SENSITIVITY ANALYSIS FOR DECISION-MAKING: FROM DECISION TREES TO ARTIFICIAL INTELLIGENCE

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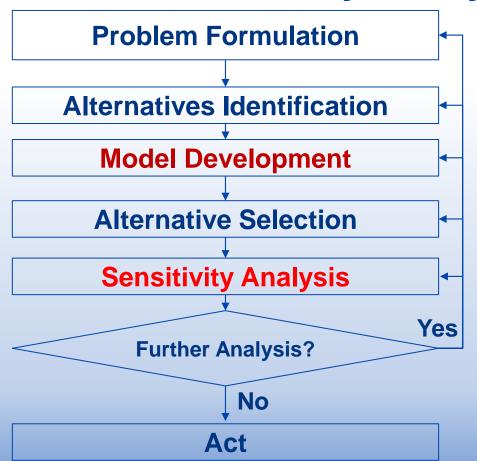
Premise

We increasingly rely on models to make decisions

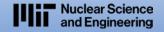




The Decision Analysis Cycle

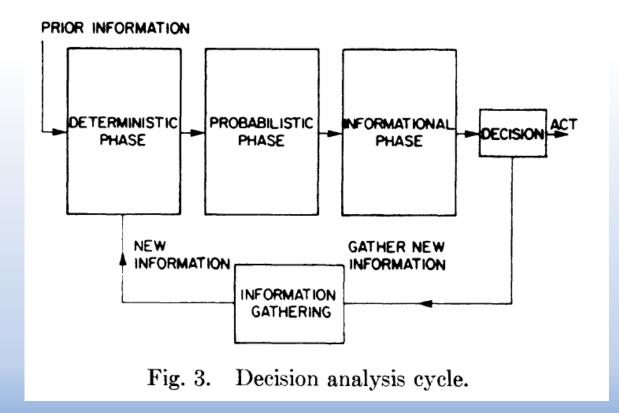


Clemen, 1997 Figure 1.1

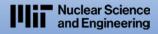




Back to Howard 1968







Sensitivity in Howard (1968)

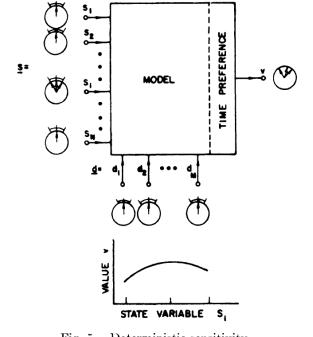
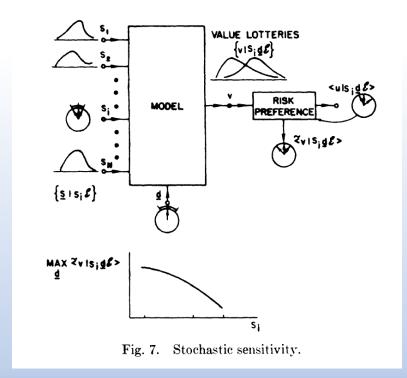
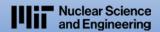


Fig. 5. Deterministic sensitivity.







