad \text{for} \quad \alpha \in \mathbb{R}_+, \beta = e^{-\alpha} \in [0, 1]$$

where $\psi$ is the pgf of $\kappa$ and $\phi_x$ is the pgf of $\xi_x$. Now consider $f(x, y) = y(A)$ for $A \subset E$, where $Mf$ is the number of points of the cluster process located in $A$. Then $Mf$ has mean and variance

$$\mathbb{E}Mf = cv(c_* a_* )$$

$$\mathbb{V}arMf = cv((c_*^2 + \delta_*^2) a_*) + (\delta^2 - c)\nu^2(c_* a_*)$$

where $a_x = \zeta_x(A)$ and Laplace transform

$$F(\alpha) = \psi(\nu \phi^A_*(\beta)) \quad \text{for} \quad \alpha \in \mathbb{R}_+, \beta = e^{-\alpha} \in [0, 1]$$

where $\phi^A_x(t) = \phi_x(a_x t + 1 - a_x)$ is the restricted pgf of $\xi_x$ to $A \subset E$.

Proof. For $f(x, y) = y(E)$, we have

$$\mathbb{E}Mf = c(\nu \times Q)f = c \int_E \nu(dx) E \mathbb{E}M_x(E) = cvc_*$$

and

$$\mathbb{V}arMf = c(\nu \times Q)f^2 + (\delta^2 - c)((\nu \times Q)f)^2$$

$$= c \int_E \nu(dx) E \mathbb{E}M_x^2(E) + (\delta^2 - c)(\nu c_*)^2$$

$$= cv(E^2 M_x(E) + \mathbb{V}ar M_x(E)) + (\delta^2 - c)(\nu c_*)^2$$

$$= cv((c_*^2 + \delta_*^2) + (\delta^2 - c)(\nu c_*)^2$$

The Laplace transform follows from

$$F(\alpha) = \psi(\nu \times Q e^{-\alpha f}) = \psi(\int_E \nu(dx) e^{-M_x(E)} = \psi(\nu \phi_*(\beta))$$

where $\beta = e^{-\alpha}$.

For $f(x, y) = y(A)$, we have

$$\mathbb{E}Mf = c(\nu \times Q)f = c \int_E \nu(dx) E \mathbb{E}M_x(A) = cv(c_* a_*)$$

and

$$\mathbb{V}arMf = c(\nu \times Q)f^2 + (\delta^2 - c)((\nu \times Q)f)^2$$

$$= cv(\mathbb{V}ar M_x(A) + E^2 M_x(A)) + (\delta^2 - c)\nu^2(c_* a_*)$$

$$= cv(c_*^2 a_* + (\delta^2 - c)a_* + c_*^2 a_*) + (\delta^2 - c)\nu^2(c_* a_*)$$

$$= cv((c_*^2 + \delta_*^2) a_*) + (\delta^2 - c)\nu^2(c_* a_*)$$
The Laplace transform follows from

\[ F(\alpha) = \psi((\nu \times Q)e^{-\alpha f}) = \psi(\nu E e^{-\alpha M(A)}) = \psi(\nu \varphi^A(\beta)) \quad \text{for} \quad \alpha \in \mathbb{R}_+ \]

In Table 5 we list some common cluster processes for choices of \( \kappa \) and \( \xi \).

| Cluster process                  | \( \kappa \) | \( \xi \) |
|----------------------------------|--------------|------------|
| Independent cluster process      | general      | general    |
| Cox cluster process              | general      | Poisson    |
| Poisson cluster process          | Poisson      | general    |
| Neyman-Scott process             | Poisson      | Poisson    |

Table 4: Cluster processes

**Remark 6 (Example).** Consider the set-up of Proposition 5. Let \((E, \mathcal{E}) = (\mathbb{R}^2, \mathcal{B}_{\mathbb{R}^2})\). Let \( \kappa \) be Poisson or Dirac. Let \( \xi \) be independent of \( \nu \) and Poisson. Let \( \zeta \) be Gaussian with mean \( \bullet \) and variance \( \sigma^2 \in \{0.01^2, 0.1^2\} \). Consider \( \nu = \text{Uniform}(0, 1]^2 \). Let \( E\kappa = 20 \) and \( E\xi = 10 \). Consider \( A = (-\infty, \frac{1}{2}] \times (-\infty, \frac{1}{2}] \) and note that \( \nu a = 1/4 \). We sample \( Mf \) for the two \( f \)'s for Poisson and Dirac. These correspond to the Neyman-Scott and Cox cluster processes respectively. In Table 5 we show the means and variances for the analytic and estimated from \( 10^5 \) random realizations. The estimated values are very close to the true values. In Figure 2 we show the distribution of \( Mf \) for the two \( f \)’s as estimated for \( \sigma^2 \in \{0.01^2, 0.1^2\} \). Dirac possesses ‘spikes’ on \( A \) for \( \sigma^2 = 0.01^2 \), corresponding to the low variance of the clusters (the spikes occurring at integers at roughly multiples of \( E\xi \)), whereas Poisson is invariant to the choice of \( \sigma^2 \), performing smoothening.

|          | \( E\, f(x,y) = y(E) \) |          | \( E\, f(x,y) = y(A) \) |
|----------|---------------------------|----------|---------------------------|
|          | \( E\, Mf \) | \( \text{Var} Mf \) | \( \text{Var} Mf \) | \( E\, Mf \) | \( \text{Var} Mf \) | \( \text{Var} Mf \) |
| Poisson  | 200 | 200.1 | 2200 | 2202.3 | 50 | 50.0 | 550 | 535.1 |
| Dirac    | 200 | 200.3 | 2000 | 2007.4 | 50 | 50.2 | 500 | 495.6 |

Table 5: Cluster random measure simulation results from \( 10^5 \) samples for \( \sigma^2 = 0.01^2 \)
2.2 High dimensional model representation, global sensitivity analysis

Suppose we have measurable space \((\mathcal{F}, \mathcal{F})\) and some mapping \(g : E \mapsto F\) that is measurable relative to \(\mathcal{E}\) and \(\mathcal{F}\). We assume that either \(F = \mathbb{R}\) or \(F\) is atomic and finite with dimension \(m\). If the first case we assume \(g \in L^2(\mathcal{E}, \mathcal{E}, \mu)\) and identify such \(g\) as a regressor. In the latter case, we identify \(g\) to a classifier. Hereafter we take \(E\) as finite with dimension \(n\). All such regressors may be decomposed into a hierarchy of high dimensional model representation (HDMR) (Rabitz and Alis [1999]) component functions

\[
g(x_1, \ldots, x_n) = g_0 + \sum_i g_i(x_i) + \sum_{i<j} g_{ij}(x_i, x_j) + \cdots + g_{1 \cdots n}(x_1, \ldots, x_n)
\]

which convey a decomposition of variance

\[
\text{Varg} = \sum_{u \subseteq \{1, \ldots, n\}} \text{Varg}_u + \sum_{u \neq v \subseteq \{1, \ldots, n\}} \text{Cov}(g_u, g_v)
\]

The component functions \(\{g_u\}\) are hierarchically orthogonal under inner product \((\cdot, \cdot)_\nu = \text{Cov}(\cdot, \cdot)\) [Hooker 2007]. This is also known as the functional ANOVA expansion or the Sobol system of \(g\). When the inputs are independent \(\nu = \prod_i \nu_i\), then the component functions are mutually orthogonal and may be recursively constructed as follows. Defining the operator

\[
M^{i_1 \cdots i_l}g(x) = \int_{\{0,1\}^{n-l}} \prod_{j \notin \{i_1, \ldots, i_l\}} \nu_j\{x_j\}g(x_1, \ldots, x_n)
\]

Figure 2: Simulated distribution of cluster process \(Mf\)
the HDMR of $g$ for $\nu = \prod_i \nu_i$ is computed recursively,
\[
\begin{align*}
g_0 &= M g(x) \\
g_i(x_i) &= M^i g(x) - g_0 \quad \text{for } i \in \{1, \cdots, n\} \\
g_{ij}(x_i, x_j) &= M^{ij} g(x) - g_i(x_i) - g_j(x_j) - g_0 \quad \text{for } i < j \in \{1, \cdots, n\} \\
&\vdots \\
g_{1 \cdots n}(x_1, \cdots, x_n) &= g(x) - g_0 - \sum_i g_i(x_i) - \sum_{i<j} g_{ij}(x_i, x_j) - \cdots
\end{align*}
\]

For the classifier $g$, we put $F = \{1, \cdots, m\}$ and introduce additional mapping $h : F \rightarrow \{0,1\}^m$ defined as
\[
h \circ g(x) = (\mathbb{I}_{\{1\}}, \cdots, \mathbb{I}_{\{m\}}) \circ g(x) \quad \text{for } x \in E
\]

Then the $m$ indicator dimensions of $h \circ g = (h_1 \circ g, \cdots, h_m \circ g) = (l_1, \cdots, l_m)$ each belong to $L^2(E,\mathcal{E},\nu)$ and may be furnished with HDMRs.

HDMR analysis conveys a global sensitivity analysis through the definition of structural and correlative sensitivity indices $\{ (S^a_u, S^b_u) : u \subseteq \{1, \cdots, n\} \}$ [Li and Rabitz 2012, Sobol 1999, 2001].

**Definition 1** (Sensitivity indices of $g$). The structural sensitivity index of subspace $u \subseteq \{1, \cdots, n\}$ is
\[
S^a_u = \frac{\text{Var}_u g}{\text{Var} g} \quad \text{for } u \subseteq \{1, \cdots, n\}, |u| \geq 1
\]
and the correlative sensitivity index is
\[
S^b_u = \sum_{v \subseteq \{1, \cdots, n\} : v \neq u} \frac{\text{Cov}(g_u, g_v)}{\text{Var}_u g} \quad \text{for } u \subseteq \{1, \cdots, n\}, |u| \geq 1
\]
so that
\[
1 = \sum_{u \subseteq \{1, \cdots, n\} : |u| \geq 1} (S^a_u + S^b_u) = S^a + S^b
\]

### 3 Random measure ANOVA of risk functionals

In Section 3.1 we decompose the variance. In Section 3.2 we decompose the mean.

#### 3.1 Variance decomposition (RM-ANOVA)

In the following result, we have that the variance of the full model is decomposed into the variance-covariance structure of the partition, obtained through the variance-covariance formulas. Based on the class of mixed binomial processes we refer to the decomposition of random measure variance in terms of partitions the random measure analysis of variance (RM-ANOVA).

**Theorem 1** (RM-ANOVA). Let $N = (\kappa, \nu)$ be a random measure on $(E, \mathcal{E})$. Let $f \in \mathcal{E}_+$ and consider disjoint partition $\{A, \cdots, B\}$ of $E$. Define $f_a = \mathbb{I}_A, \cdots, f_b = \mathbb{I}_B$. Then
\[
\text{Var} N f = \sum_{D \in \{A, \cdots, B\}} \text{Var} N f_d + \sum_{D \neq D' \in \{A, \cdots, B\}} \text{Cov}(N f_d, N f_{d'})
\]
\[
= \sum_{D \in \{A, \cdots, B\}} (\nu f_d^2 + (\delta^2 - c)(\nu f_d)^2) + \sum_{D \neq D' \in \{A, \cdots, B\}} (\delta^2 - c) \nu f_d \nu f_{d'}
\]

**Proof.** Noting that $f = \mathbb{I}_A + \cdots + \mathbb{I}_B$ and that disjointness implies that $\text{Cov}(N f_a, N f_b) = (\delta^2 - c) \nu f_a \nu f_b$, we have the decomposition using the variance and covariance formulas of the mixed binomial process.

If we normalize by the overall variance, then we retrieve a kind of sensitivity analysis.
Definition 2 (Sensitivity indices of \( Nf \)). For the random measure \( N \) and relative to the disjoint partition \( \{A, \cdots, B\} \) of \( E \), the structural sensitivity index of \( Nf \) is defined as

\[
S^a_d \equiv \frac{\text{Var}Nf_d}{\text{Var}Nf} \quad \text{for} \quad D \in \{A, \cdots, B\} \tag{11}
\]

and correlative sensitivity index is defined as

\[
S^b_d \equiv \sum_{D_i \in \{A, \cdots, B\}; D_i \neq D} \frac{\text{Cov}(Nf_d, Nf_{D_i})}{\text{Var}Nf} \quad \text{for} \quad D \in \{A, \cdots, B\} \tag{12}
\]

where

\[
1 = \sum_{D \in \{A, \cdots, B\}} (S^a_d + S^b_d) = S^a + S^b \tag{13}
\]

This gives the set of sensitivity indices \( \{(S^a_d, S^b_d) : D \in \{A, \cdots, B\}\} \).

These sensitivity indices indicate the contributions to variance of the random measure in the partitions. If \( c = \delta^2 \) for \( \kappa \), such as with Poisson (Bastian and Rempala, 2020) or an orthogonal die (Bastian and Rempala, 2020), then \( S^a = 1 \) and \( S^b = 0 \), so \( (S^a_d) \) is a probability vector, conveying a distribution of uncertainty on the partition. Otherwise, the vector is positively or negatively defective and hence loses a probabilistic interpretation.

A common setting is \( \kappa = \delta_n \) for some \( n \in \mathbb{N}_>0 \) in the binomial process \( N \). For the binomial process,

\[
S^a = \sum_{D \in \{A, \cdots, B\}} \frac{\text{Var}Nf_d}{\text{Var}Nf} = \sum_{D \in \{A, \cdots, B\}} \frac{\text{Var}f_d}{\text{Var}f} > 1 \tag{14}
\]

and

\[
S^b = \sum_{D \in \{A, \cdots, B\}} \sum_{D_i \in \{A, \cdots, B\}; D_i \neq D} \frac{-\nu f_d \nu f_{D_i}}{\text{Var}f} < 1 \tag{15}
\]

Corollary 1 (Sensitivity probability measure). For orthogonal \( N \) and \( f \in \mathcal{E}_+ \), the sensitivity probability measure \( S \) on \( (E, \mathcal{E}) \) is given by

\[
S(dx) = \frac{\nu(dx)f^2(x)}{\nu f^2} \tag{16}
\]

so that

\[
S_d \equiv \int_D S(dx) = S(D) \quad \text{for} \quad D \in \mathcal{E}
\]

For variable subset \( u \subseteq \{1, \cdots\} \), putting \( E_{-u} \equiv \bigcap_{i \in \{1, \cdots\}; i \notin u} E_i \), we have

\[
S_u(dx_u) \equiv \int_{E_{-u}} S(dx) \tag{17}
\]

3.2 Mean decomposition (MM-ANOVA)

In the following result we have a decomposition of the mean measure.

Theorem 2 (MM-ANOVA). Let \( N = (\kappa, \nu) \) be a random measure on \( (E, \mathcal{E}) \). Let \( g \in L^2(E, \mathcal{E}, \nu) \) and define \( f = (g - \nu g)^2 \in \mathcal{E}_+ \). Suppose \( E \) has dimension \( n \). Then

\[
\mathbb{E}Nf = c \sum_{u, v \subseteq \{1, \cdots, n\}} \text{Cov}(g_u, g_v) \tag{18}
\]

where the \( \{g_u\} \) are the HDMR component functions of \( g \).

