



### Explain Yourself

## Expanding and Optimizing Models to Enable Fast Shapley Value Approximations Expanding and Optimizing Models to Enable Fast Shapley<br>Approximations<br>Holger Ziekow, Peter Schanbacher and Valentin Göttisheim<br>Furtwangen University, Germany<br>Presenter: Valentin Göttisheim - email: Valentin.Goettisheim@hs-

### Holger Ziekow, Peter Schanbacher and Valentin Göttisheim Furtwangen University, Germany

### Resume



Academic Background:

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- Resume<br>Academic Background:<br>• PhD candidate Data Science, Université de Haute-Alsace since 2023.<br>• Academic staff member Data Science, Furtwangen University since 2021. **Resume**<br>Academic Background:<br>• PhD candidate Data Science, Université de Haute-Alsace since 2023.<br>• Academic staff member Data Science, Furtwangen University since 2021.<br>Research Focus: • Le Carrice<br>• PhD candidate Data Science, Université de Haute-Alsace<br>• Academic staff member Data Science, Furtwangen Univer<br>Research Focus:<br>• Explainable Artificial Intelligence (XAI)<br>• Large Language Models (LLM)<br>• In i

### Research Focus:

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- Large Language Models (LLM)
- In industrial and medical domain



# Striving for Explainable AI Models **FURTIVERS ALL ALL ASSES AND ALL ASSESS AND ALL ASSESS AND ALL AND AVERENT AVANGER AT ALL AND FURTWARGER AT ALL AND FURTWARGER AND ALL AND AND REAL ASSESS TO A LATER AND A LATER AND REAL**



Shift to inherently explainable models for trustworthy, transparent AI.



- Demand for Transparency: Transparency fosters trust, accountability, and meets regulatory demands.
- Complexity of Neural Networks: Non-linear, high-dimensional interactions complicate feature interpretation.
- Limitations of Post-Hoc Explanations: Approximate, sometimes **THE** inconsistent and difficult to interpret fully.
- Advantages of Inherent Explainability: Embedding fair feature  $\pm$ attributions directly aligns model outputs with transparency goals.

# **Striving for Explainable AI Models**<br>
Shift to inherently explainable models for trustworthy, transparent AI.<br> **Explainability embedded within the loss function**



Shift to inherently explainable models for trustworthy, transparent AI.

### Explainability embedded within the loss function



Enables the model to learn fair feature attributions during training.

Explicit trade-off between predictive performance an explainability.

Real-Time generation of predictions and Shapley values during inference.







### Agenda



Agenda<br>Explain Yourself - Expanding and Optimizing Models to Enable Fast Shaple<br>Approximations<br>1. Shapley Value Landscape<br>2. Integrated Approach: Methodology Agenda<br>
Explain Yourself - Expanding and Optimizing Models to Enable Fast Shapley Value<br>
Approximations<br> **1. Shapley Value Landscape<br>
2. Integrated Approach: Methodology<br>
3. Results from Synthetic and Real-World Data** Agenda<br>Explain Yourself - Expanding and Optimizing Models to Enable Fast Shapley Value<br>Approximations Approximations

# Approximations<br> **1. Shapley Value Landscape<br>
2. Integrated Approach: Methodology<br>
3. Results from Synthetic and Real-World Data<br>
4. Conclusion and Future Directions** 1. Shapley Value Landscape<br>2. Integrated Approach: Methodology<br>3. Results from Synthetic and Real-World Data<br>4. Conclusion and Future Directions

## **Fair Attribution**<br> **Fair Attribution**<br> **Landscape**<br>
• Fair Principles<br>
• Fair Principles<br>
• Feature Attribution<br>
• Simplifying Methods<br>
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• Simplifying Methods<br>
• Dummy:<br>
• Addi The Shapley Value Landscape

- Fair Principles
- Feature Attribution
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### Fair Attribution with Shapley Values [1,2,3]

FORESCHULE HOCHSCHULE HORE FURTHALL PRINCES<br>Quantifies a feature's contribution to model<br>predictions.<br>Fair Principles: Treats features as players in<br>a coalition. predictions.

