Random Fuzzy Sets Theory and Application to Machine Learning

Thierry Denœux

Université de technologie de Compiègne, Compiègne, France Institut Universitaire de France, Paris, France

https://www.hds.utc.fr/~tdenoeux

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A general model of uncertainty

- Modeling uncertainty: a fundamental problem in Artificial/Computational Intelligence
 - Representation of uncertain/imperfect knowledge
 - Reasoning and decision-making with uncertainty
 - Quantification of prediction uncertainty in machine learning, etc.
- As probability appeared too limited, two alternative models were introduced in the late 1970's:
 - Dempster-Shafer (DS) theory = belief functions + Dempster's rule (based on random sets, generalizes Bayesian probability theory)
 - Possibility theory = possibility measures + triangular norms (based on fuzzy sets)
- Each of these two models can be more suitable/practical than the other, depending on the available evidence (unreliable/uncertain vs. vague/fuzzy).
- The purpose of this lecture is to introduce a more general theoretical framework: Epistemic Random Fuzzy Sets, which unifies the two previous approaches and gives more flexibility in applications.

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General picture



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Classical frameworks

- Random sets and DS theory
- Fuzzy sets and possibility theory

2 Random fuzzy sets

- Definitions
- Gaussian random fuzzy numbers
- Gaussian random fuzzy vectors

3 Application to Machine Learning

- Neural network model
- Learning
- Experimental results

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Random set



- Let $(\Omega, \Sigma_{\Omega}, P)$ be a probability space, $(\Theta, \Sigma_{\Theta})$ a measurable space, and $\overline{X} : \Omega \to 2^{\Theta}$.
- The 6-tuple $(\Omega, \Sigma_{\Omega}, P, \Theta, \Sigma_{\Theta}, \overline{X})$ is a random set (RS) iff \overline{X} verifies the following measurability condition:

$$\forall B \in \Sigma_{\Theta}, \quad \{\omega \in \Omega : \overline{X}(\omega) \cap B \neq \emptyset\} \in \Sigma_{\Omega}.$$

• The images $\overline{X}(\omega)$ are called the focal sets of \overline{X} .

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Interpretation and example

- In DS theory, a RS represents a piece of evidence about a variable X taking values in set Θ (called the frame of discernment):
 - Ω is a set of interpretations of the evidence
 - If interpretation $\omega \in \Omega$ holds, we know that $X \in \overline{X}(\omega)$, and nothing more
 - ► For any $A \in \Sigma_{\Omega}$, P(A) is the (subjective) probability that the true interpretation belongs to A
- Example: unreliable sensor



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Belief and plausibility functions



• For any $B\in \Sigma_{\Theta}$, we can compute

▶ The probability that proposition " $X \in B$ " is supported by the evidence:

$$\textit{Bel}_{\overline{X}}(B) = \textit{P}(\{\omega \in \Omega : \emptyset \neq \overline{X}(\omega) \subseteq B\})$$

▶ The probability that proposition " $X \in B$ " is consistent with the evidence:

$$\begin{aligned} \mathsf{Pl}_{\overline{X}}(B) &= \mathsf{P}(\{\omega \in \Omega : \overline{X}(\omega) \cap B \neq \emptyset\}) \\ &= 1 - \mathsf{Bel}_{\overline{X}}(B^c) \end{aligned}$$

• Mappings $Bel_{\overline{X}}: \Sigma_{\Theta} \to [0, 1]$ and $Pl_{\overline{X}}: \Sigma_{\Theta} \to [0, 1]$ are called respectively, belief and plausibility functions.

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Mathematical characterization

A mapping $Bel : \Sigma_{\Theta} \mapsto [0,1]$ is a belief function (for some RS \overline{X}) iff it verifies the following properties:

- $Bel(\emptyset) = 0$
- 2 $Bel(\Theta) = 1$

③ For any $k \ge 2$ and any collection B_1, \ldots, B_k of elements of Σ_{Θ} ,

$$\textit{Bel}_{\overline{X}}\left(igcup_{i=1}^{k}B_{i}
ight)\geq\sum_{\emptyset
eq I\subseteq\{1,\ldots,k\}}(-1)^{|I|+1}\textit{Bel}_{\overline{X}}\left(igcup_{i\in I}B_{i}
ight).$$

[Complete monotonicity]

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Interpretation

In DS theory, Bel_X(B) and Pl_X(B) are interpreted, respectively, as a degree of belief that X ∈ B, and a degree of lack of belief in X ∉ B, based on some evidence. This model is more flexible than probability theory.

• Examples:

	Bel(B)	$Bel(B^c)$	PI(B)	$PI(B^c)$
evidence for B	0.9	0	1	0.1
mixed evidence for B and B^c	0.6	0.2	0.8	0.4
complete ignorance	0	0	1	1
probabilistic evidence	0.4	0.6	0.4	0.6

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Special cases

- Precise but uncertain information: if for all ω ∈ Ω, |X(ω)| = 1, RS X is said to be Bayesian. Bel_X is then a probability measure, and Pl_X = Bel_X
- Certain but imprecise information: let B ⊆ Θ; the constant RS X
 _B such that for all ω ∈ Ω, X(ω) = B corresponds to set-valued information (we know for sure that X ∈ B, and nothing more).
- In particular, if X
 ₀ is a RS such that for all ω ∈ Ω, X
 ₀(ω) = Θ, X
 ₀ is said to be vacuous: it represents complete ignorance.

