Feature Importance and Explainability

DS 6030 | Fall 2024

feature-imp.pdf

Contents

1 Intro

- **Feature Importance** is the task of understanding how important the features of a predictive model are to:
  a) making predictions, or
  b) predictive performance
- **Explainability (part of XAI)** is the task of better understanding how predictive models use the features to make predictions.

1.1 Donor Acceptance Modeling

Create a train/test split. Holding out 1000 observations for testing.

```
library(tidymodels)
n_test = 1000
set.seed(2024)
donor_data =
  donor_data_all %>%
  initial_split(prop = 1-n_test/nrow(.), strata = outcome)
donor_data
#> <Training/Testing/Total>
#> <29155/1001/30156>
```

Create a *workflow* for lightgbm boosted tree model:

```
library(bonsai)
library(lightgbm)
library(tidymodels)

#: pre-processing specs
rec_lgbm =
  recipe(outcome ~
         # Offer Features
           DISTANCE + NUM_REJECT_DON + offer_tod +
         # Donor Features
           ABNL_ECHO_CUM + COD_DON + AGE_DON + BMI_DON + CARDARREST +
           CHEST_TRAUMA + CPR_ADMIN + CPR_DURATION + CPRA + CREATININE_max +
           HRS_FROM_BD + RISK_HIV_DON + INO_count_max +
         # Candidate Features
           CAND_DIAG + prior_offers_cand + WEIGHT_CAND_KG +
           TROPONINI_max + ABO_CAND + AGE_CAND + BMI_CAND +
           STATUS_CAND + RACE_CAND + GENDER_CAND +
           ECMO_CAND + LIFE_SUPPORT_CAND + VAD_AT_LISTING_CAND +
           VENTILATOR_CAND +
           days_on_wl_active +
         # Donor/Candidate Comparison
           WEIGHT_RATIO + HEIGHT_RATIO + ABO_MATCH +
         # Center Features
           LISTING_CTR_ACCEPT_RATE_PREV + LISTING_CTR_TX_PREV
         , data = donor_data)

#: Define the lightgbm model specification
lgbm_spec =
  boost_tree(mode = "classification") %>%
  set_engine("lightgbm", num_threads = 6) %>%
  set_args(
    #: set objective/loss function
    objective = "binary",
```

```
    #: parameters to tune
    trees = tune(),            # num_iters
    num_leaves = tune(),       # maximum number of leaf nodes
    #: fixed tuning parameters
    tree_depth = 10,               # max depth of tree
    learn_rate = 0.1,              # learning_rate (shrinking)
    min_n = 10,                    # min nodes in leaf (default value)
    loss_reduction = .1,           # min_gain_to_split
    sample_size = 0.8,             # Subsample ratio
    colsample_bytree = .75,        # Column sampling
    #: random seeds
    bagging_seed = 123, # seed for sampling observations (sample_size)
    seed = 987,         # seed for sampling features (mtry)
  )

#: Create workflow (combine recipe with model specification)
lgbm_wf = workflow(preprocessor = rec_lgbm, spec = lgbm_spec)
```

Tuning for the `trees` and `num_leaves` parameters using cross-validation and Bayesian optimization

```
library(tidymodels)

#: set up 10 fold cv
set.seed(1492)
folds = training(donor_data) %>%
  rsample::vfold_cv(v = 10, strata = outcome)

#: set valid range of tuning parameters
tuning_range =
  list(
    trees = dials::trees(range = c(200L, 1000L)),
    num_leaves = dials::num_leaves(range = c(2, 50))
  )

#: bayesian optimization
opt_bayes =
  tune::tune_bayes(
  object = lgbm_wf,    # tidymodels workflow
  resamples = folds,  # tidymodels resampling object
  param_info = dials::parameters(tuning_range), # range of tuning parameters
  initial = 5,
  iter = 20,
  metrics = metric_set(mn_log_loss, brier_class, roc_auc),
  control = control_bayes(verbose = TRUE, verbose_iter = TRUE, seed = 1499)
)
```

This finds the best tuning parameters to be:

```
opt_bayes %>%
  show_best(metric = "mn_log_loss")
#> # A tibble: 5 x 9
#>   trees num_leaves .metric     .estimator  mean     n std_err .config .iter
#>   <int>      <int> <chr>       <chr>      <dbl> <int>   <dbl> <chr>   <int>
#> 1   850          3 mn_log_loss binary     0.253    10 0.00186 Iter19     19
#> 2   841          4 mn_log_loss binary     0.253    10 0.00210 Iter20     20
#> 3   789          4 mn_log_loss binary     0.253    10 0.00205 Iter17     17
#> 4   448          4 mn_log_loss binary     0.253    10 0.00167 Iter13     13
#> 5   688          4 mn_log_loss binary     0.254    10 0.00192 Iter15     15
```

This step will update the tuning parameters and refit on the entire training data

```
lgbm_fit =
  lgbm_wf %>%
  finalize_workflow(
    select_best(opt_bayes, metric = "mn_log_loss")
  ) %>%
  fit(training(donor_data))
lgbm_fit
#> == Workflow [trained] ==========================================================
#> Preprocessor: Recipe
#> Model: boost_tree()
#>
#> -- Preprocessor ----------------------------------------------------------------
#> 0 Recipe Steps
#>
#> -- Model ----------------------------------------------------------------------
#> LightGBM Model (850 trees)
#> Objective: binary
#> Fitted to dataset with 36 columns
```

2 Model specific feature importance

2.1 Linear Models

In linear models, using $\hat{f}(x) = \sum_{j=1}^{p} x_j \hat{\beta}_j$, the impact of feature j is related to $\hat{\beta}_j$. To treat each feature more equally, it is common to use the $\hat{\beta}_j$ *after standardizing* the features. It is equivalent to use $\hat{\beta}_j / \hat{\sigma}_j$ for non-standardized features.