Models

Probabilistic Risk Assessment Decision Trees/Influence Diagrams

Discrete Event Simulators Agent Based Simulators

System Dynamics Epidemiological Models

Hybrid Simulators

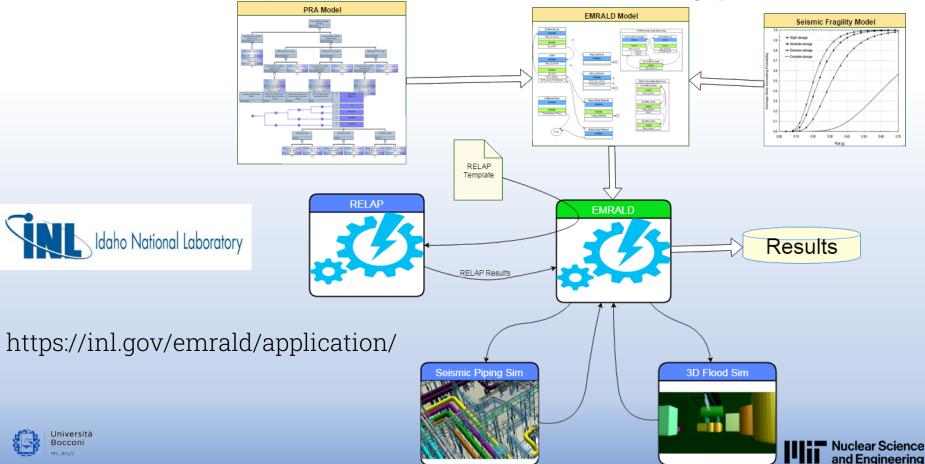
Digital Twins

Models of Phenomena



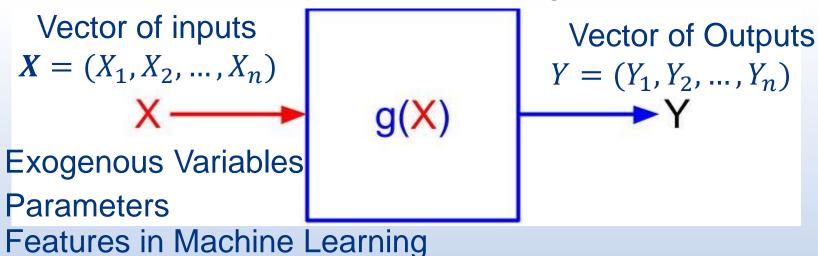


A Complex Simulator Prototype



The Setup

Input-output mapping

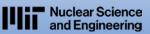




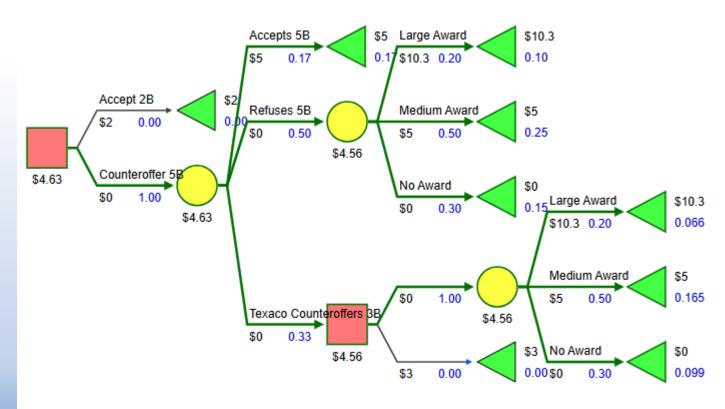


Pennzoil vs Texaco

- 1984: Pennzoil and Getty Oil agreed to merge, but Getty backed out after Texaco offered a higher price.
- Pennzoil sued Texaco for interference and won an \$11.1B judgment (later reduced to \$2B, but interest pushed it to \$10.3B).
- Texaco's CEO warned of bankruptcy if Pennzoil pursued liens and vowed to appeal up to the U.S. Supreme Court.
- In 1987, Texaco offered Pennzoil \$2B to settle before liens were filed.
- Pennzoil's chairman faced a decision: accept \$2B or
- Boccounter with \$5B as advised.



A toy Model: Pennzoil





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SPECIFIC VS GENERAL GOALS





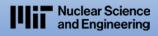
Specific Goals

- They answer a tailored sensitivity analysis question
- The answer can be problem and model-dependent
- E.g., Sensitivity of temperature on carbon emissions
- Methods can be ad-hoc

General Goals

Broad questions, with broad classes of methods

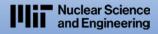




Variable Importance

- Quantify predictive contribution: On which variable does the model rely?
- Fairness: Is the model relying on variables that can create implicit bias and discrimination?
- Model Improvement: What are the areas in which further modelling efforts are needed?
- Eschenbach 1992: Factors on which to focus managerial attention during implementation
- Various Stakeholders: Inputs to prioritize in practice

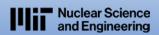




Direction of Impact

- How does the output of a model respond on the input variation?
- Is the variation causing an increase or decrease?
- Is the model monotonic, convex or periodic in the input?





Stability

- How uncertain are the model forecasts?
- Is the preferred alternative robust to the input variations?





