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Addressing the Rashomon Effect through ranking aggregation

Claudia Sessa[1], **PhD Candidate**

csessa@liuc.it

Joint work with X. Lu [2], E. Borgonovo [3], A. Cillo [1] and G.P. Crespi [1]

[1] LIUC University, 21053 Castellanza, Italy.
[2] SKEMA Business School-Université Côte d'Azur, 92150 Suresnes, France.
[3] Department of Decision Sciences, Bocconi University, Milan, Italy, MI 20136.

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The Rashomon Effect

Given a dataset and a prediction task, there may exist several prediction models that exhibit equally good performance (Breiman 2001b):

⟶ the **Rashomon Set** (Fisher, Rudin, and Dominici 2019)

⊕ Analysts can choose from a range of acceptable models to solve their prediction problem.

⊖ Models in the Rashomon Set may produce **different explanations** for the phenomenon at hand, because they are **built on alternative rationales**.

Prediction Models and the Rashomon Set

- Let $\mathbf{X} = (X_1, \ldots, X_p) \in \mathcal{X} \subseteq \mathbb{R}^p$, and $Y \in \mathcal{Y} \subseteq \mathbb{R}$ be random variables on the probability space $(\Omega, \mathcal{B}(\Omega), \mathbb{P})$.

- The data generating process (DGP) is given by $g^* : \mathcal{X} \to \mathcal{Y}$.

- A dataset $\mathcal{D} = \{\mathrm{X}, \mathrm{Y}\} = \{(\mathbf{x}^i, y^i)\}_{i=1}^n$ consists of n realizations of the DGP.

- Given a set of parameters Θ, a **prediction model** is a function $m : \mathcal{X} \times \Theta \to \mathbb{R}$ that can be used to approximate g^* and make predictions given observations of $\mathbf{X}$.

- Let $\mathcal{L}(m)$ denote the loss function used to assess the out-of-sample performance of a model m.

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Population ϵ-Rashomon Set (Fisher, Rudin, and Dominici 2019)

For a given class of machine learning models $\mathcal{F}$, the **population ϵ-Rashomon Set**, for a fixed parameter ϵ, is defined as the subset of models $m \in \mathcal{F}$ whose expected loss deviates at most ϵ from the minimum loss attained, that is:

$$\mathcal{R}(\mathcal{F}, \epsilon) := \left\{ m \in \mathcal{F} : \mathbb{E}[\mathcal{L}(m)] \leq \min_{m' \in \mathcal{F}} \mathbb{E}[\mathcal{L}(m')] + \epsilon \right\}$$

Variable Importance Measures

Variable Importance Measure

Let $\mathcal{S} = \{1, 2, \ldots, p\}$ be the set of indices of the feature vector $\mathbf{X} = (X_1, \ldots, X_p)$.

Then, an **importance measure** is a map $\Phi : \mathcal{S} \to \mathbb{R}^p_+$.

We call the image of Φ importance vector.

Two main goals of variable importance measures (Williamson et al. 2022):

- → understanding the features on which a given algorithm relies,
- → measuring the population-level predictive potential of features.

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- → measuring the population-level predictive potential of features.

Variable Importance Measures

Several indicators fall under this definition, for instance:

- **Permutation Importance** (Breiman 2001a):

$$\nu_j^{(m)} = \mathbb{E}[\mathcal{L}(Y, m(\mathbf{X_j'}))] - \mathbb{E}[\mathcal{L}(Y, m(\mathbf{X}))]$$

  where X_j' represents an independent copy of X_j, and $\mathbf{X_j'} = (X_1, \ldots, X_{j-1}, X_j', X_{j+1}, X_p)$ is the random vector where the feature X_j is substituted with an independent copy.

- **Global sensitivity measures** (Borgonovo, Hazen, and Plischke 2016):

$$\xi^{\zeta}(Y, X_j) := \mathbb{E}_{X_j}[\zeta(\mathbb{P}_Y, \mathbb{P}_{Y|X_j})]$$

  where $\mathbb{P}_Y$ and $\mathbb{P}_{Y|X_j}$ denote the marginal distribution of Y and the conditional distribution of Y given X_j, respectively, and $\zeta(\cdot, \cdot)$ is a separation measurement quantifying the discrepancy between two probability measures on the reference probability space.

Related works

Few Variable Importance approaches have been proposed that use the entire Rashomon Set:

- **Model Class Reliance** (Fisher, Rudin, and Dominici (2019))
- **Variable Importance Cloud** (Dong and Rudin (2020))
- **Method Agnostic Model Class Reliance Range** (Gunasekaran, Mistry, and Chen (2024))
- **Rashomon Importance Distribution** (Donnelly et al. (2023))

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Research Objectives

1

Clarify the connection between the coefficients of linear models in the Rashomon Set and the Permutation importance measure, exploring its relation to total indices.

