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► **To cite this version:**

Sébastien Petit, Julien Bect, Paul Feliot, Emmanuel Vazquez. Gaussian process model selection for computer experiments. MASCOT PhD student 2020 Meeting, Sep 2020, Grenoble, France. . hal-03018559

**HAL Id: hal-03018559**

**<https://centralesupelec.hal.science/hal-03018559v1>**

Submitted on 22 Nov 2020

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# Gaussian process model selection for computer experiments



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## Context

- Exploration of black-box numerical simulators  $f : \mathbb{X} \subset \mathbb{R}^d \rightarrow \mathbb{R}$  with Gaussian processes
- Given data  $D_n = (\mathcal{X}_n, f|_{\mathcal{X}_n})$ , a Gaussian process  $\xi$  can be used to make probabilistic predictions of  $f$

$$\xi(x)|D_n \sim \mathcal{N}(\hat{\xi}_\theta(x), \hat{\sigma}_\theta^2(x)) \quad (1)$$

- $\xi$  is a prior over functions
- The choice of  $\xi$  is critical for good predictions and design-of-experiments techniques

The prior  $\xi$  is often chosen within a parametric family.

- Very often: the Matérn covariance functions family is used [7]
- Many procedures have been proposed in the literature for selecting the parameters of a covariance function
- Little is known about their relative benefits

What are the most useful procedures to select the parameters of a Matérn covariance function (including or not regularity)?

- Toms 829  $C^k$  ( $k \in \{0, 1, 2\}$ ,  $d \in \{2, 5\}$ )

- Rotated Rosenbrock ( $d \in \{2, 5\}$ )

- Borehole ( $d = 8$ )

with space-filling designs  $\mathcal{X}_n$ ,  $n \in \{10d, 20d, 50d\}$ . For each case:

- We compare model selection procedures using predictions evaluated on a dense test grid

- In particular, we study the influence of the regularity parameter  $p$  of a Matérn covariance function, by setting  $p \in \{0, 1, 2, 3, 4, d, 2d, +\infty\}$  or automatically selecting its value using the selection criteria

- We present averaged results through repetitions (using random  $\mathcal{X}_n$  for instance)

## An example

Observe that

- Procedures ML, LOO-MSPE, LOO-NLPD and LOO-CRPS give similar accuracies

- The influence of  $p$  on the accuracy is strong

MSPE	ML	LOO MSPE	LOO NLPD	LOO CRPS	KA	GCV	"Best"
0	$1.08 \cdot 10^{-2}$	$1.12 \cdot 10^{-2}$	$1.07 \cdot 10^{-2}$	$1.06 \cdot 10^{-2}$	$2.16 \cdot 10^{-1}$	$1.04 \cdot 10^{-2}$	$9.74 \cdot 10^{-3}$
1	$3.27 \cdot 10^{-5}$	$3.11 \cdot 10^{-5}$	$2.78 \cdot 10^{-5}$	$2.85 \cdot 10^{-5}$	$1.71 \cdot 10^{-1}$	$2.79 \cdot 10^{-5}$	$2.45 \cdot 10^{-5}$
2	$1.17 \cdot 10^{-5}$	$1.23 \cdot 10^{-5}$	$1.29 \cdot 10^{-5}$	<b><math>1.14 \cdot 10^{-5}</math></b>	$1.59 \cdot 10^{-1}$	$1.66 \cdot 10^{-5}$	$8.68 \cdot 10^{-6}$
3	$1.54 \cdot 10^{-5}$	$1.80 \cdot 10^{-5}$	$1.81 \cdot 10^{-5}$	$1.62 \cdot 10^{-5}$	$1.36 \cdot 10^{-1}$	$2.32 \cdot 10^{-5}$	$1.26 \cdot 10^{-5}$
4	$1.90 \cdot 10^{-5}$	$2.32 \cdot 10^{-5}$	$2.30 \cdot 10^{-5}$	$2.11 \cdot 10^{-5}$	$1.23 \cdot 10^{-1}$	$3.13 \cdot 10^{-5}$	$1.60 \cdot 10^{-5}$
6	$2.36 \cdot 10^{-5}$	$3.07 \cdot 10^{-5}$	$2.90 \cdot 10^{-5}$	$2.68 \cdot 10^{-5}$	$1.12 \cdot 10^{-1}$	$4.00 \cdot 10^{-5}$	$1.99 \cdot 10^{-5}$
12	$2.60 \cdot 10^{-5}$	$3.30 \cdot 10^{-5}$	$3.04 \cdot 10^{-5}$	$2.97 \cdot 10^{-5}$	$1.03 \cdot 10^{-1}$	$4.11 \cdot 10^{-5}$	$2.16 \cdot 10^{-5}$
$+\infty$	$2.94 \cdot 10^{-5}$	$3.77 \cdot 10^{-5}$	$3.33 \cdot 10^{-5}$	$3.18 \cdot 10^{-5}$	$9.23 \cdot 10^{-2}$	$4.31 \cdot 10^{-5}$	$2.43 \cdot 10^{-5}$
$\hat{p}$	$1.17 \cdot 10^{-5}$	$1.27 \cdot 10^{-5}$	$1.29 \cdot 10^{-5}$	<b><math>1.15 \cdot 10^{-5}</math></b>	$9.23 \cdot 10^{-2}$	$1.74 \cdot 10^{-5}$	$8.68 \cdot 10^{-6}$

