# MARS via LASSO

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R package: https://github.com/DohyeongKi/regmdc

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Example: $5.3 + 2.3(x_1 - 2)_+ - 1.4(-2 - x_3)_+ + 4.7(x_1 + 3)_+(1 - x_2)_+$

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Model building strategy:

Greedy algorithm (like stepwise regression)

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Greedy algorithm (like stepwise regression)

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$\longrightarrow$ Difficult to guarantee optimality and study theoretical properties

# Our Method

We propose and study a LASSO variant of the MARS method.

Data: $(x^{(1)}, y_1), \ldots, (x^{(n)}, y_n)$ where $x^{(i)} \in [0, 1]^d$ and $y_i \in \mathbb{R}$

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Two simplifications:

- We only consider $(x_j - t_j)_+$.
  $(\because (t_j - x_j)_+ = (x_j - t_j)_+ - (x_j - 0)_+ + t_j)$
  $(x_j - t_j)_+$ is linear if $t_j = 0$.
- We assume $t_j \in [0, 1)$.

We use LASSO to fit a sparse linear combination of basis functions of the form:

$$\prod_{j \in S} (x_j - t_j)_+ \qquad \text{where } S \subseteq \{1, \ldots, d\} \text{ and } t_j \in [0, 1).$$

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We need an infinite-dimensional version of LASSO (Rosset et al. [2007], Bredies and Pikkarainen [2013], Condat [2020], ...).

- Parametrize infinite linear combinations with (signed) measures
- Measure complexity in terms of the (total) variation of the involved signed measures

# Our Function Class

$\mathcal{F}^{d,s}_{\infty-\text{mars}}$ is the collection of all the functions of the form

$$f(x_1, \ldots, x_d) = c + \sum_{\substack{\varnothing \neq S \subseteq \{1,\ldots,d\} \\ |S| \leq s}} \int_{[0,1)^{|S|}} \prod_{j \in S} (x_j - t_j)_+ \, d\nu_S(t_j, j \in S)$$

$\nu_S$ is a signed measure on $[0,1)^{|S|}$ for each $\varnothing \neq S \subseteq \{1, \ldots, d\}$ with $|S| \leq s$

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$$f(x_1) = c + \int_{[0,1)} (x_1 - t_1)_+ \, d\nu_1(t_1)$$

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(2) $d = s = 2$

$$f(x_1, x_2) = c + \int_{[0,1)} (x_1 - t_1)_+ \, d\nu_1(t_1) + \int_{[0,1)} (x_2 - t_2)_+ \, d\nu_2(t_2) + \int_{[0,1)^2} (x_1 - t_1)_+ (x_2 - t_2)_+ \, d\nu_{1,2}(t_1, t_2)$$

- The usual MARS functions are special cases.

If $\nu_S$ is supported on a finite set $\{(t^S_{\ell j}, j \in S) : \ell = 1, \dots, k_S\}$ with

$$\nu_S\big(\big\{\big(t^S_{\ell j}, j \in S\big)\big\}\big) = b^S_\ell \qquad \text{for } \ell = 1, \dots, k_S,$$

then the function becomes

$$f(x_1, \dots, x_d) = c + \sum_{\substack{\emptyset \neq S \subseteq \{1,\dots,d\} \\ |S| \leq s}} \sum_{\ell=1}^{k_S} b^S_\ell \cdot \prod_{j \in S} \big(x_j - t^S_{\ell j}\big)_+.$$

# Complexity Measure

Complexity measure for $f \in \mathcal{F}^{d,s}_{\infty-\text{mars}}$:

$$V_{\text{mars}}(f) := \sum_{\substack{\emptyset \neq S \subseteq \{1,\ldots,d\} \\ |S| \leq s}} |\nu_S| \left( [0,1)^{|S|} \setminus \{(0,\ldots,0)\} \right).$$

- The sum of the variation of the involved signed measures
- $(0,\ldots,0)$ is excluded;
  the products of linear functions are not penalized

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then

$$V_{\text{mars}}(f) = \sum_{\substack{\emptyset \neq S \subseteq \{1,\dots,d\} \\ |S| \le s}} \sum_{\ell=1}^{k_S} |b^S_\ell| \cdot \mathbf{1}\big\{\big(t^S_{\ell j}, j \in S\big) \neq (0, \dots, 0)\big\},$$

which is the sum of the absolute values of the coefficients
(the coefficients of the product of linear functions are excluded).

