Example of how to use XGBoost optimized with SERA

Use case

In this markdown two use cases are provided where three variants are taken into consideration:

- XGBoost with SERA optimization where weights are obtained automatically;
- XGBoost with SERA optimization where weights are obtained with domain knowledge;
- XGBoost with Squared Error as objective.

The first use case uses a number of intervals $I = 1000$, while the second $I = 10$.

Load required packages

```
library(ModelOptimizationIR)
library(xgboost)
library(dplyr)
library(IRon)
library(scam)
```

Load data and perform random partition

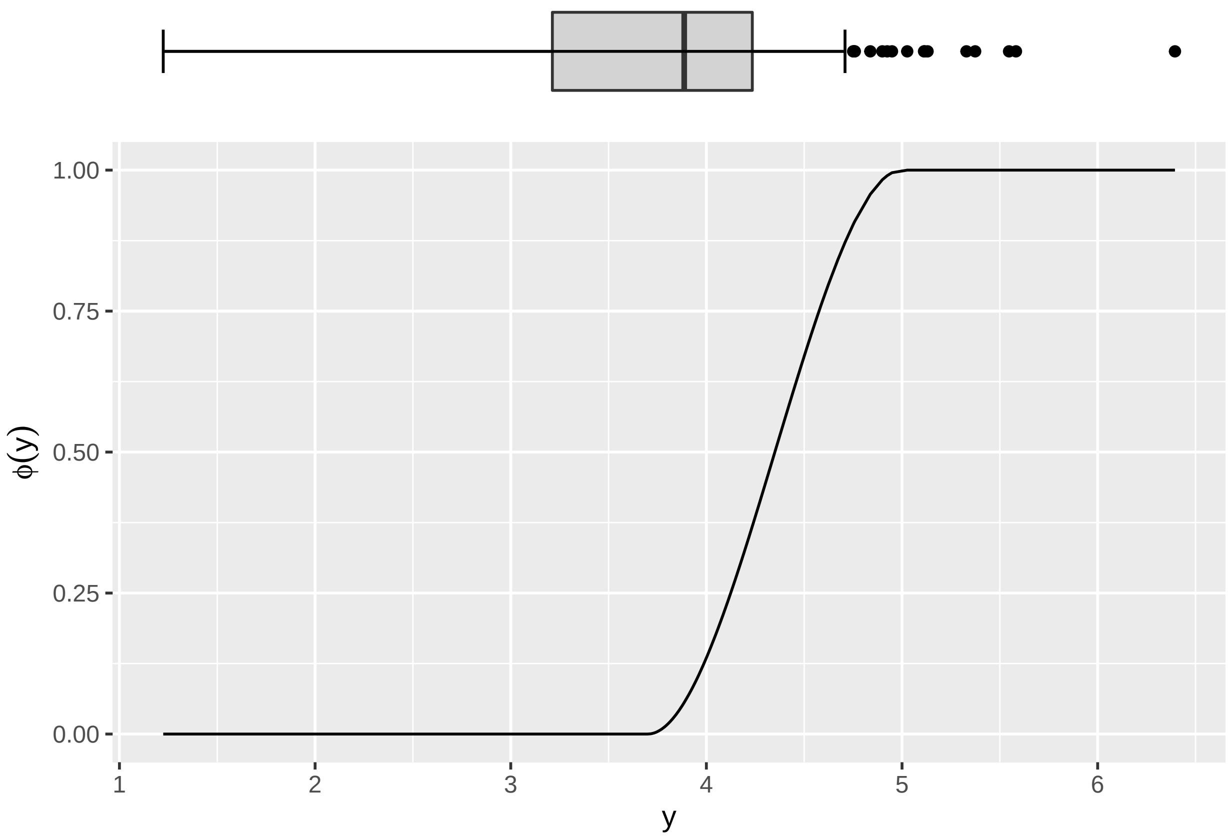
```
data("NO2Emissions")
n <- nrow(NO2Emissions)
s <- sample(1:n, size = n*0.8)

formula <- LNO2 ~ .
train <- NO2Emissions %>% dplyr::slice(s)
test <- NO2Emissions %>% dplyr::slice(-s)
```

Extract weights using domain knowledge

```
y <- train$LNO2
# Extreme points above upper fence.
control.points <- matrix(c(1.1, 0, 0, 3.7, 0, 0, 5, 1, 0), byrow = TRUE, ncol=3)

ph.ctrl <- phi.control(y = y, method="range", control.pts = control.points)
phi <- phi(y = y, phi.parms = ph.ctrl)
```

Plot with the relevance function

```
phiPlot(ds=y, phi.parms = ph.ctrl)
```



Add some hyper-parameters for modeling

```
params <- list(max_depth=7, eta=10^{-1}, gamma=10^{-2})
```

First use case $I = 1000$

Define steps to discretize SERA and calculate weights

```
I = 1000 # Default value
steps <- seq(0, 1, 1/I)
sigma <- sigma(phis = phi, steps = steps)
```