Table: Average MSPE on the validation sets for the different selection procedures and regularity choices.

## Influence of the selection criteria

We compare the selection procedures with automatically selected  $p$ . Fig. 3:  $\log(S_{\text{MSPE}})$  normalized by "Best" values; Fig. 4: interval score [4] defined by

$$S_\alpha^{\text{IS}}(l, u, x) = (u - l) + \frac{2}{\alpha}(l - x)\mathbf{1}_{x \leq l} + \frac{2}{\alpha}(x - u)\mathbf{1}_{x > u}. \quad (3)$$

## 6 Conclusions

- The regularity parameter has a strong impact on the goodness of fit
- We recommend selecting the regularity from data instead of fixing it to a "standard" value
- The choice of a reasonable selection procedure has second-order impact but ML and LOO CRPS seem to give the best performances
- All procedures have the same numerical complexity, using appropriate computations of the selection criteria and their gradients [6]

## 1 Maximum-likelihood [5]

- A very popular technique
- Choose the parameters that yield the highest value of the probability density for the observations, or equivalently, minimize

$$z^T K_\theta z + \ln(\det(K_\theta)),$$

where  $K_\theta$  is the covariance matrix of  $\xi$  at points  $\mathcal{X}_n = (x_1, \dots, x_n)$  for parameters  $\theta$  and  $z = (z_1, \dots, z_n)^T$  denotes the values of  $f$  at  $\mathcal{X}_n$

## 2 Cross-validation

Leave-one-out (LOO) [3] is a second very popular technique

- Consists in averaging *losses* for predicting one observation using the others
- We suggest using *negatively-oriented scoring rules* [4] for the loss functions
- A (negatively-oriented) scoring rule is a mapping  $S : (\mathcal{P}, \mathbb{R}) \rightarrow \mathbb{R}$  where  $\mathcal{P}$  is a class of probability distributions, with  $S(P, z)$  representing a loss for observing  $z$  while predicting  $P$
- Given a scoring rule  $S$  the corresponding LOO criterion is

$$L_S^{\text{LOO}}(\theta) = \frac{1}{n} \sum_{i=1}^n S(\mathcal{N}(\hat{\xi}_{\theta, -i}, \hat{\sigma}_{\theta, -i}^2), z_i), \quad (2)$$

where  $\mathcal{N}(\hat{\xi}_{\theta, -i}, \hat{\sigma}_{\theta, -i}^2)$  denotes LOO predictive distributions

In this work we consider the following scoring rules [4]:

- $S_{\text{MSPE}}(P, z) = (\mathbb{E}_{Z \sim P}(Z) - z)^2$
- $S_{\text{NLPD}}(P, z) = -\ln(p(z))$ , with  $p$  the pdf of  $P$
- $S_{\text{CRPS}}(P, z) = \|F - \mathbf{1}_{z \leq \cdot}\|_{L^2(\mathbb{R})}^2$ , with  $F$  the cdf of  $P$

We shall denote the resulting selection procedures by LOO-MSPE, LOO-NLPD and LOO-CRPS respectively.

## 3 Generalized cross-validation [1]

- A version of LOO-MSPE that takes the heterogeneity of the design into account

## 4 Kernel alignment [2]

- Aligns the eigenvector related to the highest eigenvalue of  $K_\theta$  with the data
- Can also be seen as a similarity between  $K_\theta$  and the covariance matrix obtained from the kernel  $(x, y) \rightarrow f(x)f(y)$

## 5 Numerical study

We use a set of 36 problems:

- Goldstein-Price ( $d \in \{1, 2\}$ )
- Mystery ( $d = 2$ )

## Influence of the regularity

We focus on two subsets of problems with different smoothness. Fig. 1: 5-dimensional Toms 829 problems; Fig. 2: 5-dimensional Rosenbrock and Borehole.