# Our Estimator

Our infinite-dimensional LASSO estimator for MARS fitting:

$$\hat{f}_{n,V}^{d,s} \in \operatorname*{argmin}_{f} \left\{ \sum_{i=1}^{n} \left(y_i - f(x^{(i)})\right)^2 : f \in \mathcal{F}_{\infty-\text{mars}}^{d,s} \text{ and } V_{\text{mars}}(f) \leq V \right\}$$

$V > 0$ is a single tuning parameter

# Existence and Computation

$\hat{f}^{d,s}_{n,V}$ exists and can be computed by applying finite-dimensional LASSO algorithms to the finite basis of functions

$$\left\{ \prod_{j \in S} (x_j - t_j)_+ : S \subseteq \{1, \dots, d\} \text{ with } |S| \le s \right.$$
$$\left. \text{and } t_j \in \{0\} \cup \left\{ x_j^{(1)}, \dots, x_j^{(n)} \right\} \right\}$$

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$x^{(i)} = (x_1^{(i)}, \ldots, x_d^{(i)})$ for the $i^{th}$ design point $x^{(i)}$

- We can find $\hat{f}^{d,s}_{n,V}$ that is a sparse linear combination of the basis functions.
- The usual MARS algorithm also works with the same finite basis although no theoretical justification is provided for this reduction.

# Approximation

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We also consider the approximate version $\tilde{f}_{n,V}^{d,s}$ that is obtained by restricting the knots $t_j$ as

$$t_j \in \left\{0, \frac{1}{N_j}, \frac{2}{N_j}, \ldots, 1\right\}$$

for some pre-specified integers $N_1, \ldots, N_d$.

# Rate of Convergence

Under the assumptions:

- data $(x^{(1)}, y_1), \ldots, (x^{(n)}, y_n)$ are generated according to the model

$$y_i = f^*(x^{(i)}) + \xi_i \qquad \text{where } \xi_i \overset{\text{i.i.d.}}{\sim} N(0, \sigma^2),$$

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- $f^* \in \mathcal{F}^{d,s}_{\infty-\text{mars}}$ with $V_{\text{mars}}(f^*) \le V$ and $\|f^*\|_\infty \le M$,
- the loss function is

$$\mathcal{L}\big(\hat{f}^{d,s}_{n,V,M}, f^*\big) := \int \big(\hat{f}^{d,s}_{n,V,M}(x) - f^*(x)\big)^2 p_0(x)\, dx,$$

we prove that

$$\mathbb{E}\mathcal{L}\left(\hat{f}^{d,s}_{n,V,M}, f^*\right) = O_{d,\sigma,V,B,M}\left(n^{-\frac{4}{5}}(\log n)^{\frac{8(s-1)}{5}}\right).$$

Remark) $d = 1$
It was proved the rate is $n^{-\frac{4}{5}}$ (see, e.g., Mammen and van de Geer [1997]).

