

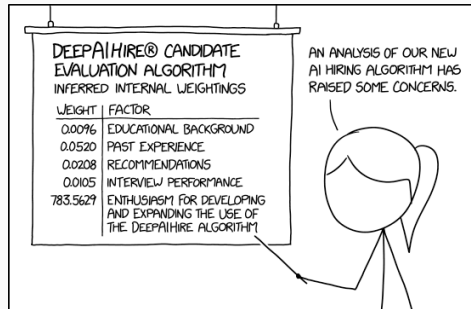
Interpretability of Supervised Learning Models

BMI 773 Clinical Research Informatics

Yuriy Sverchkov

April 27, 2015

University of Wisconsin–Madison



Why do we want to interpret models?

Why do we want to interpret models?

- Trust: having an interpretation along with a prediction can bring a practitioner to agree with a model.

Why do we want to interpret models?

- Trust: having an interpretation along with a prediction can bring a practitioner to agree with a model.
- Causality: understanding the associations driving model decisions can help uncover underlying mechanisms.

Why do we want to interpret models?

- Trust: having an interpretation along with a prediction can bring a practitioner to agree with a model.
- Causality: understanding the associations driving model decisions can help uncover underlying mechanisms.
- Transferability: understanding how a model makes decisions informs about how it will perform on a different data distribution

Why do we want to interpret models?

- Trust: having an interpretation along with a prediction can bring a practitioner to agree with a model.
- Causality: understanding the associations driving model decisions can help uncover underlying mechanisms.
- Transferability: understanding how a model makes decisions informs about how it will perform on a different data distribution
- Informativeness: pointing out evidence to support a decision (decision support systems)

What makes a model interpretable?

What makes a model interpretable?

- Simulatability: Can a person can look at the description of the model and figure out what the model's prediction about a given case would be?

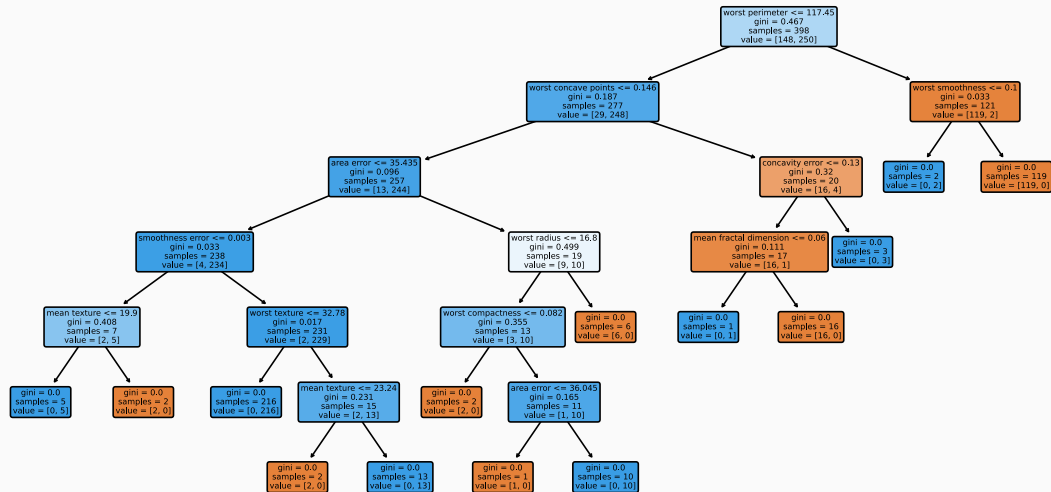
What makes a model interpretable?

- Simulatability: Can a person can look at the description of the model and figure out what the model's prediction about a given case would be?
- Decomposability: Is the model's decision made up of semantically meaningful components?

What constitutes an interpretation?

Models that are interpretable by design

Interpreting decision trees



Interpreting linear regression coefficients

Model:

$$y = \beta_0 + \sum_{i=1}^d x_i \beta_i$$

Interpretation:

An increase in the value of feature i by 1 unit corresponds to the increase in the outcome by β_i units.

Interpreting logistic regression coefficients

Model:

$$\overbrace{\log \left(\frac{P(y = 1)}{P(y = 0)} \right)}^{\text{log odds}} = \beta_0 + \sum_{i=1}^d x_i \beta_i$$

Interpretation:

An (additive) increase in the value of feature i by 1 unit corresponds to the increase in the odds of the outcome by a (multiplicative) factor of β_i .