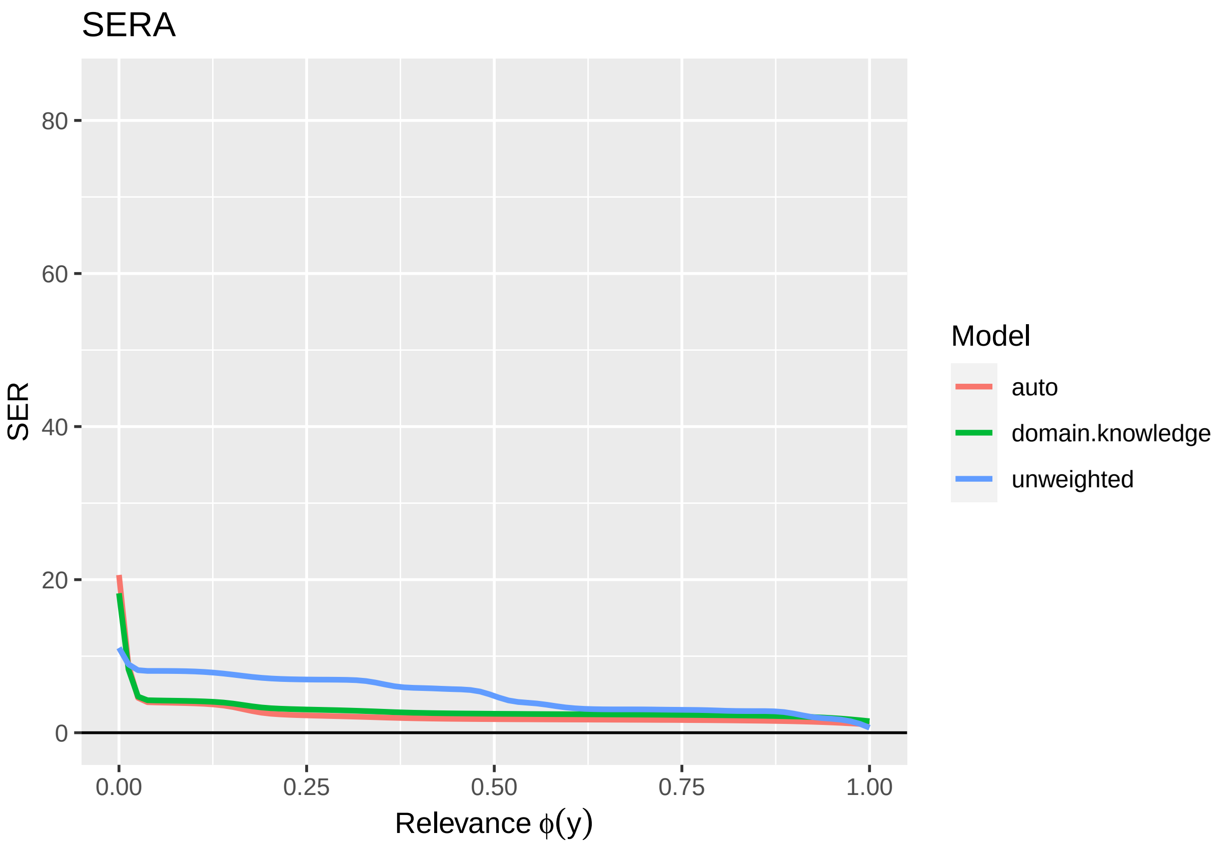
Train the models and save results

```
model_domain_knowledge <-
  XGBoost.sera(
    formula = formula,
    train = train,
    test = test,
    sigma = sigma,
    nrounds = 250,
    parameters = params
  )

model_auto <-
```

```r
  XGBoost.sera(
    formula = formula,
    train = train,
    test = test,
    nrounds = 250,
    parameters = params
  )

model_unweighted <-
  wf.XGBoost(
    formula = formula,
    train = train,
    test = test,
    nrounds = 250,
    params = params
  )

df <- tibble(
  trues = model_domain_knowledge$trues,
  `auto` = model_auto$preds,
  `domain knowledge` = model_domain_knowledge$preds,
  `unweighted` = model_unweighted$preds
)
```

Evaluate SERA

```r
sera(trues=df$trues, preds=dplyr::select(df, -trues), ph = ph.ctrl, pl=TRUE)
```




```
##            auto domain.knowledge       unweighted
##        2.256032          2.859328         4.931260
```

Evaluate MSE

```
df %>%
  summarise(across(!matches("trues"), ~mean((trues - .x)^2)))
```

```
## # A tibble: 1 x 3
##    auto `domain knowledge` unweighted
##   <dbl>              <dbl>      <dbl>
## 1 0.839              0.719      0.192
```

Second use case $I = 10$

Define steps to discretize SERA and calculate weights

```
I = 10 # Default value
steps <- seq(0, 1, 1/I)
sigma <- sigma(phis = phi, steps = steps)
```