Tornado Diagram Setup

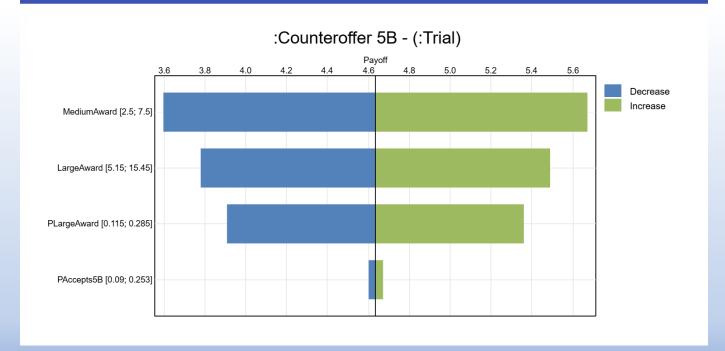






Pennzoil Tornado Diagram

Sensitivity analysis



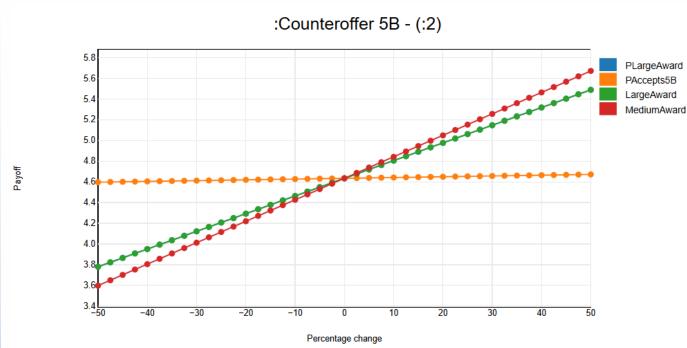




Spiderplot

Eschenbach 1992, Interfaces

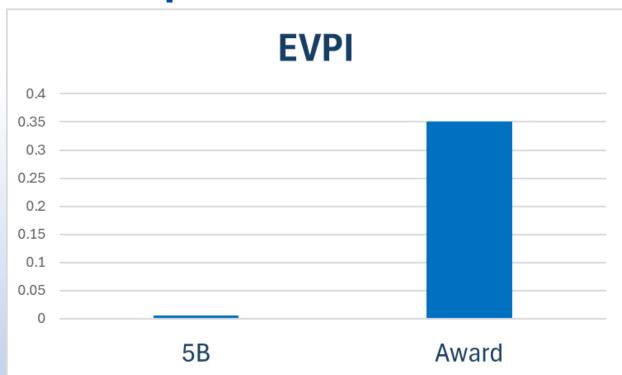
Sensitivity analysis





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Expected Value of Perfect Information

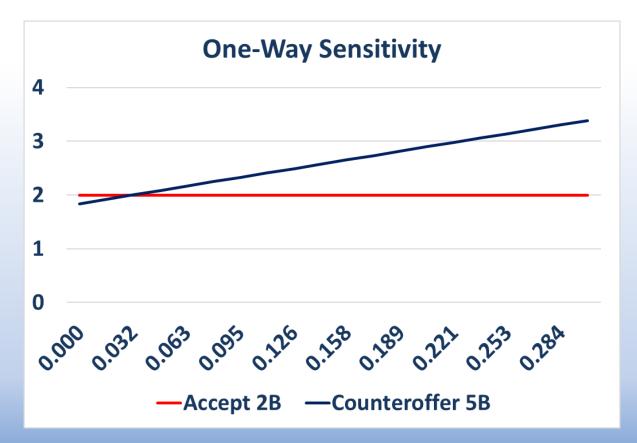


Value vs Decision Sensitivity (Hazen and Felli, 1998, MDM)

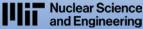




Pennzoil Stability on Pr(Accepts5B)







Structural Discovery

Is the model response the sum of the responses to the individual input variations or interactions emerge?

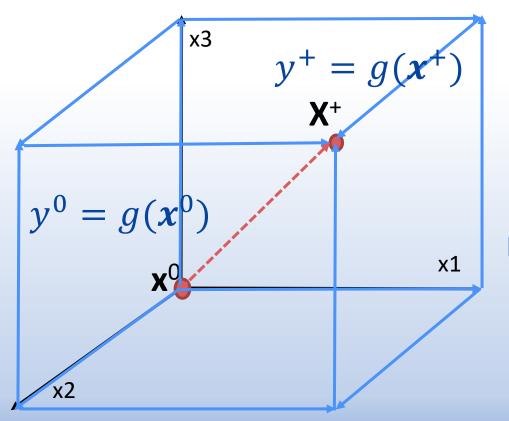
• How relevant are interactions?

• Are interactions synergistic (complementarity) or antagonistic (substitutability)?





Deterministic Sensitivity



Typically, we define ranges, $[x_i^0, x_i^+]$

Model output change:

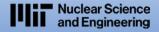
$$\Delta y = g(\mathbf{x}^+) - g(\mathbf{x}^0)$$

Model output change varying only x_i

$$\Delta_{i}y = g(x_{i}^{+}, \mathbf{x}_{-i}^{0}) - g(\mathbf{x}^{0})$$

Bar of Tornado Diagram





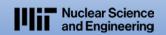
Finite-Difference Interactions

• We have:
$$\Delta y = \sum_{i=1}^{n} \phi_i + \sum_{i < j} \phi_{i,j} + \ldots + \phi_{1,2,\ldots,n}$$