Proof. Note that \( \nu f = \nu(g - \mathbb{E}g)^2 = \text{Var}g \). The HDMR decomposition of \( g \in L^2(E, \mathcal{E}, \nu) \) into component functions \( \{g_u\} \) and the associated variance decomposition finishes the proof. \( \square \)
If $\nu$ has a product form $\nu = \prod_i \nu_i$, then the component functions are mutually orthogonal and

$$\forall g = \sum_i \forall g_i + \sum_{i<j} \forall g_{ij} + \cdots + \forall g_{1\cdots n}$$

(19)

We refer to the decomposition of the mean measure using functional ANOVA (HDMR) as mean measure ANOVA (MM-ANOVA). This gives us the set of sensitivity indices $\{S_u^a, S_u^b : u \subseteq \{1, \cdots, n\}\}$. When $\nu = \prod_i \nu_i$, then similar to RM-ANOVA, we can define entropy of $f$ on $E$ through the structural sensitivity indices

$$H(f) = \sum_{u \subseteq \{1, \cdots, n\}} -S_u^a \log S_u^a$$

(20)

### 3.3 Combined (RM-MM-ANOVA)

We combine the ANOVAs of the previous sections. Let $\{A, \cdots, B\}$ be a disjoint partition of $E$. Let $f = (g - Eg)^2 \in E_+$. Let $f_a = f I_A, \cdots, f_b = f I_B$. Let $N = (\kappa, \nu)$ be the random measure on $(E, E)$ formed by STC from independency $X = \{X_i\}$ with mean and variance

$$EN_f = \kappa f = c \sum_{u,v \subseteq \{1, \cdots, n\}} \text{Cov}(g_u, g_v)$$

(21)

$$\forall N f = \kappa f^2 + (\delta^2 - c)(\nu f)^2 = \sum_{D \in \{A, \cdots, B\}} \forall N f_d + \sum_{D, \neq D_j \in \{A, \cdots, B\}} \text{Cov}(N f_d, N f_{d_j})$$

(22)

The variance is finite if $g \in L^4(E, E, \nu)$. We have respective sensitivity indices $\{S_u^a, S_u^b : u \subseteq \{1, \cdots, n\}\}$ and $\{S_d^a, S_d^b\}$. For orthogonal $N$, we have sensitivity distribution $S$ on $(E, E)$.

### 3.4 Counting distributions

The key quantity of $\kappa$ is $\delta^2 - c$. This determines the correlative structure of $N$. When $\delta^2 - c = 0$, $N$ is orthogonal. In Table 6 we give some counting distributions and indicate properties. We give pairs of counting distributions across negative, zero, and positive correlation. We indicate whether or not the random measures are closed under restriction to subspaces, as well as some limiting relations. As the orthogonal $N$ are special and we have two choices, we suggest that the orthogonal die be used whenever there is a theoretical reason for bounded support, such as a finite bound on the number of points, otherwise Poisson should be used. The orthogonal die random measure has a Poisson limit, so in many problems the distinction is meaningless.

| Name            | Support      | $\delta^2 - c$ | Closure | Limit(s)        |
|-----------------|--------------|----------------|---------|-----------------|
| Dirac(c)        | $\{c\}$     | $-c$           | No      |                 |
| Binomial(n, p)  | $\{0, \cdots, n\}$ | $-np^2$       | Yes     | Dirac, Poisson  |
| Poisson(c)      | $\mathbb{N}_{\geq 0}$ | 0             | Yes     |                 |
| Orthogonal-die(m, n) | $\{m, \cdots, n\}$ | 0             | No      | Poisson         |
| Negative-binomial(r, p) | $\mathbb{N}_{\geq 0}$ | $+r\left(\frac{p}{1-p}\right)^2$ | Yes     | Poisson         |
| Zeta(s)         | $\mathbb{N}_{\geq 0}$ | $+\frac{\zeta(s-1)\zeta(s+1) - \zeta(s)\zeta(s+1)}{\zeta(s+2)}$ for $s > 2$ | No      |                 |

Table 6: Counting measures

### 3.5 Related work

In this section we describe related work: other work that solves the same problems with different methods, work that uses the same methods to solve different problems, work that is similar to ours that solves similar problems, and a discussion of related problem domains.
Connection to functional HDMR An alternative approach to UQ of risk functionals is representation using functional HDMR (Rabitz and Alis [1999]). Taking \((E, \mathcal{E})\) as a function space, functional ANOVA of functionals has been considered in functional HDMR and functional-cut-HDMR, which project the risk functional \(f \in \mathcal{E}_+\) into functional subspaces and decomposes \(\text{Var}f\). For Dirac \(N\), we have \(\text{Var} Nf = c \text{Var} f\), and hence, assuming \(\nu = \prod_i \nu_i\), functional HDMR may be used to decompose the variance into functional subspaces

\[
\text{Var} f = \sum_i \text{Var} f_i + \sum_{i<j} \text{Var} f_{ij} + \cdots + \text{Var} f_{1\cdots n}
\]

This is distinct from RM-ANOVA, which decomposes \(\text{Var} Nf\) on a partition of disjoint subspaces.

Other UQ methods for \(g\) We describe some other UQ methods for studying the structure of \(g\) in terms of the input coordinates. Besides functional ANOVA, other approaches towards gaining functional UQ of \(g\) are variable importance and dependence measures defined by partial dependence [Friedman, 2001], derivative-based global sensitivity indices [Sobol’ and Kucherenko, 2009], entropy-based methods [Battiti, 1994; Biesiada et al., 2005], functional principal component analysis [Yao et al., 2005], and polynomial chaos expansions [Crestaux et al., 2009]. For example, for derivative-based GSA, we have functionals

\[
\eta_i = \int_E \left( \frac{\partial g(x_1, \ldots, x_n)}{\partial x_i} \right)^2 \nu(dx) \quad \text{for} \quad i \in \{1, \ldots, n\}
\]

with the relation that

\[
\sum_{u \subseteq i} S^u \leq \frac{\eta_i}{\pi^2 \text{Var} g}
\]

Other applications of mixed binomial processes Mixed binomial processes are very general and include many well-known processes such as the binomial and Poisson processes. For example, the Poisson random measure is related to the structure of Lévy processes, Markov jump processes, and the excursions of Brownian motion, and the Poisson random measure is prototypical, enabling construction of a variety of more evolved processes.

Given the mixed binomial process \(N = (\kappa, \nu)\) on \((E, \mathcal{E})\), a number of operations can be considered. One operation is restriction (thinning) of \(N\) to subspaces \(A \subset E\) with mass \(a = \nu(A) > 0\), giving restricted random measure \(N_A = (\kappa_A, \nu_A)\), where \(\nu_A(\cdot) = \nu(A \cap \cdot) / \nu(A)\) is the restricted law. The law of \(N_A\) is encoded in its Laplace functional

\[
L_A(f) = \psi(a \nu_A e^{-f} + 1 - a) \quad \text{for} \quad f \in \mathcal{E}_+
\]

Another is the image (transformation) random measure \(N \circ h^{-1} = (\kappa, \mu = \nu \circ h^{-1})\) on \((F, \mathcal{F})\) for some measurable transformation \(h : E \mapsto F\) with Laplace functional defined through

\[
L(f) = \psi(\mu e^{-f}) \quad \text{for} \quad f \in \mathcal{F}_+
\]

In the article we use a random transformation (transition probability kernel) \(Q\) where \(\mu = \nu Q\).

Other random measures The random counting measures considered here are \(\mathbb{N}_{\geq 0}\) valued. For real-valued random measures \(N\), the law of \(N\) is encoded in the characteristic functional \(\mathbb{E} e^{iNf}\) for \(f \in \{\mathcal{E} - \text{measurable functions}\}\). A prototypical real-valued additive Gaussian random measure is Wiener.
Proposition 6 (Wiener measure). Consider the $\mathbb{R}$-valued Wiener measure $W_t$ on $(\mathbb{R}_+, \mathcal{B}_{\mathbb{R}_+})$ defined as

$$W_t = \int_{[0,t]} f(s)dW_s \quad \text{for} \quad f \in L^2([0,t], \mathcal{B}_{[0,t]}, \text{Leb})$$

with characteristic functional

$$\mathbb{E}e^{iW_t} = \exp \left( -\frac{1}{2} \int_{[0,t]} f^2(s)ds \right) \quad \text{for} \quad f \in L^2([0,t], \mathcal{B}_{[0,t]}, \text{Leb})$$

Then $W_t$ is additive and for $f \in L^2([0,t], \mathcal{B}_{[0,t]}, \text{Leb})$ the random variable $W_t f$ is Gaussian with characteristic function

$$\mathbb{E}e^{irW_t} = \exp \left( -\frac{1}{2} \int_{[0,t]} f^2(s)ds \right) \quad \text{for} \quad r \in \mathbb{R}$$

mean and variance

$$\mathbb{E}W_tf = 0$$
$$\text{Var}W_tf = \int_{[0,t]} f^2(s)ds$$

and for $f, g \in L^2([0,t], \mathcal{B}_{[0,t]}, \text{Leb})$ covariance

$$\text{Cov}(W_sf, W_tg) = \int_{[0,s \wedge t]} f(u)g(u)du$$

Proof. For all choices of disjoint $f, \cdots, g$ in $L^2([0,t], \mathcal{B}_{[0,t]}, \text{Leb})$, e.g. $f = 0$, additivity follows from

$$\mathbb{E}e^{iW_t(f+\cdots+g)} = \exp \left( -\frac{1}{2} \int_{[0,t]} (f(s) + \cdots + g(s))^2ds \right) = \exp \left( -\frac{1}{2} \int_{[0,t]} (f^2(s) + \cdots + g^2(s))ds \right) = \mathbb{E}e^{iW_tf} \cdots \mathbb{E}e^{iW_tg}$$

so $W_tf, \cdots, W_tg$ are independent random variables. Similarly independence holds for orthogonal $f, \cdots, g$ in $L^2([0,t], \mathcal{B}_{[0,t]}, \text{Leb})$. The characteristic function follows from the characteristic functional as $\mathbb{E}e^{irW_t} = \mathbb{E}e^{iW_t(rf)}$, which shows $W_tf \sim \text{Gaussian}(0, \int_{[0,t]} f^2(s)ds)$. The covariance follows from Itô isometry

$$\text{Cov}(W.sf, W.tg) = \mathbb{E}W.sfW.tg = \mathbb{E} \int_{[0,s]} f(u)dW_u \int_{[0,t]} g(u)dW_u = \int_{[0,s \wedge t]} f(u)g(u)du$$

□

Other applications of HDMR Consider $n$ variate function $g(x_1, \ldots, x_n)$. Defining the $T$-order HDMR of $g$ as

$$g^T(x_1, \ldots, x_n) = \sum_{u \subseteq \{1, \ldots, n\} : |u| \leq T} g_u(x_u)$$

in many practical problems for $T \ll n$ we have $g^T \simeq g$, so $g^T$ is a reduced-order representation of $g$. Oftentimes evaluating $g$ may be expensive, whereas evaluation of the reduced-order model $g^T$ is typically fast and efficient.

Connection to bootstrap Random measure uncertainty quantification is commonly practiced through use of the binomial process $N = nF_n$ (Dirac $\kappa = \delta_n$) and its empirical distribution $F_n = 1/n N$ in the bootstrap estimator [Efron and Tibshirani 1993]. The binomial process is a degenerate mixed binomial process, so bootstrap analyses are contained within the framework of mixed binomial processes.

4 Risk functionals of input-output models

A common scenario in data science is an independency of input-output data $(X, Y) = \{(X_i, Y_i)\}$ taking values in $(E \times F, \mathcal{E} \otimes \mathcal{F})$ with distribution $\mu = \nu \times Q$ where $Q$ is a transition probability kernel from $(E, \mathcal{E})$ into $(F, \mathcal{F})$, i.e. $\mu(dx, dy) = \nu(dx)Q(x, dy)$. Let $M = (\kappa, \nu \times Q)$ be a random counting measure on $(E \times F, \mathcal{E} \otimes \mathcal{F})$. 

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4.1 Regression

For regression, consider $Mf_\theta$ for $f_\theta(x,y) = (y - g_\theta(x))^2$, where $g_\theta$ is some regressor with parameters $\theta \in \Theta$ and $F = \mathbb{R}$

$$Mf_\theta = \sum_{i=1}^{K}(Y_i - g_\theta(X_i))^2$$

with mean and variance

$$EMf_\theta = c\mu f_\theta$$

$$\text{Var}Mf_\theta = c\mu f_\theta + (\delta^2 - c)(\mu f_\theta)^2$$

Note that

$$\mu f_\theta = \int_{E \times F} \mu(dx,dy)f_\theta(x,y) = \int_E \nu(dx) \int_F Q(x,dy)f_\theta(x,y)$$

We have risk $R(\theta) = \mu f_\theta = \frac{1}{2}EMf_\theta$ so the risk estimate is attained as

$$\arg \min_{\theta \in \Theta} R(\theta)$$

Now consider a finite disjoint partition $\{A, \cdots, B\}$ of $E \times F$ and define $f_\theta^a(x,y) = f_\theta(x,y)I_A((x,y))$ and $f_\theta^b(x,y) = f_\theta(x,y)I_B((x,y))$. This gives

$$\text{Cov}(Mf_\theta^a, Mf_\theta^b) = (\delta^2 - c)\mu f_\theta^a \mu f_\theta^b$$

Therefore we have the decomposition

$$\text{Var}Mf_\theta = \sum_{D \in \{A, \cdots, B\}} \text{Var}Mf_\theta^d + \sum_{D_i \neq D_j \in \{A, \cdots, B\}} \text{Cov}(Mf_\theta^d, Mf_\theta^j)$$

(23)

This gives us the set of sensitivity indices $\{(S_\theta^a, S_\theta^b) : D \in \{A, \cdots, B\}\}$. For orthogonal $N$ the sensitivity density is defined as

$$S_\theta^a(dx_u) = \frac{1}{(\nu \times Q)f_\theta^d} \int_{E-u} \nu(dx) \int_F Q(x,dy)f_\theta^2(x,y) \quad \text{for} \quad x_u \in E_u$$

We can also define sensitivity densities on the output and input-output spaces as

$$S_\theta^a(dy) = \frac{1}{(\nu \times Q)f_\theta^d} \int_E \nu(dx)Q(x,dy)f_\theta^2(x,y) \quad \text{for} \quad y \in F$$

and

$$S_\theta^a(dx_u,dy) = \frac{1}{(\nu \times Q)f_\theta^d} \int_{E-u} \nu(dx)Q(x,dy)f_\theta^2(x,y) \quad \text{for} \quad (x_u, y) \in E_u \times F$$

For the decomposition of risk $R(\theta)$, we take $E$ with $n$ dimensions, set $c_0 = \nu g_\theta \in \mathbb{R}$ and put $F = \{c_0\}$ with

$Q(x,\cdot) = I_F(x)$. Therefore

$$R(\theta) = \mu f_\theta = \mu(g_\theta - c_0)^2 = \text{Var}g_\theta = \sum_{u,v \subseteq \{1, \cdots, n\}} \text{Cov}(g_u, g_v)$$

(24)

This gives us the set of sensitivity indices $\{(S_\theta^a, S_\theta^b) : u \subseteq \{1, \cdots, n\}\}$.

4.2 Classification

For classification, consider $Mf_\theta$ for $f_\theta(x,y) = \mathbb{I}(y \neq g_\theta(x))$ where $g_\theta$ is some classifier and $F$ is countable. We have that

$$\mu f_\theta = \int_{E \times F} \mu(dx,dy)f_\theta(x,y) = \int_E \nu(dx) \sum_{y \in F} Q(x,\{y\})f_\theta(x,y) = \mathbb{P}(y \neq g_\theta(x))$$

(25)

Risk is similarly defined. Consider the partition of $\{A, \cdots, B\}$ of $E \times F$ and define $f_\theta^a(x,y) = f_\theta(x,y)I_A((x,y))$ so that we have the vector $(Mf_\theta^a, \cdots, Mf_\theta^b)$. The $f_\theta^a, \cdots, f_\theta^b$ are disjoint. We have $\text{Cov}(Mf_\theta^a, Mf_\theta^b) = (\delta^2 - c)\mu f_\theta^a \mu f_\theta^b$.
The sensitivity distribution is given by

$$S_u(dx_u) = \frac{1}{(\nu \times Q)f_\theta} \int_{E-u} \nu(dx) \sum_{y \in F} Q(x \{y\}) f_\theta(x,y) \quad \text{for} \quad x_u \in E_u$$

We also can define a sensitivity density on $F$ as

$$S^a\{y\} = \frac{1}{(\nu \times Q)f_\theta} \int_E \nu(dx)Q(x \{y\}) f_\theta(x,y) \quad \text{for} \quad y \in F$$

and density on $E_u \times F$ as

$$S^a(dx_u, y) = \frac{1}{(\nu \times Q)f_\theta} \int_{E-u} \nu(dx)Q(x \{y\}) f_\theta(x,y) \quad \text{for} \quad (x_u, y) \in E_u \times F$$

For Dirac $\kappa$ we have

$$\text{Var} M f_\theta = c\mu_f(1 - \mu_f)$$

and sensitivity indices

$$S^a_d = \frac{\text{Var} M f^d_\theta}{\text{Var} M f_\theta} = \frac{\mu f^d_\theta(1 - \mu f^d_\theta)}{\mu_f(1 - \mu_f)} \quad \text{for} \quad D \in \{A, \cdots, B\}$$

and

$$S^b_d = \sum_{D_1 \in \{A, \cdots, B\}: D \neq D_1} \frac{\text{Cov}(M f^d_\theta, M f^d_{D_1})}{\text{Var} M f_\theta} = \sum_{D_1 \in \{A, \cdots, B\}: D \neq D_1} -\frac{\mu f^d_\theta \mu f^d_{D_1}}{\mu_f(1 - \mu_f)} \quad \text{for} \quad D \in \{A, \cdots, B\}$$

For Poisson or orthogonal die $\kappa$, we have $\delta^2 = c$ and

$$\text{Var} M f_\theta = c\nu f^d_\theta$$

and

$$S^a_d = \frac{\mu f^d_\theta}{\mu_f} \quad \text{for} \quad D \in \{A, \cdots, B\}$$

The sensitivity distribution is given by

$$S(dx, dy) = \mu(dx, dy)f_\theta(x, y)/\mu_f$$

5 Random field ANOVA

We discuss a connection between STC of mixed binomial processes and positive random fields, touching fPCA, reproducing kernel Hilbert space (RKHS), and random field theories.

