

The University of Osaka

Aggregation functions

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Motivation

- Aggregation functions
 - Link between aggregation functions and fuzzy measures
 - Non-additive measures also correspond to monotonic games (in the game theoretic sense / cooperative game theory)
- I will discuss two type of tools
 - Υ -values, with relation to Shapley values
as a tool for explainability and to approximate measures
 - Optimal Transport Problem / Wasserstein metric

Outline

1. Aggregation functions
2. Non-additive measures and games
3. Shapley and Υ Values
 - Shapley value
 - Υ values
 - Shapley vs. Υ -values
 - Approximation using distorted probabilities
4. Υ -values and explainability
5. Optimal transport problem
 - The classical problem: for probabilities
 - Our problem: for non-additive measures

Aggregation functions

Some preliminaries

Aggregation functions

- Aggregation functions for numerical data:

$\mathbb{C}(a_1, \dots, a_n)$ for $a_i \in [0, 1]$

- Monotonicity:

$$\mathbb{C}(a_1, \dots, a_n) \leq \mathbb{C}(b_1, \dots, b_n) \text{ if } a_i \leq b_i$$

- Boundary condition:

$$\mathbb{C}(a, \dots, a) = a \text{ (for all or some } a)$$

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- Choquet integral: ...

Aggregation functions

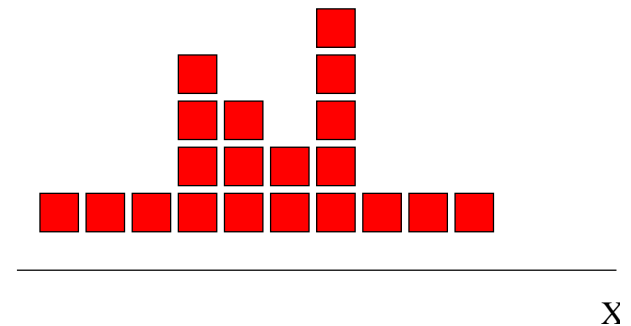
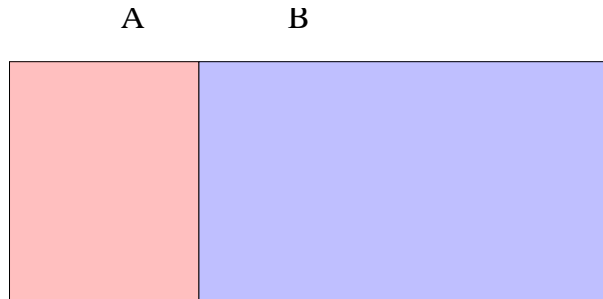
- Considerations on the weights and the aggregation functions
 - Weighted mean:
 - ▷ the weights can be seen/are a probability distribution
 - The mean is the expected value w.r.t. this probability distribution
 - The measure/probability for a set A , $\mu(A) = \sum_{x \in A} p(x)$.
 - OWA, WOWA, Choquet integral:
 - ▷ We will come back to this

Non-additive measures and games

(standard) Measures

- Axioms/requirements: set functions: $\mu(A)$ for $A \subseteq X$
 - $\mu(\emptyset) = 0$
 - $\mu(X) = 1$
 - $\mu(A \cup B) = \mu(A) + \mu(B)$ if $A \cap B = \emptyset$

- Examples:
 - Probabilities (with $\mu(X) = 1$)
 - Surface area



Non-additive measures

- Non-additive (fuzzy) measures/monotonic games/capacities are set functions: $\mu(A)$ for $A \subseteq X$
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 - We may have (positive/negative) interactions/synergies
 - ▷ $\mu(A \cup B) > \mu(A) + \mu(B)$
 - or
 - ▷ $\mu(A \cup B) < \mu(A) + \mu(B)$

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 - We may have (positive/negative) interactions/synergies
 - ▷ $\mu(A \cup B) > \mu(A) + \mu(B)$
 - or
 - ▷ $\mu(A \cup B) < \mu(A) + \mu(B)$
 - and it is also possible (for disjoint A, B, C)
 - ▷ $\mu(A) < \mu(B)$ but then $\mu(A \cup C) > \mu(B \cup C)$

Non-additive measures

- Families of measures

- Additive measures $\mu(A \cup B) = \mu(A) + \mu(B)$ (for $A \cap B = \emptyset$)

- Symmetric measures

$$\mu(A) = m(|A|)$$

- Distorted probabilities

$$\mu(A) = f(P(A))$$

- m -dimensional distorted probabilities

- Hierarchically decomposable fuzzy measures

- Arbitrary non-additive measures

Non-additive measures

- Families of measures

- The *number* of distorted probabilities is a **small proportion** of arbitrary non-additive measures.

- Number, in terms of **possible orders**

(Honda et al. 2002; Narukawa, Torra, 2005)

- ▷ Let $X = \{1, 2, \dots, m\}$ we take $\mu(\{1\}) < \mu(\{2\}) \cdots < \mu(\{m\})$.