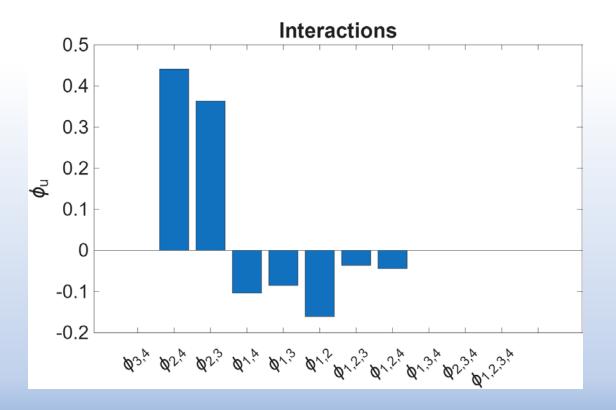
• Where:

$$\begin{cases} \phi_i = g(x_i^+; \mathbf{x}_{\sim i}^0) - g(\mathbf{x}^0) \longleftarrow & \text{First Order} \\ \phi_{i,j} = g(x_i^+, x_j^+; \mathbf{x}_{\sim i,j}^0) - \phi_i - \phi_j - g(\mathbf{x}^0) \longleftarrow & \text{Second Order} \\ \phi_{i,j,k} = g(x_i^+, x_j^+, x_k^+; \mathbf{x}_{\sim i,j,k}^0) - \phi_{i,j} - \phi_{i,k} - \phi_{j,k} - \phi_i - \phi_j - \phi_k - g(\mathbf{x}^0) \\ \dots \end{cases}$$





Pennzoil Interactions



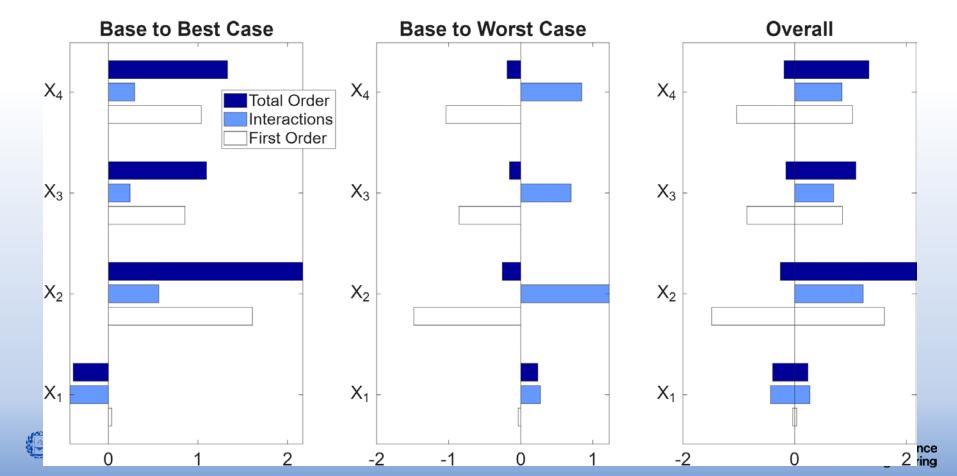


Generalized Tornado Diagrams

- Include Information on the Relevance of Interactions for each input
- Individual Effect: ϕ_i
- Total Effect: $\phi_i^T = \sum_{u:i \in u} \phi_u$
- Interaction Effect: $\phi_i^I = \phi_i^T \phi_i$
- Computational saving result by B. and Smith (2011, OR) abates the cost from 2^d to 2(d + 1).
- Just double the cost of a Tornado



Generalized Tornado Pennzoil



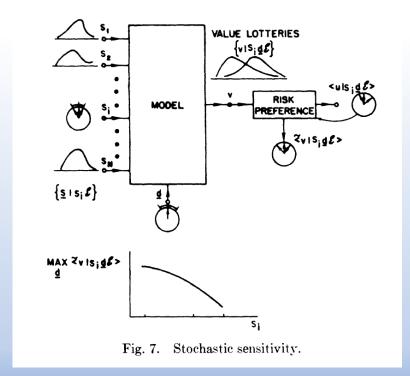
PROBABILISTIC SENSITIVITY



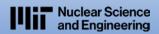


Monte Carlo Simulation

- Assign Inputs Probability Distribution
 - Delicate Step
- Propagate uncertainty through the model
 - Typically via Monte Carlo or Quasi Monte Carlo
- Evaluate Results
- Post-process Results







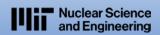
Probabilistic Sensitivity for Pennzoil



Insights

- Information on the expected value, confidence intervals
- Given the assigned ranges, the preferred alternative is "stable" (Stochastic Dominance)



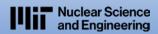


Global Importance

 When measuring importance of variables in a probabilistic sensitivity analysis setting, we can resort to several alternatives.

One important class: measures of statistical association





A Common Rationale

• Several importance measures can be written in the following form: $\xi_i = \mathbb{E}_i[d(\mathbb{P}_{\!\scriptscriptstyle Y},\mathbb{P}_{\!\scriptscriptstyle Y\mid X_i})]$

with d() a generic operator between the marginal and conditional distributions of Y.

• The above equation encompasses variance-based, kernel-based, scoring function-based global sensitivity measures, as well as value of information (B., Hazen et al 2016, RA).



