

Boosting for Classification and Regression

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Bar-Ilan
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1 Classification Application

- Margin Classifiers
- LPBoost Master Problem
- LPBoost Pricing Problem
- LPBR: Implementation of Column Generation
- Computational Results for LPBR

2 Regression Application

- Pricing Problem and RMA Formulation
- REPR: Implementation of Column Generation
- Computational Results for REPR

3 Conclusions and Improvements

Problem Setting for Two-Class Classification

- m observations, each observation has n explanatory variables
- Each observation has a response value, $y_i \in \{-1, +1\}$ for $i = 1, \dots, m$

$$\begin{cases} i \in \Omega^+ & \text{if } y_i = +1 \\ i \in \Omega^- & \text{if } y_i = -1 \end{cases} \quad \begin{cases} m_+ = |\Omega^+| \\ m_- = |\Omega^-| \end{cases}$$

- Explanatory matrix: $X \in \mathbb{R}^{m \times n}$
 - $X_i \in \mathbb{R}^n$ for $i = 1, \dots, m$ (row vector of X)
 - $x_j \in \mathbb{R}^m$ for $j = 1, \dots, n$ (column vector of X)
 - $x_{ij} \in \mathbb{R}$: $(i, j)^{th}$ element of X

	x_1	\dots	x_j	\dots	x_n	y
X_1						y_1
\vdots						\vdots
X_i			x_{ij}			y_i
\vdots						\vdots
X_m						y_m

Goal: Construct a classifier that accurately classifies positive or negative on unseen dataset

Classifier for two-class classification problems

Rule Function

Given $a, b \in \mathbb{R}^n$ with $a \leq b$,

$$r_{(a,b)}(X_i) = \begin{cases} 1 & \text{if } a \leq X_i \leq b \text{ (componentwise)} \\ 0 & \text{otherwise} \end{cases}$$

Classifier constructed by a weighted combination of rules

$$\begin{aligned} f(X_i) &= \gamma_0 + \sum_{k \in K} \gamma_k r_k(X_i) & \gamma_0, (\gamma_k)_{k \in K} &\in \mathbb{R} \\ &= \gamma_0 + \sum_{k \in K} (\gamma_k^+ r_k^+(X_i) + \gamma_k^- r_k^-(X_i)) \end{aligned}$$

$\gamma_k > 0$: a observation covered by r_k votes to classify positive, and *vice versa*

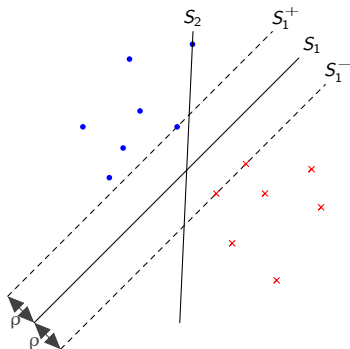
$$\text{Split } r_k(X_i) \text{ into } \begin{cases} r_k^+(X_i) = r_k(X_i) & \text{with } \gamma_k^+ \in \mathbb{R}_+ \\ r_k^-(X_i) = -r_k(X_i) & \text{with } \gamma_k^- \in \mathbb{R}_+ \end{cases}$$

Classification Rule

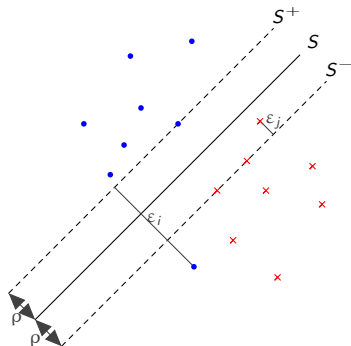
$$\text{Classify } \begin{cases} \text{positive} & \text{if } f(X_i) > 0 \text{ or } (f(X_i) = 0 \text{ and } m_+ \geq m_-) \\ \text{negative} & \text{if } f(X_i) < 0 \text{ or } (f(X_i) = 0 \text{ and } m_+ < m_-) \end{cases}$$

Margin Classifiers

Hard Margin Classifiers



Soft Margin Classifiers



Which one is a better classifier?

ρ : margin

ϵ_i : soft margin violation

Margin Classification Rule

Classify $\begin{cases} \text{positive} & \text{if } f(X_i) \geq \rho \\ \text{negative} & \text{if } f(X_i) \leq \rho \end{cases}$

LPBoost Master Problem

$$\begin{aligned} \min_{\rho, \epsilon, \gamma_0, \gamma^+, \gamma^-} \quad & -\rho + D \sum_{i=1}^m \epsilon_i^p \\ \text{s.t.} \quad & (\forall i) \quad y_i \left\{ \gamma_0 + \sum_{k \in K} (\gamma_k^+ r_k^+(X_i) + \gamma_k^- r_k^-(X_i)) \right\} + \epsilon_i \geq \rho \\ & \sum_{k \in K} (\gamma_k^+ + \gamma_k^-) = 1 \\ & \epsilon \geq 0, \quad \gamma^+, \gamma^- \geq 0 \end{aligned}$$

- $D \in \mathbb{R}_+$: a constant parameter
tradeoff between max margin and min soft margin violation
- $p = 1$ or 2

LPBoost Master Problem

$$\begin{aligned} \min_{\rho, \epsilon, \gamma_0, \gamma^+, \gamma^-} \quad & -\rho + D \sum_{i=1}^m \epsilon_i^p \\ \text{s.t.} \quad & (\forall i) \quad y_i \left\{ \underbrace{\gamma_0 + \sum_{k \in K} (\gamma_k^+ r_k^+(X_i) + \gamma_k^- r_k^-(X_i))}_{f(X_i)} \right\} + \epsilon_i \geq \rho \\ & \sum_{k \in K} (\gamma_k^+ + \gamma_k^-) = 1 \\ & \epsilon \geq 0, \quad \gamma^+, \gamma^- \geq 0 \end{aligned}$$

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 \min_{\rho, \epsilon, \gamma_0, \gamma^+, \gamma^-} \quad & \underbrace{-\rho}_{\text{max margin}} + D \underbrace{\sum_{i=1}^m \epsilon_i^p}_{\text{min soft margin violation}} && \text{Dual Variables} \\
 \text{s.t.} \quad & (\forall i) \quad y_i \left\{ \underbrace{\gamma_0 + \sum_{k \in K} (\gamma_k^+ r_k^+(X_i) + \gamma_k^- r_k^-(X_i))}_{f(X_i)} \right\} + \epsilon_i \geq \rho \leftrightarrow \mu_i \in \mathbb{R}_+ \\
 & \sum_{k \in K} (\gamma_k^+ + \gamma_k^-) = 1 && \leftrightarrow \alpha \in \mathbb{R} \\
 & \epsilon \geq 0, \quad \gamma^+, \gamma^- \geq 0
 \end{aligned}$$

- $D \in \mathbb{R}_+$: a constant parameter
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 \end{aligned}$$