- ▷ When $|X| = 2$, for DP 2 possible orderings, for arbitrary FM 2.

- ▷ When $|X| = 3$, for DP 2, for arbitrary FM 8. For DP only these orderings are possible:

$$\mu(\emptyset) < \mu(\{1\}) < \mu(\{2\}) < \mu(\{3\}) < \mu(\{1, 2\}) < \mu(\{1, 3\}) < \mu(\{2, 3\})$$

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- ▷ When $|X| = 4$, for DP 14, for arbitrary FM 70016

- ▷ When $|X| = 5$, for DP **546**, for arbitrary FM $\mathcal{O}(10^{12})$

Aggregation functions and measures

- Considerations on the weights and the aggregation functions
 - Weighted mean: weights as probability distributions (additive measures)
 - OWA, WOWA, Choquet integral:
 - ▷ OWA: **Symmetric measures**

$$\mu(A) = m(|A|)$$

- ▷ WOWA: **Distorted probabilities**

$$\mu(A) = f(P(A))$$

- ▷ Choquet integral: Arbitrary non-additive measure

Measures and games

- **games** are set functions: $\mu(A)$ for $A \subseteq X$
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- Example 1: Winning coalitions in a parliament (riksdagen)
 - X parties = V, S, MP, C, L, KD, M, SD (.SE 2022)
 - **game** for any coalition:
 - $\mu(\text{coalition}) = 1$ if and only if $\text{coalition} \geq 175$ seats
 - mandats = [24, 107, 18, 24, 16, 19, 68, 73]
349 seats, 175 are needed to pass a law

Two examples

- ▷ $\mu(\{V, S, MP, C, L, KD\}) = 1$
because $\text{sum}([24, 107, 18, 24, 16, 19]) = 208 \geq 175$
- ▷ $\mu(\{M\}) = 0$ because $\text{sum}([68]) = 68 < 175$

Measures and games

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- Explainability in AI: Game from a model in ML

Shapley and Υ Values

Motivation (to show)

- Given a game/non-additive measure μ
 - The Shapley value provides a **summary ϕ**
a summary $O(|X|)$ instead of μ on $O(2^X)$
- **Other summaries are possible?**
 - Υ -values are a summary

Motivation (to skip)

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- Motivation 1:
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 - Shapley are to a probability,
 - Υ are to symmetric measures

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- Motivation 1:
 - Shapley + numerical data is to expectation / weighted mean
 - Υ + numerical data is to linear combination of order statistics?
- Motivation 2:
 - Shapley are to a probability,
 - Υ are to symmetric measures
- All this revolves around the concept of non-additive measures (i.e., monotonic games)

Shapley value

Shapley value

- Given X ,
 - The set function μ
 - The Shapley value ϕ
- $\phi : X \rightarrow \mathbb{R}$
where $\phi(x)$ is the value associated to $x \in X$
 - The Shapley value is a power index
 - The Shapley value distributes the total gains to the players x ,
 - Shapley is an **approximation** of μ , or **summary** of μ for x
 - If μ is additive, the approximation is “perfect”
$$\mu(A) = \sum_{x \in A} \phi(x)$$
 - So, ϕ **removes interactions**

and the other value

Shapley and Υ -values

- The non-additive (fuzzy) measure perspective
 - Shapley is an approximation of μ ,
power of a variable/element in X

Shapley and Υ -values

- The non-additive (fuzzy) measure perspective
 - Shapley is an approximation of μ ,
power of a variable/element in X
 - Υ is an approximation of μ ,
power of the size of a set in X

Shapley and Υ -values

- The formula perspective. Preliminaries.
 - $A \prec B$ it means that $A \subset B$ and there are no other subsets of X between A and B .
 - **Maximal chain** on X :
 $\mathcal{C} = (C_0, C_1, \dots, C_n)$ with $C_i \subseteq X$ for $i = 1, \dots, n$.
Then, \mathcal{C} maximal chain of subsets of X if

$$\emptyset = C_0 \prec C_1 \prec \dots \prec C_{n-1} \prec C_n = X.$$

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- Example: $X = \{x_1, x_2, x_3, x_4\}$
 - $C_0 = \emptyset, C_1 = \{x_4\}, C_2 = \{x_4, x_1\}, C_3 = \{x_4, x_1, x_2\}, C_4 = X$

Shapley and Υ -values

- The formula perspective
 - Shapley is computed as

$$\begin{aligned}\phi_{x_i}(\mu) &= \sum_{S \subseteq N \setminus \{i\}} \frac{|S|! (n - |S| - 1)!}{n!} (\mu(S \cup \{i\}) - \mu(S)) \\ &= \frac{1}{n!} \sum_{C \in \mathcal{M}(X)} (\mu(C_{x_i} \cup \{x_i\}) - \mu(C_{x_i}))\end{aligned}$$

- Υ -values computed as

$$\begin{aligned}\Upsilon_i &= \frac{1}{|\mathcal{M}(X)|} \sum_{C \in \mathcal{M}(X)} (\mu(C_i) - \mu(C_{i-1})) \\ &= \frac{1}{n!} \sum_{C \in \mathcal{M}(X)} (\mu(C_i) - \mu(C_{i-1}))\end{aligned}$$

Υ -values and properties

Difference with Shapley

Υ -values: Properties

- Then, the properties:
 - An index $f : G^N \rightarrow \mathbb{R}^N$ satisfies the additivity, anonymity, the dummy player condition, and efficiency conditions if and only if f corresponds to the **the Shapley value**.