**Proposition 7** (Positive random field). Let $N = (\kappa, \nu)$ be a random measure on $(E, \mathcal{E})$ formed by independency $X = \{X_i\}$. Let $(F, \mathcal{F})$ be a measurable space and let $k : E \times F \mapsto \mathbb{R}_+$ be $\mathcal{E} \otimes \mathcal{F}$-measurable. Then

$$G(y) = \int_E N(dx)k(x, y) = \sum_{i}^{\kappa} k(X_i, y) \quad \text{for} \quad y \in F$$

defines a positive random field $G = \{G(y) : y \in F\}$ on $(F, \mathcal{F})$ with law specified by the Laplace transform

$$\mathbb{E} e^{-\alpha G} = \psi(\nu e^{-\int_F \alpha(dy) k(\cdot, y)}) \quad \text{for every finite measure } \alpha \text{ on } (F, \mathcal{F})$$

and, putting $f_y(\cdot) = k(\cdot, y) \in \mathcal{E}_+$ so that $G(y) = N f_y$ for $y \in F$, with mean and covariance

$$U(y) = \mathbb{E} G(y) = c\nu f_y \quad \text{for} \quad y \in F$$

$$C(y, z) = \text{Cov}(G(y), G(z)) = c\nu (f_y f_z) + (\delta^2 - c)\nu f_y \nu f_z \quad \text{for} \quad y, z \in F$$
Proof. The law of $G$ is specified by the finite-dimensional distributions of $(G(y_1), \ldots, G(y_n))$ for $n \geq 1$ and $y_1, \ldots, y_n \in F$ or equivalently by the Laplace transform $E e^{-\alpha G} = \mathbb{E} e^{-\int F \alpha(dy) G(y)}$ for all finite measures $\alpha$ on $(F, \mathcal{F})$. Given $N$ and $k$, the Laplace transform of $G$ follows from the Laplace functional of $N$ for test function $f_y(\cdot) = k(\cdot, y) \in \mathcal{E}_+$. The mean and covariance follow from $N$.

Remark 7 (Densities). The density of $N f_y = G(y)$, $\eta_y$, defines a transition probability kernel $\eta_y(\cdot) = Q(y, \cdot)$ from $(F, \mathcal{F})$ into $(E, \mathcal{E})$. Let $\alpha$ be a probability measure on $(F, \mathcal{F})$. Then $\alpha \times Q$ is the joint distribution on $(F \times E, \mathcal{F} \otimes \mathcal{E})$

$$(\alpha \times Q)f = \int_F \alpha(dy) \int_E Q(y, dx) f(x, y) \quad \text{for } f \in (\mathcal{F} \otimes \mathcal{E})_+$$

and $\alpha Q$ is the marginal distribution of $\alpha \times Q$ on $(E, \mathcal{E})$

$$(\alpha Q)f = \int_F \alpha(dy) \int_E Q(y, dx) f(x) \quad \text{for } f \in \mathcal{E}_+$$

We give an example for Proposition 7: consider $(F, \mathcal{F}) = (E, \mathcal{E})$ where $E$ has dimension one, $\nu$ as standard Gaussian, and the radial basis kernel $k(x, y) = e^{-\gamma (x-y)^2}$ so that

$$\nu(f_y f_z) = e^{-\frac{\gamma}{1+4\gamma} (y^2 + 2z(y-z)^2 + z^2)}$$

and

$$\nu f_y = \frac{1}{\sqrt{1+2\gamma}} e^{-\frac{\gamma}{1+2\gamma} y^2}$$

In Figure 3 we show $C$ on $[-3, 3] \times [-3, 3]$ for the radial basis kernel with $c = \gamma = 1$ for orthogonal and Dirac $N$. The random field covariance kernels are very different: in Figure 3a orthogonal has positive correlation and a single mode located at $y = z = 0$, whereas in Figure 3b Dirac has a four correlative modes, two positive and two negative, around $y, z \approx \pm 1$.

Figure 3: Random field kernel $C$ using radial basis kernel $k$ with $c = \gamma = 1$ for orthogonal and Dirac $N$

Remark 8 (Random fields on graphs). Let $(F, \mathcal{F})$ be indexed by the vertices of some graph space $(V, E)$ with distribution $\alpha$. Examples of $\alpha$ include the Markov random field and conditional random field.

Next we use the Karhunen-Loève theorem to get the eigensystem expansion of $C$. We note that KL theorem is a type of polynomial chaos expansion, where the basis is optimal in $L^2$ with respect to $\mu$. The normalized eigenvalues reveal the contributions to the variance.
Proposition 8 (fPCA expansion). Assume $C$ is continuous. Then $C$ can be decomposed

$$C(y, z) = \sum_{k \geq 1} \lambda_k \varphi_k(y) \varphi_k(z)$$

where $\{\lambda_k\}$ and $\{\varphi_k\}$ are the eigenvalues and orthonormal eigenfunctions of the operator of the form

$$f \mapsto \int_{F} \mu(dy) K(y, z) f(y)$$

$$L^2(F, \mathcal{F}, \mu) \to L^2(F, \mathcal{F}, \mu)$$

and the centered process $G - U$ can be expressed as

$$G(y) - U(y) = \sum_{k \geq 1} \xi_k \varphi_k(y)$$

where

$$\xi_k = \int_{F} \mu(dy) (G(y) - U(y)) \varphi_k(y)$$

with $\mathbb{E} \xi_k = 0$, $\text{Var} \xi_k = \lambda_k$, and $\text{Cov}(\xi_k, \xi_l) = 0$ for $k \neq l$.

Definition 3 (RF-ANOVA). Consider the random field $G$ on $(F, \mathcal{F})$ formed from random measure $N = (\kappa, \nu)$ on $(E, \mathcal{E})$ and function $k : E \times F \to \mathbb{R}_+$. Putting $\lambda = \sum_i \lambda_i$, the sensitivity indices of $G$ are the normalized variances

$$\xi_i = \frac{\lambda_i}{\lambda} \text{ for } i \in \mathbb{N}_{>0}$$

Remark 9 (Discrete approximation). The continuous eigenfunctions may be difficult to compute. In practice a finite number of eigenvalues and eigenfunctions can be attained to arbitrary precision using the eigensystem decomposition of the matrix $(C(y, z) : y, z \in \{a, \cdots, b\})$.

5.1 Related work

Random fields are ubiquitous and are tantamount to stochastic processes. There are many random field models. This section shows construction of general positive random fields $G$ with law determined by the Laplace transform, derived from the Laplace functional of $N$. Poisson random fields are canonical, although the terminology in the literature is conflicting, as ‘Poisson random field’ can sometimes mean either Poisson random measure or some other Poisson-derived quantity.

The law of real-valued random field $G$ on $(F, \mathcal{F})$ is determined by the characteristic function $\mathbb{E} e^{irG}$ for functions $r$ such that $\int_{F} r(y) G(y) dy < \infty$. A common choice is Gaussian.

6 Density identification through inversion of Laplace transforms

Let $N = (\kappa, \nu)$ be a random measure on $(E, \mathcal{E})$. For $f \in \mathcal{E}_+$, the random variable $N f$ has Laplace transform $F(\alpha)$ and distribution $\eta$. In principle $\eta$ is attained from the inverse Laplace transform of $F(\alpha)$ but in practice this can be difficult.

Remark 10 (Indicators). For indicator functions $f = \mathbb{1}_A$, $A \in \mathcal{E}$, the distribution of $N(A)$, denoted $\kappa_A$, is encoded by the pgf $\psi_A(t) = \psi(at + 1 - a)$

$$\kappa_A\{k\} = \mathbb{P}(N(A) = k) = \psi_A^{(k)}(0)/k! \text{ for } k \in \mathbb{N}_{>0}$$

We consider $f \in \mathcal{E}_+$ such that $N f \in \mathbb{R}_+$, whose law $\eta$ is encoded in the Laplace transform. We can attain $\eta$ through the method of maximum entropy using knowledge of some number of generalized moments of $N f$, described in for instance [Gzyli 2017], which are evaluations of the Laplace transform. We describe the basic set-up and application to random measures.

The basic problem of interest is the truncated moment problem

identify $\eta$ such that $F(\alpha_i) = f_i \in [0, 1]$ for $i = 1, \cdots, n$
We introduce the change of variables $Nf \mapsto y = e^{-Nf} \in [0, 1]$. Then

$$F(\alpha) = \mathbb{E}y^{\alpha} = \psi(\nu e^{-\alpha f})$$

is the generalized moment of $y$, where $y$ has distribution $\mu$. It turns out that the collection

$$\{f_i = \mathbb{E}y^{\alpha_i} : i \in \mathbb{N}_{>0}, \alpha_1 > \alpha_2 > \cdots, \sum_i \alpha_i = \infty, \lim_{i \to \infty} \alpha_i = 0\}$$

uniquely determines $\mu$. Given $\alpha_1 > \cdots > \alpha_n$, i.e. the first $n$ terms, the density $\mu(dx) = \mathbb{P}(y \in dx)$ on $[0, 1]$ can be attained using the method of maximum entropy as $\mu_n$, that is, we can use maximum entropy to invert the Laplace transform evaluated on a set of points. The maximum entropy distribution of $\mu$ given $n$ generalized moment constraints is

$$\mu_n(dy) = \frac{1}{Z(\lambda_1, \cdots, \lambda_n)} \exp(-\sum_{i=1}^n \lambda_i y^{\alpha_i}) \quad \text{for} \quad y \in [0, 1]$$

(28)

where

$$Z(\lambda_1, \cdots, \lambda_n) = \int_{[0,1]} dy \exp(-\sum_{i=1}^n \lambda_i y^{\alpha_i})$$

and $\lambda_1, \cdots, \lambda_n$ in $\mathbb{R}$ are attained as

$$\left(\lambda_1, \cdots, \lambda_n\right) = \arg\min_{(\lambda_1^*, \cdots, \lambda_n^*) \in \mathbb{R}^n} \log Z(\lambda_1^*, \cdots, \lambda_n^*) + \lambda_1^* f_1 + \cdots + \lambda_n^* f_n$$

(29)

where the function being minimized is strictly convex.

Then we can attain the maximum-entropy-derived density of $Nf$ as

$$\eta_n(dx) = \mathbb{P}(Nf \in dx) = e^{-x}(\mu_n \circ e^{-x})(dx)$$

(30)

on $(\mathbb{R}_+, \mathcal{B}_{\mathbb{R}_+})$.

If $f$ takes large values and the integral must be computed numerically, then the calculation of $F(\alpha)$ can introduce numerical problems. To circumvent this, we can introduce the normalized function $f^* = f/C$, where $C > 0$, such as $C = \nu f$. Then the density of $y = e^{-Nf^*}$ is attained as $\mu_n$, followed by that of $Nf$, given by

$$\eta_n(dx) = \mathbb{P}(Nf \in dx) = \frac{1}{C} e^{-x/C}(\mu_n \circ e^{-x/C})(dx)$$

Specific calculation Consider the gamma distribution Gamma($d, \lambda$), where $d$ is the shape parameter and $\lambda$ is the rate parameter. We have

$$F(\alpha) = \left(\frac{\lambda}{\lambda + \alpha}\right)^d$$

We draw $\alpha_i$ for $i = 1, \cdots, 10$ according to $\alpha_i \sim \text{Exponential}(1)$. Then we compute $\{F(\alpha_i)\}$ for $d = 2$ and $\lambda = 1$. Finally we estimate $\lambda_1, \cdots, \lambda_{10}$. We show the maximum entropy density $\eta_n(dx)$ below in Figure 4 in comparison to the underlying density of Gamma($2, 1$). The reconstruction is very good for a modest number ($n = 10$) of samples.
7 Examples

Here we analyze in detail two canonical functions using RM-MM-ANOVA, an elementary symmetric polynomial of \( n \) variables in Section 7.1 and a non-linear function commonly used in sensitivity analysis called the Ishigami function of three variables in Section 7.2. We compute the RM-MM-ANOVA decompositions for these problems. We describe application of the RM-MM-ANOVA framework to analyzing the risk functionals of regressors in Section 7.3 and classifiers in Section 7.4 and to adaptive randomized controlled trials in Section 7.6. We provide two additional analyses of functions in the appendices: a symmetric bivariate polynomial with correlated inputs in Section C.1 and a graph property in Section C.2. In Section 7.5 we discuss a random field model for interacting particle systems, and in Section C.3 in appendices we have a short application on the Ising model.

7.1 Elementary symmetric polynomial

As referenced in Table 1, we consider a real-valued test function \( g \) and its HDMR and global sensitivity analysis. Consider the elementary symmetric polynomial

\[
g(x_1, \ldots, x_n) = \prod_{i=1}^{n} x_i, \quad \text{iid } x, \quad \rho \equiv \sigma / \mu \neq 0
\]

with

\[
\mathbb{E}g = \mu^n
\]

\[
\mathbb{V}ar g = \mu^{2n}(1 + \rho^2)^n - 1)
\]

where \( \nu g^2 = \mu^{2n}(1 + \rho^2)^n \).

The component functions of \( g \) are linear combinations of elementary symmetric polynomials

\[
g_0 = \mu^n
\]

\[
g_i(x_i) = \mu^{n-1}x_i - g_0
\]

\[
g_{ij}(x_i, x_j) = \mu^{n-2}x_i x_j - g_i(x_i) - g_j(x_j) - g_0
\]

\[
\vdots
\]

The partition of variance is given by

\[
\mathbb{V}ar g = \sum_i \mathbb{V}ar g_i + \sum_{i<j} \mathbb{V}ar g_{ij} + \ldots + \mathbb{V}ar g_{1\ldots n},
\]
where

\[ \begin{align*}
\text{Var} x_i &= \mu^2 n \\
\text{Var} x_{ij} &= \mu^2 n^2 \\
&\vdots \\
\text{Var} x_{1\ldots n} &= \mu^2 n^{2k}.
\end{align*} \]

The sensitivity indices satisfy

\[ \sum_{i_1 < \ldots < i_k} S_{i_1 \ldots i_k} = 1 \]

and at each order follow

\[ S_{a_u}^k = \frac{n^2}{(\rho^2 + 1)^n - 1} \]

where \( \sum_{k=1}^n S_{a_u}^k = 1 \). Therefore \( P = (S_{a_u}^k) \) forms a distribution on \( \{1, \ldots, n\} \). We have

\[ \begin{align*}
E P &= \frac{n\rho^2 (\rho^2 + 1)^{n-1}}{(\rho^2 + 1)^n - 1} \\
\text{Var} P &= \frac{n\rho^2 (\rho^2 + 1)^{n-2} ((\rho^2 + 1)^n - n\rho^2 - 1)}{(\rho^2 + 1)^{n-1} - 1}^2 \\
H &= \sum_k n S_{a_u|u|=k} \log S_{a_u|u|=k}
\end{align*} \]

Below in Figure 5 we plot the sensitivity indices by subspace \((S_{a_u|u|=k} : k = 1, \ldots, n)\) for varying \(\rho\) for \(n = 100\) and the entropy as a function of \(\rho\).

Figure 5: HDMR sensitivity indices of elementary symmetric polynomial of \(n = 100\) variables in subspace dimension and entropy for varying coefficient of variation \(\rho\).

