Can We Trust a Neural Network Prediction?

Methods and Pitfalls for Explaining Black Boxes

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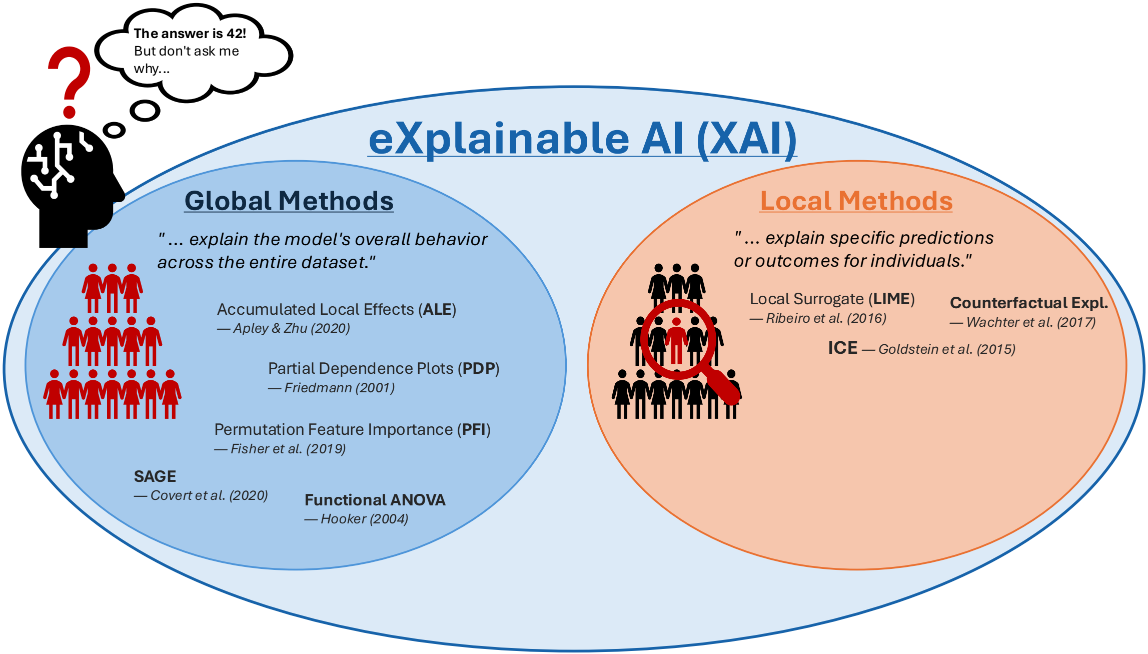
The answer is 42!
But don't ask me why...
eXplainable AI (XAI)
Global Methods
"... explain the model's overall behavior across the entire dataset."
Accumulated Local Effects (ALE)
— Apley & Zhu (2020)
Partial Dependence Plots (PDP)
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Local Methods
"... explain specific predictions or outcomes for individuals."
Local Surrogate (LIME)
— Ribeiro et al. (2016)
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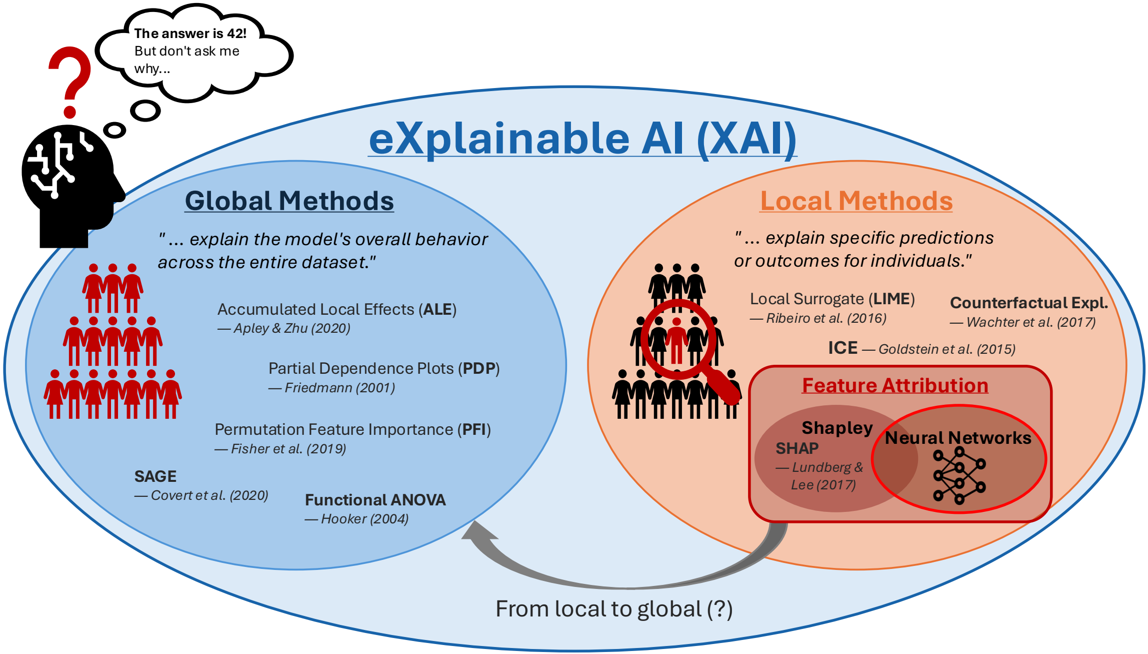
— Wachter et al. (2017)
ICE — Goldstein et al. (2015)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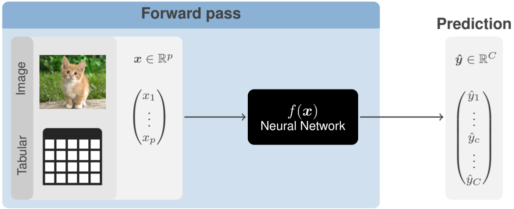
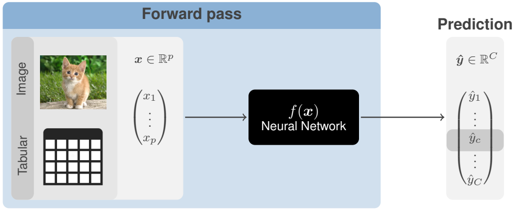
Feature Attribution
Shapley
SHAP
— Lundberg & Lee (2017)
Neural Networks
From local to global (?)


