Responsible Machine Learning with Insurance Applications

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Table of Contents

Introduction

How to explain and interpret a given model, even if it seems a black box?

Answering this question is a key aspect of responsible ML

1. Information for stakeholders
2. Detect problems in modeling process

XAI: e**X**plainable **A**rtificial **I**ntelligence

Collection of methods to explain and interpret models

Scope and Taxonomy

Scope

XAI methods for structured data and **bold** aspects below

Taxonomy of explainability

- **Global** vs. local: Describe model as a whole or around an observation.
- Model-specific vs. **model-agnostic**: Some methods are tailored to specific model classes (linear regression, tree-based), others work for all types of models.
- Intrinsic versus **post-hoc**: Simple models like a linear regression can be interpreted intrinsically, while complex models require post-hoc analysis of fitted model.

Notes

- Model-agnostic methods are always post-hoc
- Model-agnostic methods can also be applied to intrinsically interpretable models
- Won't make difference between "explainable", "interpretable", "intelligible"

XAI Outline

1. Introduction

- Notation
- Non-life insurance pricing
- Main example

2. Explaining Models

- Important post-hoc interpretation methods
- SHAP
- Improve GLM with the help of ML and XAI

3. Improving Explainability

Improve intrinsic explainability of complex models by simplifying their structure

Notation

Basic modeling situation

$$T(Y \mid \boldsymbol{x}) \approx m(\boldsymbol{x})$$

- Distributional property $T(Y \mid \boldsymbol{X} = \boldsymbol{x}) = T(Y \mid \boldsymbol{x})$ of response Y
- Model $m : \boldsymbol{x} \in \mathbb{R}^p \mapsto \mathbb{R}$ of feature vector $\boldsymbol{X} = (X^{(1)}, \ldots, X^{(p)})$ with realization $\boldsymbol{x} = (x^{(1)}, \ldots, x^{(p)})$
- m estimated by $\hat{m}$ from training data by minimizing objective criterion $\sum_{i=1}^{n} w_i L(\hat{y}_i, y_i) / \sum_{i=1}^{n} w_i + \lambda\Omega(m)$
- L: loss/scoring function, ideally strictly consistent for T; $\lambda\Omega(m)$: optional penalty
- $\boldsymbol{w} = (w_1, \ldots, w_n)^T$: vector of (optional) case weights
- $\boldsymbol{y} = (y_1, \ldots, y_n)^T$: observed values of Y
- $\hat{\boldsymbol{y}} = (\hat{y}_1, \ldots, \hat{y}_n)^T$: predicted/fitted values $\hat{y}_i = \hat{m}(\boldsymbol{x}_i)$
- $\boldsymbol{x}_1, \ldots, \boldsymbol{x}_n$: n feature vectors; $x_i^{(j)}$: value of j-th feature of i-th observation

Examples of Models

- Linear regression
- Generalized linear models (GLM)
- Generalized additive models (GAM)
- Gradient boosted trees

Will peek into them as a quick refresher and to get used to notation

Linear Regression

- Model equation postulates

$$\mathbb{E}(Y \mid \boldsymbol{x}) = m(\boldsymbol{x}) = \beta_o + \beta_1 x^{(1)} + \cdots + \beta_p x^{(p)}$$

- $(\beta_o, \beta_1, \ldots, \beta_p) \in \mathbb{R}^{p+1}$: parameter vector to be estimated
- Objective: Minimize sum of squared errors

$$\sum_{i=1}^{n} (y_i - \hat{y}_i)^2$$

  by linear least-squares
- Non-linear effects and interactions have to be added manually
- Penalized regression?
- Important extension: the generalized linear model (GLM)

Generalized Linear Model (GLM)

- Model equation postulates

$$\mathbb{E}(Y \mid \boldsymbol{x}) = m(\boldsymbol{x}) = g^{-1}(\eta(\boldsymbol{x})) = g^{-1}(\beta_o + \beta_1 x^{(1)} + \cdots + \beta_p x^{(p)})$$

- g^{-1}: inverse link, g: link function, η: linear predictor
- Parameters β_j estimated by minimizing the (possibly weighted) *average deviance*

$$\bar{S}(\hat{m}, D_{\text{train}}) = \sum_{i=1}^{n} w_i S(\hat{y}_i, y_i) / \sum_{i=1}^{n} w_i$$

over training data $D_{\text{train}} = \{(y_i, w_i, \boldsymbol{x}_i), i = 1, \ldots, n\}$

(Unit) deviance

- Distribution-specific measure: Poisson, Gamma, Bernoulli, normal, ...
- In our examples, we will often work with Poisson deviance
$S(\hat{y}_i, y_i) = 2(y_i \log(y_i/\hat{y}_i) - (y_i - \hat{y}_i))$

Generalized Additive Model (GAM)

- Extension of the GLM
- Model equation assumes

$$\mathbb{E}(Y \mid \boldsymbol{x}) = m(\boldsymbol{x}) = g^{-1}(\beta_o + f_1(x^{(1)}) + \cdots + f_p(x^{(p)}))$$

- f_j: Sufficiently nice functions (some may be fully parameteric)
- Estimated to minimize average deviance, e.g. using backfitting
- Unlike a GLM, automatically accounts for non-linear effects
- Like a GLM, a GAM can also include interaction effects

Gradient Boosted Trees

- Typical black box m
- Sum of decision trees
- In contrast to GAM, automatically picks up interactions
- Can optimize same objective criterion as GLMs/GAMs
- Using a different model structure and a different optimization technique
- Important implementations: LightGBM, XGBoost

Later, we will also work with neural nets

Non-Life Insurance Pricing

Main task: Predict *pure premium* of insurance policy

- Financial loss per year or per some other relevant exposure measure
- Used by company to optimize tariffs and to estimate expected future profit
- Predictions of statistical models fitted on historic data

Discussion

Why is it important to have good tariff?