These findings show that the effective dimension of the fractional contribution of the \(k\)-dimensional subspaces to the variance is regulated by the coefficient of variation \(\rho\) and that the distribution on subspaces is not uniform. If \(\rho = 1\), then

\[ EP = \frac{n}{2 - 2^{-n+1}} \approx \frac{n}{2} \]

if \(\rho < 1\), then \( EP < n/2 \); if \(\rho > 1\), then \( EP > n/2 \). This is an elegant result that the mean measure of squared error risk functionals of monomials admits such a decomposition.
Now consider
\[ f = (g - \mathbb{E}g)^2 = \left( \prod_{i=1}^{n} x_i - \mu^2 \right)^2 \in \mathcal{E}_+ \]
so that we have the decomposition into various subspaces
\[
\nu f = \mathbb{V} \text{arg} = \sum_{u \subseteq \{1, \cdots, n \}} \mathbb{V} \text{arg}_u = \sum_{u \subseteq \{1, \cdots, n \}, |u| \geq 1} \mu^{2n} \rho^{2|u|} = \sum_{k=1}^{n} \binom{n}{k} \mu^{2n} \rho^{2k} \tag{31}
\]

Consider random measure \( N = (\kappa, \nu) \) on \((E, \mathcal{E})\). To define the Laplace functional \( L \), note that
\[
\nu e^{-f} = \int_E \nu(dx)e^{-(\prod_{i} x_i - \mu^2)^2}
\]
This may be calculated exactly in some cases, i.e. for \( n = 1 \) and \( E = [0, 1] \) with uniform \( \nu \) we have \( \nu e^{-f} = \sqrt{\pi} \text{Erf}(\frac{1}{2}) \).
Similarly for the Laplace transform we have \( \nu e^{-\alpha f} = \sqrt{\alpha} \text{Erf} \left( \frac{\sqrt{\alpha}}{2} \right) \).

For \( f \in \mathcal{E}_+ \) the random variable \( N f \) has mean and variance
\[
\mathbb{E}N f = \nu f = c \sum_{u \subseteq \{1, \cdots, n \}} \mu^{2n} \rho^{2|u|} = c \sum_{k=1}^{n} \binom{n}{k} \mu^{2n} \rho^{2k} \tag{32}
\]
\[
\mathbb{V} \text{ar} N f = c \nu f^2 + (\delta^2 - c)(\nu f)^2 \tag{33}
\]
For the variance, we attain \( \nu f^2 \), which is the fourth central moment of \( g \),
\[
\nu f^2 = \nu(g - \mathbb{E}g)^4 = \nu g^4 - 4\mathbb{E}g \nu g^3 + 6(\mathbb{E}g)^2 \nu g^2 - 3(\mathbb{E}g)^4
\]
We have \( \nu(dx)g^j(x) = \prod_{i} \nu_i(dx_i)x_i^j \) for \( j = 1, 2, 3, 4 \). For disjoint partition \( \{A, \cdots, B\} \) of \( E \), we put \( f_a = f1_A, \cdots, f_b = f1_B \). We have
\[
\text{Cov}(N f_a, N f_b) = (\delta^2 - c)\nu f_a \nu f_b
\]
and
\[
\mathbb{V} \text{ar} N f = \sum_{D \in \{A, \cdots, B\}} \mathbb{V} \text{ar} N f_d + \sum_{D_1 \neq D_j \in \{A, \cdots, B\}} \text{Cov}(N f_d, N f_j)
\]
\[= \sum_{D \in \{A, \cdots, B\}} (\nu f_d^2 + (\delta^2 - c)(\nu f_d)^2) + \sum_{D_1 \neq D_j \in \{A, \cdots, B\}} (\delta^2 - c)\nu f_d \nu f_j
\]
For orthogonal \( N \) the sensitivity distribution in each coordinate is defined as
\[
S^q_i(dx_i) = \int_{E_1 \times \cdots \times E_{i-1} \times E_{i+1} \times \cdots \times E_n} \frac{\nu(dx)f^2(x)}{\nu f^2}
\]
**Specific calculations** For an orthogonal die or Poisson \( \kappa \), we have \( c = \delta^2 \), so structural sensitivity indices are given by
\[
S^q_d = \frac{\nu f_d^2}{\nu f^2} \quad \text{for} \quad D \in \{A, \cdots, B\} \tag{34}
\]
where
\[
\nu f_d^2 = \nu f^2 1_D = \int_D \nu(dx)(g(x) - \mathbb{E}g)^4
\]
Suppose \( n = 1 \) so that \( g(x) = x \) and let \( \nu \) on \( E = \{0, 1\} \) be Bernoulli\((p)\) with mean \( p \in [0, 1] \). To define the Laplace functional, we have
\[
\nu e^{-f} = e^{-p^2(1-p)} + e^{-(1-p)^2 p}
\]
Consider partition into the atoms $A = \{0\}$ and $B = \{1\}$. Then we have that

$$
\begin{align*}
\nu f_a^2 &= p^4(1 - p) \\
\nu f_b^2 &= (1 - p)^4 p \\
\nu f^2 &= p^4(1 - p) + (1 - p)^4 p
\end{align*}
$$

$$
\begin{align*}
S_a &= \frac{p^3}{3p^2 - 3p + 1} \\
S_b &= \frac{(1 - p)^3}{3p^2 - 3p + 1} \\
H(S_a) &= -S_a \log S_a - S_b \log S_b
\end{align*}
$$

These quantities are visualized in Figure 6. Figure 6a shows the random measure uncertainty is high for $x = 0$ when $p$ is near one and similarly for $x = 1$ when $p$ is near zero, whereas the second moment $\nu f^2$ shows interesting behavior of an inverted double-well (bistable) potential, with local maxima at $p = \frac{1}{8}(3 \pm \sqrt{3})$ and local minima at $p = \frac{1}{2}$. The potential is the uncertainty (second moment) of a point as a function of $p$ in the parameter space (unit interval). Moreover, the entropy of $N$ is shown in Figure 6c, which is symmetric and unimodal with maximum at $p = 1/2$. Being the only non-trivial partition, \{A, B\} is the maximum entropy partition of $E$.

For Dirac we have as mentioned in [14] and [15] the sensitivity indices and variance terms

$$
\begin{align*}
\nu f_a &= p^2(1 - p) \\
\nu f_b &= (1 - p)^2 p \\
\text{Var} f_a &= p^5(1 - p) \\
\text{Var} f_b &= (1 - p)^5 p \\
\text{Var} f &= p(1 - p)(1 - 2p)^2
\end{align*}
$$

$$
\begin{align*}
S_a &= \frac{\text{Var} f_a}{\text{Var} f} = \frac{p^3}{(1 - 2p)^2} \\
S_b &= \frac{\text{Var} f_b}{\text{Var} f} = \frac{(1 - p)^3}{(1 - 2p)^2} \\
S_a &= S_b = \frac{\nu f_a \nu f_b}{\text{Var} f} = \frac{p^2(1 - p)^2}{(1 - 2p)^2}
\end{align*}
$$

We see that the sensitivity indices for Dirac all have singularities at $p = 1/2$, shown in Figure 6d. The correlative terms are negative, so the structural terms do not form a probability vector but rather have positive defective mass. In Figure 6b we plot $\text{Var} f_a$, $\text{Var} f_b$, and $\text{Var} f$ as a function of $p$. These are similar to $\nu f_a^2$, $\nu f_b^2$, and $\nu f^2$ although steeper and with the overall variance less than the sum of the variances of the two restrictions. In fact the overall variance is zero at $p = 1/2$. 


Figure 6: Random measure variance restrictions, sensitivity indices, and entropy for orthogonal and Dirac $N$, Bernoulli($p$), and univariate polynomial as a function of $p$.
7.2 Ishigami function

As referenced in Table 1, we consider the Ishigami function, a non-linear continuous function

\[ g(x_1, x_2, x_3) = \sin x_1 + a \sin^2 x_2 + b x_3 \sin x_1 \quad \text{for} \quad (x_1, x_2, x_3) \in [-\pi, \pi]^3 \]

with independent uniformly distributed coordinates and parameters \( a, b \in \mathbb{R}_+ \). The mean and variance are

\[
\mathbb{E}g = \frac{a}{2} \\
\mathbb{V}arg = \frac{1}{8}a^2 + \frac{\pi^8}{18}b^2 + \frac{\pi^4}{5}b + \frac{1}{2}
\]

We organize the HDMR results into Table 9.

| Subspace \( u \) | \( g_u \) | \( \mathbb{V}arg_u \) | \( S^a_u \) |
|-----------------|-----------------|-----------------|-----------------|
| \{1\}           | \((1 + \frac{b^4}{2\pi})\sin x_1\) | \(\frac{1}{8}a^2\) | \(\frac{\pi^8}{18}b^2\) | \(\frac{\pi^4}{5}b + \frac{1}{2}\) |
| \{2\}           | \(-\frac{a}{\pi}\cos 2x_2\) | \(\frac{a^2}{8}\) | \(\frac{\pi^8}{18}b^2\) | \(\frac{\pi^4}{5}b + \frac{1}{2}\) |
| \{1, 3\}        | \(b(x_3^2 - \frac{1}{4})\sin x_1\) | \(\frac{8a^2b^2}{225}\) | \(\frac{\pi^8}{18}b^2\) | \(\frac{\pi^4}{5}b + \frac{1}{2}\) |

Table 7: HDMR of Ishigami function

Let \( f = (g - \mathbb{E}g)^2 \). We have

\[
\nu f = \mathbb{V}arg = \mathbb{V}arg_1 + \mathbb{V}arg_2 + \mathbb{V}arg_{13}
\]

(35)

For subspace \( A \subseteq E \), we put \( f_A = f I_A \) and have

\[
\nu f_A = \int_A \nu(dx)f(x)
\]

(36)

Next we calculate \( \nu f^2 \), which is the fourth central moment with value

\[
\nu f^2 = \frac{1}{24} \pi^8 (a^2 + 6)b^2 + \frac{3}{20} \pi^4 (a^2 + 2)b + \frac{3}{128} (a^4 + 16a^2 + 16) + \frac{3\pi^{16}b^4}{136} + \frac{3\pi^{12}b^3}{26}
\]

(37)

The restriction to subspace \( A \subseteq E \) is similarly given as

\[
\nu f_A^2 = \int_A \nu(dx)f^2(x)
\]

(38)

Consider the random measure \( N = (\kappa, \nu) \) on \((E, \mathcal{E})\). To define the Laplace functional, we put

\[
\nu e^{-f} = \frac{1}{(2\pi)^3} \int_{[-\pi, \pi]^3} e^{-(\sin x_1 + a \sin^2 x_2 + b x_3 \sin x_1 - \frac{2}{\pi} f)^2} dx_1 dx_2 dx_3
\]

The Laplace transform is \( F(\alpha) = \psi(\nu e^{-\alpha f}) \). For \( f \in \mathcal{E}_+ \), the random variable \( Nf \) has mean and variance

\[
\mathbb{E}Nf = c \nu f = c(\mathbb{V}arg_1 + \mathbb{V}arg_2 + \mathbb{V}arg_{13})
\]

(39)

\[
\var{Nf} = c \nu f^2 + (\delta^2 - c)(\nu f)^2
\]

(40)

The density of \( Nf, \eta_n \), can be attained from evaluations of the Laplace transform \( F \) using maximum entropy. We take \( \kappa = \text{Poisson}(100) \) and \( \alpha_i \sim \text{Exponential}(1) \) for \( i = 1, \cdots, n \) where \( n = 10 \). We have \( a = 7 \) and \( b = 0.1 \). For the integral \( \nu e^{-\alpha f} \), the variance of \( g \) is large, which introduces numerical difficulties in computing the integral, so we define \( f^* = f/\nu f \), compute \( F^*(\alpha_i) \) for \( i = 1, \cdots, n \), attain the maximum entropy distribution of \( Nf^* \leftrightarrow e^{-Nf^*} \) as \( \mu_n \), and finally attain the maximum entropy distribution of \( Nf, \eta_n \), as

\[
\eta_n(dx) = \frac{1}{\nu f} e^{-x/\nu f}(\mu_n \circ e^{-x/\nu f})(dx)
\]

In Figure 10 we show the density. In Table 8 we show the statistics compared to the exact values. The agreement is very close.
\begin{tabular}{cccc}
E\(N_f\) & \(\text{E}\eta_{10}\) & \(\text{Var}N_f\) & \(\text{Var}\eta_{10}\) \\
1 384.5 & 1 387.0 & 67 223.4 & 66 419.3 \\
\end{tabular}\\

Table 8: Mean and variance of \(N_f\) and \(\eta_n\) where \(\kappa = \text{Poisson}(100)\)

\begin{figure}[h]
\centering
\includegraphics[width=\textwidth]{figure7.png}
\caption{Density of \(N_f\), \(\eta_n\) for \(n = 10\), for \(\kappa = \text{Poisson}(100)\)}
\end{figure}

For disjoint partition \(\{A, \ldots, B\}\) of \(E\), we put \(f_a = f I_A, \ldots, f_b = f I_B\). Then we have

\[
\text{Var}N_f = \sum_{D \in \{A, \ldots, B\}} \text{Var}N_f_d + \sum_{D_i \neq D_j \in \{A, \ldots, B\}} \text{Cov}(N_f_{d_i}, N_f_{d_j})
\]

\[
= \sum_{D \in \{A, \ldots, B\}} (\nu f_d^2 + (\delta^2 - c)(\nu f_d)^2) + \sum_{D_i \neq D_j \in \{A, \ldots, B\}} (\delta^2 - c)\nu f_d \nu f_{d_j}
\]

For an orthogonal die or Poisson \(\kappa\), we have \(c = \delta^2\), so the structural sensitivity indices are given by

\[
S^a_d = \frac{\nu f_d^2}{\nu f^2} \quad \text{for} \quad D \in \{A, \ldots, B\}
\]

where

\[
\nu f_d^2 = \nu f^2 I_D = \int_D \nu(dx)(g(x) - \text{E}g)^4
\]

and its correlative are zero \(S^b_d = 0\). As such, \((S^a_d)\) forms the distribution \(P\) on \(\{A, \ldots, B\}\). The sensitivity index
density of (17) is given by

\[
\xi = 2\pi \nu f^2 = 2\pi \left( \frac{3a^4}{128} + \frac{1}{120} a^2 \left( 5\pi^8 b^2 + 18\pi^4 b + 45 \right) + \frac{3\pi^{16} b^4}{136} + \frac{3\pi^{12} b^3}{26} + \frac{\pi^8 b^2}{4} + \frac{3\pi^4 b}{10} + \frac{3}{8} \right)
\]

\[S^a(dx_1) = \frac{1}{\xi} (\alpha + \beta \sin^2(x_1) + \gamma \sin^4(x_1)) dx_1\]

\[\alpha = \frac{3a^4}{128}\]
\[\beta = \frac{1}{60} a^2 \left( 5\pi^8 b^2 + 18\pi^4 b + 45 \right)\]
\[\gamma = \frac{\pi^{16} b^4}{17} + \frac{4\pi^{12} b^3}{13} + \frac{2\pi^8 b^2}{3} + \frac{4\pi^4 b}{5} + 1\]

\[S^a(dx_2) = \frac{1}{\xi} (\alpha + \beta \cos^2(2x_2) + \gamma \cos^4(2x_2)) dx_2\]

\[\alpha = \frac{3\pi^{16} b^4}{136} + \frac{3\pi^{12} b^3}{26} + \frac{\pi^8 b^2}{4} + \frac{3\pi^4 b}{10} + \frac{3}{8}\]
\[\beta = \frac{1}{60} a^2 \left( 5\pi^8 b^2 + 18\pi^4 b + 45 \right)\]
\[\gamma = \frac{a^4}{16}\]

\[S^a(dx_3) = \frac{1}{\xi} \left( \frac{3}{128} \left( a^4 + 16 (abx_3^4 + a)^2 + 16 (bx_3^4 + a^2) \right) \right) dx_3\]

We set \(a = 7\) and vary \(b \in \{0.01, 0.05, 0.1, 0.15, 0.2\}\). We form the following partitions by subdividing each coordinate interval into \(m = 100\) disjoint equisized intervals. This gives three partitions of size 100. For the first partition \(\{A_i\}\), we take \(A_i = [-\pi + 2\pi i/m, -\pi + 2\pi (i+1)/m] \times [-\pi, \pi] \times [-\pi, \pi]\) for \(i = 0, \ldots, m-1\). In Figure 8, for each partition by a variable, we show the second moments and sensitivity indices across the intervals to reveal the uncertainties of the random measure estimator. The uncertainties are markedly different across the three coordinates: the uncertainties of the first two coordinates are periodic, with the second having higher frequency than the first, whereas the third coordinate has a ‘bathtub’ appearance. In Figure 13, we show the first-order component functions and the HDMR-derived entropy as a function of \(b\). We can see that the entropy has a maximum around \(b \approx 0.13\). We plot the entropy of the distribution defined by the random measure structural sensitivity indices as a function of \(b\), corresponding to the ranges of \(b\) used in Figure 8. All three exhibit monotonic behavior over the range of \(b\), \([0.01, 0.2]\): Coordinate 1 decreases, coordinate 2 increases, and coordinate 3 decreases.
For Dirac $\kappa$, we have $\delta^2 = 0$ so that the structural index is

\[
S_d^a = \frac{\text{Var} f_d}{\text{Var} f} \quad \text{for} \quad D \in \{A, \cdots, B\}
\] (42)

and the correlative index is

\[
S_d^b = \sum_{D_i \in \{A, \cdots, B\}: D_i \neq D} \frac{\nu f_d \nu f_i}{\text{Var} f} \quad \text{for} \quad D \in \{A, \cdots, B\}
\] (43)
We note that

\[ S_a = \sum_{D \in \{A, \ldots, B\}} S_d^a > 1 \]
\[ S_b = \sum_{D \in \{A, \ldots, B\}} S_d^b < 0 \]
\[ S_a + S_b = 1 \]

For Dirac we see that the structural terms are defined in terms of the variances of the functions, whereas for the orthogonal random measures Poisson and orthogonal die the structural terms are defined in terms of the second moments.