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Combination of independent pieces of evidence

Case 1: no conflict



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Combination of independent pieces of evidence

Case 2: conflict



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Dempster's rule of combination



We consider two RSs $(\Omega_i, \Sigma_i, P_i, \Theta, \Sigma_{\Theta}, \overline{X}_i)$, i = 1, 2 representing independent pieces of evidence. Their orthogonal sum is the RS

$$(\Omega_1 imes \Omega_2, \Sigma_1 \otimes \Sigma_2, P_{12}, \Theta, \Sigma_\Theta, \overline{X}_1 \oplus \overline{X}_2)$$

where $(\overline{X}_1 \oplus \overline{X}_2)(\omega_1, \omega_2) = \overline{X}_1(\omega_1) \cap \overline{X}_2(\omega_2)$ and P_{12} is the product measure $P_1 \times P_2$ conditioned on the set

$$\Theta^* = \{ (\omega_1, \omega_2) \in \Omega_1 \times \Omega_2 : \overline{X}_1(\omega_1) \cap \overline{X}_2(\omega_2) \neq \emptyset \}$$

Properties

• Commutativity:

$$\overline{X}_1 \oplus \overline{X}_2 = \overline{X}_2 \oplus \overline{X}_1$$

• Associativity:

$$(\overline{X}_1 \oplus \overline{X}_2) \oplus \overline{X}_3 = \overline{X}_1 \oplus (\overline{X}_2 \oplus \overline{X}_3)$$

• Neutral element: if \overline{X}_0 is vacuous,

$$\overline{X}_0 \oplus \overline{X} = \overline{X}$$

• Let $pI_{\overline{X}}: \theta \to [0,1]$ be the contour function defined by $pI_{\overline{X}}(\theta) = PI_{\overline{X}}(\{\theta\})$ for all $\theta \in \Theta$. We have

$$pl_{\overline{X}_1\oplus\overline{X}_2}\propto pl_{\overline{X}_1}pl_{\overline{X}_2}$$

• Generalization of Bayesian conditioning: if \overline{X} is a Bayesian RS and \overline{X}_B is a constant RS with focal set B, then $\overline{X} \oplus \overline{X}_B$ is a Bayesian RS, and

$$Bel_{\overline{X} \oplus \overline{X}_B} = Bel_{\overline{X}}(\cdot \mid B)$$

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Fuzzy set

- A fuzzy subset of a set Θ is a mapping $\widetilde{F}:\Theta\mapsto [0,1].$
- Example: if $\Theta = [-60, 60]$ is the range of outside air temperatures, the notion of "hot temperature" can be represented by the fuzzy subset



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Additional definitions

• The height of \widetilde{F} is

$$\mathsf{hgt}(\widetilde{F}) = \sup_{\theta \in \Theta} \widetilde{F}(heta)$$

- \widetilde{F} is normal if hgt $(\widetilde{F}) = 1$
- For any $\alpha \in [0,1]$, the α -cut of \widetilde{F} is the set

$${}^{\alpha}\widetilde{F} = \{\theta \in \Theta : \widetilde{F}(\theta) \ge \alpha\}$$

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Fuzzy sets and possibility theory

Possibility and necessity

- Let X be a variable taking values in Θ. Assume that we receive a piece of evidence telling us that "X is F", where F is a normal fuzzy subset of Θ.
- Such evidence can be seen as a flexible constraint on the true value of X. We define
 - The possibility distribution of X as $\pi_{\widetilde{F}} = \widetilde{F}$
 - ► The degree of possibility that $X \in B$ for $B \subseteq \Theta$ as

$$\Pi_{\widetilde{F}}(B) = \sup_{\theta \in B} \pi_{\widetilde{F}}(\theta)$$

• The degree of necessity that $X \in B$ as

$$N_{\widetilde{F}}(B) = 1 - \prod_{\widetilde{F}}(B^c)$$

• Example:



Possibility and necessity measures

- The mapping $\Pi_{\widetilde{F}} : 2^{\Theta} \mapsto [0, 1]$ is called a possibility measure, and $N_{\widetilde{F}} : 2^{\Theta} \mapsto [0, 1]$ is the dual necessity measure.
- Properties: for any $A, B \subseteq \Theta$,

 $\Pi_{\widetilde{E}}(A \cup B) = \max(\Pi_{\widetilde{E}}(A), \Pi_{\widetilde{E}}(B))$

$$N_{\widetilde{F}}(A \cap B) = \min(N_{\widetilde{F}}(A), N_{\widetilde{F}}(B))$$

• $N_{\tilde{F}}$ is a belief function, and $\Pi_{\tilde{F}}$ is the dual plausibility function. For this reason, it has been claimed that possibility theory is a special case of DS theory. However, the two theories have different mechanisms for combining information.

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Combination of possibility distributions

- Assume that we receive two independent pieces of information telling us that "X is \widetilde{F} " and "X is \widetilde{G} ", where \widetilde{F} and \widetilde{G} are two fuzzy subsets of Θ .
- We can deduce that "X is F ∩_⊤ G", where ∩_⊤ is a fuzzy set intersection operator based on a t-norm ⊤. The most common choices for ⊤ are the minimum and product t-norms.
- $\bullet\,$ The intersection of two normal fuzzy sets is generally not normal. We define the normalized $\top\text{-intersection}$ as

$$(\widetilde{F} \cap_{\top}^{*} \widetilde{G})(\theta) = \frac{\widetilde{F}(\theta) \top \widetilde{G}(\theta)}{\mathsf{hgt}(\widetilde{F} \cap_{\top} \widetilde{G})}$$

 When T = product, the normalized intersection is associative and is denoted by ⊙. Product intersection has a reinforcement effect that is appropriate when the information sources are assumed to be independent.

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Example

 $\widetilde{F} = hot, \ \widetilde{G} = around \ 30$



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Random fuzzy set



- Let $(\Omega, \Sigma_{\Omega}, P)$ be a probability space, $(\Theta, \Sigma_{\Theta})$ a measurable space, and \widetilde{X} a mapping from Ω to the set $[0, 1]^{\Theta}$ of fuzzy subsets of Θ .
- The 6-tuple $(\Omega, \Sigma_{\Omega}, P, \Theta, \Sigma_{\Theta}, \widetilde{X})$ is a random fuzzy set (RFS) iff for any $\alpha \in [0, 1]$, the mapping

$${}^{lpha}\widetilde{X}:\Omega
ightarrow 2^{\Theta}\ \omega\mapsto {}^{lpha}[\widetilde{X}(\omega)]=\{ heta\in\Theta:\widetilde{X}(\omega)(heta)\geqlpha\}$$

is a random set.