Forward pass
Image
Tabular
$x \in \mathbb{R}^p$
x_1
x_p
$f(x)$
Neural Network
Prediction
$\hat{y} \in \mathbb{R}^C$
$\hat{y}_1$
$\hat{y}_c$
$\hat{y}_C$



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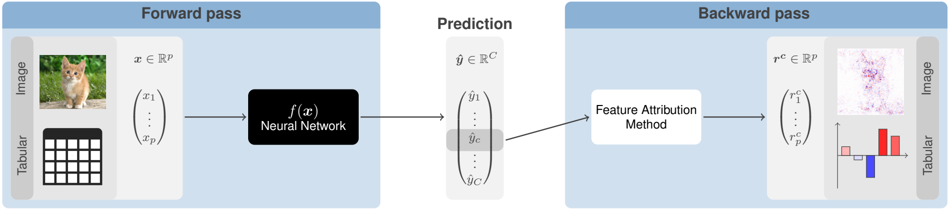
What is feature attribution?



- Assigns an attribution value of a selected output to each input variable
  - $\longrightarrow$ also known as contribution or relevance
  - $\longrightarrow$ can be positive (in red) or negative (blue)
- Utilizes the
  - $\longrightarrow$ layer-wise architecture of a neural network
  - $\longrightarrow$ automatic differentiation engine of the training
- Extremely efficient and fast
  - $\longrightarrow$ thanks to deep learning libraries like PyTorch, Keras/TensorFlow etc.
  - $\longrightarrow$ generally only one forward and one backward pass is needed (no optimization or estimation)

Which Method Should I Use?