In Figure 14 we show the decomposition of the variances and structural sensitivity indices \((S_d^a)\) across the partition for the coordinates for Dirac. The sensitivity indices exhibit distinct behavior in comparison to the sensitivity indices for orthogonal \(N\) in Figure 8; the sensitivity indices of orthogonal \(N\) are more stable, whereas the sensitivity indices of Dirac have more dramatic expression. The second moments and variances are very similar for both orthogonal and Dirac \(N\), owing to the small contribution of the first moment of \(f\) squared.

### 7.3 Regressor

As referenced in Table 1, here we have some dataset \(\mathcal{D} = (\mathbf{X}, \mathbf{y}) = \{(x_i, y_i) : i = 1, \ldots, n\}\) containing \(n\) data points in \(E \times F\) with induced distribution \(\mu = \nu \times Q\)

\[ \mu f = \frac{1}{n} \sum_{i=1}^{n} f \circ (x_i, y_i) \quad \text{for} \quad f \in (\mathcal{E} \otimes \mathcal{F})_+ \]

Let \((\mathbf{X}, \mathbf{Y}) = \{(X_i, Y_i)\}\) be the independency of values distributed according to \(\mu = \nu \times Q\) which forms the random measure \(M = (\kappa, \mu = \nu \times Q)\) on \((E \times F; \mathcal{E} \otimes \mathcal{F})\). We consider \(g\) as in the data science model as a regressor and put \(f(x, y) = (g(x) - y)^2 \in (\mathcal{E} \otimes \mathcal{F})_+\). The Laplace functional of \(M\) for \(f\) is defined through

\[ \mu e^{-f} = \int_{E \times F} \mu(dx, dy)e^{-(g(x) - y)^2} \]

The HDMR of \(g\) may be approximated with respect to the empirical random measure using tree functions, such as with Random Forest or the gradient boosting regressor. This gives an approximate MM-ANOVA decomposition of the intensity measure into subspaces. The “true” distribution is indicated by \(\tilde{\mu} = \tilde{\nu} \times \tilde{Q}\). In general \(\tilde{\nu} \neq \prod_{i=1}^{n} \tilde{\nu}_i\), so the HDMR approximation must enforce hierarchical orthogonality with respect to the empirical measure \(\nu\), such as through the QR decomposition. The sensitivity indices are \(\{(S_u^a, S_u^b) : u \subseteq \{1, \ldots, n\}\}\). Examples of such constructions for the Ishigami function using tree models are found in Section 5 and the appendices.

For the RM-ANOVA decomposition of the random measure variance into disjoint subspaces \(\{A, \ldots, B\}\), we identify the Voronoi cell partition through K-means clustering with some number of clusters and an appropriate metric, although any unsupervised clustering algorithm will do. The idea of K-means is to identify the partition that minimizes intracluster variances. The sensitivity indices are attained as \(\{(S_d^a, S_d^b) : D \in \{A, \ldots, B\}\}\). Thus the sensitivity indices reveal the random measurement uncertainty of the risk function in the various disjoint volume elements.

Let \(g_\theta\) be a Gaussian process with mean \(U_\theta\) and covariance \(K_\theta\), where \(E = \mathbb{R}^n\) and \(\mathcal{E} = \mathcal{B}_{\mathbb{R}^n}\), that is, \((g_\theta(x_1), \ldots, g_\theta(x_m))\) is Gaussian for every \(x_1, \ldots, x_m \in E\) and \(m \geq 1\). The Gaussian process is trained under an assumption of independent mean-zero additive Gaussian noise with variance \(\sigma^2\). For the point \(x \in E\), we have mean

\[ E g_\theta(x) = U_\theta(x) = K_\theta(x, \mathbf{x})(K_\theta(\mathbf{x}, \mathbf{x}) + \sigma^2 I)^{-1}\mathbf{y} \quad \text{for} \quad x \in E \]

and variance

\[ \text{Var} g_\theta(x) = K_\theta(x, x) - K_\theta(x, \mathbf{x})(K_\theta(\mathbf{x}, \mathbf{x}) + \sigma^2 I)^{-1} K_\theta(\mathbf{x}, x) \quad \text{for} \quad x \in E \]

Putting \(\alpha = (K_\theta(\mathbf{x}, \mathbf{x}) + \sigma^2 I)^{-1}\mathbf{y}\), we have the representer theorem

\[ U_\theta(x) = \sum_{i=1}^{n} \alpha_i K_\theta(x, X_i) \]
Now define $f_\theta \in (\mathcal{E} \otimes \mathcal{F})_+$ as $f_\theta(x, y) = (U_\theta(x) - y)^2$. The Laplace transform is

$$F(\alpha) = \psi(\mu e^{-\alpha f_\theta})$$

The random measure has mean and variance

$$EM_{f_\theta} = c\bar{\mu}f_\theta$$
$$\text{Var}M_{f_\theta} = c\bar{\mu}f_\theta^2 + (\delta^2 - c)(\bar{\mu}f_\theta)^2$$

For a specific calculation, consider the Ishigami function $g$ on $E = [-\pi, \pi]^3$. We construct a Gaussian process regressor with $n = 100$ random input-output samples and noise $\sigma^2 = 0$ and the radial basis function with $\gamma = 0.1$. In Table 9 we show basic diagnostics of the model, including its mean-squared-error (MSE) and the coefficient of determination (COD) (each integrated with respect to the true density to eliminate estimation error). The regressor achieves approximately 72% reconstruction fidelity. We set $Q(x, \cdot) = \delta_{g(x)}(\cdot)$. For orthogonal $M = (\kappa, \bar{\mu})$, we compute the first-order HDMR component functions, the sensitivity distributions $S_1$, $S_2$, and $S_3$ for MSE and for variance and show these in Figure 9. The sensitivity distributions are random, based on the random sample of size 100, and so for independent datasets $\mathcal{D}$ the distributions are different. In Figure 9, the sensitivities of MSE of the random measure in the coordinates can be seen to coincide with the errors in the respective component function estimates in Figures 9a and 9b. In Figures 9c, 9d, and 9e the random measure sensitivity indices of $f = (g_\theta - \mathbb{E}g_\theta)^2$ are shown in the coordinates. These are noisy versions of the true sensitivity curves seen in the earlier section on the Ishigami function.

| $Eg$ | $E_{g_\theta}$ | $\text{Var}g$ | $\text{Var}g_\theta$ | $\bar{\nu}(g_\theta - g)^2$ (MSE) | $1 - \frac{\bar{\nu}(g_\theta - g)^2}{\text{Var}g}$ (COD) |
|------|----------------|---------------|---------------------|---------------------------------|---------------------------------|
| 3.5  | 3.8617         | 13.8446       | 15.6533             | 3.8581                          | 0.7213                          |

Table 9: Gaussian process regressor performance measures for Ishigami function with $a = 7$, $b = 0.1$, $n = 100$ samples, and zero additive error $\sigma^2 = 0$
(a) HDMR Component function $g_1$

(b) HDMR Component function $g_2$

(c) Orthogonal random measure sensitivity densities of $f = (g_\theta - \mathbb{E}g_\theta)^2$ for coordinate 1

(d) Orthogonal random measure sensitivity densities of $f = (g_\theta - \mathbb{E}g_\theta)^2$ for coordinate 2

(e) Orthogonal random measure sensitivity densities of $f = (g_\theta - \mathbb{E}g_\theta)^2$ for coordinate 3

(f) Orthogonal random measure sensitivity densities of MSE $f = (g_\theta - g)^2$

Figure 9: Gaussian process regressor of the Ishigami for $a = 7$ and $b = 0.1$ using radial basis kernel with $\gamma = 0.1$ and $n = 100$ samples

7.4 Classifier

As referenced in Table 1, we suppose the same setup as the Regressor example in terms of a dataset, which forms the random measure $M = (\kappa, \mu = \nu \times Q)$ on $(E \times F, \mathcal{E} \otimes \mathcal{F})$, for a classifier. We assume $M$ is orthogonal.

Define risk function $f(x, y) = \mathbb{I}(y \neq g(x))$ for $(x, y) \in E \times F$. The Laplace functional of $f(x, y) = \mathbb{I}(y \neq g(x))$ is
defined through
\[ \mu e^{-f} = \int_{E \times F} \mu(dx, dy)e^{-\int(y \neq g(x))} \]
We are interested in \( \mu f = P(y \neq g(x)) \) and \( \mu f_a = P(y \neq g(x)|(x, y) \in D) \) so that we may attain the structural sensitivity indices \( (S_a^u) \) for some partition \( \{A, \ldots, B\} \) of \( E \times F \). We have \( \mu f_a = P(y \neq g(x)|(x, y) \in A), \ldots, \mu f_b = P(y \neq g(x)|(x, y) \in B) \).
Suppose we have a binary classifier \( g \) where \( F = \{0, 1\} \). For partitions, consider a partition on the output space, \( A = E \times \{0\} \) and \( B = E \times \{1\} \) so
\[
\mu f_a = P(y \neq g(x)|y = 0) = \int_E \nu(dx)Q(x, \{0\})f(x, 0) \\
\mu f_b = P(y \neq g(x)|y = 1) = \int_E \nu(dx)Q(x, \{1\})f(x, 1) \\
\mu f = P(y \neq g(x)) = \mu f_a + \mu f_b
\]
Interpreting the class 1 as the positive, then the sensitivity indices are
\[
S_a^u = \frac{P(y \neq g(x)|y = 0)}{P(y \neq g(x))} = \frac{\mathbb{E}FP}{\mathbb{E}FP + \mathbb{E}FN} \\
S_b^u = \frac{P(y \neq g(x)|y = 1)}{P(y \neq g(x))} = \frac{\mathbb{E}FN}{\mathbb{E}FP + \mathbb{E}FN}
\]
where \( \mathbb{E}FP \) and \( \mathbb{E}FN \) denote the expected number of false positives and negatives. The orthogonal RM-ANOVA necessarily strictly measures the false positives and false negatives in assessing estimator uncertainty for the risk function \( f(x, y) = I(y \neq g(x)) \). Maximum entropy has \( \mathbb{E}FP = \mathbb{E}FN \), i.e. balanced error across classes.
To get the usual set of HDMR sensitivity indices, define \( l = h \circ g \) per \( [\text{BL}1] \), giving for each \( x \in E \) a binary vector \( l(x) = (l_1(x), l_2(x)) \). Let
\[
\nu l = (P(g(x) = 0), P(g(x) = 1))
\]
Then the probability for each \( y \in F \) may be decomposed in terms of HDMR, giving the sensitivity indices \( \{(S_a^u(y), S_b^u(y)) : u \subseteq \{1, \ldots, n\}\} \). This gives a decomposition of the image intensity measure in terms of a partition of the elements of \( F \).
These expressions readily generalize to the multiclass setting \( F = \{y_1, \ldots, y_m\} \). Class \( y_i \in F \) has mean
\[
\mu f_i = P(y \neq g(x)|y = y_i) = \int_E \nu(dx)Q(x, \{y_i\})f(x, y_i)
\]
and sensitivity index
\[
S_i^u = \frac{P(y \neq g(x)|y = y_i)}{P(y \neq g(x))} = \frac{\mathbb{E}FP_i + \mathbb{E}FN_i}{\sum_{y_j \in F}(\mathbb{E}FP_j + \mathbb{E}FN_j)}
\]
where \( \mathbb{E}FP_i \) and \( \mathbb{E}FN_i \) are the expected number of false positives and negatives. Maximum entropy has \( \mathbb{E}FP_i + \mathbb{E}FN_i = \mathbb{E}FP_j + \mathbb{E}FN_j \) for \( y_i, y_j \in F \), i.e. balanced errors across the classes. Putting \( EF_1 = EF_1 + EFN_1 \), the maximum entropy manifold of \( (EF_1, EFN_1) \) of any class \( i \) is \( \{(x, y) \in \mathbb{R}^2_+ : x + y = EF_1\} \).

7.5 Space domain awareness of interacting particle systems

Astronomy compels the soul to look upwards and leads us from this world to another.

Plato

As referenced in Table [\text{1}], here we describe a mathematical model for space domain awareness based on random counting measures and random fields, where the points of the system are space objects, such as spacecraft, asteroids, and so on. The random field model is built using the random measure. We describe a random measure as a superposition of three (spatio-temporal) counting processes: Poisson, binomial, and negative binomial. Together, these processes can exhibit any covariance structure. We show that this modeling framework may be used to represent, for instance, spatiotemporal interaction probabilities through the random field model, provisioning an interacting particle system model.
7.5.1 Superposition random measures

Consider random measure \( N = (\kappa, \nu) \) on \((E, \mathcal{E})\). We think of the state-space as a function space \((E, \mathcal{E}) = (F, \mathcal{F})^{\mathbb{R}_+}\). Here we take element \(X_t \sim \nu\) as a space object, such as a spacecraft or asteroid, and \(F = \mathbb{R}^3\). For the counting distribution we consider the convolution \( \kappa = \kappa_- * \kappa_0 * \kappa_+ \), where \( \kappa_- \) is binomial, \( \kappa_0 \) is Poisson, and \( \kappa_+ \) is negative binomial, i.e. \( \kappa = K_- + K_0 + K_+ \), with mean \( c = c_- + c_0 + c_+ \) and variance \( \delta^2 = \delta^2_- + \delta^2_0 + \delta^2_+ \). The pgf of \( K \) is a product of the pgfs \( \psi_\theta = \psi_{\theta_-} \psi_{\theta_0} \psi_{\theta_+} \) where we put \( \theta = (\theta_-, \theta_0, \theta_+) \). The random measure \( N \) is formed through STC as

\[
 N(A) = \sum_i \mathbb{I}_A(X_i) \quad \text{for} \quad A \in \mathcal{E}
\]

The Laplace functional of \( N \) is given by

\[
 L(f) = \psi_\theta(f e^{-f}) \quad \text{for} \quad f \in \mathcal{E}_+
\]

The random measure \( N \) is orthogonal if \( c = \delta^2 \). This is equivalent to requiring \((\delta^2_- - c_-) + (\delta^2_0 - c_0) = 0\) or \( \delta^2_- + \delta^2_+ = c_- + c_+ \). The sensitivity density of \( Nf \) for \( f \in \mathcal{E}_+ \) and orthogonal \( N \) is

\[
 S(dx) = \frac{\nu(dx) f^2(x)}{\nu f^2} \quad \text{for} \quad x \in E
\]