2.2 Gain Based Feature Importance (for tree models)

Recall that the *gain* of a split in a tree model is equal to the improvement in the splitting criterion after making the split.

The importance of feature j in tree T can be expressed as:

$$\mathcal{I}_j(T) = \sum_t \text{gain}(t) \cdot \mathbb{1}(\text{split } t \text{ uses feature} j)$$

- In this equation, the importance of feature j is the total *gain* across all splits that involve feature j. Gain refers to the reduction in the chosen loss function (e.g., Gini index or mean squared error) for each split.

For an ensemble of trees (e.g., random forest, boosted trees), the importance of predictor j is the average (or sum) importance from all M trees in the ensemble:

$$\mathcal{I}_j = \frac{1}{M} \sum_{k=1}^{M} \mathcal{I}_j(T_k)$$

Averaging for random Forests

- Note: a final normalizing step may transform importance scores to sum to 1

Gain based feature importance in LightGBM

The `lgbm_fit` object from the above R code is a `workflow` (tidymodels). To use the `lightgbm::lgb.importance()` function, we need to extract the fitted model using `extract_fit_engine()`.

```
lgbm_fit %>%
  extract_fit_engine() %>%
  lightgbm::lgb.importance(percentage = FALSE) %>%
  as_tibble()
#> # A tibble: 35 x 4
#>   Feature                        Gain   Cover Frequency
#>   <chr>                         <dbl>   <int>     <int>
#> 1 NUM_REJECT_DON               10332. 1599857        84
#> 2 LISTING_CTR_ACCEPT_RATE_PREV  4613. 2165709       136
#> 3 ABNL_ECHO_CUM                 3602.  601134        39
#> 4 WEIGHT_RATIO                  2259. 2121436       127
#> 5 DISTANCE                      2118. 2012109       117
#> 6 prior_offers_cand             1882.  833302        62
#> # i 29 more rows
```

- The `Cover` is the number of observations impacted by the splits with feature j.
- The `Frequency` is the number of splits with feature j.

3 Permutation Feature Importance

An alternative, and model agnostic, approach to feature importance is to measure how much the *performance* of the predictions change if the features are manipulated. One way to do this is to modify the feature(s) and measure the change in average loss. Let $S \subseteq \{1, 2, \ldots, p\}$ be a subset of the p features. Let Z_S be a new dataset where the features in S are randomly permuted/shuffled.

But there are two primary ways to measure the performance change: (1) shuffle the data and re-fit the model and (2) use the original model and only shuffle before prediction. These are detailed below:

3.1 Approach 1: re-fit model

Let $S = j$ be a single variable.

0. Create a hold-out set X_{test}. Fit a model to the training data $\hat{f}(X)$, predict on the hold-out data, and evaluate the predictions $L(Y_{\text{test}}, \hat{f}(X_{\text{test}}))$. If we manipulate any features, the performance should decrease.
1. Create $Z_j = [X_{1:(j-1)}, P(X_j), X_{(j+1):p}]$ where $P(X_j)$ is a randomly permuted vector of X_j.
2. Re-fit model $\hat{f}_j(x)$ using data Z_j
3. Prediction on a hold-out set X_{test} and evaluate the loss $L(Y_{\text{test}}, \hat{f}_j(X_{\text{test}}))$. The change in loss is the feature importance score. I.e., importance of feature j = $L(Y_{\text{test}}, \hat{f}_j(X_{\text{test}})) - L(Y_{\text{test}}, \hat{f}(X_{\text{test}}))$.
4. Repeat steps 1:3 (or 0:3) multiple times. Also, repeat 1:3 using different features.

This approach assesses how important a feature is for making a good prediction. However, there are some issues to be aware of. Suppose you have a set of highly correlated predictors. Their importance will be near zero because you can remove any of them, and one of their correlated partners will take up the slack. If the cost of collecting features is high, then this can be a good way to remove some and maintain high predictive performance.

Of course, you can always try jointly permuting subsets $|S| > 1$ (like for Shapley values) to get the joint importance.

3.2 Approach 2: shuffle before prediction

This approach is less computational. You only shuffle the hold-out data.

1. Create a hold-out set X_{test}. Fit a model to the training data $\hat{f}(X)$, predict on the hold-out data, and evaluate the predictions $L(Y_{\text{test}}, \hat{f}(X_{\text{test}}))$. If we manipulate any features, the performance should decrease.
1. Permute one (or more) columns of the *hold-out* data.
2. Predict and evaluate performance. The change in loss is the feature importance score.
3. Repeat multiple times and take average.

This approach assesses how important each feature is to *the model learned from the training data*. So in that set of correlated predictors, maybe only one or two will get used. Those features will appear important, but the others won't.

3.3 Boruta feature selection

Boruta is a *False Selection Rate (FSR)* feature selection method originally designed for random forest (or any tree-based models).