Generalized additive models

Model:

$$g(y) = \underbrace{\beta_0 + \sum_i f_i(x_i)}_{\text{Standard GAM}} + \overbrace{\sum_{i \neq j} f_{ij}(x_i, y_j)}^{\text{Caruana, KDD 2015}}$$

Model:

$$g(y) = \underbrace{\beta_0 + \sum_i f_i(x_i)}_{\text{Standard GAM}} + \overbrace{\sum_{i \neq j} f_{ij}(x_i, y_j)}^{\text{Caruana, KDD 2015}}$$

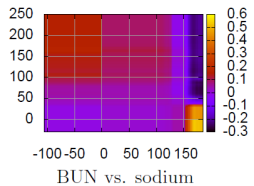
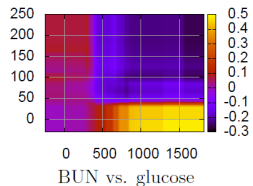
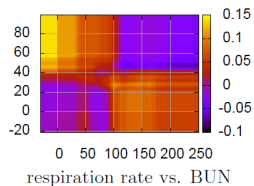
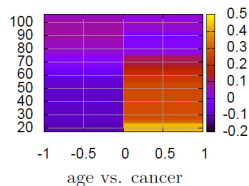
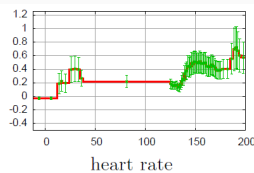
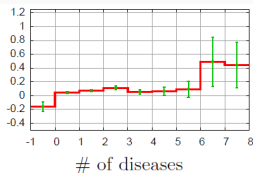
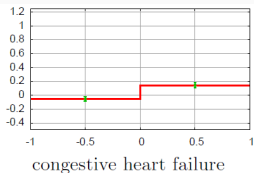
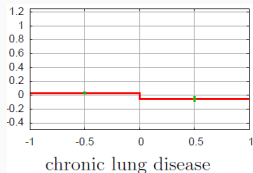
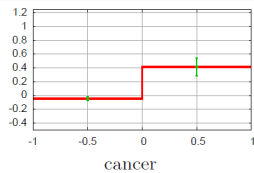
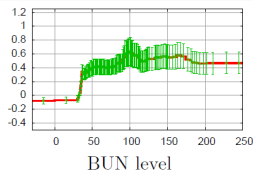
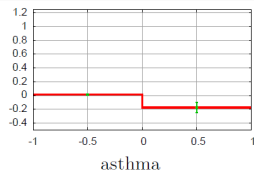
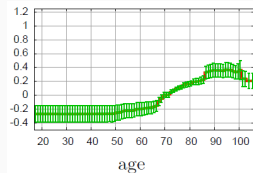
RESEARCH-ARTICLE

Intelligible Models for HealthCare: Predicting Pneumonia Risk and Hospital 30-day Readmission

Authors:  [Rich Caruana](#),  [Yin Lou](#),  [Johannes Gehrke](#),  [Paul Koch](#),  [Marc Sturm](#),  [Noemie Elhadad](#)

[Authors Info & Affiliations](#)

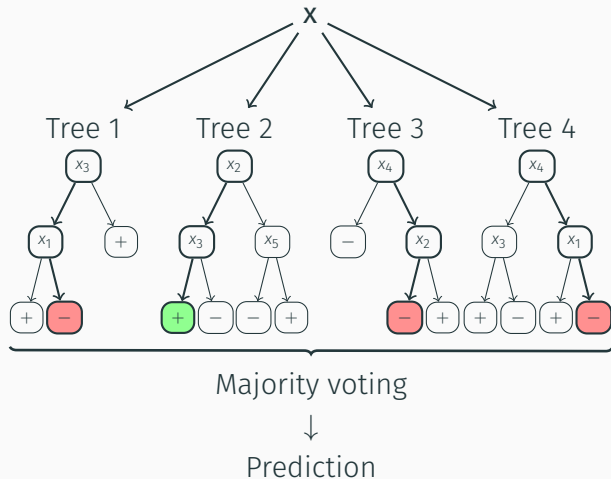
Publication: KDD '15: Proceedings of the 21th ACM SIGKDD International Conference on Knowledge Discovery and Data Mining • August 2015 • Pages 1721–1730 • <https://doi.org/10.1145/2783258.2788613>