Saliency/Gradient!!
Keep it simple

DeepLIFT!!
Need a reasonable reference

SmoothGrad!!
Smooth for clarity

IntegratedGradient!!
Need axiomatic consideration

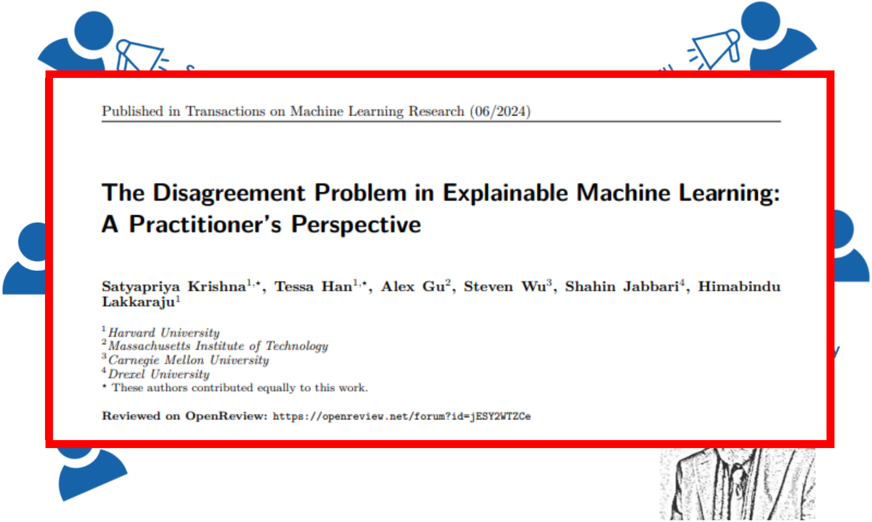
User

LRP!!
Class-sensitivity

Come on, guys!
There is only one
FAIR option.

Lloyd S. Shapley

Which Method Should I Use?



Published in Transactions on Machine Learning Research (06/2024)

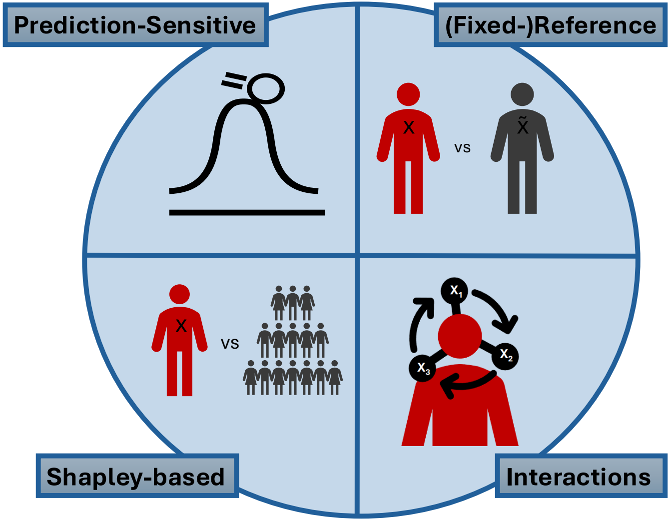
The Disagreement Problem in Explainable Machine Learning: A Practitioner's Perspective

Satyapriya Krishna[1,*], Tessa Han[1,*], Alex Gu[2], Steven Wu[3], Shahin Jabbari[4], Himabindu Lakkaraju[1]

[1] *Harvard University*
[2] *Massachusetts Institute of Technology*
[3] *Carnegie Mellon University*
[4] *Drexel University*
[*] These authors contributed equally to this work.

Reviewed on OpenReview: https://openreview.net/forum?id=jESY2WTZCe

Which Method Should I Use? – It depends...



Simulation

Features (real):

BMI, Age, Gender and HbA1c

Outcome (binary)

Diabetes (synth.)