Boruta for trees

- Introduce additional shuffled features (shadow features). This increased the number of predictor variables from p to $2p$.
- Calculate importance scores for all features (using the built-in split-based importance metrics)
- Record the "hits": all original features with importance scores greater than *max importance from all shuffled features* (these features are deemed important).
- Repeat the process M times (100 by default; or sequential).
- Determine which predictors have significantly more "hits" than expected under null of not-important.

4 Shapley (and SHAP) Values for ML

This section deals with model **Explainability** which is the task of better understanding how predictive models use features to make predictions.

4.1 Shapley Values in Cooperative Game Theory

Suppose up to $p = 4$ singers can cooperate together to make a song. Let's name the people $\{Alicia, Bob, Cardi, Drake\}$. They got together, made a album, and generated \$100M. How much should each artist receive? Is there a fair way to distribute the profits? Shapley values is one "fair" way to distribute the value (see Wikipedia: Shapley Values for the specifics).

Let $S \subseteq \{A, B, C, D\}$ be a *coalition* of the singers and $V(S)$ be the success/value (e.g., sales) of the songs they make. Pretend we can form all possible $\binom{4}{0} + \binom{4}{1} + \binom{4}{2} + \binom{4}{3} + \binom{4}{4} = 16$ coalitions and can measure the value for each one (note: implicit assumption of independence and non-stochasticity). Let the value of the empty set $V(\emptyset) = 0$.

The *shapley score* for person j is:

$$\begin{aligned}
\phi_j =& \frac{1}{\text{num of people}} \sum_{\text{coalitions not involving player } j} \frac{\text{gain when } j \text{ is added to the coalition}}{\text{number of coalitions not involving } j \text{ of this size}} \\
=& \frac{1}{p} \sum_{S: j \notin S} \binom{p-1}{|S|}^{-1} V(S \cup j) - V(S) \\
=& \frac{1}{p} \sum_{k=0}^{p-1} \binom{p-1}{k}^{-1} \sum_{S:|S|=k} V(S \cup j) - V(S)
\end{aligned}$$

For example, suppose the following coalition scores:

Coalition	Value
$\emptyset$:	\$0
Alicia:	\$40
Bob:	\$30
Cardi:	\$20
Drake:	\$10
Alicia and Bob:	\$75
Alicia and Cardi:	\$55
Alicia and Drake:	\$50
Bob and Cardi:	\$50
Bob and Drake:	\$40
Cardi and Drake:	\$25
Alicia, Bob, and Cardi:	\$95
Alicia, Bob, and Drake:	\$80
Alicia, Cardi, and Drake:	\$70
Bob, Cardi, and Drake:	\$60
Alicia, Bob, Cardi, and Drake:	\$100

Alicia	Bob	Cardi	Drake	k	V	wt
0	0	0	0	0	0	0.250
1	0	0	0	1	40	0.083
0	1	0	0	1	30	0.083
0	0	1	0	1	20	0.083
0	0	0	1	1	10	0.083
1	1	0	0	2	75	0.083
1	0	1	0	2	55	0.083
1	0	0	1	2	50	0.083
0	1	1	0	2	50	0.083
0	1	0	1	2	40	0.083
0	0	1	1	2	25	0.083
1	1	1	0	3	95	0.250
1	1	0	1	3	80	0.250
1	0	1	1	3	70	0.250
0	1	1	1	3	60	0.250
1	1	1	1	4	100	Inf

Consider all of Alicia's contributions:

Coalitions	Values	Difference
V(Alicia) - V($\emptyset$)	= 40 - 0	= 40
V(Alicia, Bob) - V(Bob)	= 75 - 30	= 45
V(Alicia, Cardi) - V(Cardi)	= 55 - 20	= 35
V(Alicia, Drake) - V(Drake)	= 50 - 10	= 40
V(Alicia, Bob, Cardi) - V(Bob, Cardi)	= 95 - 50	= 45
V(Alicia, Bob, Drake) - V(Bob, Drake)	= 80 - 40	= 40
V(Alicia, Cardi, Drake) - V(Cardi, Drake)	= 70 - 25	= 45
V(Alicia, Bob, Cardi, Drake) - V(Bob, Cardi, Drake)	= 100 - 60	= 40

$$\text{Alicia} = \frac{1}{4}\left(40 + (45 + 35 + 40)/3 + (45 + 40 + 45)/3 + 40\right) = 40.8333$$