Measures and Properties

• First order variance-Based sensitivity measures η_i^2 do not possess the zero-independence property.

$$\eta^{2}(Y,X) = \frac{\mathbb{V}[\mathbb{E}[Y|X]]}{\mathbb{V}[Y]}$$

The following do possess zero-independence (B. 2017, book):

$$\delta_i^{KL} = \mathbb{E}\left[\int_{\mathcal{Y}} f_Y(y) \ln \frac{f_Y(y)}{f_{Y|X_i}(y)} dy\right]$$

$$\delta_i = \frac{1}{2} \mathbb{E}_i \left[\int_{\mathcal{Y}} |f_Y(y) - f_{Y|X_i}(y; x_i)| \, dy \right]$$

$$\beta_i^{Ku} = \mathbb{E}_i \left[\int_{\mathcal{V}} \left(F_Y(y) - F_{Y|X_i}(y) \right)^2 dF_Y(y) \right]$$

based on the Kullback-Leibler divergence (Rahman, 2016, SIAM/ASA-JUQ)

based on the L1-norm between densities (B., 2001, RESS)

Kuiper-based (Baucells and B., 2013, MS)



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$$\beta_i^{CvM} = \mathbb{E}_i [\int_{\mathcal{V}} (F_Y(y) - F_{Y|X_i}(y))^2 dF_Y(y)]$$
MILANO

Chatterjee's new correlation coefficient (Chatterjee, 2021, JASA)

Desirable Properties

- Zero-Independence
 - Renyi (1959) postulate D: a measure of statistical dependence between Y and X should be equal to zero if and only if Y is independent of X.

- Max-Functionality
 - Renyi (1959) postulate E: The sensitivity measure should be maximal if Y=g(X)



New Indices based on Optimal Transport Theory

$$i^{\mathbf{W}_{2}^{2}}(\mathbf{Y}, X_{i}) \coloneqq \frac{\mathbb{E}\left[W_{2}^{2}(\mathbb{P}_{\mathbf{Y}}, \mathbb{P}_{\mathbf{Y}|X_{i}})\right]}{2\mathbb{V}[\%\mathbf{Y}]}$$

where W2 is the 2-squared Wasserstein distance [Wiesel, 2022, B. et al., 2025, MS].

 $0 \le i^{W_2^2} (Y, X_i) \le 1$

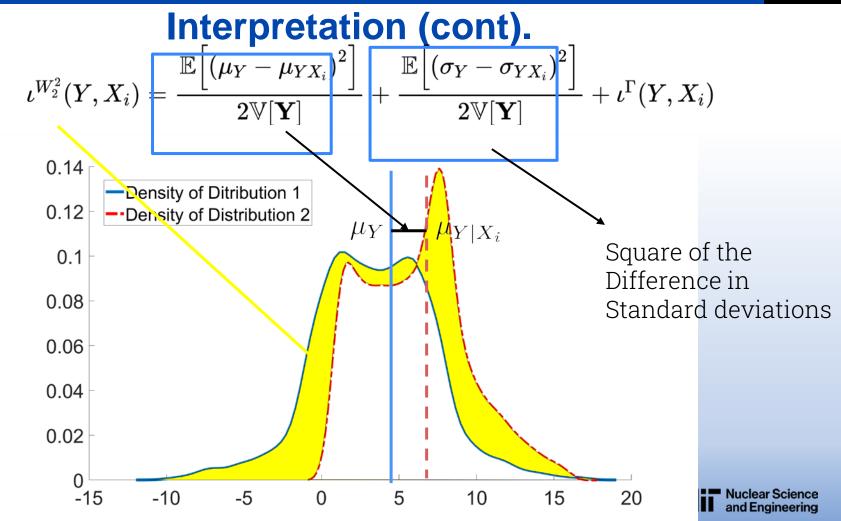
The index is normalized between 0 and 1, with 0 indicating independence and 1 indicating full functional dependence.

Moreover

 $i^{W_2^2}(\mathbf{Y}, X_i) = i^{VB}(\mathbf{Y}, X_i) + i^{\Sigma}(\mathbf{Y}, X_i) + i^{\Gamma}(\mathbf{Y}, X_i).$ Residual error term