- $D \in \mathbb{R}_+$: a constant parameter
tradeoff between max margin and min soft margin violation
- $p = 1$ or 2
- $m + 1$ constraints (except nonnegativity)
- $2 + m + 2|K|$ variables ($|K| \geq 3^n$)
- Large number of variables \Rightarrow solve by **column generation**

- Finding the smallest reduced cost (most violated dual constraints)

LPBoost Pricing Problem

$$\begin{aligned}
 z^* &= \max_{k \in K} \left\{ \sum_{i=1}^m r_k^+(X_i) y_i \mu_i, \sum_{i=1}^m r_k^-(X_i) y_i \mu_i \right\} \\
 &= \max_{k \in K} \left\{ \sum_{i=1}^m r_k^+(X_i) w_i, \sum_{i=1}^m r_k^-(X_i) w_i \right\} \\
 &= \max_{k \in K} \left\{ \sum_i r_k(X_i) w_i, - \sum_i r_k(X_i) w_i \right\} \\
 &= \max_{k \in K} \left| \sum_i r_k(X_i) w_i \right|
 \end{aligned}$$

- $w_i = y_i \mu_i$

$$= \begin{cases} \mu_i & \text{if } i \in \Omega^+ \\ -\mu_i & \text{if } i \in \Omega^- \end{cases}$$
 $i = 1, \dots, m$
- Stopping Condition:
 $z^* \leq -\alpha$

- This is RMA problem and solved by our solver
- LPBR (LPBoost with RMA)
- Maximizing the first term is finding the positive box r_k^+ s.t.
 the sum of the misclassification weights for covered positive observations
 most greatly exceeds
 the sum of the misclassification weights for covered negative observations

LPBR: Implementation of Column Generation

Restricted Master Problem:

Initially, empty K

Pricing Problem: Initially, $\mu_i = \frac{1}{m}$ (Optional: Insert initial 1D rules for all attributes)
Solved by Parallel Branch-and-Bound using PEBBL OR Greedy Heuristic

$$z^* = \max_{k \in K} \left\{ \sum_{i=1}^m r_k^+(X_i) y_i \mu_i, \sum_{i=1}^m r_k^-(X_i) y_i \mu_i \right\}$$

LPBR: Implementation of Column Generation

Restricted Master Problem:

Initially, empty K

A set of rules $r_k(\cdot)$
(can add multiple rules)



Pricing Problem:

Solved by Parallel Branch-and-Bound using PEBBL OR Greedy Heuristic

$$\max_{k \in K} \left| \sum_{i=1}^m r_k(X_i)(v_i - \mu_i) \right|$$

Stop if $z^* < -\alpha$ for Parallel Branch-and-Bound

LPBR: Implementation of Column Generation

Restricted Master Problem: Solved by GUROBI

$$\begin{aligned} \rho \in \mathbb{R}, \epsilon_i, \gamma_k^+, \gamma_k^- \in \mathbb{R}^+ \quad & r_k = \{r_k^+ \text{ or } -r_k^-\} \\ & \gamma_k = \gamma_k^+ - \gamma_k^- \quad \hat{\gamma}_k = \gamma_k^+ + \gamma_k^- \end{aligned}$$

min	$D\epsilon_1 \cdots + D\epsilon_m$	$-\rho$		
s. t.	ϵ_1	$-\rho$	$+r_1(X_1)\gamma_1$	≥ 0
	\ddots	\vdots	\vdots	\vdots
	$+ \epsilon_m$	$-\rho$	$+r_1(X_m)\gamma_1$	≥ 0
			$\hat{\gamma}_1$	$= 1$

A set of rules $r_k(\cdot)$
(can add multiple rules) ↑↑

Pricing Problem:

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$$\max_{k \in K} \left| \sum_{i=1}^m r_k(X_i)(v_i - \mu_i) \right|$$

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A set of rules $r_k(\cdot)$
(can add multiple rules)



Optimal Dual Variables
 $\mu \in \mathbb{R}_+^m, \alpha \in \mathbb{R}$

Pricing Problem:

Solved by Parallel Branch-and-Bound using PEBBL OR Greedy Heuristic

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$$z^* = \max_{k \in K} \left\{ \sum_{i=1}^m r_k^+(X_i) y_i \mu_i, \sum_{i=1}^m r_k^-(X_i) y_i \mu_i \right\}$$

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$$\max_{k \in K} \left| \sum_{i=1}^m r_k(X_i)(v_i - \mu_i) \right|$$

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s. t.	ϵ_1	$-\rho$	$+r_1(X_1)\gamma_1$	$+r_2(X_1)\gamma_2$	≥ 0
	\ddots	\vdots	\vdots	\vdots	\vdots
	$+ \epsilon_m$	$-\rho$	$+r_1(X_m)\gamma_1$	$+r_2(X_m)\gamma_2$	≥ 0
			$\hat{\gamma}_1$	$+ \hat{\gamma}_2$	$= 1$

A set of rules $r_k(\cdot)$
(can add multiple rules)



Optimal Dual Variables
 $\mu \in \mathbb{R}_+^m, \alpha \in \mathbb{R}$

Pricing Problem:

Solved by Parallel Branch-and-Bound using PEBBL OR Greedy Heuristic

$$\max_{k \in K} \left| \sum_{i=1}^m r_k(X_i)(v_i - \mu_i) \right|$$

Stop if $z^* < -\alpha$ for Parallel Branch-and-Bound

LPBR: Implementation of Column Generation

Restricted Master Problem: Solved by GUROBI

$$\begin{aligned}
 &\rho \in \mathbb{R}, \epsilon_i, \gamma_k^+, \gamma_k^- \in \mathbb{R}^+ \quad r_k = \{r_k^+ \text{ or } -r_k^-\} \\
 &\gamma_k = \gamma_k^+ - \gamma_k^- \quad \hat{\gamma}_k = \gamma_k^+ + \gamma_k^-
 \end{aligned}$$

min	$D\epsilon_1 \cdots + D\epsilon_m$	$-\rho$				
s. t.	ϵ_1	$-\rho$	$+r_1(X_1)\gamma_1$	$+r_2(X_1)\gamma_2$	\cdots	≥ 0
	\ddots	\vdots	\vdots	\vdots	\vdots	\vdots
	$+ \epsilon_m$	$-\rho$	$+r_1(X_m)\gamma_1$	$+r_2(X_m)\gamma_2$	\cdots	≥ 0
			$\hat{\gamma}_1$	$+\hat{\gamma}_2$	\cdots	$= 1$

A set of rules $r_k(\cdot)$
(can add multiple rules)



Optimal Dual Variables
 $\mu \in \mathbb{R}_+^m, \alpha \in \mathbb{R}$

Pricing Problem:

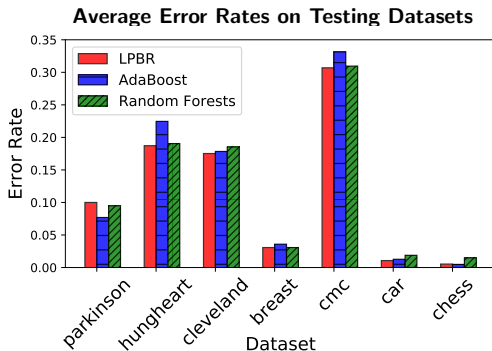
Solved by Parallel Branch-and-Bound using PEBBL OR Greedy Heuristic

$$\max_{k \in K} \left| \sum_{i=1}^m r_k(X_i)(v_i - \mu_i) \right|$$

Stop if $z^* < -\alpha$ for Parallel Branch-and-Bound

Result: LPBR has lower error rates on testing datasets

- Bi-level cross-validation to choose $D \in \{0.0001, 0.001, 0.005, 0.01\}$ with $p = 2$
- Twice of 5-fold outer and 3-fold inner cross-validations
- 100 column generation iterations (add one rule per iteration)
- Solve the subproblems by greedy RMA in general
- If the objective value of the greedy RMA satisfies the stopping condition, then solve the subproblems by the parallel branch-and-bound procedure

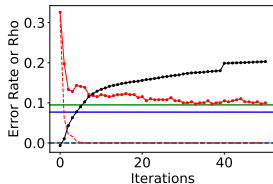


- Random Forests (R package: randomForest) with 100 trees
- AdaBoost (R package: fastAdaboost) with 100 iterations

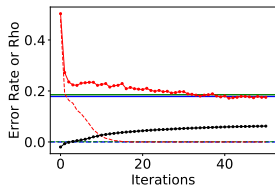
Result: Error rates decreases in each column generation iteration

- Initially generated one-dimensional greedy box-based rules
- First few rules has larger effect to minimize classification error rates
- Testing error rates decrease by increasing ρ (margin) in each iteration

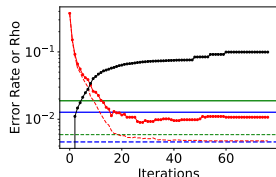
Data: parkinson



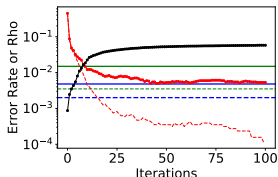
Data: cleveland



Data: car



Data: chess



Second RMA Application: Regression Model

- m observations, each observation has n explanatory variables
- Each observation has a response value, $y_i \in \mathbb{R}$ for $i = 1, \dots, m$
- Goal: Construct a prediction function $f(\cdot)$ for unseen data $(X_{i'}, y_{i'})$ such that minimizing prediction error ($\min\{f(X_{i'}) - y_{i'}\}$)
- Do not have *a priori* functional form for f

Penalized Regression with Rules

Rule Function

Given $a, b \in \mathbb{R}^n$ with $a \leq b$, $r_{(a,b)}(X_i) = \begin{cases} 1 & \text{if } a \leq X_i \leq b \text{ (componentwise)} \\ 0 & \text{otherwise} \end{cases}$

Prediction Function (Linear & Rule Regression)

For some $\beta_0, \beta_1, \dots, \beta_n, (\gamma_k)_{k \in K} \in \mathbb{R}$,

$$f(X_i) = f_{\beta_0, \beta, \gamma}(X_i) = \beta_0 + \sum_{j=1}^n \beta_j x_{ij} + \sum_{k \in K} \gamma_k r_k(X_i)$$

Rule-Enhanced Penalized Regression (REPR)

For $\beta = (\beta_1, \dots, \beta_n) \in \mathbb{R}^n$ and $\gamma \in \mathbb{R}^{|K|}$,

$$\min_{\beta_0, \beta, \gamma} \left\{ \underbrace{\sum_{i=1}^m |f_{\beta_0, \beta, \gamma}(X_i) - y_i|^p}_{\text{min prediction error}} \underbrace{+ C \|\beta\|_1}_{\text{penalize linear coefficients}} \underbrace{+ E \|\gamma\|_1}_{\text{penalize rule coefficients}} \right\}$$

$p \in \{1, 2\}$ and $C, E \geq 0$ are scalar parameters

- For $p = 2$ and $C = E > 0$, this model is the classic LASSO
- Split

$$\begin{cases} \beta = \beta^+ - \beta^- & \text{with } \beta^+, \beta^- \geq 0 \\ \gamma = \gamma^+ - \gamma^- & \text{with } \gamma^+, \gamma^- \geq 0 \end{cases}$$

REPR Master Problem

$$\min \quad \sum_{i=1}^m \epsilon_i^p + C \sum_{j=1}^n (\beta_j^+ + \beta_j^-) + E \sum_{k \in K} (\gamma_k^+ + \gamma_k^-)$$

$$\text{s. t.} \quad \beta_0 + X_i^\top (\beta^+ - \beta^-) + \sum_{k \in K} r_k(X_i)(\gamma_k^+ - \gamma_k^-) - \epsilon_i \leq y_i$$

$$(\forall i) \quad -\beta_0 - X_i^\top (\beta^+ - \beta^-) - \sum_{k \in K} r_k(X_i)(\gamma_k^+ - \gamma_k^-) - \epsilon_i \leq -y_i$$

$$\epsilon \geq 0, \quad \beta^+, \beta^- \geq 0, \quad \gamma^+, \gamma^- \geq 0$$

REPR Master Problem

$$\min \quad \sum_{i=1}^m \epsilon_i^p + C \sum_{j=1}^n (\beta_j^+ + \beta_j^-) + E \sum_{k \in K} (\gamma_k^+ + \gamma_k^-)$$

$$\text{s. t.} \quad \underbrace{\beta_0 + X_i^\top (\beta^+ - \beta^-) + \sum_{k \in K} r_k(X_i)(\gamma_k^+ - \gamma_k^-)}_{f_{\beta_0, \beta, \gamma}(X_i)} - \epsilon_i \leq y_i$$

$$(\forall i) \quad \underbrace{-\beta_0 - X_i^\top (\beta^+ - \beta^-) - \sum_{k \in K} r_k(X_i)(\gamma_k^+ - \gamma_k^-)}_{-f_{\beta_0, \beta, \gamma}(X_i)} - \epsilon_i \leq -y_i$$

$$\epsilon \geq 0, \quad \underbrace{\beta^+, \beta^-}_{-f_{\beta_0, \beta, \gamma}(X_i)} \geq 0, \quad \gamma^+, \gamma^- \geq 0$$

Overestimation constraints: $f_{\beta_0, \beta, \gamma}(X_i) - y_i \leq \epsilon_i$

Underestimation constraints: $f_{\beta_0, \beta, \gamma}(X_i) - y_i \geq -\epsilon_i$