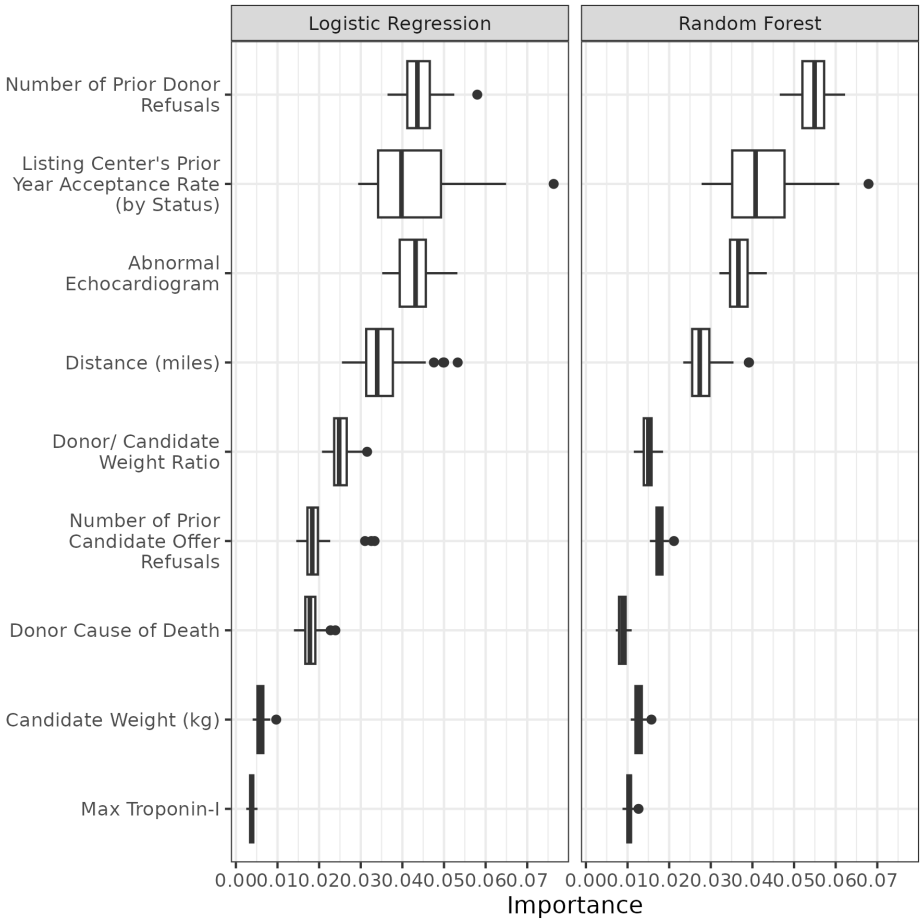
Doing the same calculations for the other players gives their Shapley values, or the proportion of the \$100 total each should receive:

Alicia	Bob	Cardi	Drake
40.83	31.67	19.17	8.33

4.2 Donor Acceptance

We built two predictive models (RF, LogReg) for estimating the probability that a pediatric donor heart is accepted by a candidate. Interest is in understanding the features clinicians use to base their Accept/Refuse decisions. There are $n = 30,156$ offers and $p = 44$ predictor variables (features).

The most important predictors[1] are:



As a running example, let's consider a particular offer:

feature	value
NUM_REJECT_DON	1.00
LISTING_CTR_ACCEPT_RATE_PREV	0.35
ABNL_ECHO_CUM	0.00
DISTANCE	441.74
WEIGHT_RATIO	1.06
prior_offers_cand	1.00
COD_DON	Head Trauma
WEIGHT_CAND_KG	38.40
TROPONINI_max	-1.00
...	...
f_hat	0.783

78.3% acceptance, but what drives this model performance?
Distance?

[1] according to SHAP importance

4.3 Shapley values for explaining a prediction

Training data D is used to build a predictive model $\hat{f}(x)$, where $x = [x_1, \ldots, x_p]$. There is a concept called SHAP (SHapley Additive exPlanations) that uses concepts from Shapley values to generate functions $\phi_0, \phi_1, \ldots, \phi_p$ such that the prediction of x can be explained by the linear sum:

$$\hat{f}(x) = \phi_0(x) + \sum_{j=1}^{p} \phi_j(x)$$

The value $\phi_j(x)$ is the SHAP value for the jth predictor variable and $\phi_0(x) = \phi_0 = E_X[\hat{f}(X)]$.

The connection to the original Shapley coalitions is that each feature is a player, and the total value of the full coalition is $\hat{f}(x)$. Let $S \subseteq \{1, 2, \ldots, p\}$ indicate the set of features in a coalition. The trick is determining how to form the value function $V_x(S)$, where the subscript x is a reminder that this is the value function for a prediction at x. This is the big idea:

$$V_x(S) = E_{\bar{S}}[f(x_S, X_{\bar{S}})] - E_X[\hat{f}(X)]$$

where $X_{\bar{S}}$ is from the distribution that is assumed independent from S. That is, we treat the values of the features in S as known, but pretend the other features values, those in the complement $\bar{S}$, are missing. The expectation is over the missing feature values. Note that $\phi_0 = E_X[\hat{f}(X)]$ is the average prediction (or the prediction when all features are missing).

Let's come back to our offer example. The average prediction is 0.116. Consider the coalition $S = \{$`NUM_REJECT_DON`, `LISTING_CTR_ACCEPT_RATE_PREV`$\}$.

Known values of coalition size 2

feature	value
NUM_REJECT_DON	1.00
LISTING_CTR_ACCEPT_RATE_PREV	0.35
ABNL_ECHO_CUM	_____
DISTANCE	_____
WEIGHT_RATIO	_____
prior_offers_cand	_____
COD_DON	_____
WEIGHT_CAND_KG	_____
TROPONINI_max	_____
All other features	...
f_hat	_____

impute → randomly select value from other observations

We need to fill in the missing feature values with their expected values. But we have some options: (i) condition on $X_S = x_S$, (ii) treat X_S and $S_{\bar{S}}$ as independent, (iii) treat all features as independent, etc.