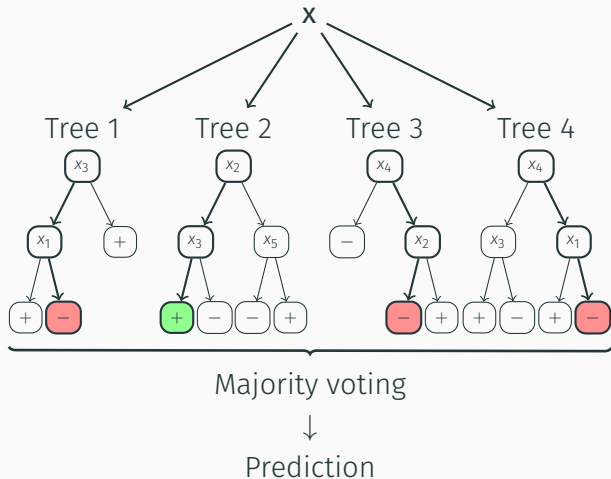
Post-hoc model-aware interpretation

- **Post-hoc** — the interpretation is not built into the predictive model
- **Model-aware** — the interpretation exploits knowledge about the model's internals

Feature importances in random forests

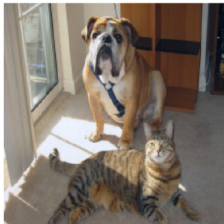


Feature importances in random forests

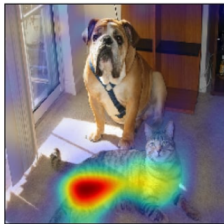


- Model-aware approach to feature importances for random forests:
 - Count the number of times a feature is selected for a split, or
 - Average the impurity score (Gini, entropy, variance) gains for each feature x_i over the all trees.
- Model-agnostic approach to feature importances: permutation (more on this later)

Saliency maps



(a) Original Image



(c) Grad-CAM 'Cat'



(i) Grad-CAM 'Dog'

Grad-CAM: Visual Explanations from Deep Networks via Gradient-based Localization

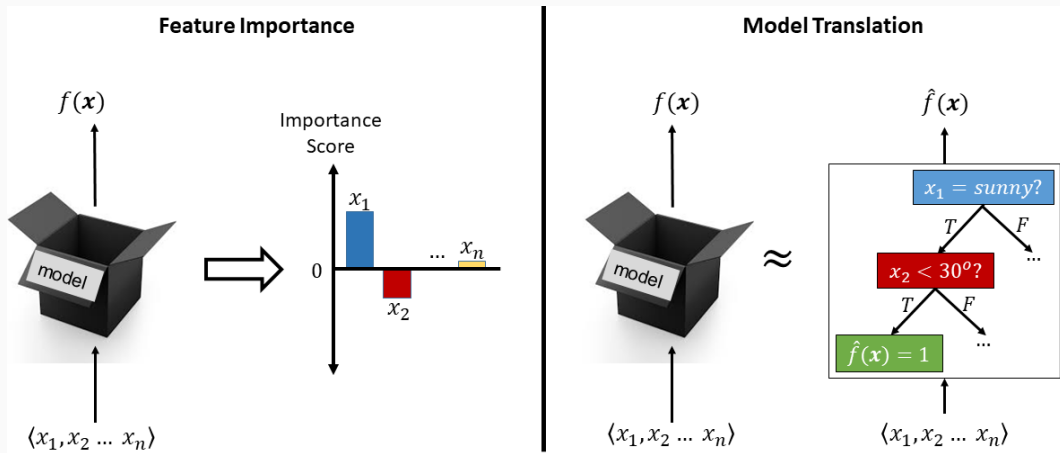
Ramprasaath R. Selvaraju · Michael Cogswell · Abhishek Das · Ramakrishna Vedantam · Devi Parikh · Dhruv Batra

- Highlight regions of the input space that drive a particular prediction
- Commonly used with image data

Post-hoc model-agnostic interpretation

- **Model-agnostic** — the interpretation assumes no knowledge about the model's internals