2

Propose an actionable methodological framework that exploits the whole Rashomon Set to obtain a unified explanation for the data.

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The Rashomon Set of Linear Models

- Let $\mathcal{D} = \{\mathrm{X}, \mathrm{Y}\}$ be a dataset. We call $m^* \in \mathcal{F}_l$ the best linear regression model trained on this dataset, characterized by the p-dimensional vector of coefficients β^*.

- Let $\mathcal{L}^*$ be the estimated mean squared loss from this model, that is $\mathcal{L}^* = \mathcal{L}(m^*) = \frac{1}{n}\sum_{i=1}^{n}(y^i - \mathbf{x}^i\beta^*)^2$.

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- The **Rashomon Set of Linear Regression models** (Semenova, Rudin, and Parr 2022) is the set of all models $m \in \mathcal{F}_l$ characterized by a vector of coefficients β that satisfies the relation:

$$\mathbb{E}[(Y - X\beta)^2] \leq (1 + \epsilon)\mathcal{L}^*.$$

- When the features are uncorrelated, the β's characterizing all models in the Rashomon Set form an ellipsoid in $\mathbb{R}^p$ centered at β^* (Dong and Rudin 2020), satisfying the following inequality

$$(\beta - \beta^*)\frac{X^\top X}{\epsilon\mathcal{L}^*}(\beta - \beta^*) \leq 1.$$

New Analytical Insights for Linear Models

- Let β_j b the coefficient associated with X_j, σ_j the standard deviation of X_j and σ_Y the standard deviation of Y.

- Let $\rho_j = \frac{Cov(Y,X_j)}{\sigma_Y \sigma_j}$ and $SRC_j = \frac{\beta_j \sigma_j}{\sigma_Y}$ be the **Pearson linear regression coefficient** and the **Standardized Regression Coefficient** between Y and X_j.

- Let $\tau_j = \sigma_Y^2 - \mathbb{E}[Var[Y|X_j]] = \frac{1}{2}\mathbb{E}\left[\left(g^*(\mathbf{X_j'}) - g^*(\mathbf{X})\right)^2\right]$ denote the **Total Index** of X_j (Homma and Saltelli 1996).

- Let $\nu_j^{(m)} = \mathbb{E}\left[\left(Y - m(\mathbf{X_j'};\beta)\right)^2\right] - \mathbb{E}\left[(Y - m(\mathbf{X};\beta))^2\right]$ denote the the **Permutation Importance** of feature X_j for model m under a quadratic loss.

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Proposition 1

Let m be a linear model with coefficients β. If m is a perfect predictor, and features are uncorrelated, then for a feature X_j

$$SRC_j^2 = \rho_j^2 = \frac{\tau_j}{\sigma_Y^2} \quad \implies \quad \nu_j^{(m)} = 2\tau_j = 2(\beta_j)^2\sigma_j^2$$

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Let m be a linear model with coefficients β. If m is a perfect predictor, and features are uncorrelated, then for a feature X_j

$$SRC_j^2 = \rho_j^2 = \frac{\tau_j}{\sigma_Y^2} \qquad \Longrightarrow \qquad \nu_j^{(m)} = 2\tau_j = 2(\beta_j)^2\sigma_j^2$$

⟶ If we fix ϵ so that models in the Rashomon Set exhibit a negligible squared error, then we expect $\nu_j^{(m)} \approx 2(\beta_j)^2\sigma_j^2$.

⟶ As the model performance worsens, the approximation does not hold and the Permutation importance $\nu_j^{(m)}$ may significantly deviate.

New Analytical Insights for Linear Models

Proposition 2

Let $\mathcal{R}(\mathcal{F}_l, \epsilon)$ be the Rashomon Set of linear models defined by the parameter ϵ, with ϵ small enough so that the squared error of the models within the Rashomon Set is negligible.

Then, under the assumption of uncorrelated features, the coefficients associated to a given feature X_j by models in $\mathcal{R}(\epsilon)$ lie within the range $\left[\beta_j^-, \beta_j^+\right]$ where

$$\beta_j^- = \beta_j^* - \delta \quad \text{and} \quad \beta_j^+ = \beta_j^* + \delta, \quad \text{with} \quad \delta = \sqrt{\frac{\epsilon L^*}{e_j^\top (X^\top X)^{-1} e_j}}((X^\top X)^{-1} e_j)_j,$$

β_j^* representing the coefficient of the best model, and e_j the unit vector in the direction j.