Let's consider option (ii), treating X_S and $S_{\bar{S}}$ as independent. We can estimate the expected value by averaging predictions from replacing the missing values with values from the training data D.

$$E[\hat{f}(X) \mid X_S = x_S, X_{\bar{S}} = \text{missing}] \approx \frac{1}{n} \sum_{i=1}^{n} \hat{f}(Z_i^S) \qquad \text{where } Z_i^S = [x_S, X_{i,\bar{S}}]$$

where $X_{i,\bar{S}}$ are feature values for $\bar{S}$ from observation i. Another way to express this for this example is $Z_i^S = xw_S + X_i(1 - w_S)$ where $w_S = [1, 1, 0, 0, \ldots, 0]$ indicates the first two features are in coalition S.

Note

You need the prediction function $\hat{f}(z)$ to be able to calculate the prediction for any z.

feature	x_S	offer: 1	offer: 2	offer: 3	offer: 4
NUM_REJECT_DON	1.00	1.00	1.00	1.00	1.00
LISTING_CTR_ACCEPT_RATE_PREV	0.35	0.35	0.35	0.35	0.35
ABNL_ECHO_CUM	_____	0.50	1.00	0.00	0.00
DISTANCE	_____	536.99	457.03	210.61	433.86
WEIGHT_RATIO	_____	0.81	1.27	0.76	2.06
prior_offers_cand	_____	0.00	0.00	0.00	0.00
COD_DON	_____	CVA	Infection (CNS)	Head Trauma	Head Trauma
WEIGHT_CAND_KG	_____	3.10	6.37	9.00	3.30
TROPONINI_max	_____	5.00	0.10	2.78	2.78
All other features	...	...	...	...	...
f_hat	_____	0.097	0.006	0.188	0.149

model prediction

If we repeat this procedure for all subsets $S \subseteq \{1, 2, \ldots, p\}$ and use the formula to calculate all the Shapley values for offer x, we get:

one offer

SHAP

feature	value	Shapley
NUM_REJECT_DON	1.00	0.094
LISTING_CTR_ACCEPT_RATE_PREV	0.35	0.202
ABNL_ECHO_CUM	0.00	0.086
DISTANCE	441.74	0.033
WEIGHT_RATIO	1.06	0.022
prior_offers_cand	1.00	0.039
COD_DON	Head Trauma	0.022
WEIGHT_CAND_KG	38.40	0.007
TROPONINI_max	-1.00	0.020
All other features	...	0.143
f_hat	0.783	0.116

increases prob of accept by 20.2%

overall avg

original prediction

Here are the Shapley values for a different offer. This offer has an estimated acceptance probability of only 0.008, lower than average.

