

Uncertainty functionals revisited: Concavity and Jensen's inequality

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Back to the early days of Bayesian experimental design

- Lindley [1956], DeGroot [1962] proposed to measure a priori the information brought by an experiment by the quantity

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- Remark: (1) is also used to construct sequential designs, using myopic (a.k.a. stepwise uncertainty reduction) approaches

Another use of uncertainty functionals

Global sensitivity analysis

Study of how **uncertainties** in a model's **inputs** propagate through the model and **contribute to the variability of its output**.

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$$S_u^{\text{cl}} = \frac{\text{var}(\mathbb{E}(Y \mid X_u))}{\text{var}(Y)} = \frac{\text{var}(Y) - \mathbb{E}(\text{var}(Y \mid X_u))}{\text{var}(Y)}.$$

Sobol' [1993], Homma and Saltelli [1996]

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Sobol' indices $\rightarrow$ “goal-oriented” generalization

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$$S_u^{\text{cl}} = \frac{\text{var}(\mathbb{E}(Y \mid X_u))}{\text{var}(Y)} = \frac{H(P^Y) - \mathbb{E}(H(P^{Y|X_u}))}{H(P^Y)}.$$

Fort et al. [2016], Borgonovo et al. [2021], Fissler and Pesenti [2023], ...

Generalization. Replace the variance with **other uncertainty measures**.

Uncertainty functionals (our definition)

Let $(\mathbb{Y}, \mathcal{Y})$ denote a measurable space (e.g., $(\mathbb{R}, \mathcal{B}(\mathbb{R}))$).

Definition

inspired by DeGroot [1962], Rao [1982b, 1984], Hainy et al. [2014], Bect et al. [2019]

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- 1 is **measurable**,[†]

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[†] $\mathbb{P}$ is equipped with the σ -algebra generated by the evaluation maps.

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- ① is measurable,
- ② **vanishes on Dirac measures:** $H(\delta_y) = 0$ for all $y \in \mathbb{Y}$,

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- ① is measurable,
- ② vanishes on Dirac measures: $H(\delta_y) = 0$ for all $y \in \mathbb{Y}$,
- ③ **decreases on average** (DoA): $H(P^Y) \geq E \left(H(P^{Y|X}) \right)^\ddagger$,

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‡ where Y is $\mathbb{Y}$ -valued and $Y|X$ admits a regular conditional distribution

Examples

1. Trace-class generalized entropies (a.k.a. ϕ -entropies) on $(\mathbb{N}, \mathcal{P}(\mathbb{N}))$

Burbea and Rao [1982], Ben-Tal and Teboulle [1986], Scarfone [2013], Tempesta [2015], ...

$$H(\nu) = \sum_{y \in \mathbb{N}} h(\nu(\{y\}))$$

with $h : [0, 1] \rightarrow \overline{\mathbb{R}}_+$ **concave**, $h(0) = h(1) = 0$.

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Examples:

- $h(p) = -p \log(p) \rightarrow$ **Shannon** (or Boltzmann-Gibbs) **entropy**,
- $h(p) = p(1 - p) \rightarrow$ **Gini-Simpson index**, Simpson [1949]
- $h(p) = (\alpha - 1)^{-1} (p - p^\alpha)$, $\alpha > 1 \rightarrow$ **α -entropy**. Havrda and Charvát [1967]
Tsallis [1988]

Examples (cont'd)

2. Regular quadratic uncertainty functionals (QUFs)

Rao [1982a, 1984], Rao and Nayak [1985], Lau [1985], Rao [2010], Hainy et al. [2014], ...

a.k.a. quadratic entropies

$$H(\nu) = \iint \rho(y, y') \nu(dy) \nu(dy')$$

with $\rho : \mathbb{Y} \times \mathbb{Y} \rightarrow \mathbb{R}_+$ symmetric, measurable, **conditionally negative definite** (CND), and vanishing on the diagonal.

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Examples:

- $\mathbb{Y} = \mathbb{R}$, $\rho(y, y') = \frac{1}{2} (y - y')^2 \rightarrow$ **variance**,
- $\mathbb{Y} = \mathbb{R}$, $\rho(y, y') = |y - y'| \rightarrow$ **Gini's mean difference**, Yitzhaki [2003]
- $\mathbb{Y} = L^2(\mu)$, μ σ -finite, $\rho(y, y') = \|y - y'\|^2 \rightarrow$ **integrated variance**,
- ... (more examples in appendix)

A foundational question

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How is this related to **concavity**?

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How can we characterize the DoA (**decreasing on average**) property?

How is this related to **concavity**?

These questions have been explored by DeGroot [1962] a long time ago, but only in the case of a *finite* set $\mathbb{Y}$...

- 1 Introduction
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From DoA to Jensen

- Recall the DoA property:

$$H\left(\mathbf{p}^Y\right) \geq \mathbb{E}\left(H\left(\mathbf{p}^{Y|X}\right)\right)$$

for all (X, Y) where Y is $\mathbb{Y}$ -valued and $Y|X$ admits a regular conditional distrib.