Moreover, the Permutation Importance ν_j of X_j, lies within the range $[\nu_j^-(\epsilon), \nu_j^+(\epsilon)]$, where

$$\begin{aligned} \nu_j^-(\epsilon) &= 2(\max\left\{0, sign\{\beta_j^- \cdot \beta_j^+\} \cdot \min\{|\beta_j^-|, |\beta_j^+|\}\right\})^2 \sigma_j^2 \quad , \\ \nu_j^+(\epsilon) &= 2(\max\{|\beta_j^-|, |\beta_j^+|\})^2 \sigma_j^2 \quad . \end{aligned}$$

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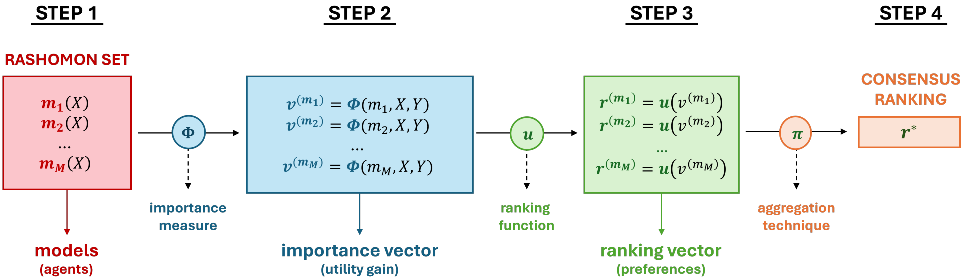
Propose an actionable methodological framework that exploits the whole Rashomon Set to obtain a unified explanation for the data.

The Proposed Methodological Framework

The proposed framework consists of 4 steps:



STEP 1

RASHOMON SET

$m_1(X)$
$m_2(X)$
$\dots$
$m_M(X)$

models
(agents)

Φ

importance measure

STEP 2

$v^{(m_1)} = \Phi(m_1, X, Y)$
$v^{(m_2)} = \Phi(m_2, X, Y)$
$\dots$
$v^{(m_M)} = \Phi(m_M, X, Y)$

importance vector
(utility gain)

u

ranking function

STEP 3

$r^{(m_1)} = u\left(v^{(m_1)}\right)$
$r^{(m_2)} = u\left(v^{(m_2)}\right)$
$\dots$
$r^{(m_M)} = u\left(v^{(m_M)}\right)$

ranking vector
(preferences)

π

aggregation technique

STEP 4

CONSENSUS RANKING

r^*

Computing the Rashomon Set (in practice)

Relatively few methods exist to compute or approximate a Rashomon Set for specific model classes:

- linear models (Dong and Rudin 2020)
- sparse decision trees (Xin et al. 2022)
- generalized additive models (Zhong et al. 2024)
- rule lists (Mata, Kanamori, and Arimura 2022)

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Empirical Rashomon Set

Let $\mathcal{D}_{train}$ and $\mathcal{D}_{test}$ be the training dataset and the test dataset, respectively, obtained by partitioning the dataset $\mathcal{D}$.

Let $\mathcal{F}$ be the set of machine learning models trained by the analyst on the dataset $\mathcal{D}_{train}$.

The **empirical Rashomon Set** is the subset of $\mathcal{F}$ containing those models whose accuracy on the test dataset, computed in terms of some measures of goodness of fit $\mathcal{A}$ (e.g. the R^2), exceeds a threshold α:

$$\tilde{\mathcal{R}}(\alpha) = \{m \in \mathcal{F} : \mathcal{A}\left(Y_{test}, m(\mathbf{X}_{test})\right) \geq \alpha\}$$

From Importance to Ranking

- For each model *m* in the empirical Rashomon Set, obtain the corresponding importance vector.

- Sort the features in descending order of importance and assign each feature its corresponding position in this order to obtain a **ranking vector**.