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Interpretation

- We use RFSs as a model of unreliable and fuzzy evidence¹:
 - Θ is the domain of an uncertain variable/quantity X
 - Ω is a set of interpretations of a piece of evidence about X
 - ► $\forall A \in \Sigma_{\Omega}$, P(A) is the probability that the true interpretation lies in A
 - If ω ∈ Ω holds, we know that "X is X̃(ω)", i.e., X is constrained by the possibility distribution X̃(ω).
- Such RFSs are called "epistemic" to stress that they represent a state of knowledge.
- $\bullet\,$ Example: a witness tells us that "the temperature was hot on Monday", and this witness is 50% reliable
 - $\Omega = {\text{rel}, \neg \text{rel}}, p(\text{rel}) = 0.5$
 - X = temperature on Monday in Celsius, $\Theta = [-60, 60]$
 - $\widetilde{X}(\text{rel}) = \text{hot (a fuzzy subset of }\Theta), \ \widetilde{X}(\neg \text{rel}) = \Theta$

Belief and plausibility functions

If interpretation ω ∈ Ω holds, the degrees of possibility and necessity that X belongs to B ∈ Σ_Θ are

$$\Pi_{\widetilde{X}(\omega)}(B) = \sup_{\theta \in B} \widetilde{X}(\omega)(\theta), \quad N_{\widetilde{X}(\omega)}(B) = 1 - \Pi_{\widetilde{X}(\omega)}(B^c)$$

• The expected necessity and possibility degrees (Zadeh, 1979) are

$$Bel_{\widetilde{X}}(B) = \int_{\Omega} N_{\widetilde{X}(\omega)}(B) dP(\omega), \quad Pl_{\widetilde{X}}(B) = \int_{\Omega} \Pi_{\widetilde{X}(\omega)}(B) dP(\omega).$$

- Function $Bel_{\tilde{X}}$ is a completely monotone capacity (a belief function), and $Pl_{\tilde{X}}$ is the dual plausibility function (Zadeh, 1979; Couso & Sánchez, 2011).
- A RFS is thus (like a random set) a way of specifying a belief function. The RFS model is more flexible.

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Example

- Continuing the previous example, what are the degrees of belief and plausibility that $X \in B = [25, 65]$?
- We have

$$\Pi_{\widetilde{X}(\mathsf{rel})}(B) = 0.75, \quad \Pi_{\widetilde{X}(\neg \mathsf{rel})}(B) = 1$$

SO

$$Pl_{\widetilde{X}}(B) = 0.5 \times 0.75 + 0.5 \times 1 = 0.875$$

Now,

$$N_{\widetilde{X}(\mathsf{rel})}(B) = 0, \quad N_{\widetilde{X}(\neg \mathsf{rel})}(B) = 0$$

SO

$$Bel_{\widetilde{X}}(B) = 0$$

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Combination of independent RFSs



- We consider two RFSs $\widetilde{X}_1 : \Omega_1 \to [0,1]^{\Theta}$ and $\widetilde{X}_2 : \Omega_2 \to [0,1]^{\Theta}$ representing independent pieces of evidence.
- if $\omega_1 \in \Omega_1$ and $\omega_2 \in \Omega_2$ both hold, we can deduce "X is $\widetilde{X}_1(\omega_1) \cap \widetilde{X}_2(\omega_2)$ ", where \cap denotes fuzzy intersection.
- We need (1) a definition of fuzzy intersection and (2) a way to handle possible conflict (inconsistency) between the two sources.

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Definition of intersection and conflict

- Fuzzy intersection: as mentioned before, the normalized product intersection is suitable for combining fuzzy information from independent sources, and it is associative.
- With fuzzy sets, conflict is a matter of degree. We define the fuzzy set of consistent pairs of interpretations as

$$\widetilde{\Theta}^*(\omega_1,\omega_2) = \sup_{\Theta} \left(\widetilde{X}_1(\omega_1) \cdot \widetilde{X}_2(\omega_2)
ight)$$

• The product measure $P_1 \times P_2$ is conditioned on fuzzy event $\widetilde{\Theta}^*$:

$$\widetilde{P}_{12}(B) = \frac{(P_1 \times P_2)(B \cap \widetilde{\Theta}^*)}{(P_1 \times P_2)(\widetilde{\Theta}^*)} = \frac{\int_{\Omega_1} \int_{\Omega_2} B(\omega_1, \omega_2) \widetilde{\Theta}^*(\omega_1, \omega_2) dP_2(\omega_2) dP_1(\omega_1)}{\int_{\Omega_1} \int_{\Omega_2} \widetilde{\Theta}^*(\omega_1, \omega_2) dP_2(\omega_2) dP_1(\omega_1)}$$

where $B(\cdot, \cdot)$ denotes the indicator function of B. This process is called soft normalization.

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Product-intersection rule

• The combined RFS is

$$(\Omega_1 imes \Omega_2, \Sigma_1 \otimes \Sigma_2, \widetilde{P}_{12}, \Theta, \Sigma_\Theta, \widetilde{X}_1 \oplus \widetilde{X}_2)$$

where

$$(\widetilde{X}_1 \oplus \widetilde{X}_2)(\omega_1, \omega_2) = \widetilde{X}_1(\omega_1) \odot \widetilde{X}_2(\omega_2)$$

and \widetilde{P}_{12} is the product measure $P_1 \times P_2$ conditioned on the fuzzy set $\widetilde{\Theta}^*(\omega_1, \omega_2)$.

This operation is called the product intersection² of X₁ and X₂ (with soft normalization). We write X₁₂ = X₁ ⊕ X₂.

²T. Denœux. Reasoning with fuzzy and uncertain evidence using epistemic random fuzzy sets: general framework and practical models. *Fuzzy Sets and Systems*:453:1–36, 2023 \ge \circ

Random fuzzy sets

Definitions

Example



- As before, let $\Theta = [-60, +60]$, $\widetilde{F} = hot$, $\widetilde{G} = around 30$.
- Evidence 1: $\Omega_1 = \{\text{rel}, \neg \text{rel}\}, p_1(\text{rel}) = 0.5, \widetilde{X}_1(\text{rel}) = \widetilde{F}, \widetilde{X}_1(\neg \text{rel}) = \Theta.$
- Evidence 2: $\Omega_2 = \{\text{rel}, \neg \text{rel}\}, p_2(\text{rel}) = 0.7, \widetilde{X}_2(\text{rel}) = \widetilde{G}, \widetilde{X}_2(\neg \text{rel}) = \Theta.$