Characterization of Insurance Policy

- $w > 0$: The exposure. Other quantities will refer to this
- N: Number of claims
- C: Total claim amount
- C/w: Pure premium
- $Y = N/w$: Claims frequency
- $Z = C/N$: Severity = avg cost per claim
- $\boldsymbol{X}$: One or more risk characteristics

Example (fictive motor third-part liability (MTPL) policies)

id	w	N	C	C/w	Y	Z	Driver's age	Horse power
1	1	0	0	0	0	-	28	80
2	0.5	2	5000	10000	4	2500	20	250
2	0.5	1	1000	2000	2	1000	21	250

Remark

Due to additivity of w, N, and C, these quantities can also be defined for multiple policies together, e.g., for the entire portfolio

Classic Pricing Models

- Instead of creating a model for $\mathbb{E}(C/w \mid \boldsymbol{x})$, decompose pure premium

$$C/w = (C/w) \cdot (N/N) = (N/w) \cdot (C/N) = YZ$$

  into product of frequency Y and severity Z
- Frequency model: $\mathbb{E}(Y \mid \boldsymbol{x}) \approx m_Y(\boldsymbol{x})$
  $\to$ Poisson GLM with log link and case weights w
- Severity model: $\mathbb{E}(Z \mid \boldsymbol{x}) \approx m_Z(\boldsymbol{x})$
  $\to$ Gamma GLM with log link and case weights N, using only rows with $N > 0$
- Assuming conditional independence of Y and Z, pure premium model is then $\mathbb{E}(C/w \mid \boldsymbol{x}) \approx m_Y(\boldsymbol{x}) m_Z(\boldsymbol{x})$

Alternative to GLMs

- Replace GLMs by GAMs or modern ML techniques
- Use same losses (deviance), weights, links

More on Non-Life Insurance Pricing

- The severity model can use different features than the frequency model
- The Gamma model with log link is slightly biased $\rightarrow$ can be fixed by applying empirical multiplicative correction factor

$$c = \sum_{i=1}^{n} y_i \Big/ \sum_{i=1}^{n} \hat{y}_i$$

  calculated on the training data
- Why using a log link for the Gamma model?
- As an alternative to model claims frequency using case weights w, directly model claim counts N without weights but using an offset of $\log(w)$
  $\rightarrow$ Same effects, but different intercept, response

Main Example

Example (French motor third-part liability (MTPL) dataset)

1. Understand data
2. Descriptive analysis
3. Build claim frequency models

The models

- Poisson GLM
- Poisson GAM
- Poisson gradient boosted trees

Notes

- Grouped train/test split
- Model interpretation

Table of Contents

Introduction

Basic workflow to inspect and explain supervised learning model m

1. Study model performance
2. Study feature importance
3. Study feature effects, ideally also interactions

Focus

Global, model-agnostic, post-hoc explainability

Analysis result

- Information gain
- Reveal problems in model/data
- Increase confidence in model and modeler

Main references

- Online book of Christoph Molnar
- Tutorial (Mayer & Lorentzen 2020)

Chapter Outline

1. Software
2. Performance
3. Excursion: grouped data
4. Variable importance
5. Effects
6. Global surrogate models
7. Improve linear models by XAI
8. SHAP

Software for Post-Hoc Interpretation

Python

- sklearn.inspection
- shap
- DALEX
- ...

R

- hstats
- DALEX
- iml
- SHAP: shapviz, fastshap, kernelshap
- ...

Performance

- Study one or more relevant performance measures
- Often: Average loss or function of it
- Gives valuable information
- Training versus test performance? $\rightarrow$ assess overfitting/optimism
- Absolute and relative measures

Also helps to detect problems

Is performance much lower than expected?

- Preprocessing errors
- Missing key feature
- Convergence problem

Is it much better?

- Data partitions not independent?
- Leakage from response to feature?

Example: Claims Frequency Models

- Calculate weighted average Poisson deviance on test data:

$$\bar{S}(\hat{m}, D_{\text{test}}) = \sum_{i=1}^{n} w_i S(\hat{y}_i, y_i) / \sum_{i=1}^{n} w_i$$

  with $S(\hat{y}_i, y_i) = 2(y_i \log(y_i/\hat{y}_i) - (y_i - \hat{y}_i))$
- Relative deviance improvement (one of many "pseudo R-squared")

$$1 - \frac{\bar{S}(\hat{m}, D_{\text{test}})}{\bar{S}(\hat{m}_{\text{trivial}}, D_{\text{test}})},$$

  where $\hat{m}_{\text{trivial}}(\boldsymbol{x}) = \sum_{D_{\text{train}}} w_i y_i / \sum_{D_{\text{train}}} w_i$ is the intercept-only model with constant predictions ideally calculated on the training data
- Repeat on training data (why?)

Excursion: Grouped Data

- Flawed validation strategy $\rightarrow$ biased performance assessment
- Detailed knowledge of data and model required $\rightarrow$ difficult to detect

Typical reason for flawed validation: Grouped data

- Pricing data
- Reserving: Models for ultimate claim amount
- Customer analytics: Browser behaviour of online visitors
- Banking: Financial transactions of clients

Grouped splitting

- Instead of random sampling of *rows*, we sample *groups*
- All rows of a group go in same data partition
- If ignored: Overfitting is being rewarded

Example and Simulation

Example (French MTPL)

- Model performance of GLM and boosted trees model without grouped splitting?
- Impact on model tuning?