**Fair Principles:** Treats features as players in a coalition.

- Efficiency: Total prediction distributed among features
- Symmetry: Equal contributions receive equal values
- Dummy: Irrelevant features have zero attribution
- **Additivity:** Supports combining contributions

Benefit: Fair feature attributions Challenge: Computational complexity



### Feature Attribution: [3]

## **Feature Att<br>
The Shapley Value<br>
Landscape**<br>
• Fair Principles<br>
• Feature Attribution<br>
• Simplifying Methods<br>
• Sinsub<br>
• Sinsub The Shapley Value Landscape

- Fair Principles
	- Feature Attribution
- 

Key Terms:

 $i \cup J$  -  $\bigvee$  -

- $\phi_i(f)$  is the Shapley value for feature  $\,$  i.
- N is the set of all features.

 $S\subseteq N\setminus\{i\}$  and the set of  $S\subseteq N\setminus\{i\}$ 

- S is a subset of features not containing i.
- $f(S)$  is the model's output with features in S.

## **Example Shapley Value**<br> **• Baseline: Replace<br>
<b>• Baseline** values (e<br> **• Marginal:** Evaluate<br> **• Marginal:** Evaluate<br> **• Conditional:** Acco<br>
via conditional explane<br>
• Simplifying Methods<br>
• Simplifying Methods<br>
• TreeSHA The Shapley Value Landscape

- Fair Principles
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- Feature-Removal Approaches: [4]<br>
 Baseline: Replace missing features with<br>
baseline values (e.g., mean, zero).<br>
 Marginal: Evaluate subsets to compute FURTHOLD<br>
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• Baseline: Replace missing features with<br>
baseline values (e.g., mean, zero).<br>• Marginal: Evaluate subsets to compute<br>
marginal effects. BREWANSEN HEU<br>
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Marginal: Evaluate subsets to compute<br>
marginal effects.<br>
Conditional: Account for featu
- marginal effects.
- $\begin{tabular}{c} \color{red} \texttt{HETU} \\ \color{red} \texttt{HETU} \\ \color{red} \texttt{Feature-Removal Approaches:} \end{tabular} \end{tabular} \vspace{-.5cm} \begin{tabular}{l} \color{red} \texttt{HETU} \\ \color{red} \texttt{HSTU} \\ \color{red} \texttt{baseline:} \end{tabular} \end{tabular} \vspace{-.5cm} \begin{tabular}{l} \color{red} \texttt{HSTU} \\ \color{red} \texttt{baseline:} \end{tabular} \end{tabular} \vspace{-.5cm} \begin{tabular}{l} \color{red} \texttt{HSTU} \\ \color{red$ Feature-Removal Approaches: [4]<br>
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• Conditional: Account for feature dependencies<br> • Baseline: Replace missing features with<br>baseline values (e.g., mean, zero).<br>• Marginal: Evaluate subsets to compute<br>marginal effects.<br>• Conditional: Account for feature dependencies<br>via conditional expectations.<br>**Efficie Baseline values (e.g., mean, zero).**<br> **Marginal:** Evaluate subsets to compute<br>
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marginal effects.<br> **Conditional:** Account for feature dependencies<br>
via conditional expectations.<br> **Exa** marginal effects.<br>
• **Conditional:** Account for feature dependencies<br>
via conditional expectations.<br> **Efficient Computation:**<br>
• **KernelSHAP**<sup>[3]</sup>: Model-agnostic; broadly<br>
applicable.<br>
• **TreeSHAP**<sup>[5]</sup>: Model-specific; o • Conditional: Account for feature dependencies<br>via conditional expectations.<br>
Efficient Computation:<br>
• KernelSHAP<sup>[3]</sup>: Model-agnostic; broadly<br>
applicable.<br>
• TreeSHAP<sup>[5]</sup>: Model-specific; optimized for<br>
decision trees