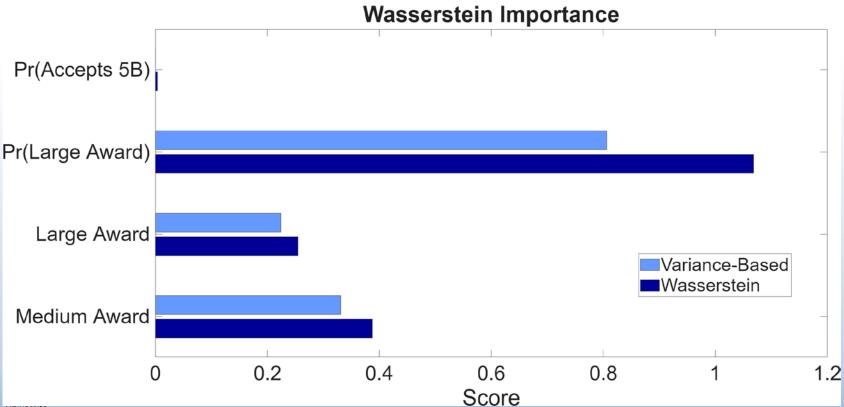


Variance-Based Impact on second moments





Pennzoil Global Sensitivity

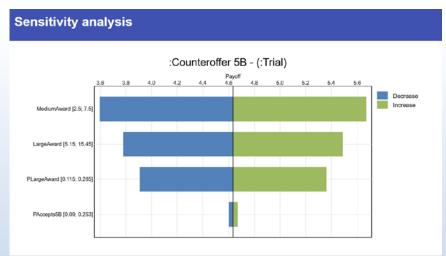


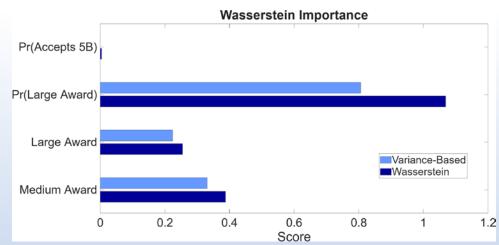


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Tornado Diagrams

Global Sensitivity Indices





Deterministic

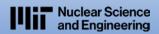
Probabilistic



Ongoing Applications

- Multivariate output large climate models (emission patterns (Chiani et al., 2025, RA)
- NASA Mars Return Program, in cooperation with NASA and Jet Propulsion Lab (Cataldo et al, 2025, RA)
- Energy Systems: in cooperation with University of North Carolina and Politecnico of Turn, (Nicoli et al., Energy, 2025)
- Modeling of Small Modular Reactors with Politecnico of Milan (Marchetti et al., Nuclear Engineering and Technology, 2025)





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MACHINE LEARNING SETUP: MODELS OF DATA

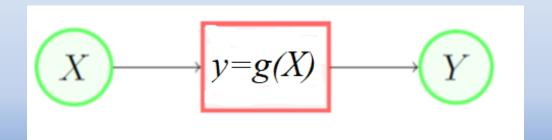




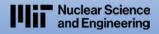
Models of Data



Machine Learning tools try to quantify the relationship under "nature" creating an input-output mapping:







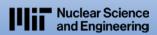
The Machine Learning Problem

Empirical Machine Learning Problem:

$$\min_{\theta \in \Theta} \mathbb{E}[\mathcal{L}(Y, \hat{g}(\mathbf{X}; \theta))]$$

• Where $\mathcal{L}(\cdot,\cdot)$ is a loss function, $\widehat{g}(\mathbf{X},\theta)$ a family of parameterized machine learning models





Models

Generalized Linear Models

Regression Trees

Neural Networks

Deep Learning

Support Vector Machines

Random Forests

XGBoost

Gaussian Process Regression

Self Orienting Maps

Models of Data



Friggs and Hartmann, 2020



The Black Box Menace

- (Begoli, Bhattacharya, and Kusnezov 2019, p. 21) underline the issue that the "Absence of Theory" makes a proper uncertainty quantification an essential ingredient in the use of black-box machine learning algorithms.
- (Guidotti et al., 2018) suggests that interpretability and explainability issues impact the use of artificial intelligent methods.
- (Saltelli, 2019) underlines that modelling quality and validity is at stake, especially as model complexity increases

Against the Black-Box Menace, we need Interpretability and Explainability



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Interpretability (I)

- (Miller, 2019) offers an insightful review on artificial intelligence explanation, without a strong distinction between intepretability and explainability
- Conversely, Rudin (2019) starts marking the distinction sharply
- Guidotti et al., 2018): A survey of methods to explain black box models
- (Murdoch et al., 2019): Interpretable Machine Learning
- (Bertsimas & Kallus, 2020): From predictive to Prescriptive Analytics
- (Rudin et al., 2022): 10 Grand Challenges in Interpretable ML
- (De Boeck et al, 2023): Explainable AI in OR





The Prejudice

	Model-based interpretability	Post hoc interpretability		
Predictive Accuracy	Generally unchanged or decrease (data-dependent)	No Effect		
Descriptive Accuracy	Increase	Increase		

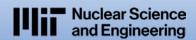


We believe that greater accuracy implies more complex models: this is **NOT** necessarily true Nuclear Scient

Explainability

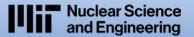
- (Guidotti et al., 2018), Saltelli (2019), suggest post-hoc explanations as essential to:
- Increase transparency
- Enhance interpretation and communication
- Increase awareness of the model behavior
- Obtain Crucial Insights