Example (Simulation)

- Random data
- Linear regression and random forest
- 80%/20% split
- Increasing proportion of duplicated rows
- Random split versus grouped split

More on Grouped Data

- We used grouping structure to create clean data splits
- Sometimes, one wants to also make use of within-group info in model
- Panel data, time-series

Examples

- Insurance of large vehicle fleets: credibility factors
- Banking: Financial transactions of client

Tricky to have clean validation strategy and to apply model correctly

Variable Importance

1. Information: Most/least important features?
2. Challenge correctness of model
   - Results as expected or not?
   - Seemingly unimportant feature is top predictor $\rightarrow$ leakage?
   - Key features not among important features $\rightarrow$ preprocessing problem, not sufficient understanding of data or modeling situation?

Model-specific variable importance measures

- Linear model: normalized coefficients, test statistics etc.
- Tree-based models: Split gain or split count

Model-agnostic measures

- Permutation importance (Breiman 2001 for random forests)
- SHAP feature importance

Permutation Importance

Permutation importance of j-th feature $X^{(j)}$, data D, and performance measure $\hat{S}$:

$$\mathrm{PVI}(j, D) = \hat{S}(\hat{m}, D^{(j)}) - \hat{S}(\hat{m}, D)$$

- $D^{(j)}$ is version of D with randomly permuted values in j-th feature column
- Read: How much $\hat{S}$ worsens after shuffling column j?
  The larger, the more important. If 0, feature is unimportant

Algorithm to calculate $\mathrm{PVI}(j, D)$ for all features

Algorithm 1: Permutation importance

scoreOriginal $\leftarrow$ performance on data
for *x in variables* **do**
  dataShuffled $\leftarrow$ data with permuted column x
  scoreShuffled $\leftarrow$ performance on dataShuffled
  importance[x] $\leftarrow$ scoreShuffled $-$ scoreOriginal
end
output : importance

Source: Mayer and Lorentzen, 2020

Remarks and Example

Remarks

- Computationally cheap $\rightarrow$ repeat m times
- Model is never refitted
- There is no formal definition of variable importance $\rightarrow$ inconsistency across methods
- Different definitions of permutation importance
- Strongly dependent features $\rightarrow$ decorrelate or analyze together
- Training or test data?

Example (French MTPL)

- PVI using exposure-weighted average Poisson deviance
- Hold-out data
- Compare with tree-split gain

Effects

Study and understand feature effects is of key importance

- How does $m(\boldsymbol{x})$ change with j-th feature?
- Often Ceteris Paribus: other components in $\boldsymbol{x}$ fixed

Advantage of intrinsically interpretable models

- (Ceteris Paribus) effect of feature $X^{(j)}$ in a linear regression

$$\mathbb{E}(Y \mid \boldsymbol{x}) \approx m(\boldsymbol{x}) = \beta_o + \beta_1 x^{(1)} + \cdots + \beta_p x^{(p)}$$

- In an additive model

$$\mathbb{E}(Y \mid \boldsymbol{x}) \approx m(\boldsymbol{x}) = \beta_o + f_1(x^{(1)}) + \cdots + f_p(x^{(p)})$$

- In a black box model?

Methods

1. Individual conditional expectation (ICE)
2. Partial dependence
3. Classic diagnostic plots
4. Interactions?
5. Later: SHAP dependence plots

Individual Conditional Expectation (ICE)

Basic thinking

- If m is additive in feature $X^{(j)}$, the Ceteris Paribus effect of $X^{(j)}$ is the same for all observations $\rightarrow$ complete description of effect / full transparency
- If complex interactions involved $\rightarrow$ approximate description only

Idea (Goldstein et al., 2015)

- Study Ceteris Paribus effect of $X^{(j)}$ for one observation
- *ICE function* for feature $X^{(j)}$ of model m and observation $\boldsymbol{x} \in \mathbb{R}^p$

$$\mathrm{ICE}_j : v \in \mathbb{R} \mapsto m(v, \boldsymbol{x}_{\setminus j})$$

- $\boldsymbol{x}_{\setminus j}$ denotes all but the j-th component of $\boldsymbol{x}$, which is replaced by v
- *ICE curve* represents graph $(v, \mathrm{ICE}_j(v))$ for grid of values $v \in \mathbb{R}$

Simple Algorithm

Algorithm to calculate $ICE_j(v)$

Algorithm 2: ICE for variable x and one observation

obs $\leftarrow$ data row
for v *in grid of values* **do**
  obs[x] $\leftarrow v$
  ice[v] $\leftarrow$ prediction for obs
end
output : ice

Source: Mayer and Lorentzen, 2020

ICE Plot: Visualize ICE curves of multiple observations

Example

Notes

- Curves with different shapes indicate interaction effects
- Parallel curves $\rightarrow$ additivity in $X^{(j)}$
- Centered ICE plots
- Usually on link scale (why?)
- ICE plots of higher dimension
- Training versus test data

Pros and Cons

\+ Simple to compute

\+ Easy to interpret (Ceteris Paribus)

\+ Gives impression about interactions

– Suboptimal when Ceteris Paribus unnatural

– Model applied to rare/impossible $\boldsymbol{x}$

– Does not show what variables are interacting

Partial Dependence Plot PDP (Friedman 2001)

- Average of many ICE curves
- Ceteris Paribus effect of $X^{(j)}$ averaged over all interaction effects

Definition

- (Empirical) partial dependence function of feature j

$$\mathrm{PD}_j(v) = \frac{1}{n}\sum_{i=1}^{n} \hat{m}(v, \boldsymbol{x}_{i,\setminus j})$$

- $\boldsymbol{x}_{i,\setminus j}$ feature vector of i-th observation without j-th component
- Estimate for $\mathbb{E}_{\boldsymbol{X}_{\setminus j}}\, m(v, \boldsymbol{X}_{\setminus j})$ (expectation runs over joint marginal distr. of $\boldsymbol{X}_{\setminus j}$)
- PDP equals graph $(v, \mathrm{PD}_j(v))$ for grid of values $v \in \mathbb{R}$
- Sum runs over reference data (=?)