7.5.2 Image random measures

Consider the mapping \( h : E \mapsto F \) as \( h(w) = w(t) \) for \( w \in E \) and \( t \in \mathbb{R}_+ \) fixed. We consider the image measure \( M_t = N \circ h^{-1} = (\kappa, \mu_t = \nu \circ h^{-1}) \) on \((F, \mathcal{F})\), where

\[
 \mu_t f = (\nu \circ h^{-1}) f = \nu(f \circ h) \quad \text{for} \quad f \in \mathcal{F}_+
\]

with Laplace functional

\[
 L(f) = \psi_\theta(\mu_t e^{-f}) \quad \text{for} \quad f \in \mathcal{F}_+
\]

formed by STC as

\[
 M_t f = \sum_i f \circ X_i(t) \quad \text{for} \quad f \in \mathcal{F}_+
\]

The sensitivity density of \( M_t f \) for \( f \in \mathcal{F}_+ \) and orthogonal \( M_t \) is

\[
 S(dx) = \frac{\mu_t(dx) f^2(x)}{\mu_t f^2} \quad \text{for} \quad x \in F
\]

7.5.3 Restricted random measures

Now consider the restriction to subspace \( A \subset F \), such as some domain of interest. For the restricted random measure \( M_A = (M_A, \mu_A) \) on \((A \cap F, \mathcal{F}_A)\), where \( \mu_A(\cdot) = \mu(A \cap \cdot / \mu(A) \) and \( \mathcal{F}_A = \{A \cap B : B \in \mathcal{F}\} \), the pgf of the counting distribution is given by

\[
 \psi_A(t) = \psi_\theta(at + 1 - a) \equiv \psi_{h_-}(at + 1 - a) \psi_{h_0}(at + 1 - a) \psi_{h_+}(at + 1 - a)
\]

where \( h_a(\theta) \) is the vector of bone mappings \((h_a(\theta_-), h_a(\theta_0), h_a(\theta_+)) \). The Laplace functional is

\[
 L_A(f) = \psi_{h_a}(\theta)(\mu_A e^{-f}) \quad \text{for} \quad f \in \mathcal{F}_+
\]

The sensitivity density of \( M_A f \) for \( f \in \mathcal{F}_+ \) and orthogonal \( M_A \) is

\[
 S_a(dx) = \frac{\mu_A(dx) f^2(x)}{\mu_A f^2} \quad \text{for} \quad x \in A
\]
7.5.4 Interacting random fields

Consider the image random measure \( M_t = (\kappa, \mu_t) \) on \( (F, \mathcal{F}) \). Now let \( k : F \times F \mapsto \mathbb{R}_+ \) be \( \mathcal{F} \otimes \mathcal{F} \) measurable and define the random field
\[
G_t(y) = \int_F M_t(dx)k(x, y) \quad \text{for} \quad y \in F
\]
with Laplace transform
\[
\mathbb{E}e^{-\alpha G_t} = \psi_\theta(\mu_t e^{-\frac{\alpha}{2} g(\cdot, \cdot)}) \quad \text{for every finite measure } \alpha \text{ on } (F, \mathcal{F})
\]
Put \( f_y(\cdot) = k(\cdot, y) \in \mathcal{F}_+ \), so that we have the mean and covariance
\[
U_t(y) = \mathbb{E}G_t(y) = c\mu_t f_y \quad \text{for} \quad y \in F
\]
\[
C_t(y, z) = \text{Cov}(G_t(y), G_t(z)) = c\mu_t (f_y f_z) + (\delta^2 - c)\mu_t f_y \mu_t f_z \quad \text{for} \quad y, z \in F
\]

For example let \( k \) be the radial basis function \( k(y, z) = e^{-\gamma ||y-z||^2} \), which we interpret as an interaction probability as a function of distance. Then \( G_t(y) \) has the interpretation of the number of interactions of space objects at some point \( y \in F \) at time \( t \in \mathbb{R}_+ \) with mean number of interactions \( U_t(y) \) and across locations \( z \in F \) interaction number covariance \( C_t(y, z) \).

7.5.5 Specific calculation

Let \( \nu \) be Wiener so that the image measure is given by
\[
\mu_t(A) = \int_{\mathbb{R}} dx \frac{1}{\sqrt{2\pi t}} e^{-\frac{x^2}{2t}} 1_A(x) \quad \text{for} \quad A \in \mathcal{B}_R
\]
This is a prototypical disequilibrium Gaussian process.

Suppose each particle pays “rent” based on its location according to \( g = \cos^2 \). The random variable \( M_t g \) is total amount of rent paid by all the particles and has Laplace transform
\[
F(\alpha) = \psi_\theta(\mu_t e^{-\alpha g}) \quad \text{for} \quad \alpha \in \mathbb{R}_+
\]
For simplicity, we assume for the moment that all the particles belong to the Poisson random measure.

Then putting \( f = (g - \mu_t g)^2 \in \mathcal{E}_+ \) and noting that \( g^{-1}(y) = \{ \pm \arccos(\pm \sqrt{y}) + 2\pi k : k \in \mathbb{Z} \} \) and \( \frac{d}{dy} g^{-1}(y) = \frac{1}{2\sqrt{y(1-y)}} \), we have
\[
\mu_t \circ g^{-1}(dy) = \sum_{k=\infty}^{\infty} dy \frac{1}{2\sqrt{2\pi ty(1-y)}} \sum_{\pm k} e^{-\frac{(\mp \arccos(\pm \sqrt{y})+2\pi k)^2}{2t}}
\]
\[
\mu_t g = e^{-t} \cosh(t) \xrightarrow{t \to \infty} \frac{1}{2}
\]
\[
\mu_t f = \frac{1}{8} e^{-8t} (e^{4t} - 1)^2 \xrightarrow{t \to \infty} \frac{1}{8}
\]
\[
\mu_t f^2 = \frac{1}{4} e^{-16t} \sinh^4(2t)(4\sinh(4t) + \sinh(8t) + 8\cosh(4t) + 2\cosh(8t) + 5) \xrightarrow{t \to \infty} \frac{3}{128}
\]
\[
S(dx) = \frac{\mu_t(dx) f^2(x)}{\mu_t f^2}
\]
Hence the statistics all admit stationary solutions.

We identify the density of \( M_t g \), denoted by \( \eta_t \), where \( \kappa = \text{Poisson}(100) \), by evaluating \( F(\alpha_i) \) for \( i = 1, \ldots, n \) with \( \alpha_i \sim \text{Exponential}(1) \) and attaining the density by maximum entropy. For \( n = 10 \) we show the density in Figure 10.

We show the statistics compared to the exact values. The agreement is very close.
| EM$_{tg}$ | E$\eta_{10}$ | Var$M_{tg}$ | Var$\eta_{10}$ |
|----------|------------|------------|------------|
| 56.7668  | 56.7667    | 44.2710    | 44.2624    |

Table 10: Mean and variance of $M_{tg}$ and $\eta_n$ where $\kappa =$ Poisson(100)

We take $k : E \times E \rightarrow \mathbb{R}_+$ as the radial basis kernel for interaction probability. Putting $f_y(\cdot) = k(\cdot, y) \in \mathcal{E}_+$, this gives expected interaction probability

$$U_t(y) = \mu_t f_y = \frac{e^{-\frac{\gamma y^2}{2\gamma t + 1}}}{\sqrt{2\gamma t + 1}} \xrightarrow{t \to \infty} 0$$

and covariance term

$$\mu_t(f_y, f_z) = \frac{e^{-\gamma \frac{(2\gamma (y-z)^2 + y^2 + z^2)}{2\gamma t + 1}}}{\sqrt{2\gamma t + 1}}$$

We have that $U_t$ is maximized at time $\hat{t}$ with value $U_{\hat{t}}$

$$\hat{t} = \max\{y^2 - \frac{1}{2\gamma}, 0\}$$

$$U_{\hat{t}} = \begin{cases} 
\frac{1}{\sqrt{2\gamma}} \hat{t} > 0 \\
 e^{-\gamma y^2} \hat{t} = 0 
\end{cases}$$

These results show that the time of maximum interaction probability increases quadratically in interaction distance $O(y^2)$, whereas the maximum interaction probability decreases with interaction distance $O(1/|y|)$.

We have covariance

$$C_t(y, z) = \frac{c}{\sqrt{4\gamma t + 1}} e^{-\gamma \frac{(2\gamma (y-z)^2 + y^2 + z^2)}{2\gamma t + 1}} + \frac{\delta^2 - c}{2\gamma t + 1} e^{-\gamma \frac{y^2 + z^2}{2\gamma t + 1}}$$

A higher-order interaction random field can be defined through defining $k : E \times E^n \rightarrow \mathbb{R}_+$. For example, suppose $k$ is defined through a correlated bivariate radial basis function

$$k(x, (y, z)) = \exp - \frac{1}{2(1-\rho^2)} \left( \frac{(x-y)^2}{\sigma_y^2} - 2\rho \frac{x-y}{\sigma_y} \frac{x-z}{\sigma_z} + \frac{(x-z)^2}{\sigma_z^2} \right)$$

Putting $f_{yz}(\cdot) = k(\cdot, (y, z)) \in \mathcal{E}_+$, we have mean

$$U_t(y, z) = \mu_t f_{yz} = \frac{\exp - \left( \frac{t(y-z)^2 + \sigma_y^2 + \sigma_z^2 - 2\rho \sigma_y \sigma_z y z}{2(1-\rho^2)\sigma_y^2 + 2t(\sigma_y^2 + \sigma_z^2 - 2\rho \sigma_y \sigma_z)} \right)}{1 + t \frac{\sigma_y^2 + \sigma_z^2 - 2\rho \sigma_y \sigma_z}{(1-\rho^2)\sigma_y^2 + 2t(\sigma_y^2 + \sigma_z^2 - 2\rho \sigma_y \sigma_z)}} \xrightarrow{t \to \infty} 0$$
This reveals the expected probability of interaction of a particle with two correlated points.

In Figures 11a and 11b, we show the sensitivity indices for the random measure for $M_t$ for $t \in \{1, 5\}$. They are markedly different for the times and are each multimodal. This follows from the exponential dampening of periodic $g$. In Figure 11c, we show the random field sensitivity indices, estimated from the eigenvalues of the covariance matrix on a grid on $[-5, 5] \times [-5, 5]$, each coordinate containing 100 equispaced values, and we take $c = \delta^2 = \gamma = 1$.

As shown in Figure 11d, as time increases, the effective dimension increases. Figures 11e and 11f show the covariance reconstruction using the principal eigenvector and eigenvalue $\lambda_1 \varphi_1^T \varphi$ at $t = 1$ for orthogonal and Dirac $M_t$. These are first-order approximations to the kernels of Figures 3a and 3b.

**Specific calculation: drift and initial condition**

Suppose we have $N = (\kappa, \nu)$ on $(E, \mathcal{E})$ where $\nu$ is Wiener. Now introduce an initial condition $X_0 \in \mathbb{R}$ and drift constant $D \in \mathbb{R}$ with joint distribution $\eta$. The triple $(X, X_0, D)$ forms the random measure $M = (\kappa, \mu = \nu \times \eta)$. Now consider the function $h(X, X_0, D) = X(t) + X_0 + Dt$ for $t \in \mathbb{R}_+$ fixed. Then the image measure $\mu_t = \mu \circ h^{-1}$ is given by

$$
\mu_t(A) = \int_{\mathbb{R} \times \mathbb{R}} \eta(dx_0, dD) \int_{\mathbb{R}} dx \frac{1}{\sqrt{2\pi t}} e^{-\frac{(x-x_0-Dt)^2}{2t}} I_A(x) \quad \text{for} \quad A \in \mathcal{B}_{\mathbb{R}}
$$

If $\eta$ is Gaussian with hyperparameters for $X_0$ as $\mu_0$ and $\sigma_0^2$ and for $D$ as $\mu_D$ and $\sigma_D^2$ and correlation $\rho [−1, 1]$, then

$$
\mu_t(A) = \int_{\mathbb{R}} dx \frac{1}{\sqrt{2\pi(\sigma_0^2 + t + \sigma_D^2 t^2 + 2\sigma_0 \sigma_D t \rho)}} \exp\left(-\frac{(x-\mu_0-\mu_D t)^2}{2(\sigma_0^2 + t + \sigma_D^2 t^2 + 2\sigma_0 \sigma_D t \rho)}\right) I_A(x)
$$

so $\mu_t = \text{Gaussian}(\mu_0 + \mu_D t, \sigma_0^2 + t + \sigma_D^2 t^2 + 2\sigma_0 \sigma_D t \rho)$. The random field mean and covariance are similar to the case without drift, with additional parameters.

For interactions such as collisions which generate debris fields, the interaction can define a transition into a cluster process, of the non-vaporized components and their drifts, with initial locations at the location of the object undergoing spallation.
(a) Random measure sensitivity density $S(dx)$ for $t = 1$

(b) Random measure sensitivity density $S(dx)$ for $t = 5$

(c) Orthogonal $M_t$: Random field sensitivity indices $\{S_i\}$

(d) Orthogonal $M_t$: effective dimension of random field as a function of time $t$

(e) Orthogonal $M_t$: Random field covariance reconstruction $\lambda_1 \varphi_1^T \varphi_1$ at $t = 1$

(f) Dirac $M_t$: Random field covariance reconstruction $\lambda_1 \varphi_1^T \varphi_1$ at $t = 1$

Figure 11: Wiener interaction probability analysis
7.5.6 Identification

We recount the quantities that comprise the random measure and field models. Both are described through the tuple \( \Xi = (\kappa, \mu_t, k) \). For each such tuple, there exists an indexed collection of restrictions \( \Upsilon(\Xi) = \{ (\kappa_A, \mu_{tA}, k) : A \subseteq F \} \).

7.5.7 Generalizations

All manner of generalizations can be had. We can assume the spacecraft are marked with properties, such as flag (country or company), and we can introduce additional complexity into the function \( k \) by allowing interaction probability to depend on additional dimensions and to have different interaction types. Interactions could be collisions (the collision probability resulting from the uncertainty of the particle’s position at some time), the experience of space weather events (having spatiotemporal uncertainty), confrontation / dispute (where the particles are combatants), and so on. We can also consider interacting random fields for various restrictions of the system into subspaces. For example we could form restrictions through some clustering / partition of the domain and of space object marks / properties. With humanity’s increasing expression of space-faring activities, e.g. [Musk (2017)], the models here can serve as canonical representations of the information it generates, i.e. the filtration \((\mathcal{F}_t)_{t \in \mathbb{R}_+}\) generated by \( M \),

\[
\mathcal{F}_t = \sigma\{M_s : s \leq t\}.
\]

7.6 Adaptive randomized controlled trials

As referenced in Table 1, we discuss a framework for adaptive randomized controlled trials using random measures that mitigates the phenomenon of under or over-powered trials at final analysis time that is based on superpositions of orthogonal die random measures. The injection of counting noise by the orthogonal dice into trial design does not negatively impact type I or II error probabilities and eliminates effect correlation across groups caused by a fixed trial size. The normalized uncertainties (variances) may be interpreted as probabilities, which provides insight into the distribution of uncertainty of the random measure across groups.