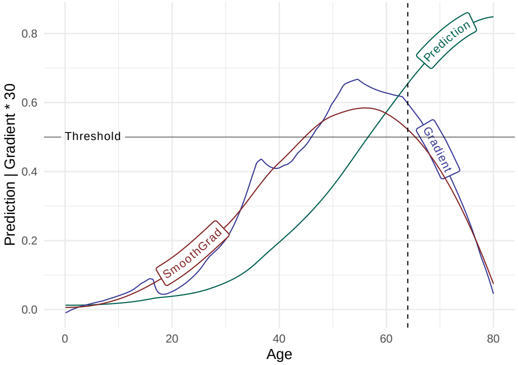
Prediction-Sensitive Methods

"How sensitive is the prediction w.r.t. this feature?"

Gradient[1]: $\frac{\partial f(\boldsymbol{x})}{\partial x_i}$ **SmoothGrad**[2]: $\sum_{k=1}^{K} \frac{\partial f(\boldsymbol{x} + \boldsymbol{\varepsilon^{(k)}})}{\partial x_i + \varepsilon_i^{(k)}} \quad \left(\varepsilon^{(k)} \sim \mathcal{N}(0, I\sigma)\right)$

Interpretation:

- Increasing patient's age increases model's prediction for diabetes



[1] Simonyan et al. (2014) ● [2] Smilkov et al. (2017)

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Interpretation:

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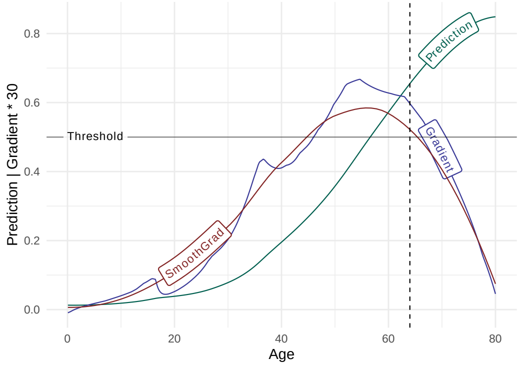
Pitfalls:

- Show output sensitivity, not attributions!
- Depend on feature scaling

  $\rightarrow$ complicating comparisons for tabular data
- Provide point-specific insights
- **SmoothGrad**
  - Reduces noise ("area-gradient") but depends on smoothing parameters
  - Is Gaussian noise always the best choice?



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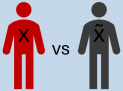
(Fixed-)Reference Methods



"What are the features' contributions for predicting $f(x)$ instead of $f(\tilde{x})$?"

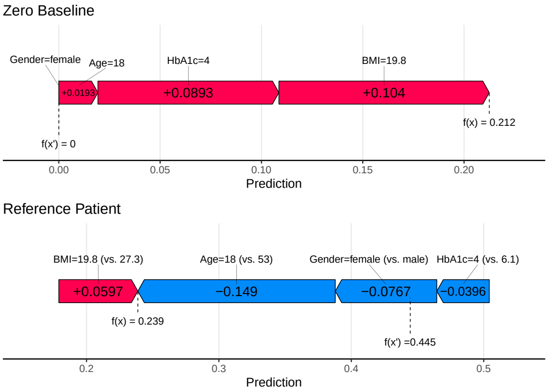
*Grad×Input[3]: $\frac{\partial f(\boldsymbol{x})}{\partial x_i} \cdot x_i$ **IntGrad**[5]: $(x_i - \tilde{x}_i) \int_{\alpha=0}^{1} \frac{\partial f(\tilde{\boldsymbol{x}} + \alpha(\boldsymbol{x} - \tilde{\boldsymbol{x}}))}{\partial x_i} d\alpha$

***LRP**[4] **DeepLIFT**[3]

*Approximation and fixed reference ($\tilde{x} = 0$)

Interpretation:

- Decomposition of $f(x) - f(\tilde{x})$ in feature-wise effects
- Did this feature change (from x to $\tilde{x}$) argue against or for an increase?