- $\widetilde{\Theta}^*(\text{rel}, \text{rel}) = 0.5$, $\widetilde{\Theta}^*(\text{rel}, \neg \text{rel}) = \widetilde{\Theta}^*(\neg \text{rel}, \text{rel}) = \widetilde{\Theta}^*(\neg \text{rel}, \neg \text{rel}) = 1$
- $(P_1 \times P_2)\widetilde{\Theta}^*) = 0.35 \times 0.5 + 0.15 \times 1 + 0.35 \times 1 + 0.15 \times 1 = 0.825$
- $\tilde{p}_{12}(\text{rel}, \text{rel}) = 0.35 \times 0.5/0.825$, $\tilde{p}_{12}(\neg \text{rel}, \text{rel}) = 0.35/0.825$, $\tilde{p}_{12}(\text{rel}, \neg \text{rel}) = 0.15/0.825$, $\tilde{p}_{12}(\neg \text{rel}, \neg \text{rel}) = 0.15/0.825$
- $(\widetilde{X}_1 \oplus \widetilde{X}_2)(\text{rel}, \text{rel}) = \widetilde{F} \odot \widetilde{G}$, $(\widetilde{X}_1 \oplus \widetilde{X}_2)(\text{rel}, \neg \text{rel}) = \widetilde{F}$, $(\widetilde{X}_1 \oplus \widetilde{X}_2)(\text{rel}, \neg \text{rel}) = \widetilde{G}$, $(\widetilde{X}_1 \oplus \widetilde{X}_2)(\neg \text{rel}, \neg \text{rel}) = \Theta$.

Properties

- Commutativity, associativity
- Generalization of Dempster's rule and the normalized product intersection of possibility distributions
- Multiplication of contour functions

$$\mathsf{pl}_{\widetilde{X}_1 \oplus \widetilde{X}_2} \propto \mathsf{pl}_{\widetilde{X}_1} \mathsf{pl}_{\widetilde{X}_2}$$

• Generalization of conditioning of a probability measure by a fuzzy event: if \overline{X} is a Bayesian RS and $\widetilde{X}_{\widetilde{B}}$ is a constant RF with fuzzy focal set \widetilde{B} , then $\overline{X} \oplus \widetilde{X}_{\widetilde{B}}$ is a Bayesian RS, and

$$\mathit{Bel}_{\overline{X} \oplus \widetilde{X}_{\widetilde{B}}} = \mathit{Bel}_{\overline{X}}(\cdot | \widetilde{B})$$

i.e.

$$\forall A \in \Sigma_{\Theta}, \quad \textit{Bel}_{\overline{X} \oplus \widetilde{X}_{\widetilde{B}}}(A) = \frac{\int_{A} \widetilde{B}(\theta) \textit{dBel}_{\overline{X}}(\theta)}{\int_{\Theta} \widetilde{B}(\theta) \textit{dBel}_{\overline{X}}(\theta)}$$

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Motivation

- In probability theory and statistics, the Gaussian probability distribution is widely used because it allows for simple calculations and easy manipulation (conditioning, marginalization, etc.)
- Until now, a similar workable model has been missing in DS theory to represent uncertainty on continuous variables (possibility distributions or p-boxes are not closed under Dempster's rule)
- Gaussian random fuzzy numbers (GRFNs) and extensions are simple models of RFSs making it possible to define families of belief functions on ℝ, ℝ^p, [a, b], etc., which can be easily combined by the product-intersection operator ⊕.

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Gaussian fuzzy numbers



• A Gaussian fuzzy number (GFN) is a normal fuzzy subset of ${\mathbb R}$ with membership function

$$\varphi(x; m, h) = \exp\left(-\frac{h}{2}(x-m)^2\right),$$

where $m \in \mathbb{R}$ is the mode and $h \in [0, +\infty]$ is the precision. It is denoted by GFN(m, h).

• Property: $\operatorname{GFN}(m_1, h_1) \odot \operatorname{GFN}(m_2, h_2) = \operatorname{GFN}(m_{12}, h_{12})$ with

$$m_{12} = rac{h_1 m_1 + h_2 m_2}{h_1 + h_2}$$
 and $h_{12} = h_1 + h_2.$

Gaussian random fuzzy numbers



- A Gaussian random fuzzy number (GRFN)³ is a GFN whose mode is a Gaussian random variable (GRV): it can be seen as an uncertain GFN or as a fuzzy GRV.
- Formally: a GRFN with mean μ , variance σ^2 and precision h is a RFS $\widetilde{X} : \Omega \mapsto [0, 1]^{\mathbb{R}}$ defined as $\widetilde{X}(\omega) = \operatorname{GFN}(M(\omega), h)$ where $M \sim N(\mu, \sigma^2)$. We write $\widetilde{X} \sim \widetilde{N}(\mu, \sigma^2, h)$.

³T. Denœux. Fuzzy Sets and Systems 453:1–36, 2023

Special cases

- If h = 0, $\widetilde{X}(\omega) = \mathbb{R}$ for all ω : \widetilde{X} induces the vacuous belief function on \mathbb{R} ; it represents complete ignorance
- If $h = +\infty$, \widetilde{X} is equivalent to a GRV with mean μ and variance σ^2 :

$$\widetilde{N}(\mu, \sigma^2, +\infty) = N(\mu, \sigma^2)$$

• If $\sigma^2 = 0$, \widetilde{X} is equivalent to a Gaussian possibility distribution:

 $\widetilde{N}(\mu, 0, h) = GFN(\mu, h)$

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Contour function



• The contour function of \widetilde{X} is

$$pl_{\widetilde{X}}(x) = rac{1}{\sqrt{1+h\sigma^2}} \exp\left(-rac{h(x-\mu)^2}{2(1+h\sigma^2)}
ight)$$

• Remarks: (1) for all x, $pI_{\widetilde{X}}(x) \to 0$ when $\sigma^2 \neq 0$ and $h \to \infty$; (2) when $\sigma^2 = 0$, $pI_{\widetilde{X}}$ is the possibility distribution of $\widetilde{X} \sim GFN(\mu, h)$.