From Importance to Ranking

- For each model *m* in the empirical Rashomon Set, obtain the corresponding importance vector.
- Sort the features in descending order of importance and assign each feature its corresponding position in this order to obtain a **ranking vector**.
- **Ranking aggregation**: combining multiple rankings into a single, representative *consensus ranking* that synthesize information from input rankings.
- Several ranking aggregation techniques are available in the literature:
  - **Heuristic techniques** (e.g. *CombMIN*, *CombMAX*, *CombSUM* (Fox and Shaw 1994), *Borda counts* (Borda 1953), *Condorcet method* (De Condorcet et al. 1785))
  - **Optimization-based techniques** (e.g. minimizing Kendall's tau (Kendall 1948) or Spearman's footrule similarity (Spearman 1987))
  - **Distribution-based techniques** (e.g. *MC4*, *MCT* (DeConde et al. 2006), *Robust Rank Aggregation* (Kolde et al. 2012))

Numerical Experiments

Simulated data

Hooker test case

- 10 features, linear DGP
- Permutation Importance
- Two empirical Rashomon Sets of Linear Regressions based on the R^2 with respectively $\alpha = 0.94$ and $\alpha = 0.89$

Friedman test case

- 6 features (1 irrelevant)
- 2-Wasserstein Sensitivity Index
- Classification task
- Empirical Rashomon Set based on Accuracy with $\alpha = 0.8$

Real data

Boston Housing

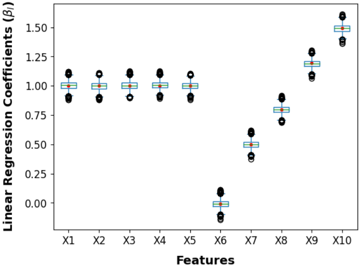
- 13 features
- Permutation Importance
- Empirical Rashomon Set based on the R^2 with $\alpha = 0.8$

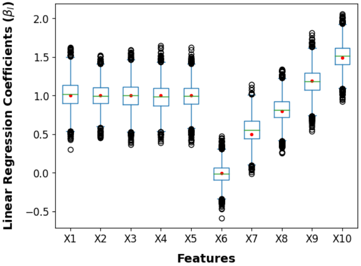
Procedure

1. Compute the empirical Rashomon Set
2. Choose one importance measure and compute the importance vector and importance ranking vector
3. Aggregate rankings to compute the consensus ranking using different aggregation techniques

Hooker test case (Hooker, Mentch, and Zhou 2021)

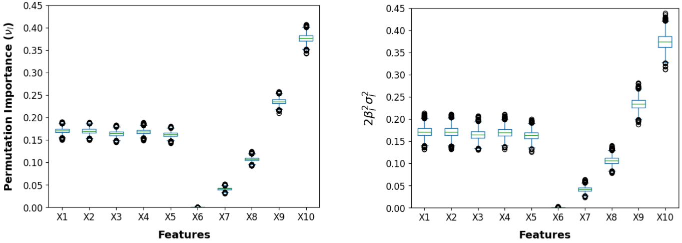
- $X_j \sim \text{Uniform}[0, 1], \quad \text{for } j = 1, ..., 10$
- $Y = X_1 + X_2 + X_3 + X_4 + X_5 + 0X_6 + 0.5X_7 + 0.8X_8 + 1.2X_9 + 1.5X_{10} + \eta, \quad \text{with } \eta \sim N(0, 0.1^2)$
- Training test: 10000 observations
- Test set: 5000 observations
- Two empirical Rashomon Sets of Linear Regressions based on the R^2, with $\alpha = 0.94$ and $\alpha = 0.89$:



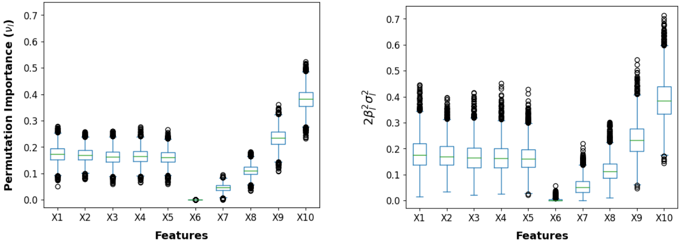


Hooker test case (Hooker, Mentch, and Zhou 2021)

$\alpha = 0.94$



$\alpha = 0.89$



Friedman test case (Donnelly et al. 2023)

- $X_j \sim \text{Uniform}[0,1]$ for $j = 1, \dots, 6$
- $Y = \mathbb{1}[10\sin(\pi X_1 X_2) + 20(X_3 - 0.5)^2 + 10X_4 + 5X_5 + \eta \geq 15], \quad \text{with } \eta \sim Normal(0, 1^2)$
- Training test: 10000 observations
- Test set: 5000 observations
- Epirical Rashomon Set made of 24 classification models whose accuracy is greater than or equal to 80%
- Importance measure:

2-Wasserstein Sensitivity Index (Borgonovo, Figalli, et al. 2024)

Let $Y \in \mathbb{R}$ and let $Q_Y(u)$ and $Q_{Y|X_j}(u)$ represent the u^{th} quantile of the distribution of Y and of Y given X_j, respectively. Then, the **2-Wasserstein Sensitivity Index** is defined as:

$$\iota(Y, X_j) = (2\mathbb{V}[Y])^{-1}\mathbb{E}\left[\int_0^1 \left(Q_Y(u) - Q_{Y|X_j}(u)\right)^2 du\right]$$