REPR Master Problem

$$\begin{aligned}
 \min \quad & \underbrace{\sum_{i=1}^m \epsilon_i^p}_{\text{min prediction error}} + C \underbrace{\sum_{j=1}^n (\beta_j^+ + \beta_j^-)}_{\text{penalize linear coefficients}} + E \underbrace{\sum_{k \in K} (\gamma_k^+ + \gamma_k^-)}_{\text{penalize rule coefficients}} \\
 \text{s. t.} \quad & \underbrace{\beta_0 + X_i^\top (\beta^+ - \beta^-) + \sum_{k \in K} r_k(X_i)(\gamma_k^+ - \gamma_k^-) - \epsilon_i}_{f_{\beta_0, \beta, \gamma}(X_i)} \leq y_i \\
 & (\forall i) \quad \underbrace{-\beta_0 - X_i^\top (\beta^+ - \beta^-) - \sum_{k \in K} r_k(X_i)(\gamma_k^+ - \gamma_k^-) - \epsilon_i}_{-f_{\beta_0, \beta, \gamma}(X_i)} \leq -y_i \\
 & \epsilon \geq 0, \quad \beta^+, \beta^- \geq 0, \quad \gamma^+, \gamma^- \geq 0
 \end{aligned}$$

Overestimation constraints: $f_{\beta_0, \beta, \gamma}(X_i) - y_i \leq \epsilon_i$

Underestimation constraints: $f_{\beta_0, \beta, \gamma}(X_i) - y_i \geq -\epsilon_i$

REPR Master Problem

$$\begin{aligned}
 \min \quad & \underbrace{\sum_{i=1}^m \epsilon_i^p}_{\text{min prediction error}} + C \underbrace{\sum_{j=1}^n (\beta_j^+ + \beta_j^-)}_{\text{penalize linear coefficients}} + E \underbrace{\sum_{k \in K} (\gamma_k^+ + \gamma_k^-)}_{\text{penalize rule coefficients}} && \text{Dual Variables} \\
 \text{s. t.} \quad & \underbrace{\beta_0 + X_i^\top (\beta^+ - \beta^-) + \sum_{k \in K} r_k(X_i)(\gamma_k^+ - \gamma_k^-) - \epsilon_i}_{f_{\beta_0, \beta, \gamma}(X_i)} \leq y_i && \Leftrightarrow \mu_i \in \mathbb{R}_+ \\
 & \underbrace{(\forall i) \quad -\beta_0 - X_i^\top (\beta^+ - \beta^-) - \sum_{k \in K} r_k(X_i)(\gamma_k^+ - \gamma_k^-) - \epsilon_i}_{-f_{\beta_0, \beta, \gamma}(X_i)} \leq -y_i && \Leftrightarrow \nu_i \in \mathbb{R}_+ \\
 & \epsilon \geq 0, \quad \beta^+, \beta^- \geq 0, \quad \gamma^+, \gamma^- \geq 0
 \end{aligned}$$

Overestimation constraints: $f_{\beta_0, \beta, \gamma}(X_i) - y_i \leq \epsilon_i$

Underestimation constraints: $f_{\beta_0, \beta, \gamma}(X_i) - y_i \geq -\epsilon_i$

Overestimated: $\mu_i > 0, \nu_i = 0$

Underestimated: $\mu_i = 0, \nu_i > 0$

REPR Master Problem

$$\begin{aligned}
 \min \quad & \underbrace{\sum_{i=1}^m \epsilon_i^p}_{\text{min prediction error}} + C \underbrace{\sum_{j=1}^n (\beta_j^+ + \beta_j^-)}_{\text{penalize linear coefficients}} + E \underbrace{\sum_{k \in K} (\gamma_k^+ + \gamma_k^-)}_{\text{penalize rule coefficients}} && \text{Dual Variables} \\
 \text{s. t.} \quad & \underbrace{\beta_0 + X_i^\top (\beta^+ - \beta^-) + \sum_{k \in K} r_k(X_i)(\gamma_k^+ - \gamma_k^-) - \epsilon_i}_{f_{\beta_0, \beta, \gamma}(X_i)} \leq y_i && \Leftrightarrow \mu_i \in \mathbb{R}_+ \\
 & \underbrace{(\forall i) \quad -\beta_0 - X_i^\top (\beta^+ - \beta^-) - \sum_{k \in K} r_k(X_i)(\gamma_k^+ - \gamma_k^-) - \epsilon_i}_{-f_{\beta_0, \beta, \gamma}(X_i)} \leq -y_i && \Leftrightarrow \nu_i \in \mathbb{R}_+ \\
 & \epsilon \geq 0, \quad \beta^+, \beta^- \geq 0, \quad \gamma^+, \gamma^- \geq 0
 \end{aligned}$$

Overestimation constraints: $f_{\beta_0, \beta, \gamma}(X_i) - y_i \leq \epsilon_i$

Underestimation constraints: $f_{\beta_0, \beta, \gamma}(X_i) - y_i \geq -\epsilon_i$

Overestimated: $\mu_i > 0, \nu_i = 0$

Underestimated: $\mu_i = 0, \nu_i > 0$

- $2m$ constraints (except nonnegativity)
- $1 + m + 2n + 2|K|$ variables ($|K| \geq 3^n$)
- Large number of variables \Rightarrow solve by **column generation**

Pricing Problem and RMA Formulation

- Finding the smallest reduced cost (most violated dual constraints)

REPR Pricing Problem

[Link: Reduced Cost](#)

$$\max_{k \in K} \left| \sum_{i=1}^m r_k(X_i)(v_i - \mu_i) \right|$$

- This is \mathcal{NP} -hard Rectangular Maximum Agreement (RMA) problem

Rectangular Maximum Agreement (RMA) Problem

$$\begin{array}{ll} \max_{a, b \in \mathbb{R}^n} & |w(\text{Cover}_X(a, b))| \\ \text{s. t.} & a, b \in \mathbb{R}^n \end{array}$$

- REPR pricing problem reduces to RMA with

$$\begin{cases} w_i &= \mu_i - v_i \quad (\forall i) \\ \Omega^+ &= \{i \in \{1, \dots, m\} \mid \mu_i \geq v_i\} & \text{Overestimated } (\mu_i > 0, v_i = 0) \\ \Omega^- &= \{i \in \{1, \dots, m\} \mid \mu_i < v_i\} & \text{Underestimated } (\mu_i = 0, v_i > 0) \end{cases}$$