Belief and plausibility of intervals

$$\begin{aligned} Bel_{\widetilde{X}}([x,y]) &= \Phi\left(\frac{y-\mu}{\sigma}\right) - \Phi\left(\frac{x-\mu}{\sigma}\right) - \\ pl_{\widetilde{X}}(x) \left[\Phi\left(\frac{(x+y)/2-\mu}{\sigma\sqrt{h\sigma^2+1}}\right) - \Phi\left(\frac{x-\mu}{\sigma\sqrt{h\sigma^2+1}}\right) \right] - \\ pl_{\widetilde{X}}(y) \left[\Phi\left(\frac{y-\mu}{\sigma\sqrt{h\sigma^2+1}}\right) - \Phi\left(\frac{(x+y)/2-\mu}{\sigma\sqrt{h\sigma^2+1}}\right) \right] \end{aligned}$$

$$\begin{aligned} \mathsf{Pl}_{\widetilde{X}}([x,y]) &= \Phi\left(\frac{y-\mu}{\sigma}\right) - \Phi\left(\frac{x-\mu}{\sigma}\right) + \mathsf{pl}_{\widetilde{X}}(x)\Phi\left(\frac{x-\mu}{\sigma\sqrt{h\sigma^2+1}}\right) + \\ \mathsf{pl}_{\widetilde{X}}(y)\left[1 - \Phi\left(\frac{y-\mu}{\sigma\sqrt{h\sigma^2+1}}\right)\right] \end{aligned}$$

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Lower and upper distribution functions



In particular, the lower and upper cdfs of $\widetilde{X}\sim \widetilde{\textit{N}}(\mu,\sigma^2,h)$ are

$$\mathsf{Bel}_{\widetilde{X}}((-\infty,y]) = \Phi\left(rac{y-\mu}{\sigma}
ight) - \mathsf{pl}_{\widetilde{X}}(y)\Phi\left(rac{y-\mu}{\sigma\sqrt{h\sigma^2+1}}
ight)$$

and

$$Pl_{\widetilde{X}}((-\infty, y]) = \Phi\left(\frac{y-\mu}{\sigma}\right) + pl_{\widetilde{X}}(y)\left[1 - \Phi\left(\frac{y-\mu}{\sigma\sqrt{h\sigma^2 + 1}}\right)\right].$$

Combination of GRFNs



Given two GRFNs $\widetilde{X}_1 \sim \widetilde{N}(\mu_1, \sigma_1^2, h_1)$ and $\widetilde{X}_2 \sim \widetilde{N}(\mu_2, \sigma_2^2, h_2)$, we have

$$\widetilde{X}_1 \oplus \widetilde{X}_2 \sim \widetilde{N}(\widetilde{\mu}_{12}, \widetilde{\sigma}_{12}^2, h_1 + h_2)$$

(Equations on next slide)

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Combination of GRFNs

Equations⁴

$$\widetilde{\mu}_{12} = \frac{h_1\widetilde{\mu}_1 + h_2\widetilde{\mu}_2}{h_1 + h_2}, \quad \widetilde{\sigma}_{12}^2 = \frac{h_1^2\widetilde{\sigma}_1^2 + h_2^2\widetilde{\sigma}_2^2 + 2\rho h_1 h_2\widetilde{\sigma}_1\widetilde{\sigma}_2}{(h_1 + h_2)^2}$$

with

$$\begin{split} \widetilde{\mu}_{1} &= \frac{\mu_{1}(1 + \overline{h}\sigma_{2}^{2}) + \mu_{2}\overline{h}\sigma_{1}^{2}}{1 + \overline{h}(\sigma_{1}^{2} + \sigma_{2}^{2})}, \quad \widetilde{\mu}_{2} &= \frac{\mu_{2}(1 + \overline{h}\sigma_{1}^{2}) + \mu_{1}\overline{h}\sigma_{2}^{2}}{1 + \overline{h}(\sigma_{1}^{2} + \sigma_{2}^{2})}\\ \widetilde{\sigma}_{1}^{2} &= \frac{\sigma_{1}^{2}(1 + \overline{h}\sigma_{2}^{2})}{1 + \overline{h}(\sigma_{1}^{2} + \sigma_{2}^{2})}, \quad \widetilde{\sigma}_{2}^{2} &= \frac{\sigma_{2}^{2}(1 + \overline{h}\sigma_{1}^{2})}{1 + \overline{h}(\sigma_{1}^{2} + \sigma_{2}^{2})}\\ \rho &= \frac{\overline{h}\sigma_{1}\sigma_{2}}{\sqrt{(1 + \overline{h}\sigma_{1}^{2})(1 + \overline{h}\sigma_{2}^{2})}} \quad \text{and} \quad \overline{h} = \frac{h_{1}h_{2}}{h_{1} + h_{2}} \end{split}$$

⁴T. Denœux. Reasoning with fuzzy and uncertain evidence using epistemic random fuzzy sets: general framework and practical models. *Fuzzy Sets and Systems*:453:1-36, 2023 = -9

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Classical frameworks

- Random sets and DS theory
- Fuzzy sets and possibility theory

2 Random fuzzy sets

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- Gaussian random fuzzy vectors

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Gaussian fuzzy vectors



A *p*-dimensional Gaussian fuzzy vector (GFV) with mode $\boldsymbol{m} \in \mathbb{R}^{p}$ and symmetric and positive semidefinite precision matrix $\boldsymbol{H} \in \mathbb{R}^{p \times p}$ is defined as the fuzzy subset of \mathbb{R}^{p} with membership function

$$\varphi(\mathbf{x}; \mathbf{m}, \mathbf{H}) = \exp\left(-\frac{1}{2}(\mathbf{x} - \mathbf{m})^T \mathbf{H}(\mathbf{x} - \mathbf{m})\right).$$

It is denoted as $GFV(\boldsymbol{m}, \boldsymbol{H})$.

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Product intersection of GFVs



$$\mathsf{GFV}(\boldsymbol{m}_1, \boldsymbol{H}_1) \odot \mathsf{GFV}(\boldsymbol{m}_2, \boldsymbol{H}_2) = \mathsf{GFV}(\boldsymbol{m}_{12}, \boldsymbol{H}_{12}),$$

with

$$m_{12} = (H_1 + H_2)^{-1}(H_1m_1 + H_2m_2)$$
 and $H_{12} = H_1 + H_2$.