All goals remain valid

- Variable importance
- Direction of Impact
 - ALE Plots, Partial Dependence Plots, developed in machine learning
- Structural Discovery
- Stability Analysis



Type of "Explanations"

- Local explanations
 - Prediction by prediction
- Dataset level explanations
 - One Single Number
- Data generating process
- Model predictions

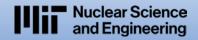




Some Local Explanation Methods

- LIME (Ribeiro et al, 2016)
- Shapley-value based:
 - SHAPs (Lundberg and Lee, 2017)
 - Baseline Shapley Values (Sundararajan, 2020, B. and Rabitti, 2023)
 - Cohort Shapley Values (Mase and Owen, 2022)





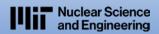
Permutation Feature Importance

■ Breiman's feature importance of X_i is defined as:

$$\widehat{\nu}_{j} = \frac{1}{N} \sum_{n=1}^{N} \mathcal{L}\left(\mathbf{y}^{n}, \widehat{g}(\mathbf{x}_{j,\pi}^{n}; \theta^{*})\right) - \underbrace{\frac{1}{N} \sum_{n=1}^{N} \mathcal{L}\left(\mathbf{y}^{n}, \widehat{g}(\mathbf{x}^{n}; \theta^{*})\right)}_{\text{Loss after}}$$

$$\mathbf{X_{i} \ permuted}$$
Original
Loss





Total Indices

■ Total indices (Homma and Saltelli, 1996):

$$\tau_j = \mathbb{V}_{-j}[\mathbb{E}_j[Y|\mathbf{X}_{-j}]] = \mathbb{V}[Y] - \mathbb{E}_{-j}[\mathbb{V}_j[Y|\mathbf{X}_{-j}]],$$

- Expected residual variance after we fix all features by X_i
- Jansen (1999) shows that they can be written as

$$\tau_{j} = \frac{1}{2} \left(\mathbb{E} \left[\left(g(X'_{j}, \mathbf{X}_{-j}) - g(\mathbf{X}) \right)^{2} \right] \right),$$

Which is equivalent to:

$$\tau_{j} = \frac{1}{2} \int_{\mathcal{X}} \int_{\mathcal{X}_{j}} \left(g\left(x_{j}', \mathbf{x}_{-j}\right) - g\left(\mathbf{x}\right) \right)^{2} dF_{X_{j}|\mathbf{X}_{-j}}(x_{j}'|\mathbf{x}_{-j}) dF_{\mathbf{X}}(\mathbf{x}).$$
The the correlation between \mathbf{X}_{j} and \mathbf{X}_{j} , we get the Verdinelli and Wasserman

■ If we ignore the correlation between X_j and X_{-j}, we get the Verdinelli and Wasserman index

$$\tau'_{j} = \frac{1}{2} \int_{\mathcal{X}} \int_{\mathcal{X}_{i}} \left(g\left(x'_{j}, \mathbf{x}_{-j}\right) - g\left(\mathbf{x}\right) \right)^{2} \overline{dF_{X_{j}}(x'_{j})} dF_{\mathbf{X}}(\mathbf{x}).$$

Proposition

If $\mathcal{L}(\cdot, \cdot)$ is the quadratic loss and if the model is a perfect predictor, then 1)

$$\nu_{j} = \mathbb{E}\left[\left(\widehat{g}(\mathbf{X}; \theta^{*}) - \widehat{g}(X_{j}^{'}, \mathbf{X}_{-j}; \theta^{*})\right)^{2}\right]. \tag{1}$$

2) If X'_j is sampled independently of \mathbf{X}_{-j} , then

$$u_j = 2\tau$$
, Non Classical total index(2)

where τ'_j is the Ψ_{DLoco} total index in Verdinelli and Wassermann (2023).

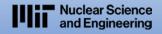
3) If X'_{j} is sampled conditionally on \mathbf{X}_{-j} , then

$$\nu_j = 2\tau$$
, Classical total index (3)

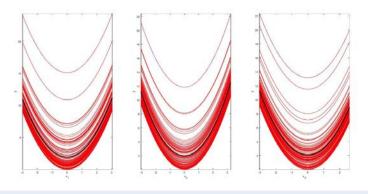
where τ_i is the classical total index

Direction of Change

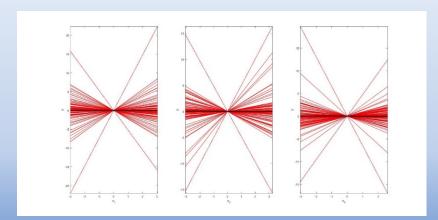




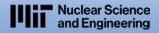
DOES Y BEHAVE LIKE THIS?



OR LIKE THIS?