Υ -values: Properties

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- It was possible to **characterize** the Υ -values also (**Theorem 1¹**):
 - An index $f : G^N \rightarrow \mathbb{R}^N$ satisfies **additivity, absolute anonymity, dummy cardinality**, and **efficiency** if and only if f correspond to the Υ -values.

¹V. Torra (2024) Υ -values: power indices à la orness for non-additive measures, IEEEETFS.

Υ -values: Properties

- What are these properties and how they differ with Shapley?
 - Index f and **additivity**:
 - when for any pair of measures μ and ν on X it holds that

$$f(\mu + \nu) = f(\mu) + f(\nu).$$

- Property for both Shapley and Υ -values

Υ -values: Properties

- What are these properties and how they differ with Shapley?
 - Index f and **efficiency**:
 - when for any measure μ on X it holds

$$\sum_{i=1}^n f_i = \mu(X)$$

if $\mu(\emptyset) = 0$; otherwise the total is $\mu(X) - \mu(\emptyset)$.

- Property for both Shapley and Υ -values

Υ -values: Properties

- What are these properties and how they differ with Shapley?
 - Index f , dummy players and dummy cardinality:
 - **Dummy player** x : $\mu(S \cup \{x\}) = \mu(S) + \mu(\{x\})$
for all $S \subseteq (X \setminus \{x\})$.
 - **f dummy player property**: for all dummy players $x \in X$,
 $f_{i(x)}(\mu) = \mu(\{x\})$ for all measures μ .

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for all $|S \cup \{x\}| = i$, s.t. $S \subseteq (X \setminus \{x\})$, and h_i a constant.
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- Shapley: dummy player property; Υ : dummy cardinality

Υ -values: Properties

- What are these properties and how they differ with Shapley?
 - Index f , anonymity and absolute anonymity
 - f satisfies the **anonymity** property when given a permutation π on X , we have

$$f(\mu^\pi) = \pi^*(f(\mu))$$

where $\pi^*(x) = (\pi_{\pi(1)}^*(x), \dots, \pi_{\pi(|X|)}^*(x))$ and $\pi_{\pi(k)}^*(x) = x_K$.

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- Shapley: anonymity property; Υ : absolute anonymity property

Approximation using distorted probabilities

Summaries of μ , and approximations of μ

- Additive
 - If μ additive (e.g. probability), Shapley value is the probability
- Symmetric measures
 - if $\mu(A) = \mu(B)$ when $|A| = |B|$
(only set size matters)
 - Then, (characterization) there exist w_1, \dots, w_n such that

$$\mu(A) = \sum_{i=1}^{|A|} w_i$$
 - If μ is symmetric, $\Upsilon_i = w_i$
- If μ is a distorted probability,
approximation by $\Upsilon_i = w_i, P = \phi$

Summaries of μ , and approximations of μ

- How the approximation is built? $\mu' = f \circ P$
 - Compute $\langle \phi, \Upsilon \rangle$ from the measures
 - $P := \phi$ (i.e., ϕ represents the probabilities)
 - $w^*(\alpha) = f(k) = \sum_{i=1}^k w_i = \sum_{i=1}^k \Upsilon_i$
for $\alpha = |A|/|X| = k/n$
 - Complete w^* interpolating² the points already established.
 - $\mu' = w^* \circ \phi = f \circ P$.

- NOTE:
This is WOWA's interpolation approach from weights p and w .