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Gaussian random fuzzy vectors



A Gaussian random fuzzy vector (GRFV) $\widetilde{X} \sim \widetilde{N}(\mu, \Sigma, H)$ with covariance matrix Σ and precision matrix H is random fuzzy set $\widetilde{X} : \Omega \to [0, 1]^{\mathbb{R}^{\rho}}$ defined as

$$\widetilde{X}(\omega) = \mathsf{GFV}(oldsymbol{M}(\omega),oldsymbol{H}) \hspace{0.3cm} ext{with} \hspace{0.3cm}oldsymbol{M} \sim \mathcal{N}(oldsymbol{\mu},oldsymbol{\Sigma})$$

Combination of GRFVs



Let $\widetilde{X}_1 \sim \widetilde{N}(\mu_1, \boldsymbol{\Sigma}_1, \boldsymbol{H}_1)$ and $\widetilde{X}_2 \sim \widetilde{N}(\mu_2, \boldsymbol{\Sigma}_2, \boldsymbol{H}_2)$ be two independent GRFVs such that matrices $\boldsymbol{\Sigma}_1, \boldsymbol{\Sigma}_2, \boldsymbol{H}_1$ and \boldsymbol{H}_2 are all positive definite. We have

$$\widetilde{X}_1 \oplus \widetilde{X}_2 \sim \widetilde{N}(\widetilde{\mu}_{12}, \widetilde{\boldsymbol{\Sigma}}_{12}, \boldsymbol{H}_1 + \boldsymbol{H}_2)$$

(Equations on next slide)

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Combination of GRFVs Equations⁵

$$\widetilde{\mu}_{12} = \boldsymbol{A}\widetilde{\mu}$$
 and $\widetilde{\boldsymbol{\Sigma}}_{12} = \boldsymbol{A}\widetilde{\boldsymbol{\Sigma}}\boldsymbol{A}^{\mathsf{T}}$

where **A** is the constant $p \times 2p$ matrix defined as

$$oldsymbol{A} = oldsymbol{H}_{12}^{-1} egin{pmatrix} oldsymbol{H}_1 & oldsymbol{H}_2 \end{pmatrix}$$

$$\widetilde{\boldsymbol{\Sigma}} = \begin{pmatrix} \boldsymbol{\Sigma}_1^{-1} + \overline{\boldsymbol{H}} & -\overline{\boldsymbol{H}} \\ -\overline{\boldsymbol{H}} & \boldsymbol{\Sigma}_2^{-1} + \overline{\boldsymbol{H}} \end{pmatrix}^{-1}$$

$$\widetilde{\mu} = \begin{pmatrix} \overline{H}^{-1} \Sigma_1^{-1} + I_p & -I_p \\ -I_p & \overline{H}^{-1} \Sigma_2^{-1} + I_p \end{pmatrix} \begin{pmatrix} \overline{H}^{-1} \Sigma_1^{-1} & \mathbf{0} \\ \mathbf{0} & \overline{H}^{-1} \Sigma_2^{-1} \end{pmatrix} \begin{pmatrix} \mu_1 \\ \mu_2 \end{pmatrix}$$

and

$$\overline{\boldsymbol{H}} = (\boldsymbol{H}_1^{-1} + \boldsymbol{H}_2^{-1})^{-1}.$$

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 $^{^{5}}$ T. Denœux. Reasoning with fuzzy and uncertain evidence using epistemic random fuzzy sets: general framework and practical models. *Fuzzy Sets and Systems*:453:1=36, 2023 \ge \circ

Extension of the GRFN model

- The GRFN model can be extended to allow the definition of random fuzzy numbers and vectors with
 - Different supports ([a, b], [$a, +\infty$), probability simplex, etc.)
 - Different "shapes" (skewed, heavy-tailed etc.)

while maintaining the closure property under the product-intersection rule.

- This can be achieved by composing a RFS X̃ : Ω → [0,1]^Θ with a one-to-one mapping from Θ to another space Λ, to obtain a a RFS Ỹ : Ω → [0,1]^Λ.
- More details in my paper "Belief Functions on the Real Line defined by Transformed Gaussian Random Fuzzy Numbers" to be presented on Tuesday, August 15, session "Fuzzy Machine Learning", 8:00-10:00, Room #113.

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Evidential Machine Learning



- Evidential Machine Learning (ML): an approach to ML in which uncertainty is quantified by belief functions.
- Previous work has mainly focussed on clustering and classification because these learning tasks only require belief functions on finite frames.
- With models for defining and combining belief functions on continuous frames, it is now possible to tackle other learning tasks, such as regression.

The ENNreg model

- We consider a regression problem: the task is to predict a continuous random response variable Y from p input variables X = (X₁,..., X_p), based on a learning set {(x_i, y_i)}ⁿ_{i=1}.
- We propose a neural network model⁶ (ENNreg), which for an observed input vector $\mathbf{X} = \mathbf{x}$ computes a GRFN $\widetilde{Y}(\mathbf{x})$ with associated belief function $Bel_{\widetilde{Y}(\mathbf{x})}$ representing uncertainty about Y.
- ENNreg is based on prototypes. The distances to the prototypes are treated as independent pieces of evidence about the response and are combined by the product-intersection rule

⁶T. Denœux. Quantifying Prediction Uncertainty in Regression using Random Fuzzy Sets: the ENNreg model. *IEEE Transactions on Fuzzy Systems*, 2023. a + () + (

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Propagation equations (1/2)

- Let w_1, \ldots, w_K denote K vectors in the *p*-dimensional input space, called prototypes.
- The similarity between input vector \boldsymbol{x} and prototype \boldsymbol{w}_k is measured by

$$s_k(\mathbf{x}) = \exp(-\gamma_k^2 \|\mathbf{x} - \mathbf{w}_k\|^2)$$

where $\gamma_k > 0$ is a scale parameter.

• The evidence from prototype \boldsymbol{w}_k is represented by a GRFN

$$\widetilde{Y}_k(oldsymbol{x})\sim \widetilde{N}(\mu_k(oldsymbol{x}),\sigma_k^2,oldsymbol{s}_k(oldsymbol{x})h_k)$$

where σ_k^2 and h_k are variance and precision parameters, and

$$\mu_k(\mathbf{x}) = \boldsymbol{\beta}_k^T \mathbf{x} + \beta_{k0}$$

where β_k is a *p*-dimensional vector of coefficients, and β_{k0} is a scalar parameter.

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Propagation equations (2/2)

• The output $\widetilde{Y}(x)$ for input x is computed as

$$\widetilde{Y}(\boldsymbol{x}) = \widetilde{Y}_1(\boldsymbol{x}) \boxplus \ldots \boxplus \widetilde{Y}_{\mathcal{K}}(\boldsymbol{x})$$

where \boxplus denotes product intersection without the normalization step (to simplify calculations).