- **Model-agnostic** — the interpretation assumes no knowledge about the model's internals



Eliciting feature importances from black-box models

1. Given a black-box model $f : \mathcal{X} \rightarrow \mathcal{Y}$

Eliciting feature importances from black-box models

1. Given a black-box model $f : \mathcal{X} \rightarrow \mathcal{Y}$
2. and a training instance $(\mathbf{x}^{(j)}, y^{(j)})$,

Eliciting feature importances from black-box models

1. Given a black-box model $f : \mathcal{X} \rightarrow \mathcal{Y}$
2. and a training instance $(\mathbf{x}^{(j)}, y^{(j)})$,
3. compute a loss function $L(f(\mathbf{x}^{(j)}), y^{(j)})$.

Eliciting feature importances from black-box models

1. Given a black-box model $f : \mathcal{X} \rightarrow \mathcal{Y}$
2. and a training instance $(\mathbf{x}^{(j)}, y^{(j)})$,
3. compute a loss function $L(f(\mathbf{x}^{(j)}), y^{(j)})$.
4. Construct a *perturbed* training instance $\mathbf{x}_{\sim i}^{(j)} = \langle x_1^{(j)}, \dots, x_{i-1}^{(j)}, z_i, x_{i+1}^{(j)}, \dots, x_d^{(j)} \rangle$ in which we replaced the value of the i -th feature

Eliciting feature importances from black-box models

1. Given a black-box model $f : \mathcal{X} \rightarrow \mathcal{Y}$
2. and a training instance $(\mathbf{x}^{(j)}, y^{(j)})$,
3. compute a loss function $L(f(\mathbf{x}^{(j)}), y^{(j)})$.
4. Construct a *perturbed* training instance $\mathbf{x}_{\sim i}^{(j)} = \langle x_1^{(j)}, \dots, x_{i-1}^{(j)}, z_i, x_{i+1}^{(j)}, \dots, x_d^{(j)} \rangle$ in which we replaced the value of the i -th feature
 - The best perturbation is domain-dependent (zeroing out, random/permuted values, population mean).

Eliciting feature importances from black-box models

1. Given a black-box model $f : \mathcal{X} \rightarrow \mathcal{Y}$
2. and a training instance $(\mathbf{x}^{(j)}, y^{(j)})$,
3. compute a loss function $L(f(\mathbf{x}^{(j)}), y^{(j)})$.
4. Construct a *perturbed* training instance $\mathbf{x}_{\sim i}^{(j)} = \langle x_1^{(j)}, \dots, x_{i-1}^{(j)}, z_i, x_{i+1}^{(j)}, \dots, x_d^{(j)} \rangle$ in which we replaced the value of the i -th feature
 - The best perturbation is domain-dependent (zeroing out, random/permutated values, population mean).
5. Compute the loss on the perturbed instance $L(f(\mathbf{x}_{\sim i}^{(j)}), y^{(j)})$

Eliciting feature importances from black-box models

1. Given a black-box model $f : \mathcal{X} \rightarrow \mathcal{Y}$
2. and a training instance $(\mathbf{x}^{(j)}, y^{(j)})$,
3. compute a loss function $L(f(\mathbf{x}^{(j)}), y^{(j)})$.
4. Construct a *perturbed* training instance $\mathbf{x}_{\sim i}^{(j)} = \langle x_1^{(j)}, \dots, x_{i-1}^{(j)}, z_i, x_{i+1}^{(j)}, \dots, x_d^{(j)} \rangle$ in which we replaced the value of the i -th feature
 - The best perturbation is domain-dependent (zeroing out, random/permuted values, population mean).
5. Compute the loss on the perturbed instance $L(f(\mathbf{x}_{\sim i}^{(j)}), y^{(j)})$
6. Consider average difference in loss across the training set

$$\frac{1}{n} \sum_{j=0}^n \left(L(f(\mathbf{x}_{\sim i}^{(j)}), y^{(j)}) - L(f(\mathbf{x}^{(j)}), y^{(j)}) \right)$$