²Interpolation with a continuous monotonic function

Approximations of μ as a way to visualize the measure

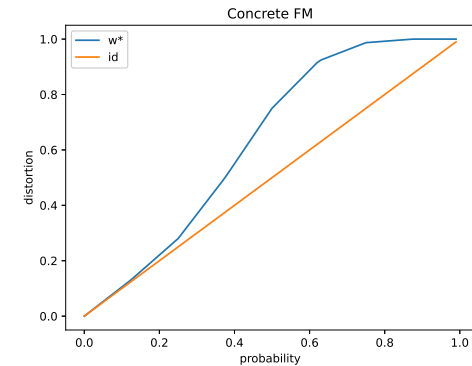
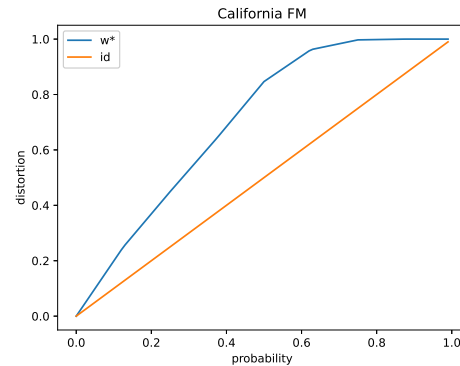
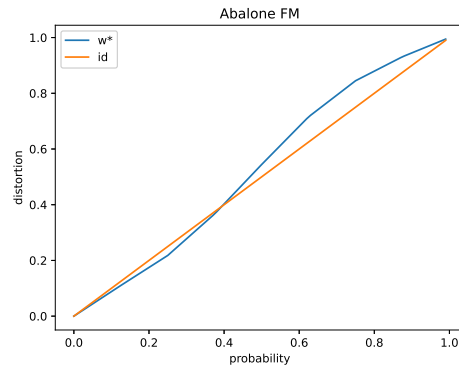
- Arbitrary non-additive measures are not easy to grasp
 - Measures are defined by $2^{|X|}$ values
 - Distorted probabilities are interpretable in terms of p and f
- Interpretation of an arbitrary measure through a distorted probability

Approximations of μ as a way to visualize the measure

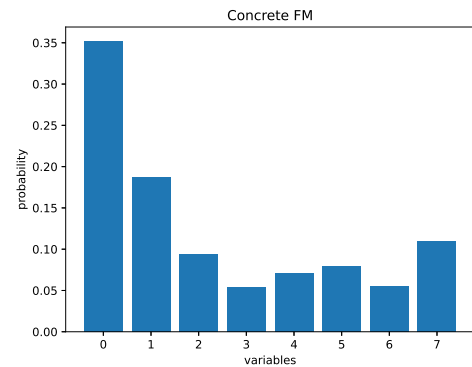
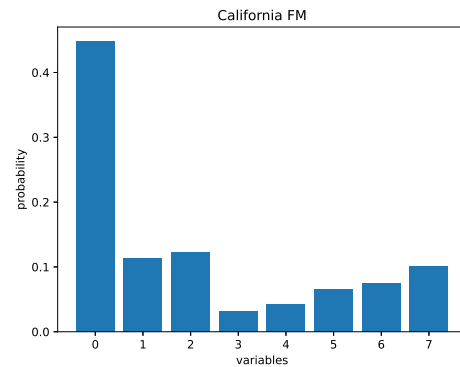
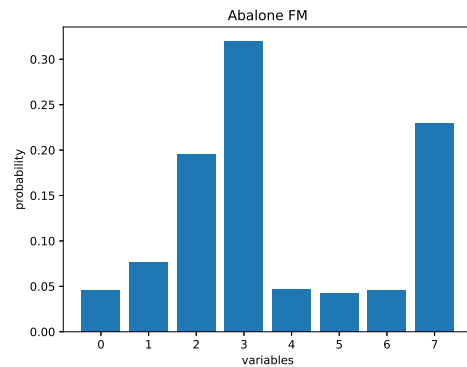
- Some examples.
 - Learn an arbitrary fuzzy measure (using a Choquet integral-based ML model)
 - Approximate the measure by a distorted probability
- Data used:
 - Abalone. 4177 records, 8 inputs, 1 output.
 - California. 20640 records, 8 inputs, 1 output.
 - Concrete. 1030 records, 8 inputs, 1 output.

Approximations of μ as a way to visualize the measure

Distortion functions w^* associated to Υ values.



Probability distributions associated to Shapley values.

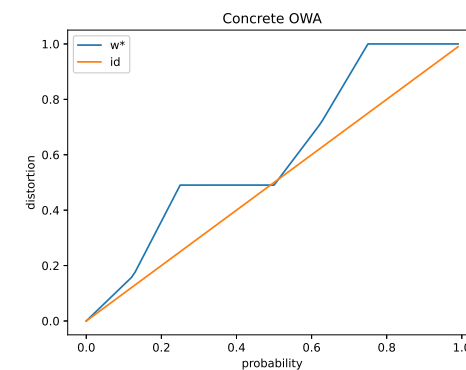
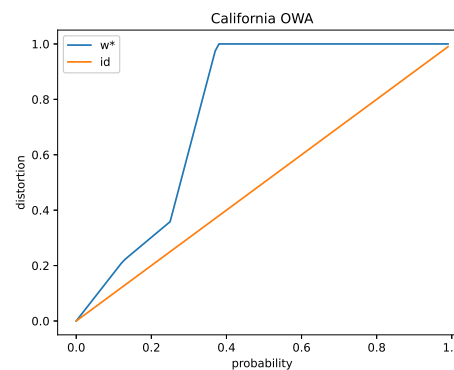
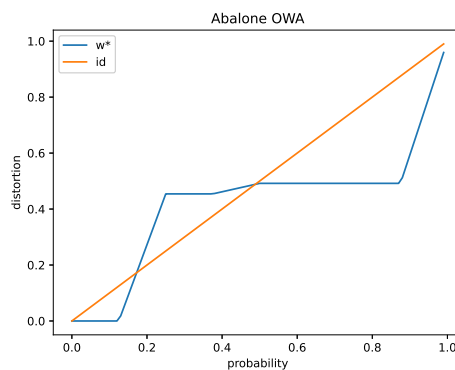


Approximations of μ as a way to visualize the measure

- Properties of the approximation (from ϕ and Υ)

Data set	orness Υ	orness w
Abalone	0.533	0.411
California	0.735	0.796
Concrete	0.653	0.621

Distortion functions w^* associated to **optimal OWA** parameters w .