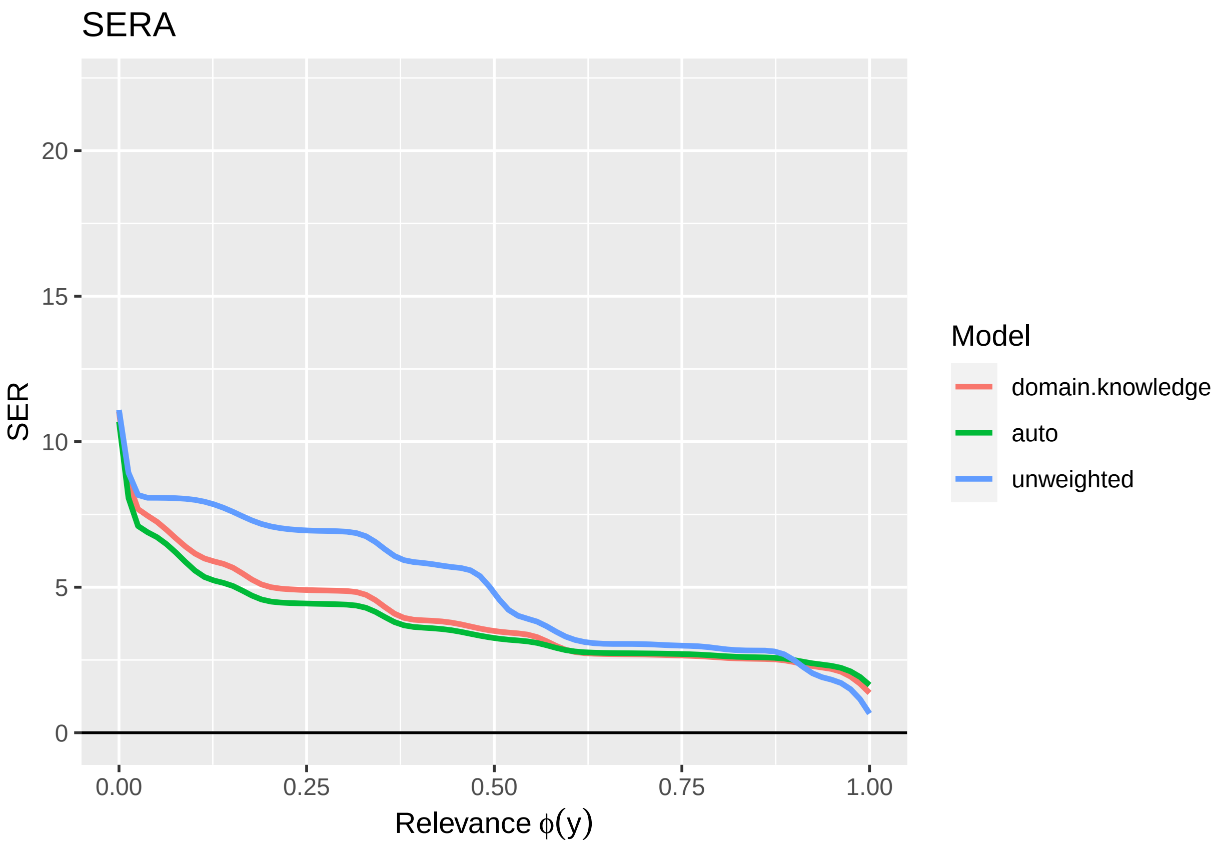
Train the models and save results

```
model_domain_knowledge <-
  XGBoost.sera(
    formula = formula,
```

```
    train = train,
    test = test,
    sigma = sigma,
    nrounds = 250,
    parameters = params
  )

model_auto <-
  XGBoost.sera(
    formula = formula,
    train = train,
    test = test,
    nrounds = 250,
    parameters = params,
    I = 10
  )

model_unweighted <-
  wf.XGBoost(
    formula = formula,
    train = train,
    test = test,
    nrounds = 250,
    params = params
  )

df <- tibble(
  trues = model_domain_knowledge$trues,
  `domain knowledge` = model_domain_knowledge$preds,
  `auto` = model_auto$preds,
  `unweighted` = model_unweighted$preds
)
```

Evaluate SERA

```
sera(trues=df$trues, preds=dplyr::select(df, -trues), ph = ph.ctrl, pl=TRUE)
```




```
## domain.knowledge             auto       unweighted
##         3.924750         3.713635         4.931260
```

Evaluate MSE

```
df %>%
  summarise(across(!matches("trues"), ~mean((trues - .x)^2)))
```

```
## # A tibble: 1 x 3
##   `domain knowledge`  auto unweighted
##                <dbl> <dbl>      <dbl>
## 1              0.216 0.221      0.192
```

Better generalization was achieved, but at the cost of worst predictive focus on extreme values.