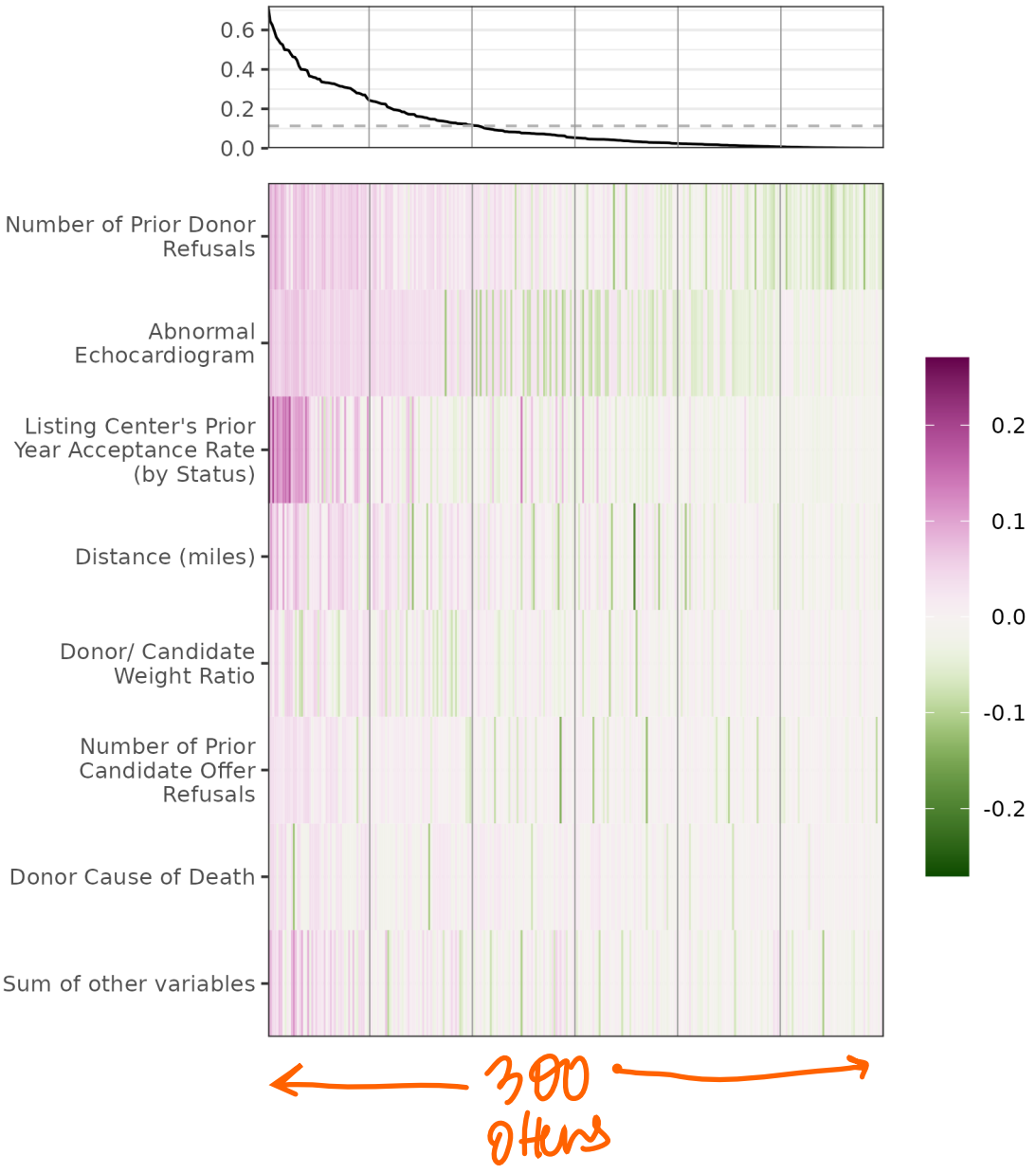
another offer

feature	value	Shapley
NUM_REJECT_DON	24.00	-0.046
LISTING_CTR_ACCEPT_RATE_PREV	0.05	-0.020
ABNL_ECHO_CUM	0.00	0.012
DISTANCE	634.54	-0.019
WEIGHT_RATIO	0.93	0.001
prior_offers_cand	0.00	0.010
COD_DON	Anoxia	-0.006
WEIGHT_CAND_KG	23.65	-0.008
TROPONINI_max	5.41	-0.009
All other features	...	-0.021
f_hat	0.008	0.116

24 prior rejections lowered P(Accept) by 4.6%

original prob

Here are the Shapley values for a sample of 300 random offers:



4.3.1 Estimating Shapley Values

There are too many features ($p = 44$) to exhaustively calculate all subsets (at least for my level of patience). Also, note that we need to make repeated calls to the prediction function, so the speed of prediction will play a role in estimating the Shapley values.

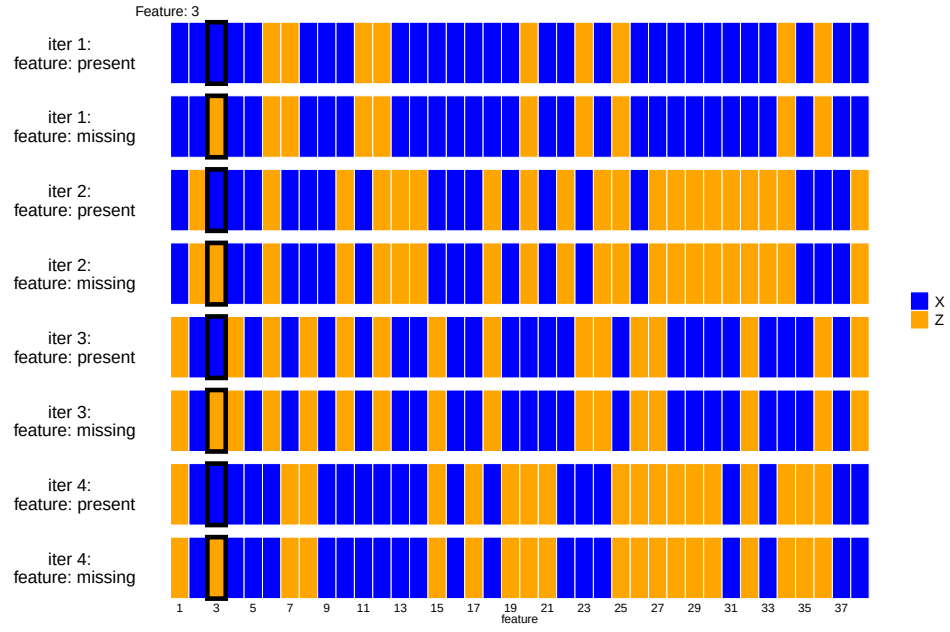
1. Shapley Sampling

Štrumbelj and Kononenko (2014) propose an approximation with Monte-Carlo sampling (see IML book 9.5.3.3):

$$\hat{\phi}_j(x) = \frac{1}{M}\sum_{m=1}^{M} \hat{f}(Z_m^{S_m \cup j}) - \hat{f}(Z_m^{S_m})$$

where S_m is a random subset. For each iteration, two samples are drawn (i) random data instance (i.e., a row of data) (ii) random set of features S_m that does not include j. Form $Z_m^{S_m \cup j}$ and make a prediction. Then replace feature j with x_j and make another prediction. The difference between the two predictions is the gain/importance of feature j to the prediction.