Additive and symmetric measures

- If we compute $CI_\mu(f)$, approximations
 - through Shapley, (expectation) and the weighted mean

$$wm_\phi(f)$$

- through Υ , linear combination of order statistics (owa)

$$owa_\Upsilon(f)$$

Υ -values and explainability

Υ -values and explainability

- Model M at instance u
 - **Game:** $\mu(S) = M(u^S) - M(u^\emptyset)$
 - Shapley: compute ϕ_x relevance and importance for $x \in X$
 - $M(u) = \mu(X) + M(u^\emptyset) = \sum_x \phi_i(\mu) + M(u^\emptyset)$
 - Υ : compute Υ_i relevance and importance³ for i
 - ▷ $M(u) = \mu(X) + M(u^\emptyset) = \sum_i \Upsilon_i(\mu) + M(u^\emptyset)$
 - ▷ Also, a summary of the information in M at u .

³V.Torra, The complementary role of Shapley and Υ -values in explainability, submitted.

Υ -values and explainability

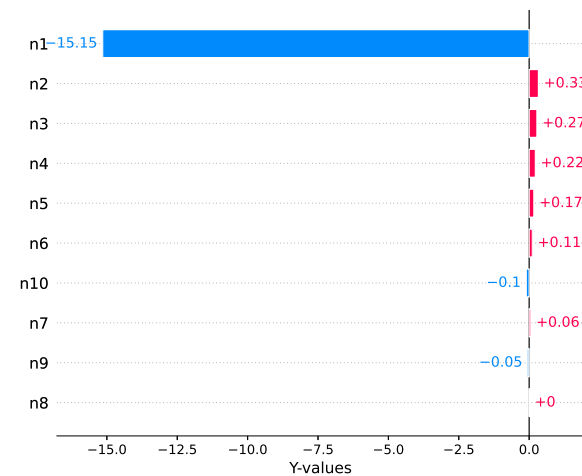
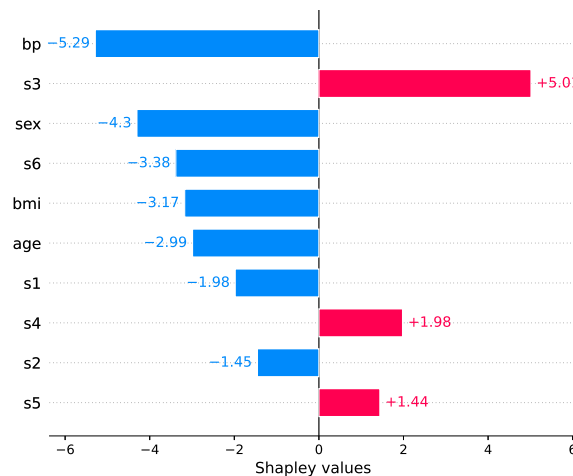
- Model M at instance u
 - **Game:** $\mu(S) = M(u^S) - M(u^\emptyset)$
 - Shapley: compute ϕ_x relevance and importance for $x \in X$
 - $M(u) = \mu(X) + M(u^\emptyset) = \sum_x \phi_i(\mu) + M(u^\emptyset)$
 - Υ : compute Υ_i relevance and importance³ for i
 - ▷ $M(u) = \mu(X) + M(u^\emptyset) = \sum_i \Upsilon_i(\mu) + M(u^\emptyset)$
 - ▷ Also, a summary of the information in M at u .
 - **Summary in Shapley \neq summary in Υ of the same model**

³V.Torra, The complementary role of Shapley and Υ -values in explainability, submitted.