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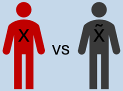

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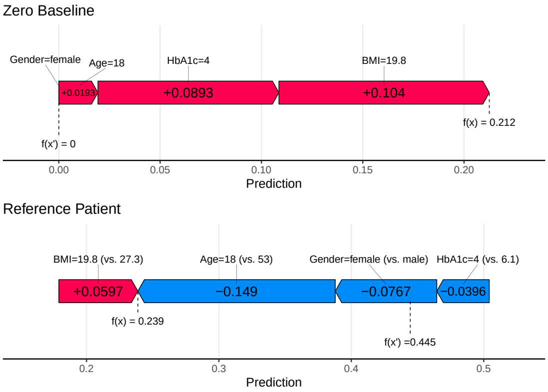
Pitfalls:

- Explanations are highly sensitive to the choice of reference
- Other reference means other question
- Grad$\times$Input and LRP struggle with non-linearity[6]
- Typical references (e.g., 0) often fall outside data distribution



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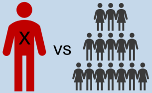
Shapley-based Methods



"What are the features' contributions for predicting $f(x)$ compared to $\mathbb{E}_X\left[f(X)\right]$?"

GradSHAP[7]: $\mathbb{E}_{\substack{\tilde{x}\sim X \\ \alpha\sim\mathcal{U}[0,1]}}\left[(x_i-\tilde{x}_i)\frac{\partial f(\tilde{x}+\alpha(x-\tilde{x}))}{\partial x_i}\right]$

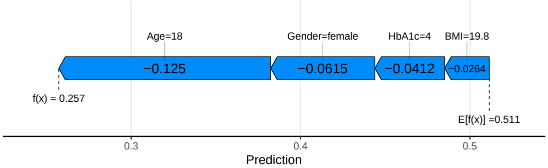
DeepSHAP[8] (rescale or reveal-cancel)

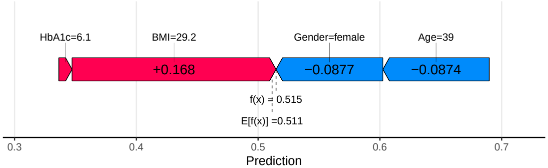
Interpretation:

- Decomposition of $f(x) - \mathbb{E}\left[f(X)\right]$ in feature-wise effects
- What is the marginal contribution of this feature?

  $\rightarrow$ answers a more natural question

  $\rightarrow$ axiomatic and theoretical foundation





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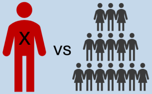

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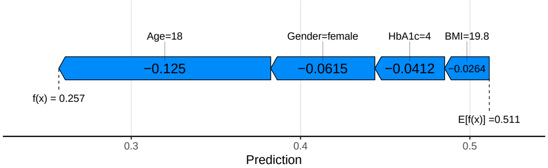
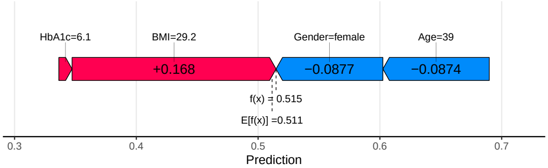
Pitfalls:

- Still marginal (no conditional Shapley values)
- Higher computational costs
- Requires suitable (reference) dataset





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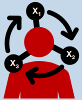
Interaction-based Methods



"Is there a combined effect of features on $f(x)$?"