• We have $\widetilde{Y}(\boldsymbol{x}) \sim \widetilde{\textit{N}}(\mu(\boldsymbol{x}), \sigma^2(\boldsymbol{x}), h(\boldsymbol{x}))$, with

$$\mu(\mathbf{x}) = \frac{\sum_{k=1}^{K} s_k(\mathbf{x}) h_k \mu_k(\mathbf{x})}{\sum_{k=1}^{K} s_k(\mathbf{x}) h_k}$$

$$\sigma^{2}(\boldsymbol{x}) = \frac{\sum_{k=1}^{K} s_{k}^{2}(\boldsymbol{x}) h_{k}^{2} \sigma_{k}^{2}}{\left(\sum_{k=1}^{K} s_{k}(\boldsymbol{x}) h_{k}\right)^{2}} \text{ and } h(\boldsymbol{x}) = \sum_{k=1}^{K} s_{k}(\boldsymbol{x}) h_{k}$$

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Neural network architecture



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Negative log-likelihood loss (probabilistic forecasts)

• In the case of a probabilistic forecast with pdf \hat{f} , we typically measure the prediction error (or loss) by the negative log-likelihood

$$\mathcal{L}(y,\widehat{f}) = -\ln \widehat{f}(y)$$

• We actually never observe a real number y with infinite precision, but an interval $[y]_{\epsilon} = [y - \epsilon, y + \epsilon]$ centered at y. The probability of that interval is

$$\widehat{P}([y]_{\epsilon}) = \widehat{F}(y+\epsilon) - \widehat{F}(y-\epsilon) \approx 2\widehat{f}(y)\epsilon,$$

So, $\mathcal{L}(y, \hat{f}) = -\ln \widehat{P}([y]_{\epsilon}) + \text{cst.}$

• Generalization in the case of prediction in the form of a belief function?

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Extension

- $\mathcal{L}_{\epsilon}(y, \widetilde{Y}) = -\ln Bel_{\widetilde{Y}}([y]_{\epsilon})$ does not work (does not reward imprecision).
- $\mathcal{L}_{\epsilon}(y, \widetilde{Y}) = -\ln Pl_{\widetilde{Y}}([y]_{\epsilon})$ also does not work (minimized when \widetilde{Y} is vacuous). Proposal:

$$\mathcal{L}_{\lambda,\epsilon}(y,\widetilde{Y}) = -\lambda \ln \operatorname{Bel}_{\widetilde{Y}}([y]_{\epsilon}) - (1-\lambda) \ln \operatorname{Pl}_{\widetilde{Y}}([y]_{\epsilon})$$

with $\lambda \in [0, 1]$ and $\epsilon > 0$.

• Smaller values of λ correspond to more cautious predictions.

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Influence of λ



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Training

• The network is training by minimizing the regularized average loss

$$C_{\lambda,\epsilon,\xi,\rho}^{(R)}(\Psi) = \underbrace{\frac{1}{n} \sum_{i=1}^{n} \mathcal{L}_{\lambda,\epsilon}(y_i, \widetilde{Y}(\boldsymbol{x}_i; \Psi))}_{C_{\lambda,\epsilon}(\Psi)} + \underbrace{\frac{\xi}{K} \sum_{k=1}^{K} h_k}_{R_1(\Psi)} + \underbrace{\frac{\rho}{K} \sum_{k=1}^{K} \gamma_k^2}_{R_2(\Psi)},$$

where

- \triangleright $R_1(\Psi)$ has the effect of reducing the number of prototypes used for the prediction (setting $h_k = 0$ amounts to discarding prototype k)
- $R_2(\Psi)$ shrinks the solution towards a linear model (setting $\gamma_k = 0$ for all k vields a linear model).
- Heuristics: $\lambda = 0.9$, $\epsilon = 0.01 \hat{\sigma}_{Y}$, ξ and ρ tuned using a validation set or cross-validation.

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Calibration

- For any $\alpha \in (0,1]$, we define an α -level belief prediction interval (BPI) as an interval $\mathcal{B}_{\alpha}(\mathbf{x})$ centered at $\mu(\mathbf{x})$, such that $Bel_{\widetilde{Y}(\mathbf{x})}(\mathcal{B}_{\alpha}(\mathbf{x})) = \alpha$.
- The predictions will be said to be calibrated if, for all $\alpha \in (0, 1]$, α -level BPIs have a coverage probability at least equal to α , i.e.

$$\forall \alpha \in (0,1], \quad P_{\boldsymbol{X},Y} \left(Y \in \mathcal{B}_{\alpha}(\boldsymbol{X}) \right) \geq \alpha$$
(1)

- As in the probabilistic case, the calibration of evidential predictions can be checked graphically using a calibration plot (see infra).
- The precision output h(x) can be multiplied by a constant c > 0 to ensure (1) with predictions as precise as possible.

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Example

We consider iid data with one-dimensional input $X \sim \text{Unif}(-2,2)$ and

$$Y = X + (\sin 3X)^3 + \frac{X+2}{4\sqrt{2}}U, \quad U \sim N(0,1)$$



- Learning and validation sets of size n = 300.
- Network with *K* = 30 prototypes initialized by the k-means algorithm.
- ξ and ρ determined by minimizing the validation MSE.
- Shown: expected values μ(x) (red) with BPIs at levels 0.5, 0.9 and 0.99

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Calibration curves



Calibration curves for the probabilistic PIs $\mu(x) \pm u_{(1+\alpha)/2}\sigma(x)$ (in blue) and the BPIs (in red)

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Data sets

	п	р	response
Boston	506	13	medv
Energy	768	8	Y2
Concrete	1030	8	strength
Yacht	308	6	Y
Wine	1599	11	quality
kin8nm	8192	8	V9
Crime	1994	100	ViolentCrimesPerPop
Residential	372	103	V10
Airfoil	1503	5	Y
Bike	731	9	cnt

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Comparison with classical methods (RMS)