$\longrightarrow$ Similar results can be proved for the approximate version $\tilde{f}^{d,s}_{n,V,M}$

# Minimax Lower Bound

Under the same assumption, we prove that the minimax rate under the loss function $\mathcal{L}$ over the class

$$\left\{f \in \mathcal{F}^{d,s}_{\infty-\text{mars}} : V_{\text{mars}}(f) \le V \text{ and } \|f^*\|_\infty \le M\right\}$$

is bounded from below by

$$n^{-\frac{4}{5}}(\log n)^{\frac{8(s-1)}{5}}.$$

# Connection to Smoothness Constrained Estimation

$d = s = 1$

The **total variation** of a function $g : [0,1] \to \mathbb{R}$ is defined by

$$V(g) := \sup_{0=u_0<u_1<\cdots<u_k=1} \sum_{i=0}^{k-1} \left| g(u_{i+1}) - g(u_i) \right|$$

where the supremum is over all $k \geq 1$ and partitions $0 = u_0 < u_1 < \cdots < u_k = 1$ of $[0,1]$.

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Then, somewhat loosely, we can describe the estimator $\hat{f}^{1,1}_{n,V}$ as

$$\hat{f}^{1,1}_{n,V} \in \operatorname*{argmin}_f \left\{ \sum_{i=1}^{n} \left(y_i - f(x^{(i)})\right)^2 : V(f') \leq V \right\}.$$

Corresponding penalized version:

$$\underset{f}{\operatorname{argmin}} \left\{ \sum_{i=1}^{n} \left(y_i - f(x^{(i)})\right)^2 + \lambda V(f') \right\}$$

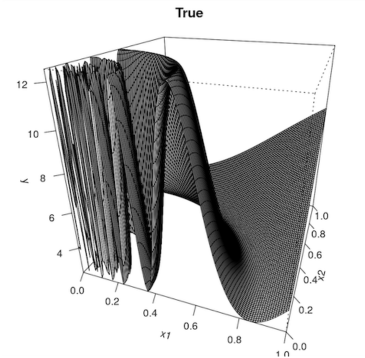
The piecewise linear **locally adaptive regression spline** (LARS) estimator of Mammen and van de Geer [1997]

# Example

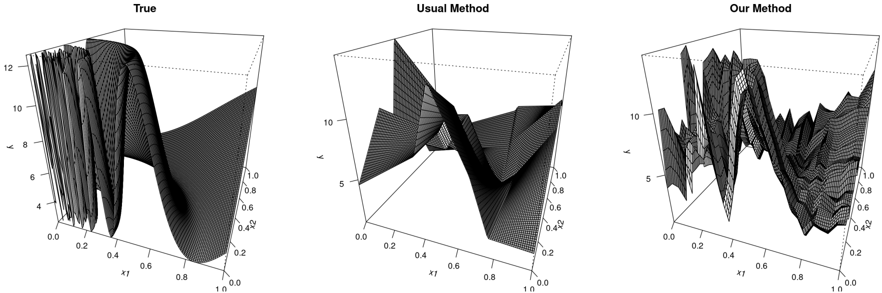
A function with locally varying smoothness (Doppler function):

$$y_i = 5 \cdot \sin\left(4/(\sqrt{(x_1^{(i)})^2 + (x_2^{(i)})^2} + 0.001)\right) + 7.5 + \xi_i$$

for $i = 1, \ldots, n$, where $\xi_i \overset{\text{i.i.d.}}{\sim} N(0, 1)$.



$n = 800$, $s = 2$, $N_j = 25$, $V$ is chosen by 10-fold cross validation




Average loss over 25 repetitions

| | Usual Method | Our Method |
|---|---|---|
| Average loss (Standard error) | 3.28 (0.07) | 1.51 (0.06) |

More examples (simulated data and real data) are in
https://github.com/DohyeongKi/mars-lasso-paper

# Conclusion

- We propose and study an infinite-dimensional LASSO estimator for MARS.
- Our estimator can be computed with finite dimensional LASSO algorithms.
- Our estimator achieves the rate $n^{-\frac{4}{5}}(\log n)^{\frac{8(s-1)}{5}}$ under the standard nonparametric regression setting.

- The dependence on the dimension of the exponent of the log factor is inevitable.
- It can be considered as a multivariate generalization of the piecewise linear locally adaptive regression spline estimator of Mammen and van de Geer [1997].

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