- Solve RMA by a specialized parallel branch-and-bound procedure

Some Insight into Column Generation

Link: REPR Dual

$$\begin{aligned}
 \min \quad & \sum_{i=1}^m \epsilon_i^p + C \sum_{j=1}^n (\beta_j^+ + \beta_j^-) + E \sum_{k \in K} (\gamma_k^+ + \gamma_k^-) \\
 \text{s. t.} \quad & (\forall i) \quad \beta_0 + X_i^\top (\beta^+ - \beta^-) + \sum_{k \in K} r_k(X_i)(\gamma_k^+ - \gamma_k^-) - \epsilon_i \leq y_i \quad \longleftrightarrow \quad \mu_i \\
 & (\forall i) \quad -X_i^\top (\beta^+ - \beta^-) - \sum_{k \in K} r_k(X_i)(\gamma_k^+ - \gamma_k^-) - \epsilon_i \leq -y_i \quad \longleftrightarrow \quad \nu_i \\
 & \epsilon \geq 0, \quad \beta^+, \beta^- \geq 0, \quad \gamma^+, \gamma^- \geq 0
 \end{aligned}$$

$$p = 1 \quad \begin{cases} w_i = \mu_i = 1 & \text{when observation } i \text{ is } \mathbf{overestimated} \\ w_i = -\nu_i = -1 & \text{when observation } i \text{ is } \mathbf{underestimated} \end{cases}$$

Pricing problem: find a box in which overestimated observations most outnumber underestimated ones or *vice versa*

$$p = 2 \quad \begin{cases} w_i = \mu_i = 2\epsilon_i & \text{when observation } i \text{ is } \mathbf{overestimated} \\ w_i = -\nu_i = -2\epsilon_i & \text{when observation } i \text{ is } \mathbf{underestimated} \end{cases}$$

Pricing problem: find a box that the sum of overestimation errors most greatly exceeds the sum of underestimation errors or *vice versa*

REPR: Implementation of Column Generation

Restricted Master Problem: Solved by GUROBI; Initially, empty K

$$\epsilon_i, \beta_j^+, \beta_j^-, \gamma_k^+, \gamma_k^- \in \mathbb{R}^+ \quad \hat{\beta}_j = \beta_j^+ + \beta_j^-$$

$$\beta_j = \beta_j^+ - \beta_j^-$$

min	$\epsilon_1^p \cdots + \epsilon_m^p$	$+C\hat{\beta}_1 \cdots + C\hat{\beta}_n$		
s. t.	ϵ_1	$+\beta_0 + x_{11}\beta_1 \cdots + x_{1n}\beta_n$		$\leq y_1$
	\ddots	\vdots		\vdots
	$+\epsilon_m$	$+\beta_0 + x_{m1}\beta_1 \cdots + x_{mn}\beta_n$		$\leq y_m$
	$-\epsilon_1$	$-\beta_0 - x_{11}\beta_1 \cdots - x_{1n}\beta_n$		$\leq -y_1$
	\ddots	\vdots		\vdots
	$-\epsilon_m$	$-\beta_0 - x_{m1}\beta_1 \cdots - x_{mn}\beta_n$		$\leq -y_m$

REPR: Implementation of Column Generation

Restricted Master Problem: Solved by GUROBI

$$\epsilon_i, \beta_j^+, \beta_j^-, \gamma_k^+, \gamma_k^- \in \mathbb{R}^+ \quad \hat{\beta}_j = \beta_j^+ + \beta_j^-$$

$$\beta_j = \beta_j^+ - \beta_j^-$$

min	$\epsilon_1^p \cdots + \epsilon_m^p$	$+C\hat{\beta}_1 \cdots + C\hat{\beta}_n$		
s. t.	ϵ_1	$+\beta_0 + x_{11}\beta_1 \cdots + x_{1n}\beta_n$		$\leq y_1$
	\vdots	\vdots		\vdots
	$+\epsilon_m$	$+\beta_0 + x_{m1}\beta_1 \cdots + x_{mn}\beta_n$		$\leq y_m$
	$-\epsilon_1$	$-\beta_0 - x_{11}\beta_1 \cdots - x_{1n}\beta_n$		$\leq -y_1$
	\vdots	\vdots		\vdots
	$-\epsilon_m$	$-\beta_0 - x_{m1}\beta_1 \cdots - x_{mn}\beta_n$		$\leq -y_m$

\Downarrow Optimal Dual Variables
 $\mu, \nu \in \mathbb{R}^m$

REPR: Implementation of Column Generation

Restricted Master Problem: Solved by GUROBI

$$\epsilon_i, \beta_j^+, \beta_j^-, \gamma_k^+, \gamma_k^- \in \mathbb{R}^+ \quad \hat{\beta}_j = \beta_j^+ + \beta_j^-$$

$$\beta_j = \beta_j^+ - \beta_j^-$$

min	$\epsilon_1^p \cdots + \epsilon_m^p$	$+ C \hat{\beta}_1 \cdots + C \hat{\beta}_n$		
s. t.	ϵ_1	$+ \beta_0 + x_{11} \beta_1 \cdots + x_{1n} \beta_n$		$\leq y_1$
	\vdots	\vdots		\vdots
	$+ \epsilon_m$	$+ \beta_0 + x_{m1} \beta_1 \cdots + x_{mn} \beta_n$		$\leq y_m$
	$-\epsilon_1$	$-\beta_0 - x_{11} \beta_1 \cdots - x_{1n} \beta_n$		$\leq -y_1$
	\vdots	\vdots		\vdots
	$-\epsilon_m$	$-\beta_0 - x_{m1} \beta_1 \cdots - x_{mn} \beta_n$		$\leq -y_m$

\Downarrow Optimal Dual Variables
 $\mu, \nu \in \mathbb{R}^m$

Pricing Problem:

Solved by Parallel Branch-and-Bound using PEBBL OR Greedy Heuristic

$$z^* = \max_{k \in K} \left| \sum_{i=1}^m r_k(X_i) (\nu_i - \mu_i) \right|$$

Stop if $z^* < E$ for Parallel Branch-and-Bound

REPR: Implementation of Column Generation

Restricted Master Problem: Solved by GUROBI

$$\epsilon_i, \beta_j^+, \beta_j^-, \gamma_k^+, \gamma_k^- \in \mathbb{R}^+ \quad \hat{\beta}_j = \beta_j^+ + \beta_j^-$$

$$\beta_j = \beta_j^+ - \beta_j^-$$

min	$\epsilon_1^p \cdots + \epsilon_m^p$	$+ C \hat{\beta}_1 \cdots + C \hat{\beta}_n$		
s. t.	ϵ_1	$+ \beta_0 + x_{11} \beta_1 \cdots + x_{1n} \beta_n$		$\leq y_1$
	\vdots	\vdots		\vdots
	$+ \epsilon_m$	$+ \beta_0 + x_{m1} \beta_1 \cdots + x_{mn} \beta_n$		$\leq y_m$
	$-\epsilon_1$	$-\beta_0 - x_{11} \beta_1 \cdots - x_{1n} \beta_n$		$\leq -y_1$
	\vdots	\vdots		\vdots
	$-\epsilon_m$	$-\beta_0 - x_{m1} \beta_1 \cdots - x_{mn} \beta_n$		$\leq -y_m$