7.6.1 Randomized controlled trials

A randomized controlled trial is a random realization of a random counting measure. Let \( N = (\kappa, \nu) \) be a random counting measure on a clinical trial design space \((E, \mathcal{E})\), where \( \kappa \) is a counting distribution with mean \( c \) and variance \( \delta^2 \) and \( \nu \) is a probability measure on \((E, \mathcal{E})\). In the simplest case, \( E = \{C, T\} \) contains control and treatment groups with equal probability, i.e. \( \nu\{C\} = \nu\{T\} = 1/2 \). Enrollees are materialized \( \mathbf{X} = \{X_i\} \) and measurements are attained from the enrollees \( \mathbf{Y} = \{Y_i\} \) in measurement space \((F, \mathcal{F})\) according to transition probability kernel \( Q \) from \((E, \mathcal{E})\) into \((F, \mathcal{F})\), i.e. \( Y_i \sim Q(X_i, \cdot) \). For simplicity, we assume \((F, \mathcal{F}) = (\mathbb{R}_+, \mathcal{B}_{\mathbb{R}_+})\). The random measure \( M = (\kappa, \nu \times Q) \) on \((E \times F, \mathcal{E} \otimes \mathcal{F})\) is formed from \((\mathbf{X}, \mathbf{Y})\) by stone throwing construction as

\[
Mf = \sum_{i=1}^{K} f \circ (X_i, Y_i) \quad \text{for} \quad f \in (\mathcal{E} \otimes \mathcal{F})_+.
\]

Put \( f_T(x, y) = \mathbb{1}_{\{T\}}(x) \) and \( f_C(x, y) = \mathbb{1}_{\{C\}}(x) \). These are disjoint functions. In general, the random variables \( Mf_T \) and \( Mf_C \) are correlated, where

\[
\text{Cov}(Mf_T, Mf_C) = (\delta^2 - c)(\nu \times Q)f_T(\nu \times Q)f_C
\]

with mean

\[
\mathbb{E}Mf_T = c(\nu \times Q)f_T
\]

and variance

\[
\text{Var}Mf_T = c(\nu \times Q)f_T^2 + (\delta^2 - c)(\nu \times Q)f_T^2
\]

The variance of the random measure describes its uncertainty. We have

\[
(\nu \times Q)f_T = \int_E \nu(dx)\mathbb{1}_{\{T\}}(x) \int_F Q(x, dy)y = \frac{1}{2} \int_F Q(\{T\}, dy)y = \frac{1}{2} c_T
\]

and

\[
(\nu \times Q)f_T^2 = \int_E \nu(dx)\mathbb{1}_{\{T\}}(x) \int_F Q(x, dy)y^2 = \frac{1}{2} \int_F Q(\{T\}, dy)y^2 = \frac{1}{2} (c_T^2 + \delta_T^2)
\]

40
The null hypothesis is that \((\nu \times Q)f_T = (\nu \times Q)f_C\) and depends on the mean measure. This is equivalent to \(EMf_T = EMf_C\). The typical setting is \(\kappa = \text{Dirac}(c)\) for \(c \in \mathbb{N} > 0\). This random measure has minimum variance with \(\delta^2 = 0\). The covariance is negative due to the fixed sample size,

\[
\text{Cov}(Mf_T, Mf_C) = -\frac{c}{4}c_Tc_C
\]

and

\[
\text{Cov}(\frac{1}{c}Mf_T, \frac{1}{c}Mf_C) = -\frac{1}{4c}c_Tc_C
\]

which decays to zero as \(c \to \infty\).

When \(\kappa\) is orthogonal, the covariance is zero for any mean sample size \(c \in (0, \infty)\), the variance is given by

\[
\text{Var}Mf_T = c(\nu \times Q)f_T^2
\]

and the normalized variances form a sensitivity distribution

\[
S_T = \frac{\nu \times Q}{f_T^2} = \frac{c_T^2 + \delta_T^2}{c_T^2 + \delta_T^2 + c_C^2 + \delta_C^2}
\]

where \(S_T + S_C = 1\).

For example, consider a randomized controlled trial testing vaccine efficacy. The measurement is an indicator of infection of the underlying disease being vaccinated against over the period of the trial. Then \(c_T = \mathbb{P}(T)\) and \(c_C = \mathbb{P}(C)\) are the probabilities of infection based on group assignment and the variance is

\[
\text{Var}Mf_T = c\mathbb{P}(T) + (\delta^2 - c)\mathbb{P}^2(T)
\]

and the covariance is

\[
\text{Cov}(Mf_T, Mf_C) = (\delta^2 - c)\mathbb{P}(T)\mathbb{P}(C)
\]

For Dirac, this is

\[
\text{Var}Mf_T = c\mathbb{P}(T)(1 - \mathbb{P}(T))
\]

and

\[
\text{Cov}(Mf_T, Mf_C) = -c\mathbb{P}(T)\mathbb{P}(C)
\]

For orthogonal \(\kappa\) the variance is

\[
\text{Var}Mf_T = c\mathbb{P}(T)
\]

and the sensitivity index in \(T\) is

\[
S_T = \frac{\mathbb{P}(T)}{\mathbb{P}(T) + \mathbb{P}(C)}
\]

When \(\mathbb{P}(T) \ll \mathbb{P}(C)\), then the uncertainty of the effects is dominated by the infections of the control group, \(S_T \ll S_C\).

In Figure [12] we show the entropy of \(S\) in \(\mathbb{P}(C)\) and \(\mathbb{P}(T)\), i.e.

\[
H(S) = -S_C \log(S_C) - S_T \log(S_T)
\]

Clinical trials of efficacious vaccines against infectious diseases have low entropy of uncertainty.
7.6.2 Adaptation using superpositions of orthogonal dice

We take $M$ to be a superposition of independent random measures that are constructed sequentially. Here we consider for simplicity two random measures with superposition counting law

$$
\kappa = \kappa_1 * \kappa_2
$$

Because the random measures are independent, the superposition law of the random measure is described through the product of the Laplace functionals of the respective random measures. If these random measures are orthogonal, then the superposition random measure is orthogonal.

Let $c_1$ be the initial total size informed by power analysis: that is, the minimum number of enrollees at some effect size (with some assumed type I and II error probabilities). We fractionate the design by some factor $a$, such as $a = 1/2$. We take $K_1 \sim \kappa_1$ as the first orthogonal die with support $\text{supp}(K_1) = \{m, \cdots, n\}$ with $m \geq ac_1$. $K_1$ is the number of enrollees in the first random measure. Then, based on the collection of the data and observation of effects in this first batch, power analysis with the empirical effect gives the imputed total number of new enrollees for the desired significance level, which we denote as $c_2$. If $c_2 > K_1$, then additional data is generated, through new independent enrollees, to prevent an underpowered design. In this case, to construct $\kappa_2$, we choose the first orthogonal die with lower support $m \geq c_2 - K_1$. Then $K_2 \sim \kappa_2$ is sampled and the enrollees materialized. Then we have that $K_1 + K_2 \geq c_2$, so we have achieved or exceeded our type I and II error probabilities. Because $\kappa_1$ and $\kappa_2$ are independent and orthogonal, then $\kappa$ is orthogonal. In analysis of effects across treatment and control groups, the group effects are approximately compound Poisson random variables due to weak convergence of orthogonal die random measure to the Poisson random measure.

The first 15 orthogonal dice are shown below in Table 11. There are an infinite number of orthogonal dice, and their support size $n - m + 1$ is coprime to 2 and 3, i.e. their sizes enumerate all primes greater than or equal to 5 and their products. Please see [Bastian and Rempala (2020)] for more information about the orthogonal dice and weak convergence of the orthogonal die random measure to the Poisson random measure.
Here we expand the randomized controlled trial space to incorporate a mark-space. We suppose each enrollee has some independent mark-space \((H, \mathcal{H})\), containing properties such as demographics, genome, contact network properties, etc., with distribution \(\eta\). Now let \(Q\) be a transition kernel from \((E \times H, \mathcal{E} \otimes \mathcal{H})\) into \((F, \mathcal{F}) = (\mathbb{R}_+, \mathbb{B}_{\mathbb{R}_+})\). The random measure \(M = (\kappa, \nu \times \eta \times Q)\) on \((E \times H \times F, \mathcal{E} \otimes \mathcal{H} \otimes \mathcal{F})\) is formed by \((X, Y, Z)\) through STC.

Consider again the set-up of a randomized controlled trial testing vaccine efficacy. We retrieve the existing analysis with \(f_T(x, y, z) = I\{T\}(x)z\) and \(f_C(x, y, z) = I\{C\}(x)z\), e.g., the mean is

\[
\mathbb{E}Mf_T = c(\nu \times \eta \times Q)f_T = c \int_E \nu(dx)I\{T\}(x) \int_H \eta(dy) \int_F Q((x, y), dz)z
\]

\[
= c \int_H \eta(dy) \int_F Q((\{T\}, y), dz)z
\]

\[
= c \int_H \eta(dy)\mathbb{P}(T, y)
\]

\[
= c \mathbb{P}(T)
\]

Now suppose we have a partition \(A, \cdots, B\) of \(H\). We define \(f_T^A(x, y, z) = I\{T\}(x)I_A(y)z\) and \(f_C^A(x, y, z) = I\{C\}(x)I_A(y)z\). The mean is

\[
\mathbb{E}Mf_T^A = \frac{c}{2}\mathbb{P}_A(T)
\]

Suppose we have some classifier \(g : E \times H \mapsto \{0, 1\}\) that predicts infection, trained on input-output samples \(\{(X_i, Y_i, Z_i)\}\). Let \(f(x, y, z) = (g(x, y) - z)^2\). Let \(Q((x, y), \cdot) = \delta_{\mathbb{E}g}(\cdot)\) so that \(f(x, y, z) = (g(x, y) - \mathbb{E}g)^2\). Then

\[
\mathbb{E}Mf = c(\nu \times \eta \times Q)f = c\text{Var}g
\]

The HDMR of \(g\) attains the hierarchy of component functions in \(E \times H\). The classifier \(g\) has real-world application to pharmaceutical development: the United States Food and Drug Administration (FDA) has an Accelerated Approval program for “serious conditions that fill an unmet medical need” [10]. If (a) the classifier is trained on independent input-output samples, such as from some other trial or design, and if (b) the relation between the marks and the measurement has a strong clinical foundation, and if (c) the classifier is highly predictive, then in some cases the predicted outcomes may be used as surrogates for the actual outcomes to attain provisional acceptance until the actual outcomes may be measured. Similar hold for regressors and continuous measurements.

### Table 11: First 15 orthogonal dice

| m | n | c | n − m + 1 |
|---|---|---|-----------|
| 0 | 4 | 2 | 5         |
| 1 | 7 | 4 | 7         |
| 5 | 15| 10| 11        |
| 8 | 20| 14| 13        |
| 16| 32| 24| 17        |
| 21| 39| 30| 19        |
| 33| 55| 44| 23        |
| 40| 64| 52| 25        |
| 56| 84| 70| 29        |
| 65| 95| 80| 31        |
| 85| 119|102|35       |
| 96| 132|114|37       |
| 120|160|140|41       |
| 133|175|154|43       |
| 161|207|184|47       |
8 Discussion and conclusions

We describe a general integrated framework RM-MM-RF-ANOVA for uncertainty quantification, which furnishes first and second-order statistics and enables construction of general positive random fields. The first-order MM-ANOVA analysis is a functional ANOVA decomposition of the intensity measure of the squared loss functional into subspaces, whereas the second-order RM-ANOVA analysis is decomposition of random measure variance into subspaces. For orthogonal random measures, RM-ANOVA furnishes a sensitivity distribution which may be attained in all marginals. Positive random fields may be constructed from the random measures, and RF-ANOVA decomposes the field.

This UQ framework is based on the variance-covariance structure of the mixed binomial process. As such it generalizes the binomial process, also known as the empirical random measure or the Dirac random counting measure, and its bootstrap estimator. The generalization is through a degree-of-freedom gain with the instantiation of a counting distribution \( \kappa \). We show that for the squared loss function, the mean (intensity) measure may be decomposed using HDMR. Other loss functions may be used, such as absolute loss, thereby forsaking functional ANOVA for representation of the intensity measure. The random field model may be used to construct interacting particle systems. The method of maximum entropy allows the density of the random variable \( Nf \) (formed by the random measure \( N \) and test function \( f \in \mathcal{E}_+ \)) to be attained from a collection of evaluations of the Laplace transform. This gives a general, scalable method to attain the density of \( Nf \).

The examples illuminate some interesting findings and are suggestive. We find that the effective dimension of the HDMR of the symmetric polynomial is regulated by the coefficient of variation \( \rho \) of the input variables, with maximum entropy at \( \rho = 1 \). Its HDMR is dense in subspaces. For a univariate polynomial with Bernoulli input, the orthogonal random measure variance exhibits strong dependence on \( p \), with maximum entropy at \( p = 1/2 \). Moreover we find the second moment, corresponding to the variance of the orthogonal random measure, to have the structure of an inverted double-well potential. We also see that the structural sensitivity indices for the binomial process (Dirac random counting measure) each possess a singularity. In the second example, we find that the Ishigami function has a non-monotone entropy profile in the second parameter for \( a = 7 \) and that the orthogonal random measure uncertainty on partitions by each of the coordinates are markedly different across the coordinates: two are periodic while the other has a “bath-tub” appearance. Their entropies are monotone. In the third and fourth examples, we describe applications to regression and classification. In the regression example, we derive the uncertainty measures for a Gaussian process regressor trained on a small number of samples (\( n = 100 \)) from the Ishigami function. Despite the small sample size, the GPR is able to accurately reconstruct the HDMR component functions, and the sensitivity density is noisy. For classification, we find that the orthogonal random measure sensitivity indices depend on the number of incorrect classifications. Maximum entropy of the orthogonal random measure is achieved with equal errors across classes. The example of interacting particle systems illustrates how spatiotemporal interaction probabilities may be attained from traffic flow random measure models. For the specific example, the sensitivity distribution exhibits multi-modal behavior, and the random field enables construction of the covariance and its reconstruction through the truncated eigensystem. The example of adaptive randomized controlled trials shows that the injection of counting noise into trial design does not negatively impact type I or II error probabilities and confers an orthogonal design, which enables the sensitivity distribution to be attained in the effects. Adaptation through superpositions of orthogonal dice mitigates the phenomenon of under- or over-powered trials at final analysis time.

Across the examples, we calculate virtually all the quantities analytically and suggest these may be useful and canonical for UQ by random measures. These examples also underscore the significance of the orthogonal mixed binomial processes, that is, those random counting measures whose counting distributions have mean equals variance. For orthogonal \( N \), the structural sensitivity indices define a probability measure on partitions, conferring a probabilistic interpretation of uncertainty and enabling calculation of entropy. Therefore we suggest UQ practitioners to employ orthogonal random measures, such as Poisson or the orthogonal dice, as a substitute for empirical random measures, in order to gain probabilistic insight into the UQ exercise. The examples indeed show that, at the cost of increasing the uncertainty of the random measure through orthogonal \( N \) (\( \kappa \) having positive variance equal to mean), one gets a return of an interpretation of the normalized random measure variances as probabilities.

References

Bastian, C. D. and Rabitz, H. (2018). High Dimensional Model Representation as a Glass Box in Supervised Machine Learning.  *arXiv e-prints*, page arXiv:1807.10320.

Bastian, C. D. and Rempala, G. A. (2020). Orthogonal Die Random Measures, Primes, and Applications.  *arXiv e-prints*, page arXiv:2009.10503.
Bastian, C. D. and Rempala, G. A. (2020). Throwing stones and collecting bones: Looking for Poisson-like random measures. *Mathematical Methods in the Applied Sciences*, n/a(n/a).

Battiti, R. (1994). Using mutual information for selecting features in supervised neural net learning. *IEEE Transactions on Neural Networks*, 5(4):537–550.

Biesiada, J., Duch, W., Kachel, A., Maczka, K., and Palucha, S. (2005). Feature ranking methods based on information entropy with parzen windows. In *International Conference on Research in Electrotechnology and Applied Informatics*.

Cinlar, E. (2011). *Probability and Stochastics*. Springer-Verlag New York.

Crestaux, T., Le Maître, O., and Martinez, J.-M. (2009). Polynomial chaos expansion for sensitivity analysis. *Reliability Engineering & System Safety*, 94(7):1161–1172.

Efron, B. and Tibshirani, R. J. (1993). *An Introduction to the Bootstrap*. Number 57 in Monographs on Statistics and Applied Probability. Chapman & Hall/CRC, Boca Raton, Florida, USA.

FDA (2016). Accelerated approval program.

Friedman, J. H. (2001). Greedy function approximation: A gradient boosting machine. *Ann. Statist.*, 29(5):1189–1232.

Gzyl, H. (2017). Superresolution in the maximum entropy approach to invert laplace transforms. *Inverse Problems in Science and Engineering*, 25(10):1536–1545.

Hooker, G. (2007). Generalized functional anova diagnostics for high-dimensional functions of dependent variables. *Journal of Computational and Graphical Statistics*, 16(3):709–732.

Kallenberg, O. (2017). *Random Measures, Theory and Applications*. Springer.

Li, G. and Rabitz, H. (2012). General formulation of hdmr component functions with independent and correlated variables. *Journal of Mathematical Chemistry*, 50(1):99–130.

Musk, E. (2017). Making humans a multi-planetary species. *New Space*, 5(2):46–61.

Rabitz, H. and Alis, O. F. (1999). General foundations of high dimensional model representations. *Journal of Mathematical Chemistry*, 25(2-3):197–233.