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Proposition

H is DoA iff it satisfies **Jensen's inequality** (concave version):

$$H(\bar{\nu}) \geq E(H(\nu))$$

for all random probability measures ν on $(\mathbb{Y}, \mathcal{Y})$.

From Jensen's inequality to concavity

Let $H : \mathbb{P} \rightarrow \overline{\mathbb{R}}$ denote a measurable (signed) probability functional.

Theorem (part 1)

If H satisfies **Jensen's inequality** on $\mathbb{P}$ (concave version), then H is **concave**:
for all $\lambda \in (0, 1)$ and all $\nu_1, \nu_2 \in \text{dom}(H) = \{\nu \in \mathbb{P} \mid H(\nu) > -\infty\}$,

$$H(\lambda\nu_1 + (1 - \lambda)\nu_2) \geq \lambda H(\nu_1) + (1 - \lambda)H(\nu_2).$$

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Proof. Let $X \sim \text{Ber}(\lambda)$. Consider the random measure

$$\nu = \nu_1 \mathbb{1}_{X=1} + \nu_2 \mathbb{1}_{X=0}.$$

Then we have

$$\begin{aligned}\bar{\nu} &= \lambda \nu_1 + (1 - \lambda) \nu_2, \\ E(H(\nu)) &= \lambda H(\nu_1) + (1 - \lambda) H(\nu_2),\end{aligned}$$

which proves the claim. □

The case of finite spaces

DeGroot [1962] also observed that the converse holds when $\mathbb{Y}$ is finite.

Theorem (part 2)

If $\mathbb{Y}$ is **finite** and H is **concave**, then H satisfies **Jensen's inequality** on $\mathbb{P}$.

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If $\mathbb{Y}$ is finite and H is concave, then H satisfies Jensen's inequality on $\mathbb{P}$.

Proof. Assume that $\mathbb{Y} = \{1, \dots, m\}$. Then $\mathbb{P}$ can be identified with the $(m-1)$ -dimensional probability simplex in $\mathbb{R}^m$:

$$\Sigma_{m-1} = \left\{ \nu \in \mathbb{R}^m \mid \sum_{i=1}^m \nu_i = 1, \nu_i \geq 0, \text{ for } i = 1, \dots, m \right\},$$

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What if $\mathbb{Y}$ is not finite?

Main result

Theorem

Assume that $(\mathbb{Y}, \mathcal{Y}) \cong (\mathbb{R}, \mathcal{B}(\mathbb{R})) \otimes (\mathbb{Y}', \mathcal{Y}')$, for some measurable space $(\mathbb{Y}', \mathcal{Y}')$.

Remarks

- $(\mathbb{Y}, \mathcal{Y})$ must be “rich enough”.

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- $(\mathbb{Y}, \mathcal{Y})$ must be “rich enough”. We **don't know** if the result holds for $(\mathbb{N}, \mathcal{P}(\mathbb{N}))$.
- It has been known since **Perlman [1974]** that Jensen's inequality does not hold in general in finite-dimensional spaces.
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- Remark: Let $\nu_y = \nu(\{y\})$. Let $D_{\nu} = \{y \in \mathbb{R} \mid \nu_y > 0\}$. Then

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- H is nonnegative, measurable, **concave**, and vanishes on Dirac measures. But we will show that it **violates Jensen's inequality**.

Proof (cont'd)

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- $\bar{\nu}$ is a Laplace distribution, which has no atom, therefore

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- Thus **Jensen's inequality does not hold:**

$$H(\bar{\nu}) \not\geq \mathbb{E}(H(\nu)).$$



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A sufficient condition

Proposition

Let $\mathbb{D}$ be a non-empty set, and $L : \mathbb{Y} \times \mathbb{D} \rightarrow \overline{\mathbb{R}}_+$ be a function such that, for all $d \in \mathbb{D}$, $L(\cdot, d)$ is measurable.

A sufficient condition: Uncertainty as Bayes risk

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$$H(\nu) = \inf_{d \in \mathbb{D}} \int L(y, d) \nu(dy), \quad \nu \in \mathbb{P}, \quad \rightarrow \text{min ?}$$

defines a non-negative measurable probability functional $H : \mathbb{P} \rightarrow \overline{\mathbb{R}}_+$ that satisfies Jensen's inequality.

(well known; see, e.g., [Bect et al. \[2019\]](#))

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Proof. For any random probability measure ν and any $d \in \mathbb{D}$,

$$\mathbb{E} \left(\int_{\mathbb{Y}} L(y, d) \nu(dy) \right) = \int_{\mathbb{Y}} L(y, d) \bar{\nu}(dy).$$

The result then follows from the property $\inf_d (\mathbb{E}(\cdot)) \geq \mathbb{E}(\inf_d (\cdot))$. □

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Connection with ...

When the infimum is attained, we obtain an interesting class of functionals.