Hessian: $\frac{\partial^2 f(x)}{\partial x_i \, \partial x_j}$

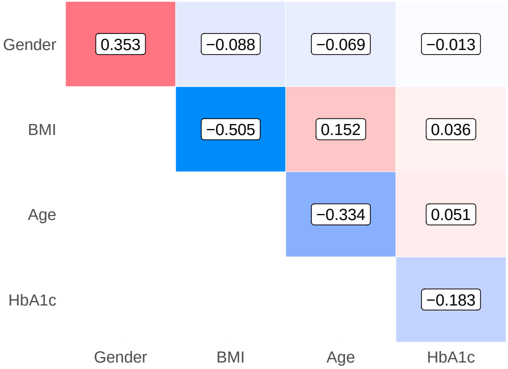
ExpectedHessian[9]

IntHessian[9]: $(x_i - \tilde{x}_i)\,(x_j - \tilde{x}_j) \int_0^1 \int_0^1 \alpha\beta \frac{\partial^2 f(\tilde{x} + \alpha\beta(x - \tilde{x}))}{\partial x_i \, \partial x_j} \, d\alpha \, d\beta$

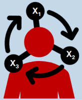
Interpretation:

- Decomposition of $f(x) - f(\tilde{x})$ / $f(x) - \mathbb{E}_X\left[f(X)\right]$ in feature-wise main (diagonal) and two-way interaction effects (**IntHessian**/ **ExpHessian**)
- Reveals local interaction effects and strength (**Hessian**)

f(x) = 0.039 vs. f(x') = 0.569



Interaction-based Methods



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Pitfalls:

- Higher computational costs
- Not possible for ReLU networks

  $\longrightarrow$ vanishing 2nd derivative
- (similar to the other three groups)

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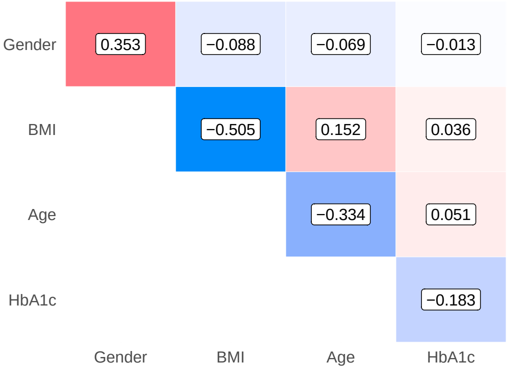
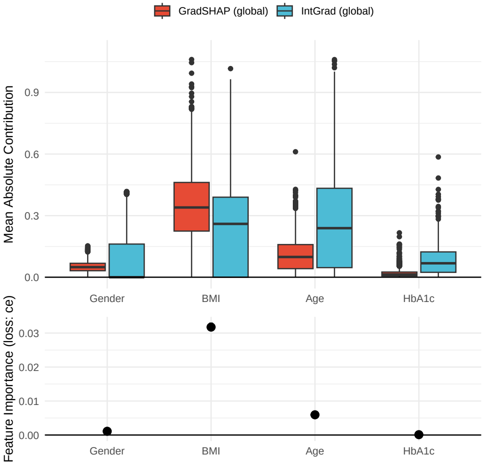


[9] Janizek et al. (2021)

From Local to Global Explanations

- **So far:** Only explanations of individuals
- Aggregating local explanations for global insights (Lundberg et al. (2020))
- Gives relative importance among features
- Can we do so for other feature attribution methods?
  - Prediction-sensitive: Global feature's sensitivity (but depends on scaling)
  - Reference-based: Global effect against single reference
  - Shapley-based: Marginal global effect

$\Rightarrow$ Only explaining the model's prediction (not necessarily aligning with data-based or loss-based importance measures)



Key Takeaways & Future Work

Key Takeaways:

- Feature Attribution Method $\neq$ *feature attribution* $\rightarrow$ answer different questions!
- Choice of method depends on the question: sensitivity, (baseline/marginal) attribution, or interaction
- Each reference value answers another question
- No recommendation for vague approximations (like LRP, Grad$\times$Input)
- Can be aggregated to global importance measures $\rightarrow$ feature selection
- Prediction-based! $\rightarrow$ *"What does the model see for the prediction" – not true to the data*

Future Work:

- Adopting methods for loss-based insights $\rightarrow$ performance attribution
- Extending methods for conditional (not marginal) values

Thank you for your attention!

Slides, references and reproduction material

R Package `innsight`

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