A set of rules $r_k(\cdot)$
(can add multiple rules)



Optimal Dual Variables
 $\mu, \nu \in \mathbb{R}^m$

Pricing Problem:

Solved by Parallel Branch-and-Bound using PEBBL OR Greedy Heuristic

$$\max_{k \in K} \left| \sum_{i=1}^m r_k(X_i)(\nu_i - \mu_i) \right|$$

Stop if $z^* < E$ for Parallel Branch-and-Bound

REPR: Implementation of Column Generation

Restricted Master Problem: Solved by GUROBI

$$\epsilon_i, \beta_j^+, \beta_j^-, \gamma_k^+, \gamma_k^- \in \mathbb{R}^+ \quad \hat{\beta}_j = \beta_j^+ + \beta_j^- \quad \hat{\gamma}_j = \gamma_k^+ + \gamma_k^- \\ \beta_j = \beta_j^+ - \beta_j^- \quad \gamma_k = \gamma_k^+ - \gamma_k^-$$

min	$\epsilon_1^p \cdots + \epsilon_m^p$	$+C\hat{\beta}_1 \cdots + C\hat{\beta}_n$	$+D\hat{\gamma}_1$	
s. t.	ϵ_1	$+\beta_0 + x_{11}\beta_1 \cdots + x_{1n}\beta_n$	$+r_1(X_1)\gamma_1$	$\leq y_1$
	\ddots	\vdots	\vdots	\vdots
	$+\epsilon_m$	$+\beta_0 + x_{m1}\beta_1 \cdots + x_{mn}\beta_n$	$+r_1(X_m)\gamma_1$	$\leq y_m$
	$-\epsilon_1$	$-\beta_0 - x_{11}\beta_1 \cdots - x_{1n}\beta_n$	$-r_1(X_1)\gamma_0$	$\leq -y_1$
	\ddots	\vdots	\vdots	\vdots
	$-\epsilon_m$	$-\beta_0 - x_{m1}\beta_1 \cdots - x_{mn}\beta_n$	$-r_1(X_m)\gamma_1$	$\leq -y_m$

A set of rules $r_k(\cdot)$
(can add multiple rules)



Optimal Dual Variables
 $\mu, \nu \in \mathbb{R}^m$

Pricing Problem:

Solved by Parallel Branch-and-Bound using PEBBL OR Greedy Heuristic

$$\max_{k \in K} \left| \sum_{i=1}^m r_k(X_i)(v_i - \mu_i) \right|$$

Stop if $z^* < E$ for Parallel Branch-and-Bound

REPR: Implementation of Column Generation

Restricted Master Problem: Solved by GUROBI

$$\epsilon_i, \beta_j^+, \beta_j^-, \gamma_k^+, \gamma_k^- \in \mathbb{R}^+ \quad \hat{\beta}_j = \beta_j^+ + \beta_j^- \quad \hat{\gamma}_j = \gamma_j^+ + \gamma_j^- \\ \beta_j = \beta_j^+ - \beta_j^- \quad \gamma_k = \gamma_k^+ - \gamma_k^-$$

min	$\epsilon_1^p \cdots + \epsilon_m^p$	$+C\hat{\beta}_1 \cdots + C\hat{\beta}_n$	$+D\hat{\gamma}_1$	
s. t.	ϵ_1	$+\beta_0 + x_{11}\beta_1 \cdots + x_{1n}\beta_n$	$+r_1(X_1)\gamma_1$	$\leq y_1$
	\ddots	\vdots	\vdots	\vdots
	$+\epsilon_m$	$+\beta_0 + x_{m1}\beta_1 \cdots + x_{mn}\beta_n$	$+r_1(X_m)\gamma_1$	$\leq y_m$
	$-\epsilon_1$	$-\beta_0 - x_{11}\beta_1 \cdots - x_{1n}\beta_n$	$-r_1(X_1)\gamma_0$	$\leq -y_1$
	\ddots	\vdots	\vdots	\vdots
	$-\epsilon_m$	$-\beta_0 - x_{m1}\beta_1 \cdots - x_{mn}\beta_n$	$-r_1(X_m)\gamma_1$	$\leq -y_m$

A set of rules $r_k(\cdot)$
(can add multiple rules)



Optimal Dual Variables
 $\mu, \nu \in \mathbb{R}^m$

Pricing Problem:

Solved by Parallel Branch-and-Bound using PEBBL OR Greedy Heuristic

$$\max_{k \in K} \left| \sum_{i=1}^m r_k(X_i)(\nu_i - \mu_i) \right|$$

Stop if $z^* < E$ for Parallel Branch-and-Bound

REPR: Implementation of Column Generation

Restricted Master Problem: Solved by GUROBI

$$\epsilon_i, \beta_j^+, \beta_j^-, \gamma_k^+, \gamma_k^- \in \mathbb{R}^+ \quad \hat{\beta}_j = \beta_j^+ + \beta_j^- \quad \hat{\gamma}_j = \gamma_k^+ + \gamma_k^- \\ \beta_j = \beta_j^+ - \beta_j^- \quad \gamma_k = \gamma_k^+ - \gamma_k^-$$

min	$\epsilon_1^p \cdots + \epsilon_m^p$	$+C\hat{\beta}_1 \cdots + C\hat{\beta}_n$	$+D\hat{\gamma}_1$	
s. t.	ϵ_1	$+\beta_0 + x_{11}\beta_1 \cdots + x_{1n}\beta_n$	$+r_1(X_1)\gamma_1$	$\leq y_1$
	\vdots	\vdots	\vdots	\vdots
	$+\epsilon_m$	$+\beta_0 + x_{m1}\beta_1 \cdots + x_{mn}\beta_n$	$+r_1(X_m)\gamma_1$	$\leq y_m$
	$-\epsilon_1$	$-\beta_0 - x_{11}\beta_1 \cdots - x_{1n}\beta_n$	$-r_1(X_1)\gamma_0$	$\leq -y_1$
	\vdots	\vdots	\vdots	\vdots
	$-\epsilon_m$	$-\beta_0 - x_{m1}\beta_1 \cdots - x_{mn}\beta_n$	$-r_1(X_m)\gamma_1$	$\leq -y_m$

A set of rules $r_k(\cdot)$
(can add multiple rules)



Optimal Dual Variables
 $\mu, \gamma \in \mathbb{R}^m$

Pricing Problem:

Solved by Parallel Branch-and-Bound using PEBBL OR Greedy Heuristic

$$z^* = \max_{k \in K} \left| \sum_{i=1}^m r_k(X_i)(v_i - \mu_i) \right|$$

Stop if $z^* < E$ for Parallel Branch-and-Bound

REPR: Implementation of Column Generation

Restricted Master Problem: Solved by GUROBI

$$\epsilon_i, \beta_j^+, \beta_j^-, \gamma_k^+, \gamma_k^- \in \mathbb{R}^+ \quad \hat{\beta}_j = \beta_j^+ + \beta_j^- \quad \hat{\gamma}_j = \gamma_j^+ + \gamma_j^- \\ \beta_j = \beta_j^+ - \beta_j^- \quad \gamma_k = \gamma_k^+ - \gamma_k^-$$

min	$\epsilon_1^p \cdots + \epsilon_m^p$	$+C\hat{\beta}_1 \cdots + C\hat{\beta}_n$	$+D\hat{\gamma}_1$	
s. t.	ϵ_1	$+\beta_0 + x_{11}\beta_1 \cdots + x_{1n}\beta_n$	$+r_1(X_1)\gamma_1$	$\leq y_1$
	\vdots	\vdots	\vdots	\vdots
	$+\epsilon_m$	$+\beta_0 + x_{m1}\beta_1 \cdots + x_{mn}\beta_n$	$+r_1(X_m)\gamma_1$	$\leq y_m$
	$-\epsilon_1$	$-\beta_0 - x_{11}\beta_1 \cdots - x_{1n}\beta_n$	$-r_1(X_1)\gamma_0$	$\leq -y_1$
	\vdots	\vdots	\vdots	\vdots
	$-\epsilon_m$	$-\beta_0 - x_{m1}\beta_1 \cdots - x_{mn}\beta_n$	$-r_1(X_m)\gamma_1$	$\leq -y_m$

A set of rules $r_k(\cdot)$
(can add multiple rules)



Optimal Dual Variables
 $\mu, \gamma \in \mathbb{R}^m$

Pricing Problem:

Solved by Parallel Branch-and-Bound using PEBBL OR Greedy Heuristic

$$\max_{k \in K} \left| \sum_{i=1}^m r_k(X_i)(v_i - \mu_i) \right|$$

Stop if $z^* < E$ for Parallel Branch-and-Bound

REPR: Implementation of Column Generation

Restricted Master Problem: Solved by GUROBI

$$\epsilon_i, \beta_j^+, \beta_j^-, \gamma_k^+, \gamma_k^- \in \mathbb{R}^+ \quad \hat{\beta}_j = \beta_j^+ + \beta_j^- \quad \hat{\gamma}_j = \gamma_k^+ + \gamma_k^- \\ \beta_j = \beta_j^+ - \beta_j^- \quad \gamma_k = \gamma_k^+ - \gamma_k^-$$

min	$\epsilon_1^p \cdots + \epsilon_m^p$	$+C\hat{\beta}_1 \cdots + C\hat{\beta}_n$	$+D\hat{\gamma}_1$	$+D\hat{\gamma}_2$	
s. t.	ϵ_1	$+\beta_0 + x_{11}\beta_1 \cdots + x_{1n}\beta_n$	$+r_1(X_1)\gamma_1$	$+r_2(X_1)\gamma_2$	$\leq y_1$
	\ddots	\vdots	\vdots	\vdots	\vdots
	$+\epsilon_m$	$+\beta_0 + x_{m1}\beta_1 \cdots + x_{mn}\beta_n$	$+r_1(X_m)\gamma_1$	$+r_2(X_m)\gamma_2$	$\leq y_m$
	$-\epsilon_1$	$-\beta_0 - x_{11}\beta_1 \cdots - x_{1n}\beta_n$	$-r_1(X_1)\gamma_0$	$-r_2(X_1)\gamma_2$	$\leq -y_1$
	\ddots	\vdots	\vdots	\vdots	\vdots
	$-\epsilon_m$	$-\beta_0 - x_{m1}\beta_1 \cdots - x_{mn}\beta_n$	$-r_1(X_m)\gamma_1$	$-r_2(X_m)\gamma_2$	$\leq -y_m$

A set of rules $r_k(\cdot)$
(can add multiple rules)



Optimal Dual Variables
 $\mu, \nu \in \mathbb{R}^m$

Pricing Problem:

Solved by Parallel Branch-and-Bound using PEBBL OR Greedy Heuristic

$$\max_{k \in K} \left| \sum_{i=1}^m r_k(X_i)(\nu_i - \mu_i) \right|$$

Stop if $z^* < E$ for Parallel Branch-and-Bound

REPR: Implementation of Column Generation

Restricted Master Problem: Solved by GUROBI

$$\epsilon_i, \beta_j^+, \beta_j^-, \gamma_k^+, \gamma_k^- \in \mathbb{R}^+ \quad \hat{\beta}_j = \beta_j^+ + \beta_j^- \quad \hat{\gamma}_j = \gamma_k^+ + \gamma_k^- \\ \beta_j = \beta_j^+ - \beta_j^- \quad \gamma_k = \gamma_k^+ - \gamma_k^-$$

min	$\epsilon_1^p \cdots + \epsilon_m^p$	$+C\hat{\beta}_1 \cdots + C\hat{\beta}_n$	$+D\hat{\gamma}_1$	$+D\hat{\gamma}_2$	\cdots	
s. t.	ϵ_1	$+\beta_0 + x_{11}\beta_1 \cdots + x_{1n}\beta_n$	$+r_1(X_1)\gamma_1$	$+r_2(X_1)\gamma_2$	\cdots	$\leq y_1$
	\ddots	\vdots	\vdots	\vdots	\vdots	\vdots
	$+\epsilon_m$	$+\beta_0 + x_{m1}\beta_1 \cdots + x_{mn}\beta_n$	$+r_1(X_m)\gamma_1$	$+r_2(X_m)\gamma_2$	\cdots	$\leq y_m$
	$-\epsilon_1$	$-\beta_0 - x_{11}\beta_1 \cdots - x_{1n}\beta_n$	$-r_1(X_1)\gamma_0$	$-r_2(X_1)\gamma_2$	\cdots	$\leq -y_1$
	\ddots	\vdots	\vdots	\vdots	\vdots	\vdots
	$-\epsilon_m$	$-\beta_0 - x_{m1}\beta_1 \cdots - x_{mn}\beta_n$	$-r_1(X_m)\gamma_1$	$-r_2(X_m)\gamma_2$	\cdots	$\leq -y_m$

A set of rules $r_k(\cdot)$
(can add multiple rules)



Optimal Dual Variables
 $\mu, \nu \in \mathbb{R}^m$

Pricing Problem:

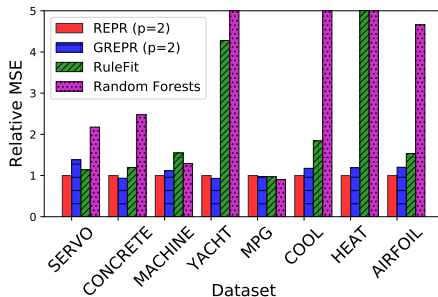
Solved by Parallel Branch-and-Bound using PEBBL OR Greedy Heuristic

$$\max_{k \in K} \left| \sum_{i=1}^m r_k(X_i)(\nu_i - \mu_i) \right|$$

Stop if $z^* < E$ for Parallel Branch-and-Bound

Result: REPR has lower relative MSE on testing datasets

- Bi-level cross-validation (inner cross-validation to choose $C = E$), $p = 2$
- 150 column generation iterations (add one rule per iteration)
- **REPR**: Pricing by parallel branch and bound
- **GREPR**: Pricing by greedy heuristic (serial)