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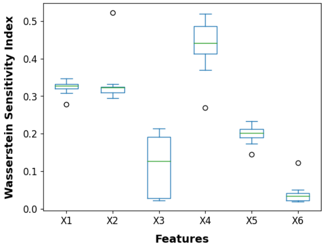
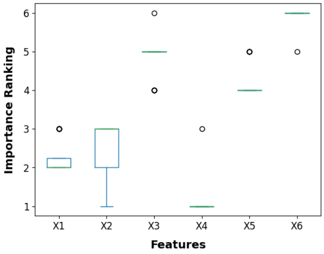
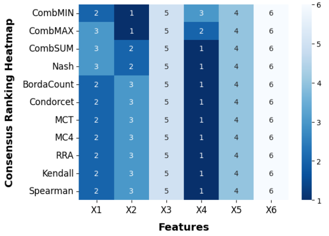


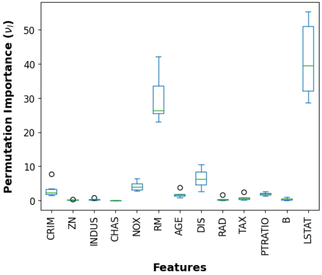


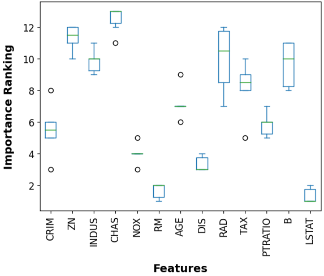


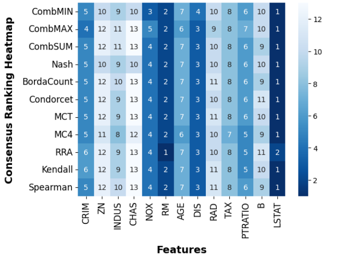
	X1	X2	X3	X4	X5	X6
CombMIN	2	1	5	3	4	6
CombMAX	3	1	5	2	4	6
CombSUM	3	2	5	1	4	6
Nash	3	2	5	1	4	6
BordaCount	2	3	5	1	4	6
Condorcet	2	3	5	1	4	6
MCT	2	3	5	1	4	6
MC4	2	3	5	1	4	6
RRA	2	3	5	1	4	6
Kendall	2	3	5	1	4	6
Spearman	2	3	5	1	4	6

Boston Housing dataset

- 506 observations of 13 features capturing information about houses and their surrounding neighborhoods
- Output variable: **MEDV**, the median value of owner-occupied homes
- Train-test split: 80% train, 20% test
- Epirical Rashomon Set made of 6 tree-based models: a gradient boosting ($R^2 = 92\%$), an XGBoost ($R^2 = 91\%$), a bagging regressor ($R^2 = 91\%$), a light gradient boosting machine (LGBM) ($R^2 = 89\%$), an extra-trees regressor ($R^2 = 88\%$) and a random forest ($R^2 = 88\%$)







	CRIM	ZN	INDUS	CHAS	NOX	RM	AGE	DIS	RAD	TAX	PTRATIO	B	LSTAT
CombMIN	5	10	9	10	3	2	7	4	10	8	6	10	1
CombMAX	4	12	11	13	5	2	6	3	9	8	7	10	1
CombSUM	5	12	11	13	4	2	7	3	10	8	6	9	1
Nash	5	10	9	10	4	2	7	3	10	8	6	10	1
BordaCount	5	12	10	13	4	2	7	3	11	8	6	9	1
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MC4	5	11	8	12	4	2	6	3	10	7	5	9	1
RRA	6	12	9	13	4	1	7	3	10	8	5	11	2
Kendall	6	12	9	13	4	2	7	3	11	8	5	10	1
Spearman	5	12	10	13	4	2	7	3	11	8	6	9	1

Conclusions

Contributions

- We established a theoretical connection between linear models' coefficients and Permutation Importance that facilitates interpretation
- We introduced a framework that uses the Rashomon Set to derive a unique feature importance ranking
- Our approach offers an intuitive means for practitioners to interpret model outputs in real-world contexts, where decision-makers may lack advanced technical expertise

Limitations

- The choice of the rank aggregation technique is crucial to achieve a reliable consensus
- We do not address the issue of explanation multiplicity

Thank You!

Claudia Sessa

PhD Candidate at LIUC University

csessa@liuc.it

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