Algorithm

Calculate $PD_j(v)$ on grid of values for v

Algorithm 3: Partial dependence profile for variable x

$n \leftarrow$ number of observations
$m \leftarrow$ grid size for variable x
iceProfiles $\leftarrow$ matrix with n rows and m columns
for i *in* 1 *to* n **do**
  iceProfiles$[i, :] \leftarrow$ ice curve for ith obs and variable x
end
pd $\leftarrow$ column means of iceProfiles
output : pd

Source: Mayer and Lorentzen, 2020

Example

More on Partial Dependence

Remarks

- 2-dimensional PDP of $X^{(j)}$ and $X^{(k)}$:

$$\mathrm{PD}_{jk}(v_j, v_k) = \frac{1}{n}\sum_{i=1}^{n} \hat{m}(v_j, v_k, \boldsymbol{x}_{i,\setminus\{j,k\}})$$

- Accumulated local effects (ALE)

Pros and Cons

+ Simple to compute
+ Easy to interpret (Ceteris Paribus)
– Suboptimal when Ceteris Paribus unnatural
– Model applied to rare/impossible $\boldsymbol{x}$
– No information about interactions

Classic Diagnostic Plots

Related plots

1. Response versus covariate
   $\rightarrow$ Descriptive marginal effects
2. Predicted versus covariate
   $\rightarrow$ Modeled marginal effects
3. Residual versus covariate:
   $\rightarrow$ Bias assessment

Remarks

- Small and large datasets
- Binning of feature values
- Training versus test data?
- Relation to PDP?
- Pros and Cons?

Example

Interaction Effects

- Including interactions: Additive models versus black box models
- ICE plot for $X^{(j)}$ gives impression of total interaction effects associated with $X^{(j)}$

Pairwise interaction strength: Friedman's H^2

If model is additive in $X^{(j)}$ and $X^{(k)}$, then

$$\mathrm{PD}_{jk}(x_i^{(j)}, x_i^{(k)}) = \mathrm{PD}_j(x_i^{(j)}) + \mathrm{PD}_k(x_i^{(k)})$$

for all $\mathbf{x}_i$ in reference data D, assuming PD functions are mean-centered over D. Thus,

$$H_{jk}^2 = \frac{\sum_{i=1}^n \left[\mathrm{PD}_{jk}(x_i^{(j)}, x_i^{(k)}) - \mathrm{PD}_j(x_i^{(j)}) - \mathrm{PD}_k(x_i^{(k)})\right]^2}{\sum_{i=1}^n \left[\mathrm{PD}_{jk}(x_i^{(j)}, x_i^{(k)})\right]^2}$$

measures (relative) deviation from additivity, where sums run over D

- Interpretation of H^2? When close to 0 or 1?

Absolute Interaction Strength

Friedman's H^2 is a relative measure $\rightarrow$ absolute measure?

$$\tilde{H}_{jk} = \sqrt{\frac{1}{n}\sum_{i=1}^{n}\left[\mathrm{PD}_{jk}(x_i^{(j)}, x_i^{(k)}) - \mathrm{PD}_j(x_i^{(j)}) - \mathrm{PD}_k(x_i^{(k)})\right]^2}$$

Remarks on H^2 and $\tilde{H}$

- Find out *how* features are interacting?
  $\rightarrow$ Conditional PDP/ICE, 2D PDP, SHAP
- Computational burden?
- Usually, one works on link scale

Example

Global Surrogate Models

Idea

- Fit intrinsically interpretable model m_I to predictions of $\hat{m}$
- Usually a small decision tree
- $\hat{m}_I$ is called (global) surrogate model for $\hat{m}$
- Objective function and R-squared of $\hat{m}_I$?

Remarks

- Training or test data?
- Variable importances of $\hat{m}_I$?

Example

Improve Linear Models by XAI

Workflow

- Build strong GLM by the help of ML and XAI
- Why not directly use ML model?

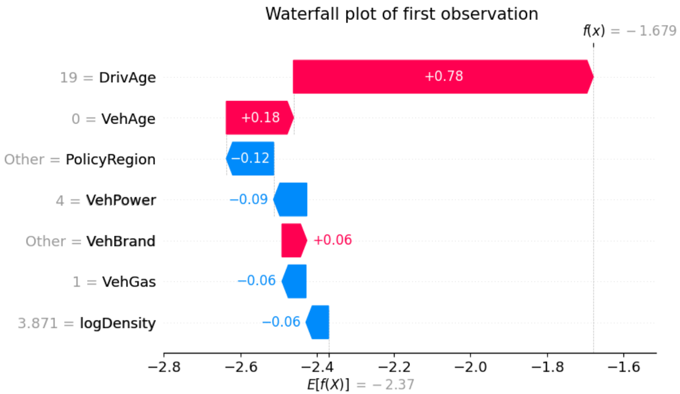
Compare XAI aspects

1. Performance: Difference between GLM and ML model large or small?
2. Variable importance: Similar features important?
3. Main effects: Similar or not? $\rightarrow$ Change representation in GLM
4. Interaction effects: Add strong meaningful interactions to GLM

Example

SHAP: SHapley Additive exPlanations

- Local explanations
- Basic idea of SHAP?
- LIME: Local Interpretable Model-agnostic Explanations



Shapley Values

- $\mathcal{M}$: Set of $p = |\mathcal{M}|$ players
- Playing cooperative game with numeric payoff
- Contribution of subset $\mathcal{L} \subseteq \mathcal{M}$ of players measured by function $v : \mathcal{L} \mapsto \mathbb{R}$

How to distribute payoff fairly among players?