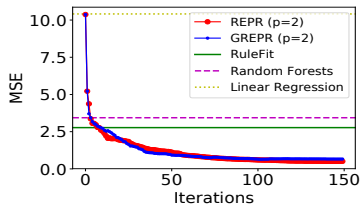


- REPR average MSE normalized to 1
- Some bars truncated
- Random Forests, RuleFit, and Linear Regression were implemented by their R packages with default setting (default parameters)

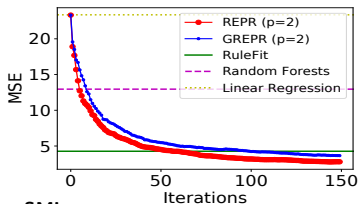
Result: MSE decreases in each column generation iteration (No obvious overfitting)

- First iteration of REPR is the same as LASSO
- First few rules have larger effect to minimize MSE on testing datasets

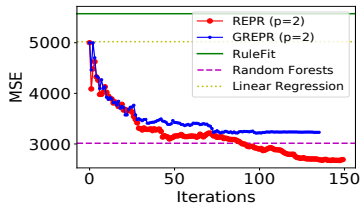
Data: HEAT



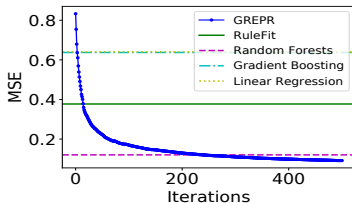
Data: AIRFOIL



Data: MACHINE



Data: SML



Conclusion

- LPBR constructs competitive classification models
- REPR makes more accurate and robust predictions than the other methods such as RuleFit and Random Forests

Improvement

- Try using larger datasets
- Dimensional reduction
- More parallel procedures
- Smarter parameter choices

$p = 1$

$$\begin{aligned}
 & \max_{\mu \geq 0, \alpha} && \alpha \\
 \text{s. t.} &&& - \sum_{i=1}^m \mu_i y_i r_k^+(X_i) \geq \alpha, && k \in K \\
 &&& - \sum_{i=1}^m \mu_i y_i r_k^-(X_i) \geq \alpha, && k \in K \\
 &&& \sum_{i=1}^m y_i \mu_i = 0, \quad \sum_{i=1}^m \mu_i = 1 \\
 &&& 0 \leq \mu_i \leq D, && i = 1, \dots, m
 \end{aligned}$$

$p = 2$

$$\begin{aligned}
 & \max_{\mu \geq 0, \alpha} && \alpha + \sum_{i=1}^m \left(\frac{\mu_i}{2} - \frac{\mu_i^2}{2D} \right) \\
 \text{s. t.} &&& - \sum_{i=1}^m \mu_i y_i r_k^+(X_i) \geq \alpha, && k \in K \\
 &&& - \sum_{i=1}^m \mu_i y_i r_k^-(X_i) \geq \alpha, && k \in K \\
 &&& \sum_{i=1}^m y_i \mu_i = 0, \quad \sum_{i=1}^m \mu_i = 1
 \end{aligned}$$

- **Reduced cost:** rate at which optimal objective changes as you increase the value of a variable

Reduced Cost

$$\text{rc}[\gamma_k^+] = E - \sum_{i=1}^m r_k(X_i) v_i + \sum_{i=1}^m r_k(X_i) \mu_i$$

$$\text{rc}[\gamma_k^-] = E + \sum_{i=1}^m r_k(X_i) v_i - \sum_{i=1}^m r_k(X_i) \mu_i$$

- Finding the smallest reduced cost
 - most violated dual constraints
 - variable whose introduction improves the objective fastest

REPR Pricing Problem

$$\max_{k \in K} \left| \sum_{i=1}^m r_k(X_i) (v_i - \mu_i) \right|$$

Dual Formulation of RPER

[Link: Insight](#)

$p = 1$

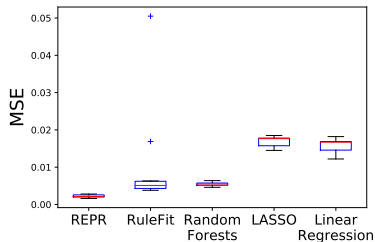
$$\begin{aligned} \max_{\mu, \nu \geq 0} \quad & \sum_{i=1}^m y_i (\nu_i - \mu_i) \\ \text{s. t.} \quad & \sum_{i=1}^m (\mu_i - \nu_i) = 0 \\ & \mu_i + \nu_i \leq 1, \quad i = 1, \dots, m \\ & \left| \sum_{i=1}^m \nu_i x_{ij} - \sum_{i=1}^m \mu_i x_{ij} \right| \leq C, \quad j = 1, \dots, n \\ & \left| \sum_{i=1}^m \nu_i r_k(X_i) - \sum_{i=1}^m \mu_i r_k(X_i) \right| \leq E, \quad k \in K \end{aligned}$$

$p = 2$

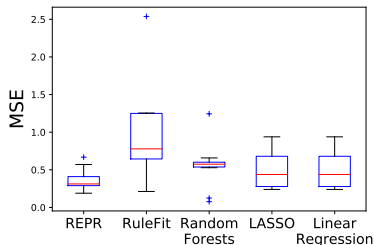
$$\begin{aligned} \max_{\mu, \nu \geq 0} \quad & \sum_{i=1}^m y_i (\nu_i - \mu_i) - \frac{1}{4} \sum_{i=1}^m (\nu_i + \mu_i)^2 \\ \text{s. t.} \quad & \sum_{i=1}^m (\mu_i - \nu_i) = 0 \\ & \left| \sum_{i=1}^m \nu_i x_{ij} - \sum_{i=1}^m \mu_i x_{ij} \right| \leq C, \quad j = 1, \dots, n \\ & \left| \sum_{i=1}^m \nu_i r_k(X_i) - \sum_{i=1}^m \mu_i r_k(X_i) \right| \leq E, \quad k \in K \end{aligned}$$

Result: REPR has Lower MSE Variance across Folds

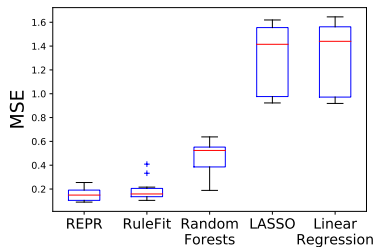
Data: HEAT



Data: MACHINE



Data: SERVO



Data: CONCRETE