### • Feature Attribution **Efficient Computation:**

- **KernelSHAP** [3]: Model-agnostic; broadly applicable.
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### Integrated Shapley Values

| Integrated Shapley Values   |                       |
|---|-----------------------|
| Neural Network Architecture & Methodology   |                       |
| $g = arg min E \left[ (y - g_0(x))^2 + \frac{\lambda}{2} \sum_{i=1}^{N} \left( \phi_i(x) - \hat{\phi}_i(x) \right)^2 \right]$ |                       |
| How $\hat{\phi}_i(x)$ is Derived  |                       |
| Utilize KernelExplainer to compute real Shapley   |                       |
| Utilize KernelExplainer to compute real Shapley   |                       |
| Values $\phi_i(x)$ during training.   |                       |
| Learning Approximation:   | Low $\lambda$ Values: |
| 1: Priorities prediction accuracy and Shapley value attributes.   |                       |
| 1: Proritizes prediction accuracy.  |                       |
| 2: Proritizes prediction accuracy.  |                       |
| 3: Prortives prediction accuracy.   |                       |
| 4: NonUCiss   |                       |
| 5: Prortizes prediction accuracy.   |                       |
| 6: NonUCiss   |                       |
| 7: Prortizes prediction accuracy.   |                       |
| 8: NonCiss  |                       |
| 9: A balances the emphasis between prediction accuracy and Shapley value attention.   |                       |
| 1: NonUCiss   |                       |
| 1: Prortizes prediction error with minimal emphasis   |                       |
| 1: NonUCiss   |                       |
| 2: Prortizes prediction error with minimal emphasis   |                       |
| 3: An output  |                       |
| 4: Learning to predict $\hat{\phi}_i(x)$ by minimizing the difference between $\phi_i(x)$ and $\hat{\phi}_i(x)$               |                       |
| 5: Enances Shapley value precision and explainability loss, improving<br>feature distribution accuracy.                       |                       |

### How  $\overline{\boldsymbol{\phi}}_i(x)$  is Derived

values  $\phi_i(x)$  during training.

### Learning Approximation:

- The model integrates Shapley approximations  $\cdot$ as an output
- Learning to predict  $\hat{\phi}_i(x)$  by minimizing the difference between  $\phi_i(x)$  and  $\hat{\phi}_i(x)$

### Mechanism of  $\lambda$

λ balances the emphasis between prediction accuracy and Shapley value attributions.

### Low λ Values:

- Prioritizes prediction accuracy.
- Minimizes prediction error with minimal emphasis on Shapley values.

### High λ Values:

- $\mathcal{L}_i(x)$  external term on the number of the precision and explainability.
	- Increases the weight of explainability loss, improving feature attribution accuracy.



# **FREAL-World Data (FREAD ACT)**<br> **Architecture and Training**<br>
Input Layer: 3 nodes (one for each feature).<br>
Hidden Layers:<br>
• Layer 1: 16 neurons, Leaky ReLU activation.<br>
• Layer 2: 8 neurons, Leaky ReLU activation.<br> **Outp** Results from Synthetic and Real-World Datament HFU

Experimental Design to Evaluate Shapley Integration

### Experimental Setup

**Objective:** Demonstrate the impact of embedding<br>Shapley values on accuracy and interpretability by<br>varying the  $\lambda$  parameter. **Experimental Setup**<br> **Chapter Conduces on accuracy and interpretability by**<br>
Synthetic Dataset:<br>
• Created to observe trade-offs between prediction<br>
• Created to observe trade-offs between prediction<br>
• Created to observ

### Synthetic Dataset:

- Created to observe trade-offs between prediction accuracy and explainability.
- Includes controlled linear and complex feature relationships.

### Real-World Dataset (Wine Quality):

- 
- 

### Architecture and Training

Input Layer: 3 nodes (one for each feature).