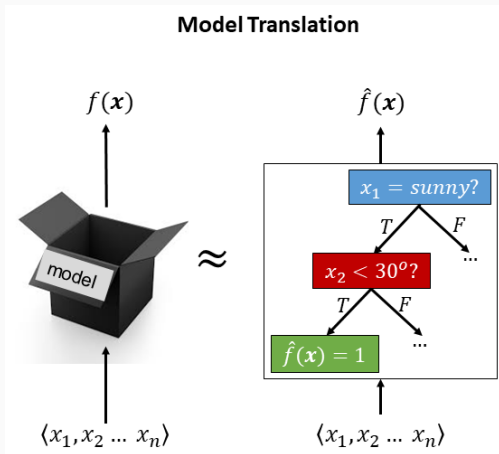
Eliciting feature importances from black-box models

1. Given a black-box model $f : \mathcal{X} \rightarrow \mathcal{Y}$
2. and a training instance $(\mathbf{x}^{(j)}, y^{(j)})$,
3. compute a loss function $L(f(\mathbf{x}^{(j)}), y^{(j)})$.
4. Construct a *perturbed* training instance $\mathbf{x}_{\sim i}^{(j)} = \langle x_1^{(j)}, \dots, x_{i-1}^{(j)}, z_i, x_{i+1}^{(j)}, \dots, x_d^{(j)} \rangle$ in which we replaced the value of the i -th feature
 - The best perturbation is domain-dependent (zeroing out, random/permutated values, population mean).
5. Compute the loss on the perturbed instance $L(f(\mathbf{x}_{\sim i}^{(j)}), y^{(j)})$
6. Consider average difference in loss across the training set

$$\frac{1}{n} \sum_{j=0}^n \left(L(f(\mathbf{x}_{\sim i}^{(j)}), y^{(j)}) - L(f(\mathbf{x}^{(j)}), y^{(j)}) \right)$$

- This gives an importance score for feature i .

Learning high-fidelity mimic models



- Learn an interpretable model that has high fidelity to the black box
- **Fidelity:** how well the interpreting model's outputs match the black box output (given the same inputs)
- Instead of learning only from a training set, learning is also based on the black box's outputs
- The black box is queried throughout the learning process

Black box → decision tree

Black box → decision tree

- Decision trees learned using the black-box model as an oracle
- Better results than learning a decision tree from the training data
- Craven and Shavlik 1995
- Breiman and Shang 1996
- Bastani et al. 2017
- Frosst and Hinton 2017

Appears in *Advances in Neural Information Processing Systems, Vol. 8.*
MIT Press, Cambridge, MA, 1996.

Extracting Tree-Structured Representations of Trained Networks

Mark W. Craven and Jude W. Shavlik
Computer Sciences Department
University of Wisconsin-Madison

Table 2: Test-set accuracy and fidelity.

domain	accuracy				fidelity
	networks	C4.5	ID2-of-3	TREPAN	TREPAN
heart	84.5%	71.0%	74.6%	81.8%	94.1%
promoters	90.6	84.4	83.5	87.6	85.7
protein coding	94.1	90.3	90.9	91.4	92.4
voting	92.2	89.2	87.8	90.8	95.9

Black box \rightarrow (locally) linear

Black box \rightarrow (locally) linear

“Why Should I Trust You?” Explaining the Predictions of Any Classifier

Marco Tulio Ribeiro
University of Washington
Seattle, WA 98105, USA
marcotcr@cs.uw.edu

Sameer Singh
University of Washington
Seattle, WA 98105, USA
sameer@cs.uw.edu

Carlos Guestrin
University of Washington
Seattle, WA 98105, USA
guestrin@cs.uw.edu

$$\underset{g}{\operatorname{argmin}} \underbrace{\mathcal{L}(f, g, \pi_x)}_{\text{fidelity loss around } x} + \underbrace{\Omega(g)}_{\text{complexity}}$$

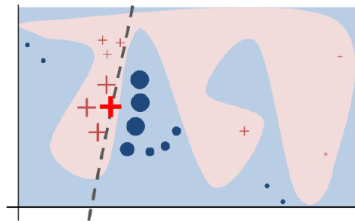


Figure 3: Toy example to present intuition for LIME. The black-box model’s complex decision function f (unknown to LIME) is represented by the blue/pink background, which cannot be approximated well by a linear model. The bold red cross is the instance being explained. LIME samples instances, gets predictions using f , and weighs them by the proximity to the instance being explained (represented here by size). The dashed line is the learned explanation that is locally (but not globally) faithful.