Global trend indicators

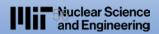
Conditional Regression Curves (Wooldridge 2013)

$$r_i(x_i) = \mathbb{E}[g(\mathbf{X})|X_i = x_i] = \int_{\mathcal{X}_{\sim z}} g((\mathbf{x}_{-i}; x_i)) dF_{\mathbf{X}|X_i}(\mathbf{x}_{-i}; x_i)$$

Partial dependence functions (Friedman 2001)

$$h_i(x_i) = \int_{\mathcal{X}_{\sim i}} g(x_i; \mathbf{x}_{\sim i}) dF_{\mathbf{X}_{\sim i}}(\mathbf{x}_{\sim i})$$



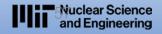


Global trend indicators (II)

ALE plots (Apley and Zhu, 2021, JRSSB)

$$ALE_i(x_i) = \int_{x_{i,\min}}^{x_i} \mathbb{E}[g_i'(\mathbf{X})|X_i = z_i]dz_i$$

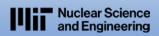




Consistent Indicators

- Determine whether the indicators correctly report properties of the original input-output mapping
- Monotonicity Consistency
- Convexity Consistency
- Lipschitz consistency



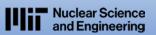


A Summary

Indicator	Symbol	Monotonicity consistency	Lipschitz consistency	Concavity consistency	Discrete inputs	Handles distributions
Gradients/Hessians	$g_i'(\mathbf{X})$	Yes	Yes	N/A	Yes	No
Tornado	$\Delta g_i^+, \Delta g_i^-$	Yes	Yes	N/A	Yes	No
One-way function	$g(x_i; \mathbf{x}_{-i}^0)$	Yes	Yes	Yes	Yes	No
Correlation coefficient	$ ho_{Y,X_i}$	Independent	N/A	N/A	Yes	Yes
Conditional expectation	$r_i(x_i)$	Independent	No	Independent	Yes	Yes
Partial dependence function	$PD_i(x_i)$	Yes	Yes	Yes	Yes	Yes
ALE function	$ALE_i(x_i)$	Independent	No	Independent	Yes	Yes

From B., Baucells et al., 2025, Risk Analysis

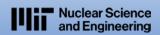




PD-One-way Plots

- ICE plots overlap "individual conditional expectations" and partial dependence functions
- It turns out that partial dependence functions are averages of one-way sensitivity functions of spiderplots
- and individual conditional expectations are one-way sensitivity functiond

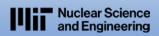




Two indices

- •Flatness Index: A partial dependence function can be flat even if Y depends on X_i
- Discrepancy index: Does the average hide the individual behavior in each of the one-way sensitivity functions?
- Insights on additivity





PD-One-way Plots for Pennzoil

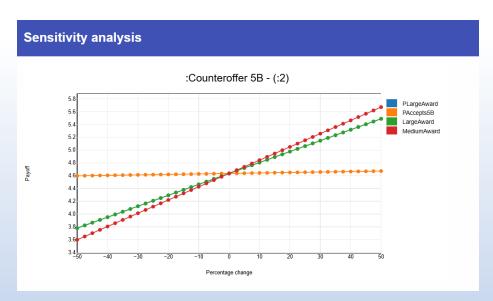
Discrepancy 0.34, Flatness 1.00 Discrepancy 0.00, Flatness 0.00 Discrepancy 0.01, Flatness 0.04 8 8 $>^6$ >6 >6 0.15 0.2 0.25 0.15 0.2 0.25 12 14 Pr(Accepts 5B) Pr(Large Award) Large Award Discrepancy 0.00, Flatness 0.00 8 <u>></u>6 **Medium Award**

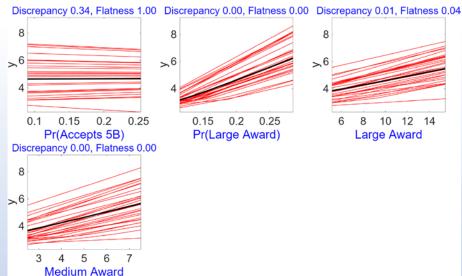


Nuclear Science and Engineering

Spiderplots

PD-Oneway Plots

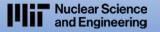




Deterministic

Probabilistic





Some Quotes

- The judicious application of sensitivity analysis techniques appears to be the key ingredient needed to draw out the maximum capabilities of mathematical modeling (Rabitz, 1989), p. 221.
- Sensitivity Analysis for Modelers: Would you go to an orthopedist who did not use X-Ray? (Fuerbringer, 1996).
- In order for the analysis to be useful it must provide information concerning the way in which our equilibrium quantities will change as a result of changes in the parameters (Samuelson, 1941).



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Github

https://github.com/emanueleborgonovo/SensitivityDecisionMaking/tree/main



Github



Thank You for Your Attention!