Answer by Lloyd Shapley (1953): Player j should receive "Shapley value"

$$\phi_j(v) = \phi_j = \sum_{\mathcal{L} \subseteq \mathcal{M} \setminus \{j\}} \underbrace{\frac{|\mathcal{L}|!(p - |\mathcal{L}| - 1)!}{p!}}_{\text{Shapley weight}} (\underbrace{v(\mathcal{L} \cup \{j\}) - v(\mathcal{L})}_{\text{Contribution of j to } \mathcal{L}}).$$

- Weighted average contribution over all coalitions $\mathcal{L} \subseteq \mathcal{M} \setminus \{j\}$
- Average contribution over all $p!$ permutations $(\underbrace{\ldots}_{\mathcal{L}}, j, \underbrace{\ldots}_{\text{not playing}})$

What means Fair?

Shapley values are only way to distribute total winnings fairly in this sense:

Efficiency

$v(\mathcal{M}) = \phi_o + \sum_{j=1}^{p} \phi_j$, where $\phi_o = v(\emptyset)$ denotes non-distributed payoff

Symmetry

If $v(\mathcal{L} \cup \{i\}) = v(\mathcal{L} \cup \{j\})$ for every $\mathcal{L} \subseteq \mathcal{M} \setminus \{i, j\}$, then $\phi_i = \phi_j$

Dummy player

If $v(\mathcal{L} \cup \{j\}) = v(\mathcal{L})$ for all coalitions $\mathcal{L} \subseteq \mathcal{M} \setminus \{j\}$, then $\phi_j = 0$

Linearity

Consider two cooperative games with gain functions v and w. Then,
$\phi_j(v + w) = \phi_j(v) + \phi_j(w)$ and $\phi_j(\alpha v) = \alpha \phi_j(v)$ for all $1 \leq j \leq p$ and $\alpha \in \mathbb{R}$

Shapley Values in Statistics and ML

Early idea

Lipovetsky and Conklin (2001): Fair decomposition of *R-squared* in linear regression

Nowadays: Štrumbelj and Kononenko (2010, 2014), Lundberg and Lee (2017)

- Decompose *predictions* fairly into $m(\boldsymbol{x}) = \phi_o + \sum_{j=1}^{p} \phi_j, \quad \phi_o = \mathbb{E}(m(\boldsymbol{X}))$
- Fair only if ϕ_j are Shapley values
- Natural contribution function: $v(\mathcal{L}) = m(\boldsymbol{x}_\mathcal{L})$, $\boldsymbol{x}_\mathcal{L}$ are components in $\mathcal{L} \subseteq \mathcal{M}$
- But: Features cannot be turned off in $m \rightarrow$ use statistics to estimate it

Situations where no estimation is required

- $p = 1$: Then $\phi_1 = m(\boldsymbol{x}) - \phi_o$
- Linear regression without correlations:

$$m(\boldsymbol{x}) = \underbrace{\beta_0}_{\phi_o} + \underbrace{\beta_1 x^{(1)}}_{\phi_1} + \cdots + \underbrace{\beta_p x^{(p)}}_{\phi_p}$$

How to Estimate Contribution Function

Controversy in estimating $m(\boldsymbol{x}_{\mathcal{L}})$

- Causal inference: Marginal expectations $\mathbb{E}(m(\boldsymbol{x}_{\mathcal{L}}, \boldsymbol{X}_{\mathcal{M}\setminus\mathcal{L}}))$
- Statistically more natural: Conditional expectations $\mathbb{E}(m(\boldsymbol{x}_{\mathcal{L}}, \boldsymbol{X}_{\mathcal{M}\setminus\mathcal{L}}) \mid \boldsymbol{X}_{\mathcal{L}} = \boldsymbol{x}_{\mathcal{L}})$

Algorithms

1. Monte Carlo sampling: For each j and many $\mathcal{L}$, contributions $v(\mathcal{L} \cup \{j\}) - v(\mathcal{L})$ are evaluated using marginal expectations and then plugged into Shapley's Eq.
2. Kernel SHAP: For many $\mathcal{L}$, evaluate $v(\mathcal{L})$ using marginal expectations. Then use weighted regression to get all Shapley values without plugging into Shapley's Eq.
3. TreeSHAP: Uses properties of trees to directly calculate $v(\mathcal{L})$ for all $\mathcal{L} \subseteq \mathcal{M}$ and then plugging into Shapley's Eq.

Example

From Local to Global Explanations

Decompose n predictions, not just one

- X: $(n \times p)$ feature matrix with elements x_{ij}, $1 \leq i \leq n$, $1 \leq j \leq p$
- Φ: $(n \times p)$ matrix of SHAP values with elements ϕ_{ij}
- $\phi_o = \frac{1}{n} \sum_{i=1}^{n} \hat{m}(\boldsymbol{x}_i)$
- $\hat{m}(\boldsymbol{x}_i) = \phi_o + \sum_{j=1}^{p} \phi_{ij}$ for n feature vectors $\boldsymbol{x}_i$

Example

Strategy to understand model as a whole

- SHAP feature importance: $I_j = \frac{1}{n} \sum_{i=1}^{n} |\phi_{ij}|$
- SHAP dependence plots: $\{(x_{ij}, \phi_{ij}), 1 \leq i \leq n\}$
- Interactions: Use $x_{ik}, k \neq j$ to add color to SHAP dependence plot (alternative?)