### Hidden Layers:

- 
- 

### Output Layer:

- 1 Target Prediction  $\nu$
- 3 Shapley Value Approximations  $(\phi^1(x),\phi^2(x),\phi^3(x))$

### Training Configurations:

- $(x), \phi^2(x), \phi^3(x)$ <br>phasis on Shapley  $(x), \phi^3(x))$ <br>on Shapley  $\cdot$   $\lambda$  = 0: Accuracy-focused, with minimal emphasis on Shapley values.
- $\lambda$  = 1: Balanced, with equal weight on prediction accuracy and explainability.
- $\lambda$  = 1000: Shapley-focused, prioritizing interpretability over prediction accuracy.

### Experiment I.



corresponding Shapley values (green, red, orange).

### Experiment I.<br>
Synthetic Dataset<br>
Pregion: Learning Curves with MSE for<br>
Synthetic Dataset<br>
Design:<br>
Target  $y = 2 \cdot x_1 + \frac{1}{2}e$  where  $x_1$  is the<br>
main feature with noise  $\epsilon$ .<br>  $\therefore x_2$ : Independent, however, non-linea  $-1$  $\frac{1}{2} \epsilon$  where  $x_1$  is the  $\frac{1}{2} \epsilon \frac{1}{2} \frac{1}{$  $-0.5$  $-2$ .  $0.0$  $0.4$  $0.6$  $0.8$  $1.0$  $0.6$  $0.8$  $0.2$  $1.0$  $1.2$  $0.5$  $\Omega$  $-1$  $0.0$  $0.0$  $-2$  $-0.5$  $1.0$  $0.0$  $0.4$ 0.6  $0.8$  $0.0$  $0.2$  $0.4$  $0.6$  $0.8$  $1.0$  $0.6$  $0.8$  $1.0$  $1.2$  $0.1$  $0.05$  $0.5$  $0.0$  $-0.1$  $0.00$  $-0.2$  $0.05$  $-0.3$  $0.0$  $0.4$  $0.6$  $0.8$  $1.0$  $0.0$  $0.2$  $0.4$  $0.6$  $0.8$  $1.0$  $0.6$  $0.8$  $1.2$  $0<sub>2</sub>$  $1.0$

SHAP values for y=A vs feature<br>Figure: Shapley values of features (left to right) of models  $\lambda \in 0.1,100$  (top to bottom).

### Synthetic Dataset

### Design:

- $\frac{1}{2}$  subsequently is the  $\sim$ main feature with noise  $\epsilon$ .
- $x_2$ : Independent, however, non-linear transformation of  $x_1$  and  $y$ .
- $x_3$ : Independent, uniformly distributed.  $\begin{bmatrix} 1 & 0.2 \\ 0 & 0.2 \end{bmatrix}$

### Findings:

- Higer  $\lambda$ :
	- Correct attributions, improving<br>explainability.<br>• Reduces MSE for Shapley values. explainability.
	- Reduces MSE for Shapley values.  $\sum_{-0.5}^{11}$
- Trade-off in prediction accuracy vs. interpretability

### Experiment II.



Figure: Learning Curves with MSE for  $\lambda \in \{0.1, 1000\}$  models (left to right) for the outcome of interest y (blue) and the corresponding Shapley values (green, red, orange).

### Wine Quality Dataset

### Data Source:

• Wine-quality-red dataset from  $\frac{1}{8}$   $\frac{0.5}{0.0}$ OpenML [6]. .

### Features Used:

• 'sulphates,' 'alcohol,' and 'total<br>sulfur dioxide' chosen by<br> $\frac{1}{6}$   $\frac{1}{6}$   $\frac{1}{6}$ sulfur dioxide' chosen by explorative analysis  $\sum_{n=1}^{\infty}$ 

### Findings:

• Partial dependency plots reveal<br>more stable Shapley values at<br>higher  $\lambda$ more stable Shapley values at higher λ



**Figure:** Shapley values of features (left to right) of models  $\lambda \in 0.1,1000$  (top to bottom)



### Conclusion

- Embedding Shapley values aligns feature attributions to fair principles during training.
- Adjusting λ enables a flexible tradeoff between accuracy and interpretability.
- Both synthetic and real-world experiments show that increasing  $\lambda$ enhances explainability.