Υ -values and explainability

- Examples

- Summary in Shapley \neq summary in Υ of the same model

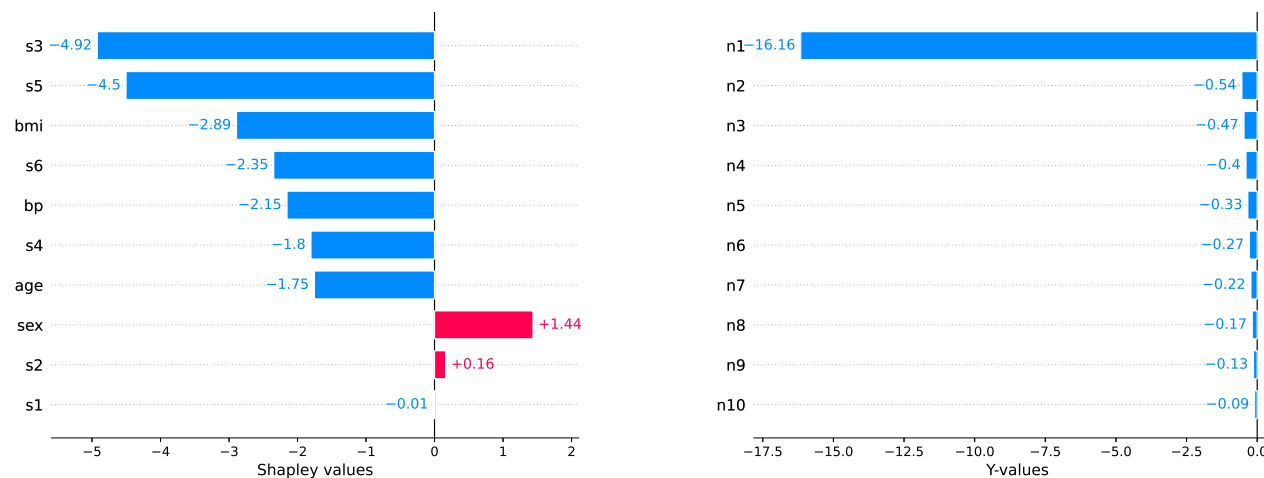


Shapley (left) and Υ -values (right) for a record of the Diabetes data set (record 1 in the test set) computed from a model extracted using SVM/SVR.

Υ -values and explainability

- Examples

- Summary in Shapley \neq summary in Υ of the same model

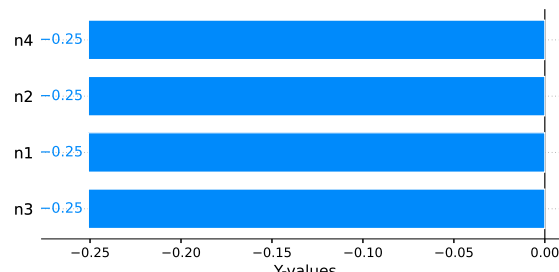


Shapley (left) and Υ -values (right) for a record of the Diabetes data set (record 4 in the test set) computed from a model extracted using SVM/SVR.

Υ -values and explainability

- Properties

- Summary in Shapley \neq summary in Υ of the same model
- Υ can show the (non-)linearity of the model, Shapley cannot
- If the model is linear,
 - ▷ Shapley = coefficients
 - ▷ $\Upsilon = 1/|X|$
- Example:



Explanations via Υ -values for a record in the Iris data set with output in class 1, and a linear regression model.

Optimal transport problem

Classical problem

- Optimal transport problem between two probabilities
- Wasserstein distance is based on the optimal transport

The classical problem: Optimal transport for probabilities

Classical problem

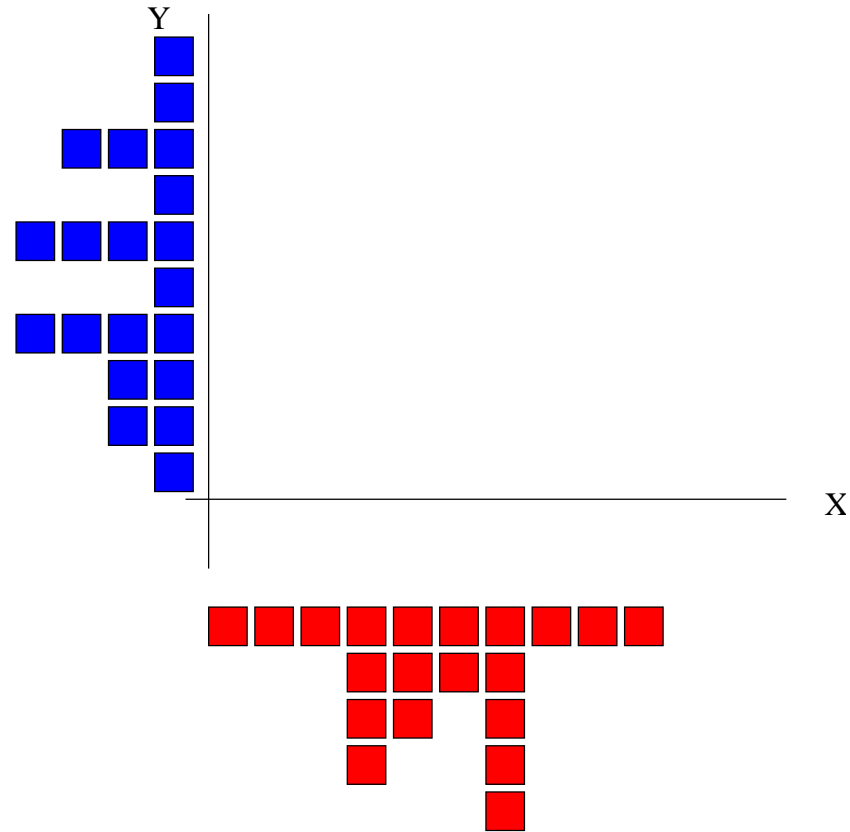
Optimal transport problem: The case of probabilities