Here is an example using four samples:



2. KernSHAP

Recognizing that the Shapley values can be specified in a linear model

$$\hat{f}(x) = \phi_0(x) + \sum_{j=1}^{p} \phi_j(x)$$

KernelSHAP is an approach to estimate the Shapley values using weighted linear regression:

$$\hat{\phi}(x) = \underset{\phi_0,\phi_j}{\arg\min} \sum_{S} w(S) \left(\hat{f}(x_S) - \phi_0 - \sum_{j} \phi_j \right)^2$$

using the weight function

$$w(S) = \frac{1-p}{\binom{p}{k_S} k_S (p - k_S)}$$

3. Model specific methods

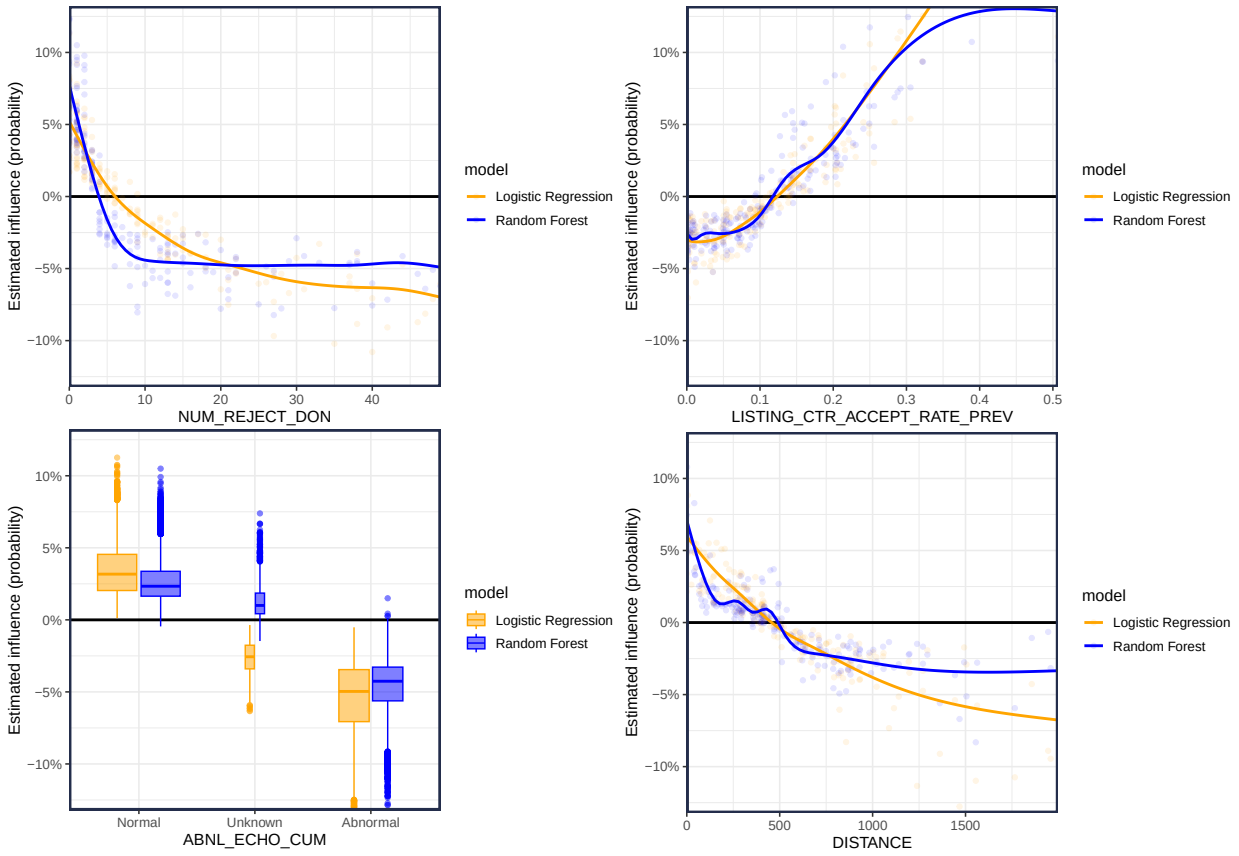
TreeSHAP, DeepSHAP, MaxSHAP

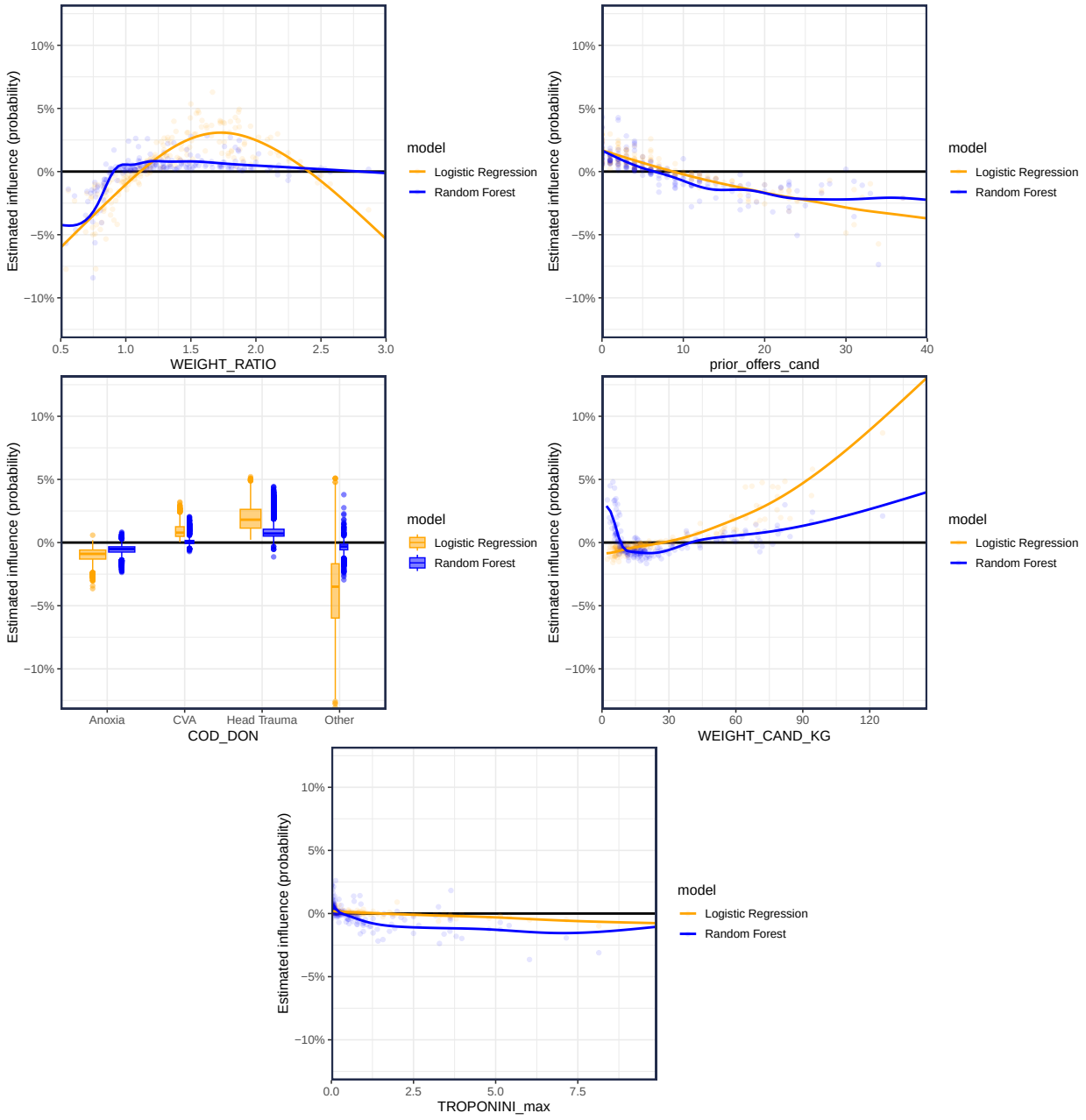
4.4 SHAP Effects Plots

We can estimate the SHAP values for a sample of the data and make marginal effects plots. The following scatterplots are formed from

$$\{x_{ij}, \phi_{ij}\}$$

where x_{ij} is from the data and ϕ_{ij} is the jth SHAP value for observation i.





4.5 SHAP Feature Importance

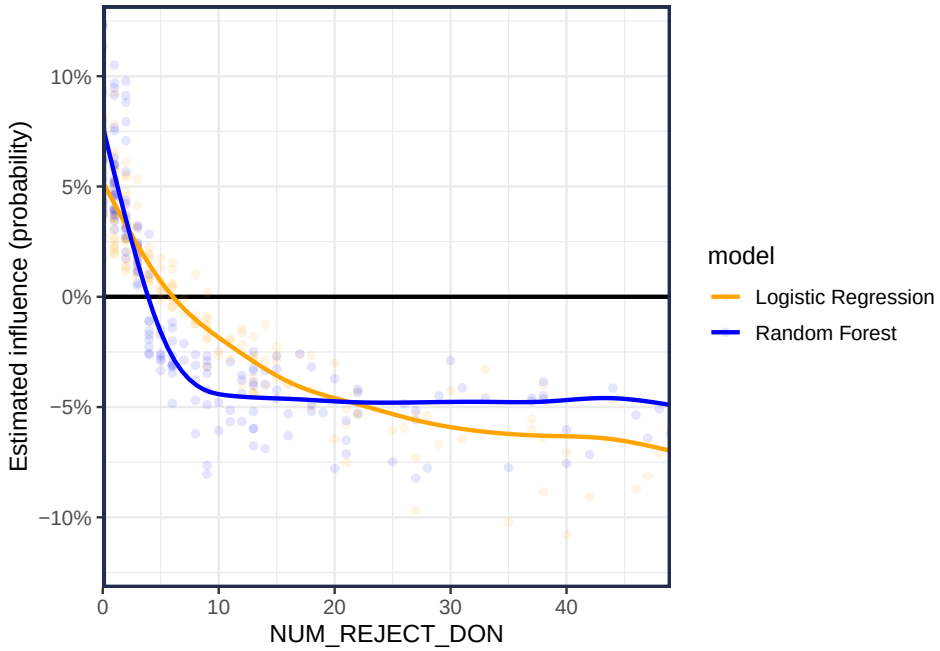
Permutation and gain based feature importance measures how much the *performance* changes if the features are manipulated. Alternatively, SHAP feature importance measures how much the *predictions* change if the features are manipulated (i.e., treated as missing).

The larger a feature's absolute value of the Shapley values (in the data) the more influence it has on the predictions. The SHAP feature importance score is given by the average absolute value (over the data).

$$I_j = \frac{1}{n}\sum_{i=1}^{n} |\phi_{ij}|$$

I think variance or standard deviation would also be a good metric for variable importance.

Looking back up to the plots. The feature importance is a measure of the average deviation from the points (shapley values) and the horizontal line at 0.



4.6 Other Explanable ML methods

Interpretable Machine Learning by Christoph Molnar describes several other methods to help *explain* the predictions from an ML model (e.g., PDP, LIME).