SHAP Analysis to Improve Linear Model

Revisit strategy

- A lot of info on ML black box can be generated very quickly
- Use to build strong GLM

Example

Remember

SHAP has a solid theoretical foundation. In practice, some of it is lost because statistics is not mathematics.

Table of Contents

Introduction

"The best explanation of a simple model is the model itself" (Lundberg and Lee, 2017)

Two main strategies in XAI

- Model is black box $\rightarrow$ interpret it post-hoc
- Make model less opaque / improve intrinsic explainability

Basic hierarchy of intrinsic explainability

1. Linear additive models (like GLMs)
2. Additive models (like GAMs)
3. Black box models (like boosted trees or neural nets)

Note

- To link or not?
- Single decision tree

Boundaries are Blurred

Examples

- GLMs can have non-linear effects
- GLMs and GAMs can have interactions
- A complex GLM can be (almost) as black box as a boosted trees model
- Boosted trees models can have all or some features additive
- Neural nets can have all or some features additive

Partly additive models = Additive with (possibly complex) interactions

- Additive time effects: $m(\boldsymbol{x}) = f(\text{Time}) + f'(\text{other features})$
- Additive gender effects: $m(\boldsymbol{x}) = f(\text{Gender}) + f'(\text{other features})$
- Additive model with non-additive location effects:
  $m(\boldsymbol{x}) = f_1(x^{(1)}) + \cdots + f_{p_1}(x^{(p_1)}) + f(\text{location features})$

Chapter Outline

Structuring boosted trees

- Additive models
- Partly additive models
- Monotonicity

Structuring neural nets

- Additive models
- Partly additive models

(Tune boosted trees models)

Structuring Boosted Trees

Interpreting boosted trees models

- Single decision trees m_k are simple to interpret
- Boosted trees m are sums of K decision trees

$$m(\boldsymbol{x}) = m_1(\boldsymbol{x}) + \cdots + m_K(\boldsymbol{x})$$

- Interpretation only post-hoc

Let's add structure to boosted trees!

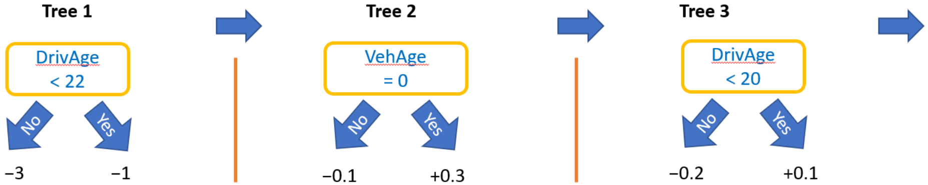
Additive Boosted Trees

What is a tree stump?

- Decision tree m_k with only one split (assume on j-th feature)
- $m_k(\boldsymbol{x}) = v_1 + (v_2 - v_1)\mathbb{I}(x^{(j)} \leq s)$; $(v_1, v_2, s = ?)$

Boosted tree stumps are additive

- f_j: sum of those m_k that split on j-th feature
- $m(\boldsymbol{x}) = f_1(x^{(1)}) + \cdots + f_p(x^{(p)})$



More on Boosted Tree Stumps

- Additivity $\rightarrow$ full description of feature effects via ICE/PDP
- SHAP dependence plot? (Mayer 2022)
- Discussion: Pros and cons versus classic GAM?
- References: Lou et al. (2012), Nori et al. (2019)

Example

Partly Additive Boosted Trees

- Grow trees of depth 2 $\rightarrow$ pairwise interactions
- Partly additive model via *interaction constraints* (Lee et al. 2015)

Interaction constraints

- $IC = \{F_1, \ldots, F_K\}$
- Each F_k is feature subset allowed to interact

How do they work?

- Consider a decision tree
- Each branch will use features only from one $F_k \in IC$.
- Rule: Each split considers features only from those F_k that contain all previous split variables of the branch. First split?
- Translates to tree and to sum of trees.

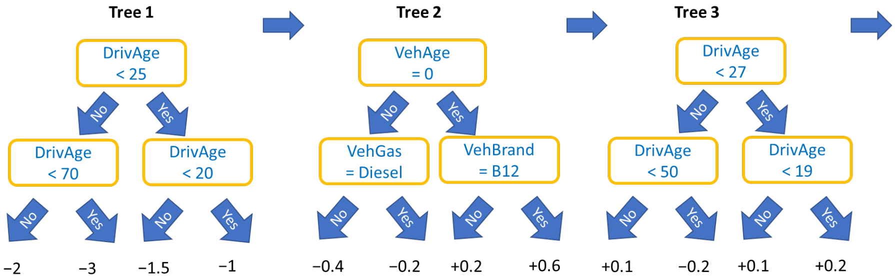
Partly Additive Models via Interaction Constraints

How to set IC so that model is additive in j-th feature?

- $F_1 = \{X^{(j)}\}$
- $X^{(j)} \notin F_k$, for $k > 1$

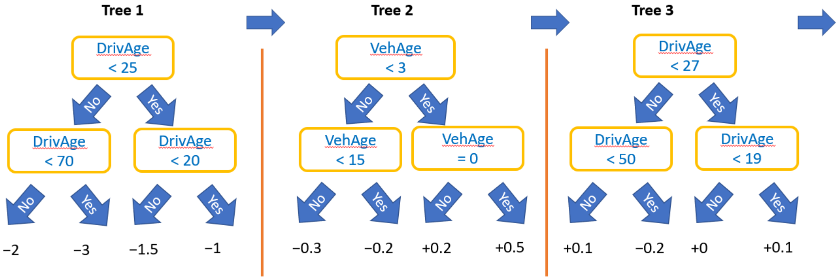
Example

$IC = \{\{\text{DrivAge}\}, \{\text{logDensity}\}, \{\text{PolicyRegion}\}, \{\text{VehAge}, \text{Brand}, \text{Gas}, \text{Power}\}\}$



More on Interaction Constraints

- If all elements in IC are disjoint, each tree uses features from only one F_k
- $IC = \{\{X^{(1)}\}, \ldots, \{X^{(p)}\}\}$ gives additive model:



- Difference to boosted tree stumps?