	ENNreg	RBF	RVM	SVM	GP	RF	MLP
Boston	$\textbf{2.87} \pm \textbf{0.14}$	3.31 ± 0.19	3.42 ± 0.17	3.17 ± 0.15	3.70 ± 0.22	$\textbf{3.11} \pm \textbf{0.14}$	$\textbf{3.14} \pm \textbf{0.14}$
Energy	1.06 ± 0.05	2.06 ± 0.08	1.79 ± 0.05	1.39 ± 0.06	2.58 ± 0.07	1.75 ± 0.06	$\textbf{0.95} \pm \textbf{0.16}$
Concr.	5.10 ± 0.12	6.30 ± 0.19	6.38 ± 0.16	5.62 ± 0.13	6.93 ± 0.13	$\textbf{4.64} \pm \textbf{0.12}$	$\textbf{4.82} \pm \textbf{0.16}$
Yacht	$\textbf{0.44}\pm\textbf{0.04}$	2.00 ± 0.20	1.88 ± 0.20	1.93 ± 0.11	6.12 ± 0.31	0.96 ± 0.08	0.50 ± 0.05
Wine	0.63 ± 0.01	0.63 ± 0.01	0.80 ± 0.02	0.61 ± 0.01	0.61 ± 0.01	$\textbf{0.56} \pm \textbf{0.01}$	0.77 ± 0.01
kin8nm	0.08 ± 0.00	0.11 ± 0.00	_	0.09 ± 0.00	0.08 ± 0.00	0.14 ± 0.00	$\textbf{0.07} \pm \textbf{0.00}$
Crime	$\textbf{0.14}\pm\textbf{0.00}$	0.14 ± 0.00	$\textbf{0.14}\pm\textbf{0.00}$	$\textbf{0.14}\pm\textbf{0.00}$	$\textbf{0.14}\pm\textbf{0.00}$	$\textbf{0.14}\pm\textbf{0.00}$	$\textbf{0.14} \pm \textbf{0.00}$
Resid.	$\textbf{0.11}\pm\textbf{0.01}$	0.16 ± 0.01	0.17 ± 0.01	0.15 ± 0.01	0.22 ± 0.01	0.16 ± 0.01	0.14 ± 0.01
Airfoil	$\textbf{1.46} \pm \textbf{0.03}$	1.70 ± 0.04	2.58 ± 0.04	2.37 ± 0.04	2.49 ± 0.04	$\textbf{1.44}\pm\textbf{0.04}$	1.53 ± 0.04
Bike	$\textbf{6.59} \pm \textbf{0.19}$	$\textbf{6.49} \pm \textbf{0.15}$	$\textbf{6.64} \pm \textbf{0.14}$	7.11 ± 0.16	7.55 ± 0.14	6.86 ± 0.17	9.68 ± 0.20

Comparison with SOTA methods (RMS & NLL)

	RMS					
	ENNreg	PBP	MC-dropout	Deep ens.	Deep ev. reg.	
Boston	$\textbf{2.87} \pm \textbf{0.14}$	$\textbf{3.01} \pm \textbf{0.18}$	$\textbf{2.97} \pm \textbf{0.19}$	$\textbf{3.28} \pm \textbf{1.00}$	$\textbf{3.06} \pm \textbf{0.16}$	
Energy	$\textbf{1.06} \pm \textbf{0.05}$	1.80 ± 0.05	1.66 ± 0.04	2.09 ± 0.29	2.06 ± 0.10	
Concr.	$\textbf{5.10} \pm \textbf{0.12}$	5.67 ± 0.09	$\textbf{5.23} \pm \textbf{0.12}$	6.03 ± 0.58	5.85 ± 0.15	
Yacht	$\textbf{0.44} \pm \textbf{0.04}$	1.02 ± 0.05	1.11 ± 0.09	1.58 ± 0.48	1.57 ± 0.56	
Wine	$\textbf{0.63} \pm \textbf{0.01}$	$\textbf{0.64} \pm \textbf{0.01}$	$\textbf{0.62} \pm \textbf{0.01}$	$\textbf{0.64} \pm \textbf{0.04}$	$\textbf{0.61} \pm \textbf{0.02}$	
kin8nm	$\textbf{0.08} \pm \textbf{0.00}$	0.10 ± 0.00	0.10 ± 0.00	0.09 ± 0.00	0.09 ± 0.00	

	NLL					
	ENNreg	PBP	MC-dropout	Deep ens.	Deep ev. reg.	
Boston	2.53 ± 0.07	2.57 ± 0.09	$\textbf{2.46} \pm \textbf{0.06}$	$\textbf{2.41} \pm \textbf{0.25}$	$\textbf{2.35} \pm \textbf{0.06}$	
Energy	$\textbf{1.14} \pm \textbf{0.07}$	2.04 ± 0.02	1.99 ± 0.02	$\textbf{1.38} \pm \textbf{0.22}$	1.39 ± 0.06	
Concr.	3.38 ± 0.13	3.16 ± 0.02	$\textbf{3.04} \pm \textbf{0.02}$	$\textbf{3.06} \pm \textbf{0.18}$	$\textbf{3.01} \pm \textbf{0.02}$	
Yacht	$\textbf{0.13} \pm \textbf{0.12}$	1.63 ± 0.02	1.55 ± 0.03	1.18 ± 0.21	$1.03\ {\pm}0.19$	
Wine	$\textbf{0.94} \pm \textbf{0.01}$	0.97 ± 0.01	$\textbf{0.93} \pm \textbf{0.01}$	$\textbf{0.94} \pm \textbf{0.12}$	$\textbf{0.89} \pm \textbf{0.05}$	
kin8nm	-1.19 \pm 0.00	-0.90 \pm 0.01	-0.95 \pm 0.01	-1.20 \pm 0.02	$\textbf{-1.24}\pm0.01$	

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Calibration plots



Probabilistic predictions (blue), raw evidential predictions (red) and adjusted evidential predictions (green).

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Calibration plots



Probabilistic predictions (blue), raw evidential predictions (red) and adjusted evidential predictions (green).

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Summary

- The theory of epistemic RFSs is a very general framework, generalizing both possibility theory and DS theory. It allows one to represent and reason with uncertain, imprecise and vague information.
- Practical models of RFNs and RFVs indexed by 3 parameters (mode, variance and precision) make it possible to define belief functions on continuous frames that can be easily manipulated and combined, overcoming a limitation of DS theory.
- The ENNreg model is a regression neural network based on the combination of GRFNs. The network output for input vector **x** is a GRFN defined by three numbers:
 - a point prediction $\mu(\mathbf{x})$
 - a variance $\sigma^2(\mathbf{x})$ measuring random uncertainty
 - a precision h(x) representing epistemic uncertainty
- Experimental results show that ENNreg performs as well as, or better than state-of-the-art regression methods, while providing conservative (cautious) predictions.

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