### Future Research Directions

- Change approach to align feature attributions to improve scalability.
- Extending experiments to complex architectures and broader data sets could expand application potential.
- Evaluating performanceinterpretability trade-off.

## Questions? Valentin Göttisheim – Valentin.Gottisheim@hs-furtwangen.de

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### Backup: House Price Prediction Example

### Model Prediction: \$440,000

- 1.Square Footage (120m²): \$120,000
- 
- 3.Bedrooms (4): \$120,000
- 4.Proximity to Park (100m): \$0

- 1.Efficiency: All features
- 2.Symmetry: Square Footage and Location

…

3.Dummy: Proximity to Park

Efficiency: Total contribution equals the model's prediction.

**2. Location (Valencia):** \$200,000  $+ \phi_{proximity\ to\ Park}$ <br>= 120.000 + 200.000 + 120.000 + 0 = 440.000  $\phi$  Square Footage +  $\phi$  Location +  $\phi$  Bedrooms  $+$   $\phi$  *Proximity to Park* **ion Example**<br> **ion:**<br> **ion:**<br> **p**<br> **ion:**<br> **p**<br> **o**<br> **ion:**<br> **p**<br> **ion:**<br> **i**<br> **p**<br> **i**<br> **p**<br> **ion:**<br> **ion:** 

Symmetry: Features with equal contributions receive equal attribution.

**Assumptions of Fair Attribution:**  $f(Location \cup Square Footage) - f(Location) = 120,000$ **Criticiency:** Total contribution equals the model's<br>
Dependence of the model of the model of the syntax = 120,000 + 200,000 + 120,000 + 0 = 440,000<br>
Symmetry: Features with equal contributions<br>
eceive equal attribution.<br> **LOTT LAATITPLE**<br> **Lecation:**<br>  $\phi_{Square\cdot Footage} + \phi_{Location} + \phi_{Bedrooms} + \phi_{Proximity\cdot to Park} + \phi_{Proximity\cdot to Park}$ <br>
= 120,000 + 200,000 + 120,000 + 0 = 440,000<br> **mmetry:** Features with equal contributions<br> *Location* ∪ *Square Footage*) –  $f(Location) = 120,000$ <br>  $f$ **ency:** Total contribution equals the model's<br>
tion.<br>  $\frac{\partial Square \cdot F} {\partial x} = \frac{\partial S}{\partial x} + \frac{\partial S}{\partial y}$ <br>  $\frac{\partial S}{\partial y} = \frac{\partial S}{\partial x} + \frac{\partial S}{\partial y}$ <br>  $\frac{\partial S}{\partial x} = \frac{\partial S}{\partial y} + \frac{\partial S}{\partial y}$ <br>  $\frac{\partial S}{\partial y} = \frac{\partial S}{\partial x}$ <br>  $\frac{\partial S}{\partial y} = \frac{\partial S}{\partial y}$ <br>  $\frac{\partial$ rediction.<br>  $\phi_{Square\cdot Footage} + \phi_{Location} + \phi_{Bedrooms}$ <br>  $+ \phi_{Proximity\, to \, Park}$ <br>
= 120,000 + 200,000 + 120,000 + 0 = 440,000<br> **ymmetry:** Features with equal contributions<br>
secive equal attribution.<br>  $\mathcal{E}(Location \cup Square\, Footage) - \mathcal{E}(Location) = 120,000$ <br>  $\mathcal{E}(Location \cup Bed$ botage +  $\Phi$  Location +  $\Phi$  Bedrooms<br>+  $\Phi$  Proximity to Park<br>- 200,000 + 120,000 + 0 = 440,000<br>atures with equal contributions<br>ttribution.<br>uare Footage) -  $f$  (Location) = 120,000<br>Bedrooms) -  $f$  (Location) = 120,000<br>r

Dummy: Features with no impact receive zero attribution.

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