Monotonic Constraints

- Monotonicity of $m(\boldsymbol{x})$ in j-th feature is another aspect of interpretability
- Violated natural monotonicity can have dramatic impact on trustworthiness
- Example: car *collision* model
- How is it implemented?
- Translates to tree ensembles

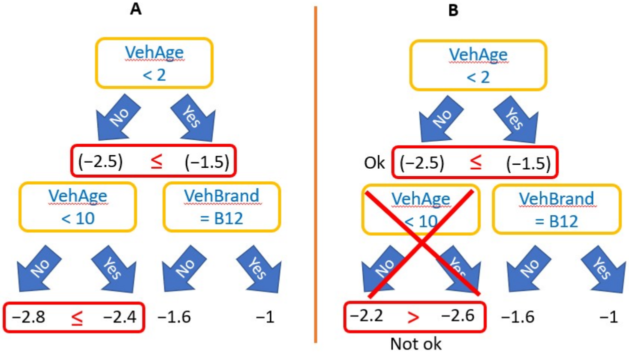
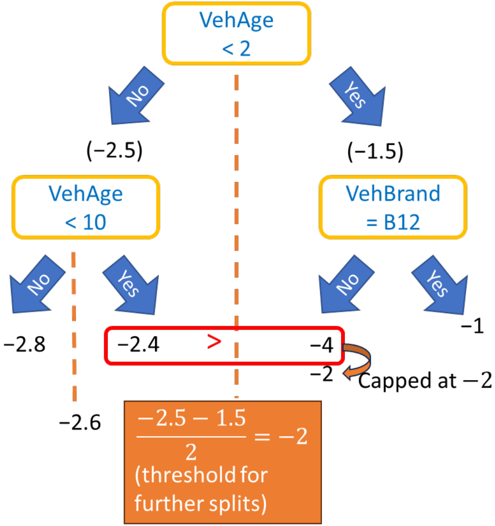


Figure: Monotone decreasing predictions in vehicle age

Enforcing Monotonicity: Capping logic



More on Monotonic Constraints

- Be careful when imposing monotonicity (why?)
- Can help to reduce wiggliness of effect
- Monotonicity for other model classes like GLMs, GAMs, neural nets?
- Monotonicity and outlying feature values

Example

Structuring Neural Nets

Swiss army knife of ML: Neural nets can

- mimic GLMs and GAMs,
- learn interactions and non-linear effects,
- fit data larger than RAM (e.g. images, videos),
- use multidimensional input and output,
- use input and output of mixed dimensionality,
- fit models with millions of parameters,
- perform non-linear dimension reduction,
- ...

How to create

1. linear,
2. complex,
3. additive, and
4. partly additive

neural nets?

Some Notes on Neural Nets

- Why haven't we worked with neural nets so far?
- Neural nets versus boosted trees?
- TensorFlow (with Keras), PyTorch
- Keras: sequential versus functional API
- Keras in R

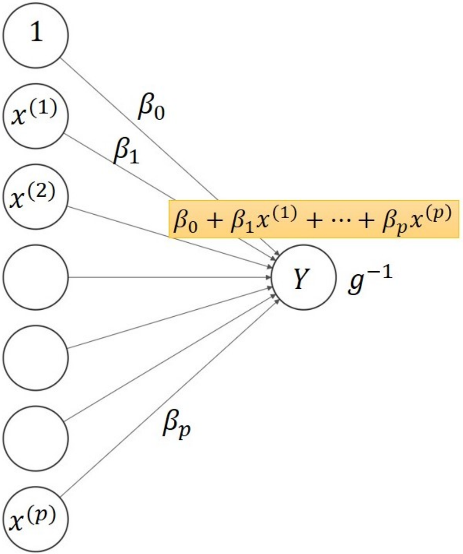
A Simple Neural Net: GLM

Some slang

- Input and output layer?
- Nodes and node values?
- Fully connected / dense layer
- Exponential activation function

Example

- Scaling
- Callbacks
- Integer encoding



Mini-Batch Gradient Descent with Backpropagation

Notation: Neural net m_β; its total loss on data D and loss function L:

$$Q(m_\beta, D) = \sum_{(y_i, \boldsymbol{x}_i) \in D} L(m_\beta(\boldsymbol{x}_i), y_i)$$

1. Init: Randomly initialize parameter vector β by $\hat{\beta}$
2. Forward: Calculate $Q(m_{\hat{\beta}}, D_{\text{batch}})$ on batch
3. Backprop: Modify $\hat{\beta}$ to improve $Q(m_{\hat{\beta}}, D_{\text{batch}})$
   3.1 Calculate partial derivatives $\nabla\hat{\beta} = \frac{\partial Q(m_\beta, D_{\text{batch}})}{\partial \beta} \mid_{\beta=\hat{\beta}}$ using backprop (=?)
   3.2 Gradient descent: Move slightly into right direction: $\hat{\beta} \leftarrow \hat{\beta} - \lambda \cdot \nabla\hat{\beta}$
4. Repeat Steps 2 and 3 until one epoch is over
5. Repeat Step 4 until some stopping criterion triggers