Sobol, I. (2001). Global sensitivity indices for nonlinear mathematical models and their monte carlo estimates. *Mathematics and Computers in Simulation*, 55(1-3):271–280.

Sobol, I. M. (1990). On sensitivity estimation for nonlinear mathematical models. *Matem. Mod.*, 2(1):112–118.

Sobol’, I. M. and Kucherenko, S. (2009). Derivative based global sensitivity measures and their link with global sensitivity indices. *Mathematics and Computers in Simulation*, 79(10):3009–3017.

Yao, F., Muller, H.-G., and Wang, J.-L. (2005). Functional linear regression analysis for longitudinal data. *Ann. Statist.*, 33(6):2873–2903.
A Supplementary figures

A.1 Ishigami function

Figure 13: Ishigami first-order component functions $g_1$ and $g_2$ for $a = 7$ and $b = 0.1$; Ishigami function orthogonal random measure entropy for partitions by coordinates as a function of $b$; HDMR entropy as a function of $b$ for $a = 7$. 
Figure 14: Ishigami function for Dirac \(N\): variances \((\text{Var}_d)\) and structural sensitivity indices \((S^a_d)\) for partitions by coordinates into 100 intervals for \(a = 7\) and \(b \in \{0.01, 0.05, 0.1, 0.15, 0.2\}\)

B  Fubini’s Theorem

A foundational theorem of random measures is Fubini’s Theorem.
Theorem 3 (Measure-kernel-function). Let $Q$ be a transition kernel from $(E, \mathcal{E})$ into $(F, \mathcal{F})$. Then

$$Qf(x) = \int_{F} Q(x, dy) f(y) \quad \text{for} \quad x \in E$$

defines a function $Qf$ that is in $\mathcal{E}_+$ for every function $f$ in $\mathcal{F}_+$;

$$\nu Q(B) = \int_{E} \nu(dx) Q(x, B) \quad \text{for} \quad B \in \mathcal{F}$$

defines a measure $\nu Q$ on $(F, \mathcal{F})$ for each measure $\nu$ on $(E, \mathcal{E})$; and

$$(\nu Q)f = \nu(Qf) = \int_{E} \nu(dx) \int_{F} Q(x, dy) f(y)$$

for every measure $\nu$ on $(E, \mathcal{E})$ and function $f$ in $\mathcal{F}_+$.

Remark 11 (Random measure). The random measure $N = (\kappa, \nu)$ on $(E, \mathcal{E})$ is a transition kernel from $(\Omega, \mathcal{H})$ into $(E, \mathcal{E})$. Then

$$Nf(\omega) = \int_{E} N(\omega, dx) f(x) \quad \text{for} \quad \omega \in \Omega$$

defines a positive random variable $Nf$ for every function $f$ in $\mathcal{E}_+$;

$$c\nu(B) = EN(B) = \int_{\Omega} \mathbb{P}(d\omega) N(\omega, B) \quad \text{for} \quad B \in \mathcal{E}$$

defines a measure $c\nu = EN$ on $(E, \mathcal{E})$ for each measure $\mathbb{P}$ on $(\Omega, \mathcal{H})$ called the mean or intensity measure; and

$$ENf = c\nu f = \int_{\Omega} \mathbb{P}(d\omega) \int_{E} N(\omega, dx) f(x)$$

for every measure $\mathbb{P}$ on $(\Omega, \mathcal{H})$ and function $f$ in $\mathcal{E}_+$.

C Additional examples

C.1 Symmetric polynomial with correlation

As referenced in Table 1, here we consider correlation in a bivariate symmetric polynomial. Suppose we have $E = \mathbb{R}^2$ and $\nu = \text{Gaussian}([0, 0], \begin{bmatrix} 1 & \rho \\ \rho & 1 \end{bmatrix})$ and the polynomial $g(x_1, x_2) = 1 + x_1 + x_2 + x_1x_2$. This has mean and variance

$$\mathbb{E}g = 1 + \rho$$
$$\mathbb{V}ar g = 3 + 2(\rho + 1)$$
This admits a HDMR analysis

\[ g_1(x_1) = x_1 + \left(\frac{\rho}{\rho^2 + 1}\right)(x_1^2 - 1) \]

\[ g_2(x_2) = x_2 + \left(\frac{\rho}{\rho^2 + 1}\right)(x_2^2 - 1) \]

\[ g_{12}(x_1, x_2) = \frac{\rho^2 x_1 x_2 - \rho (x_1^2 + x_2^2 - 1) + x_1 x_2 - \rho^3}{\rho^2 + 1} \]

\[ \text{Var} g_1 = \text{Var} g_2 = \frac{\rho^4 + 4\rho^2 + 1}{(\rho^2 + 1)^2} \]

\[ \text{Cov}(g_1, g_2) = \frac{\rho (\rho^2 (\rho (\rho + 2) + 2) + 1)}{(\rho^2 + 1)^2} \]

\[ \text{Var} g_{12} = \frac{(1 - \rho^2)^2}{\rho^2 + 1} \]

\[ S_1^a = S_2^a = \frac{\rho^4 + 4\rho^2 + 1}{(\rho^2 + 1)^2 (3 + \rho (\rho + 2))} \]

\[ S_1^b = S_2^b = \frac{\rho (\rho^2 (\rho (\rho + 2) + 2) + 1)}{(\rho^2 + 1)^2 (3 + \rho (\rho + 2))} \]

\[ S_{12}^a = \frac{(1 - \rho^2)^2}{(\rho^2 + 1) (3 + \rho (\rho + 2))} \]

\[ ED = \frac{2 (\rho^4 + \rho^3 + \rho^2 + \rho + 2)}{(\rho^2 + 1) (3 + \rho (\rho + 2))} \]

with decomposition of variance

\[ \text{Var} g = \text{Var} g_1 + \text{Var} g_2 + 2 \text{Cov}(g_1, g_2) + \text{Var} g_{12} \]

where we note that \( \text{Cov}(g_{12}, g_1) = \text{Cov}(g_{12}, g_2) = 0 \) due to hierarchical orthogonality, so \( S_{12}^b = 0 \).

In Figure 15 we show the first and second order HDMR sensitivity indices. The sensitivity indices show behavior whereby the second-order subspace vanishes and first-order achieve unity as \( |\rho| \to 1 \). The effective dimension is unimodal, so too is the entropy. Interestingly these quantities all have local maxima and minima around \( \rho \approx -0.106 \) and none are symmetric, despite \( g \) being symmetric.
Figure 15: First and second order HDMR sensitivity indices for polynomial model with correlated inputs; effective dimension; entropy on subspace dimension; all as a function of correlation coefficient $\rho$

For the random measure $N = (\kappa, \nu)$ on $(E, \mathcal{E})$ and for the function $f = (g - \mathbb{E}g)^2 \in \mathcal{E}_+$, we have the decomposition of $Nf$ of the mean

$$E N f = \nu f = \nu \text{arg} = \nu \text{arg} + 2 \text{Cov}(g_1, g_2) + \nu \text{arg}_{12}$$

and for the disjoint partition $\{A, \cdots, B\}$ of $E$, putting $f_d = f^D$ for $D \in \{A, \cdots, B\}$, the decomposition of the variance as

$$\text{Var} N f = \nu f^2 + (\delta^2 - c)(\nu f)^2$$

$$= \sum_{D \in \{A, \cdots, B\}} \text{Var} N f_d + \sum_{D_i \neq D_j \in \{A, \cdots, B\}} \text{Cov}(N f_{d_i}, N f_{d_j})$$

$$= \sum_{D \in \{A, \cdots, B\}} (\nu f_d^2 + (\delta^2 - c)(\nu f_d)^2) + \sum_{D_i \neq D_j \in \{A, \cdots, B\}} (\delta^2 - c)\nu f_{d_i} \nu f_{d_j}$$

The second moment is

$$\nu f^2 = 3\rho(3\rho(\rho + 4) + 46) + 36 + 57$$

The Laplace functional is defined through

$$\nu e^{-f} = \int_{\mathbb{R}^2} d\nu(x_1, x_2) e^{-f(x_1, x_2)} = \int_{\mathbb{R}^2} dx_1 dx_2 e^{-\left(\frac{1}{2(1 - \rho^2)}(x_1^2 + x_2^2 - 2\rho x_1 x_2) + (x_1 x_2 + x_1 + x_2 - \rho)^2\right)} \frac{1}{2\pi \sqrt{1 - \rho^2}}$$
The sensitivity distribution of coordinate $i \in \{1, 2\}$ is analytically computed.

In Figure 16 we plot the density $S^a_i$ for coordinate $i$ and its entropy. The density shows complex behavior, moving from bimodal to unimodal as $\rho$ ranges from $-1$ to $1$. Entropy has a maximum around $\rho \approx -0.64$. For the maximum entropy, we change the measure to a product of uniform distributions $\nu = \text{Uniform}[-1,1] \times \text{Uniform}[-1,1]$ so that $g$ takes values on $[0,4]$. The maximum entropy distribution is approximated using Metropolis-Hastings, where 125,000 samples were simulated, with the first 25,000 discarded as burn-in. We see that the coordinate uncertainty by sensitivity indices approximates the maximum entropy distribution in the coordinate.

![Figure 16: Bivariate polynomial for orthogonal $N$: structural sensitivity density $S^a_i$ for coordinate $i$, entropy, and maximum entropy](image)

(C.2 Graph property)

As referenced in Table 1, let $G(n,p)$ be the Erdős-Renyi (ER) graph space with $n$ vertices and edge probability $p$. We have $E = \{0,1\}^{(n\choose 2)}$ with measure $\nu = \prod_i \nu_i$ where $\nu_i = \text{Bernoulli}(p)$

$$\nu\{x\} = \prod_i \nu_i\{x_i\} = \prod_i p^{x_i}(1-p)^{1-x_i} = p^{\sum x_i}(1-p)^{\binom{n}{2} - \sum x_i} \quad \text{for} \quad x \in E$$

Hence the law $\nu$ is defined in terms of the number of edges. Denote $E_i = \{0,1\}^i$ for $i \in \{1, \cdots, \binom{n}{2}\}$. Suppose we partition $E$ into sets by the number of edges $\{A_0, \cdots, A_{\binom{n}{2}}\}$ where $A_0 = \{(0, \cdots, 0)\}$ with zero edges and
\( A_n = \{(1, \cdots, 1)\} \) with \( \binom{n}{2} \) edges. Putting \( y = \sum_i x_i \), we define

\[
\nu(A_y) = \left( \binom{n}{2} \right)^y (1-p)^{\binom{n}{2} - y} = \text{Binomial}(\binom{n}{2}, p) \quad \text{for} \quad y \in \{0, 1, \cdots, \binom{n}{2}\}
\]

so the distribution of the number of edges is binomial. Suppose for each \( x \in E \), we compute the spectral gap \( g(x) \in \mathbb{R}_+ \) of the graph Laplacian, where we define \( g((0, \cdots, 0)) = 0 \). We compute the mean and variance as

\[
\mathbb{E}g = \sum_{x \in E} \nu\{x\} g(x)
\]
\[
\mathbb{V}arg = \sum_{x \in E} \nu\{x\} g^2(x) - (\mathbb{E}g)^2
\]

In possession of the component functions \( \{g_u\} \), we compute the variances (\( \mathbb{V}arg_u \)) and sensitivity indices (\( S_u \)). The sensitivity indices form a probability measure on the subspaces, and we compute its entropy. In Figure 17 for \( n = 5 \) we plot the mean, variance, sensitivity indices, and entropy as a function of \( p \). Mean and variance generally increase in \( p \), whereas entropy increases then decreases, with a maximum near \( p \approx 0.5 \).

![Figure 17: Spectral gap of graph Laplacian of Erdős-Renyi \( G(n = 5, p) \): Mean, variance, sensitivity indices, and entropy as a function of \( p \)](image-url)
Now consider the random measure $N = (\kappa, \nu)$ on $(E, \mathcal{E})$ and consider risk function $f = (g - \mathbb{E}g)^2 \in \mathcal{E}_+$. The Laplace functional is defined through

$$\nu e^{-f} = \int_E \nu(dx)e^{-(g(x) - \mathbb{E}g)^2}$$

Then the mean and variance are computed as

$$\mathbb{E}Nf = c\nu f = c\nu \mathbb{E}g$$
$$\mathbb{V}ar Nf = c\nu f^2 - (\delta^2 - c)(\nu f)^2$$

As before we consider Dirac and orthogonal $N$. For each coordinate $i$, we take the partition \{A_i, B_i\} of $E$, where $A_i = E_1 \times \cdots \times E_{i-1} \times \{0\} \times E_{i+1} \times \cdots \times E_n$ and $B_i = E_1 \times \cdots \times E_{i-1} \times \{1\} \times E_{i+1} \times \cdots \times E_n$ for the $i \in \{1, \cdots, n\}$.

We take $n = 5$ and plot the spectral gap RM analysis in Figure 18 of the variances, second moments, and sensitivity indices. The Dirac and orthogonal $N$ are similar, with non-linear surfaces. Entropy has two modes.
(a) Orthogonal $N$: $(\nu f^2_d)$ for coordinate 1

(b) Orthogonal $N$: $(S^o_d)$ for coordinate 1

(c) Dirac $N$: $(\text{Var}f_d)$ for coordinate 1

(d) Dirac $N$: $(S^o_d)$ for coordinate 1

(e) Entropy of $(S^o_d)$ for coordinate 1 as a function of $p$

(f) $\nu f^2$ and $\text{Var}f$ as a function of $p$

Figure 18: Spectral gap of graph Laplacian of Erdős-Renyi $G(n = 5, p)$ for orthogonal and Dirac $N$: second moments $(\nu f^2_d)$, variances $(\text{Var}f_d)$, and structural sensitivity indices $(S^o_d)$ for partitions by coordinates
C.3 Ising random field

As referenced in Table 1, we give an example for Remark 8 for the nearest neighbor Ising model on a lattice. Let
\( N = (\kappa, \nu) \) be a random measure on \((E, \mathcal{E})\). Consider measurable space \((F, \mathcal{F})\), where \( F = \{-1, 1\}^{2^{|V|}} \) with dimension \(2^{|V|}\) and discrete \(\sigma\)-algebra \(\mathcal{F} = 2^F\).

Let \( k : E \times F \to \mathbb{R}_+ \) be \( E \otimes \mathcal{F} \) measurable. Consider the random field \( G \) on \((F, \mathcal{F})\) formed by \( G(y) = N f_y \) for \( y \in F \) where \( f_y(\cdot) = k(\cdot, y) \in \mathcal{E}_+ \). Define the Hamiltonian function
\[
H(y) = - \sum_{i \sim j} y_i y_j
\]
and put
\[
Z_\beta = \sum_{y \in F} e^{-\beta H(y)}
\]
where \( \beta \in \mathbb{R}_+ \). The density is defined as
\[
\lambda_\beta \{ y \} = \frac{e^{-\beta H(y)}}{Z_\beta} \quad \text{for} \quad y \in F
\]
To define the Laplace transform of \( G \), we define \( f_\beta \in \mathcal{E}_+ \) as
\[
f_\beta(x) = \sum_{y \in F} \lambda_\beta \{ y \} k(x, y) \quad \text{for} \quad x \in E
\]
and compute \( \nu e^{-f_\beta} \). Let \(|V| = n \in \mathbb{N}_{>0}\).

The average spin (magnetization) is
\[
g(y) = \frac{1}{n} \sum_{i} y_i \quad \text{for} \quad y \in F
\]
Let \( \nu = \text{Uniform}[-1, 1] \) with \((E, \mathcal{E}) = ([1, 1], \mathcal{B}_{[1,1]})\). Define \( k \) as
\[
k(x, y) = (x - g(y))^2 \quad \text{for} \quad (x, y) \in E \times F
\]
The random field \( G \) has the interpretation of magnetization distance on lattice points. We have
\[
\nu f_y = g^2(y) + \frac{1}{3} \quad \text{for} \quad y \in F
\]
and
\[
\nu(f_y f_z) = \frac{1}{15} \left( 5g^2(y) (3g^2(z) + 1) + 20g(y)g(z) + 5g^2(z) + 3 \right) \quad \text{for} \quad y, z \in F
\]
In Figure 19 we plot the kernel \( K \) for orthogonal and Dirac \( N \) and \( c = 1 \).
Figure 19: Random field kernel $K$ for orthogonal and Dirac $N$