- Inputs:
 - X , and probability measure P on X (with prob. dist. p)
 - Y , and probability measure Q on Y (with prob. dist. q)
(on X and subsets of X , assume X finite)
- Output:
 - Assignment from P to Q
 - A cost of the assignment: optimal

Classical problem

Optimal transport problem: The case of probabilities

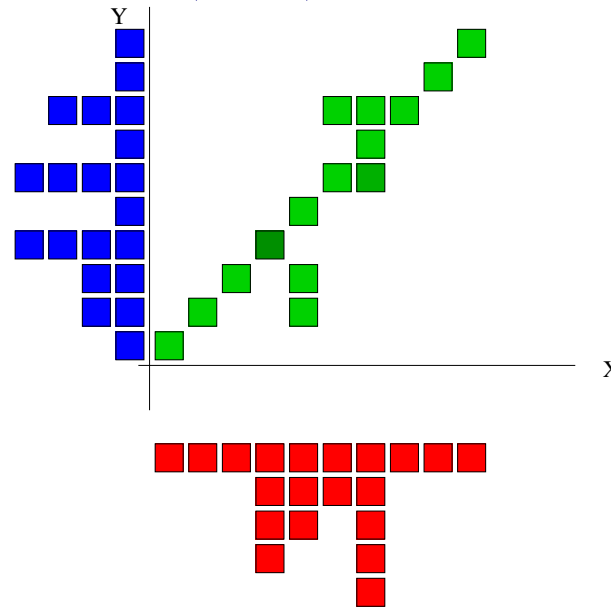
- Probability distributions on X and Y



Classical case

Optimal transport problem: The case of probabilities

- **Assignment** of probabilities $\gamma(x, y)$



- γ positive, and marginals should be p and q

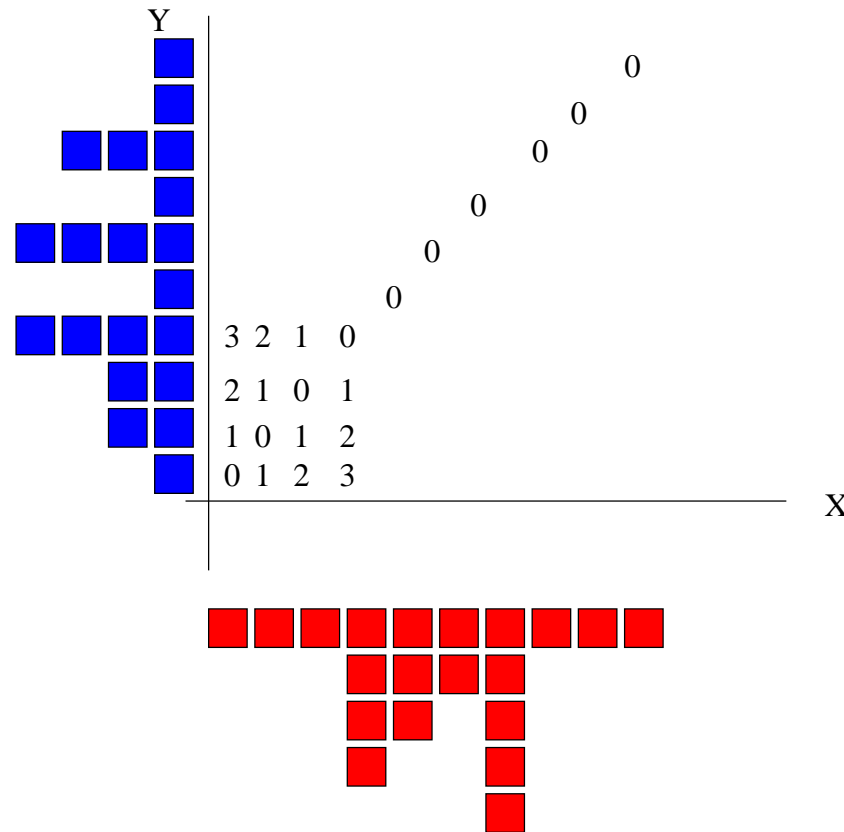
$$p(x) = \sum_{y \in Y} \gamma(x, y)$$

$$q(y) = \sum_{x \in X} \gamma(x, y)$$

Classical case

Optimal transport problem: a cost function

- $c : X \times Y \rightarrow \mathbb{R}^+$



- Cost: $\sum_{x \in X} \sum_{y \in Y} c(x, y) \gamma(x, y)$
- Distance: using **the assignment with minimum cost.**

Optimal transport and non-additive measures

Optimal transport

Optimal transport problem: The case of non-additive measures

- input:
 - X , and non-additive measure μ on X
 - Y , and non-additive measure ν on Y
- Output:
 - **Assignment** from μ to ν
 - A cost of the assignment: optimal

Optimal transport

How to proceed?