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A probability functional H admits the previous representation, in which **the infimum** over $\mathbb{D}$ is **attained** for every $\nu \in \mathbb{P}$:

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if and only if it is the **generalized entropy function** associated with a proper, non-negative, negatively oriented **scoring rule** $S : \mathbb{Y} \times \mathbb{P} \rightarrow \overline{\mathbb{R}}_+$:

$$H(\nu) = \min_{\nu' \in \mathbb{P}} \int S(y, \nu') \nu(dy).$$

Grünwald and Dawid [2004]

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$$H(\nu) = \min_{d \in \mathbb{D}} \int L(y, d) \nu(dy)$$

if and only if it is the generalized entropy function associated with a proper, non-negative, negatively oriented scoring rule $S : \mathbb{Y} \times \mathbb{P} \rightarrow \overline{\mathbb{R}}_+$:

$$H(\nu) = \min_{\nu' \in \mathbb{P}} \int S(y, \nu') \nu(dy).$$

Grünwald and Dawid [2004]

Proof. Take $S(y, \nu) = L(y, d^*(\nu))$ with $d^*(\nu) \in \operatorname{argmin}_d \int L(y, d) \nu(dy)$.

Example: Gini's mean difference

- Recall **Gini's mean difference** on $\mathbb{Y} = \mathbb{R}$:

$$H(\nu) = \mathbb{E}_{\nu} (|Y - Y'|), \quad Y, Y' \stackrel{\text{iid}}{\sim} \nu.$$

This is the **regular QUF** with CND kernel $\rho(y, y') = |y - y'|$.

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- Representation as a “**generalized variance**”: if $H(\nu) < +\infty$,

$$H(\nu) = \min_{t \in \mathbb{H}} \mathbb{E}_\nu \left(\|\psi(Y) - t\|_{\mathbb{H}}^2 \right)$$

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$$H(\nu) = \min_{\nu' \in \mathbb{P}} E_{\nu} (S(Y, \nu'))$$

where $S(y, \nu) = 2 \text{CRPS}(y, \nu) = 2 \int (F_{\nu}(y') - \mathbb{1}_{y' \leq y})^2 dy'$.

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- 1 Introduction
- 2 Jensen's inequality and concavity
- 3 Sufficient conditions
- 4 Summary & open problems

One problem (almost) solved, two more to go...

Let $H : \mathbb{P} \rightarrow \overline{\mathbb{R}}_+$ be measurable and vanish on the diagonal.

H is concave



H is decreasing on average ($\Leftrightarrow$ satisfies Jensen's inequality)



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$\Uparrow$ $\Downarrow$ if $\mathbb{Y}$ is “rich enough”

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TTBOOK all the existing examples of uncertainty functionals are in the last class!

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Appendices

Conditionally negative definite kernel

Definition

A **measurable symmetric** function $\rho : \mathbb{Y} \times \mathbb{Y} \rightarrow \mathbb{R}_+$,

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$$\sum_{k,l}^m \lambda_k \lambda_l \rho(y_k, y_l) \leq 0.$$

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Characterization of ρ

Any CND kernel ρ vanishing on the diagonal admits a Hilbertian representation: there exist a Hilbert space $\mathbb{H}$ and a map $\psi : \mathbb{Y} \rightarrow \mathbb{H}$ such that

$$\rho(y, y') = \|\psi(y) - \psi(y')\|_{\mathbb{H}}^2, \quad \forall y, y' \in \mathbb{Y}.$$

Conversely, kernels defined this way are CND and vanish on the diagonal.

Some examples of regular QUFs

$\mathbb{Y}$	CND kernel ρ	Regular QUF $H(\nu)$	Name
$\{0, 1\}$	$\frac{1}{2} \mathbb{1}_{y \neq y'}$	$\nu_1 (1 - \nu_1)$	Bernoulli variance
$\mathbb{N}$	$\mathbb{1}_{y \neq y'}$	$1 - \sum_{y \in \mathbb{N}} \nu_y^2$	Gini-Simpson index ⁽¹⁾
$\mathbb{R}$	$\frac{1}{2} (y - y')^2$	$\text{var}_\nu (Y)$	variance
$\mathbb{R}$	$ y - y' $	$E_\nu (Y - Y')$	Gini's mean diff. ⁽²⁾
$\mathbb{R}$	$ y - y' ^\beta \text{ (}\dagger\text{)}$	$E_\nu (Y - Y' ^\beta)$	Fract. Brownian var. ⁽³⁾
$\mathbb{R}$	$1 - e^{-(y-y')^2}$	$E_\nu (1 - e^{-(Y-Y')^2})$	(unnamed ?)
$L^2(\mu)$	$\ y - y'\ ^2$	$\int \text{var}_\nu (Y(s)) \mu(ds)$	integrated variance

Notations: $\nu \in \mathbb{P}$; $\nu_y = \nu(\{y\})$ for all $y \in \mathbb{Y}$; $(\dagger) 0 < \beta < 2$; $Y, Y' \stackrel{\text{iid}}{\sim} \nu$;

μ σ -finite. Refs: ⁽¹⁾ Simpson [1949], ⁽²⁾ Yitzhaki [2003], ⁽³⁾ Székely and Rizzo [2013]