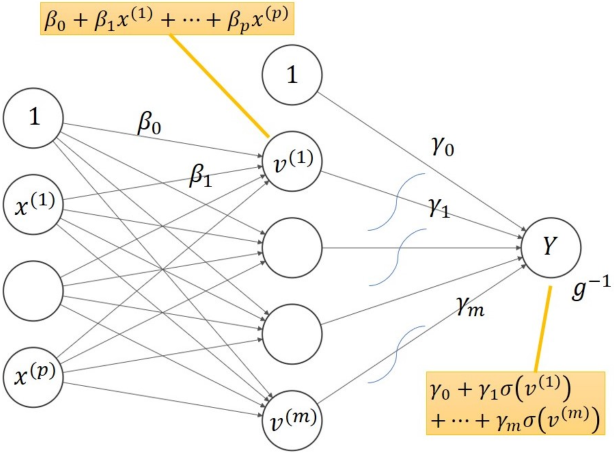
More Complex Models

Some additional slang

- Hidden layers
- Representational learning
- Activation functions:
  two purposes
- How to choose architecture?
- How to choose number of parameters/weights?

Example

- Three hidden layers
- 561 parameters

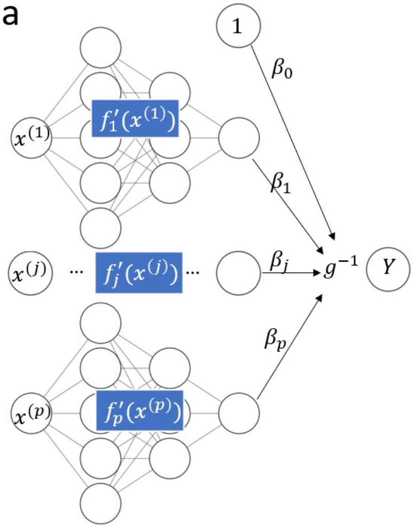


Additive Neural Nets (Agarwal et al. 2020)

- Represent each feature by single-output net
- Directly connected to output layer
- Linear components?
- Unordered categorical features?

Example

- ‘VehBrand’, ‘PolicyRegion’: 1-D embedding
- ‘VehGas’ and ‘logDensity’: Scaled and represented by linear function
- Rest: Scaled and represented by small net each
- Similar structure as our original GAM



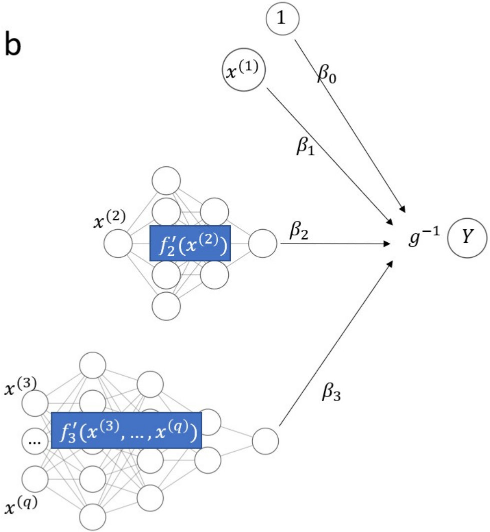
Source: Fig 1a in
https://www.mdpi.com/1911-8074/15/5/193

Partly Additive Models

- Pairwise interactions?
- How constructed?

Example: Additive driver effects?

- 'logDensity': Scaled and represented as linear function
- 'DrivAge': Scaled and represented by a small sub-network
- 'PolicyRegion': 1-D embedding
- Vehicle features: sub-network with different inputs and five outputs



Source: Fig 1b in https://www.mdpi.com/1911-8074/15/5/193

Excursion: Tuning Boosted Trees

Model tuning in general

- How to choose hyperparameters of ML models?
- Each model class (GLMs, GAMs, random forests, boosted trees, neural nets, ...) has specialities that should be respected
- Examples?

Why focussing on boosted trees?

- Usually among best performing models for tabular data
- Boosting + SHAP $\to$ strong GLMs
- It takes some practice

Aspects

1. Objective and evaluation metric
2. Number of boosting rounds
3. Learning rate
4. Further parameters

Objective and Metric

Ideal choice of loss function

- Meaningful for task
- Strictly consistent for target functional T

Translation to objective and metric

- Objective: average loss on training data (plus regularization) used for model training
- Evaluation metric: average (cross-)validation loss used for model comparison and selection

Example

Number of Boosting Rounds

Very important to select reasonable number of boosting rounds

- Boosting round = tree
- Too few rounds $\rightarrow$ underfitting
- Too many rounds $\rightarrow$ overfitting
- Heavily depends on choice of other parameters, thus difficult to choose

"Early stopping" as standard solution

- How does it work?
- Why is it so convenient?

Learning Rate

- Weight of each tree in final model
- Often between wide range of 1 and 0.005
- Good value heavily depends on number of boosting rounds
- Trick: select it so that early stopping ends after $100 - 1000$ trees (why?)
- Halving the number of trees means doubling the learning rate for comparable performance

Regularization Parameters

Additional parameters to select

- number of leaf nodes
- tree depth
- loss penalties
- different types of subsampling rates
- ...

Choose them by (cross-)validation

- One by one
- Grid-search
- Random search

Note

- Early-stopping often compensates for suboptimal choice of other parameters
- Very different parameter combinations may lead to similar performance

Overall Strategy

Three steps

1. Choose strictly consistent and meaningful loss for functional T
   $\rightarrow$ objective and evaluation metric
2. Choose learning rate to get $100 - 1000$ trees with early stopping
3. Select remaining parameters manually or by random search via (cross-)validation

Simplification

When to skip expensive Step 3?

Example

- French MTPL
- Speciality: grouped partitions