- **Option 0.** We consider a cost function on $X \times Y$ and a Choquet integral of measures on $X \times Y$ with marginals μ and ν .
 - For all non-additive measures in $X \times Y$, minimum CI

Optimal transport

How to proceed?

- **Option 0.** We consider a cost function on $X \times Y$ and a Choquet integral of measures on $X \times Y$ with marginals μ and ν .
 - For all non-additive measures in $X \times Y$, minimum CI
- The problem seems difficult in practice
 - The **Fubini theorem does not apply** in general for Choquet integral
 - **Margins, also Choquet integrals (?)**

Transforms

Measures and transforms: $\mu \leftrightarrow \tau_\mu$

- $(\max, +)$ -transform⁴

$$\tau_\mu(B) = \mu(B) - \max_{A \subset B} \mu(A)$$

- The $(\max, +)$ -transform is **always positive** in $[0,1]$
- If μ **additive** $\tau_\mu(B) = \min_{x_i \in B} \mu(\{x_i\})$.

⁴V. Torra, (Max, \oplus) -transforms and genetic algorithms for fuzzy measure identification, Fuzzy Sets and Systems 28 (2022) 253-265

Optimal transport

- **Option 3.** Definition through the $(max, +)$ -transform, cost $c_a : 2^X \times 2^X \rightarrow [0, 1]$
 - Find $assg : 2^X \times 2^X \rightarrow [0, 1]$ such that
 - ▷ $assg(\emptyset, \emptyset) = 0$
 - ▷ $\tau_\mu(A) = \sum_{B' \subseteq X} assg(A, B')$ for all $A \neq \emptyset$
 - ▷ $\tau_\nu(B) = \sum_{A' \subseteq X} assg(A', B)$ for all $B \neq \emptyset$
 - Cost of the assignment:
 - ▷ $cost(c_a, assg) = \sum_{A \subseteq X} \sum_{B \subseteq X} c_a(A, B) assg(A, B).$

Optimal transport

- **Option 3.** Then, we can define:
 - Optimal transport: Assignment **with minimal cost**
 - **Wasserstein-like discrepancy:**

$$d_{c_a}(\mu, \nu) = \inf_{assg \in \Pi(\tau_\mu, \tau_\nu)} \sum_{A \subseteq X} \sum_{B \subseteq X} c_a(A, B) assg(A, B)$$

Optimal transport

- **Option 3.** Example, μ is additive, ν is not, $(\max, +)$ -transforms τ_μ and τ_ν , feasible assignment:

$\nu(B)$	τ_ν	<i>set</i>	<i>lackν</i>							
1	0.8	X	0	0	0.3	0.5	0	0	0	0
0	0	$\{x_2, x_3\}$	0	0	0	0	0	0	0	0
0.2	0	$\{x_1, x_3\}$	0	0	0	0	0	0	0	0
0.2	0	$\{x_1, x_2\}$	0	0	0	0	0	0	0	0
0	0	$\{x_3\}$	0	0	0	0	0	0	0	0
0	0	$\{x_2\}$	0	0	0	0	0	0	0	0
0.2	0.2	$\{x_1\}$	0	0.2	0	0	0	0	0	0
<i>lackμ</i>		\emptyset	--	0	0	0	0.1	0.1	0.4	0.1
<i>set</i>			\emptyset	$\{x_1\}$	$\{x_2\}$	$\{x_3\}$	$\{x_1, x_2\}$	$\{x_1, x_3\}$	$\{x_2, x_3\}$	X
τ_μ	--		--	0.2	0.3	0.5	0.1	0.1	0.4	0.1
$\mu(A)$			--	0.2	0.3	0.5	0.4	0.6	0.9	1.0

Optimal transport

- Properties⁵:
 - This is a proper generalization
 - When our FM solution is a probability solution?
 - ▷ assignment on X, Y vs. assignment on $2^X, 2^Y$
 - ▷ cost on X, Y vs. cost on $2^X, 2^Y$
 - Results on
 - ▷ A cost function that is independent on the measures
 - ▷ A cost function that depends on the measures

⁵V. Torra (2023) The transport problem for non-additive measures, Euro. J Oper. Res. 311 679-689

Optimal transport

- **Implementation: Linear problem with linear constraints**
 - 1. Linear problem with linear constraints (case belief functions)
OT with 2^X variables
 - 2. Linear problem with linear constraints (case Möbius transform)
 Same but: transformation of $|t|$ into two additional constraints
 $+t \leq t', -t \leq t'$. So, **$2 \cdot 2^{2|X|}$ additional constraints**
 - 3. Linear problem with linear constraints (case $(\max, +)$ -transform)
OT with 2^X variables.
 Software: <http://www.mdai.cat/code/>
- ▷ What is an appropriate cost function?

Summary

Summary

- Tools for measures and games
 - Υ -values and their characterization
 - ϕ and Υ -values for explainability
 - Optimal transport problem for non-additive measures

Thank you

References

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