We compare  $\log S_{\text{MSPE}}$  normalized by "Best" values both with automatically selected or fixed- $p \in \{0, 1, 2, 3, 4, d, 2d, +\infty\}$ .

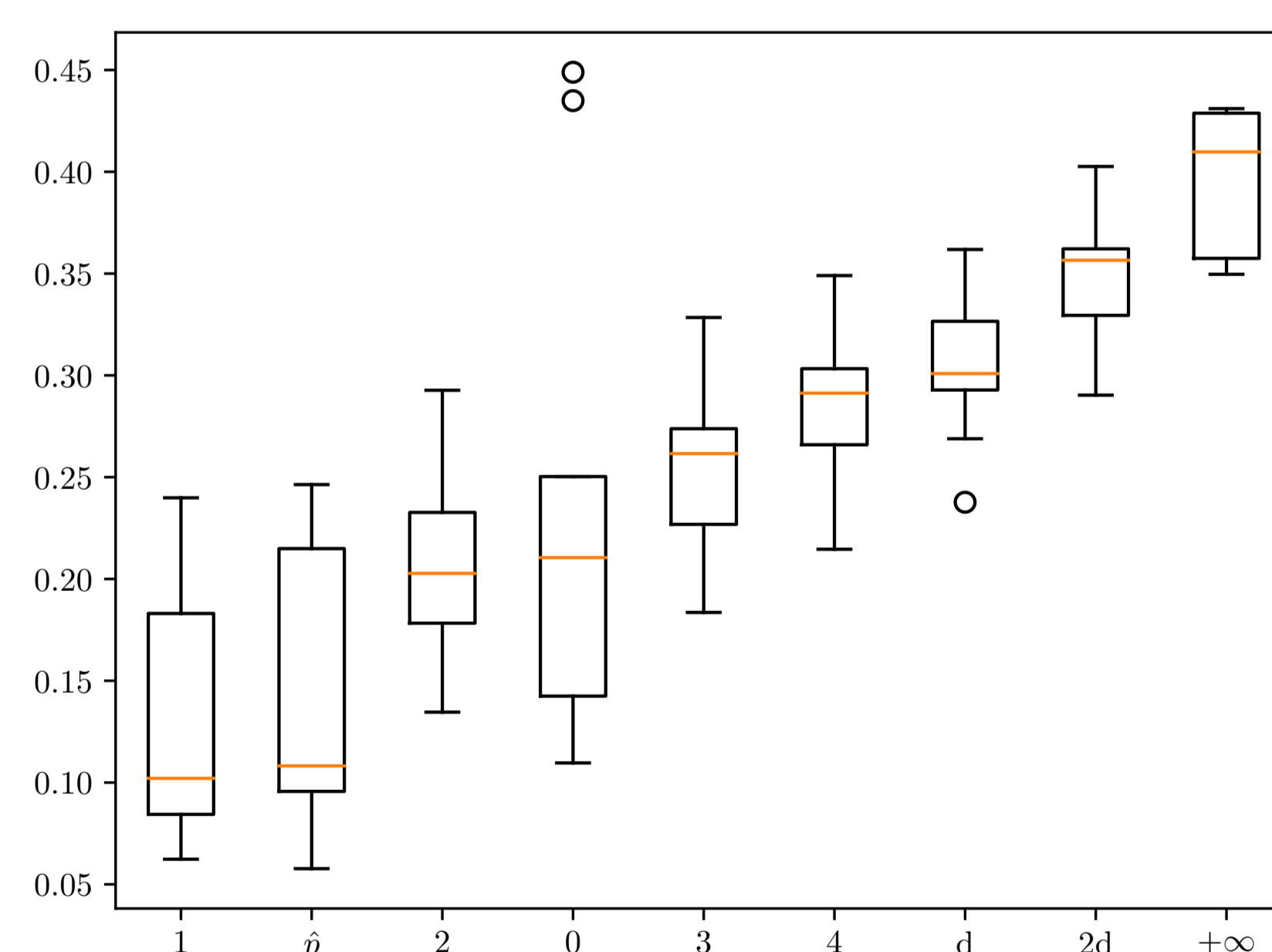


Fig. 1: Influence of the regularity on the loss for non-smooth problems.

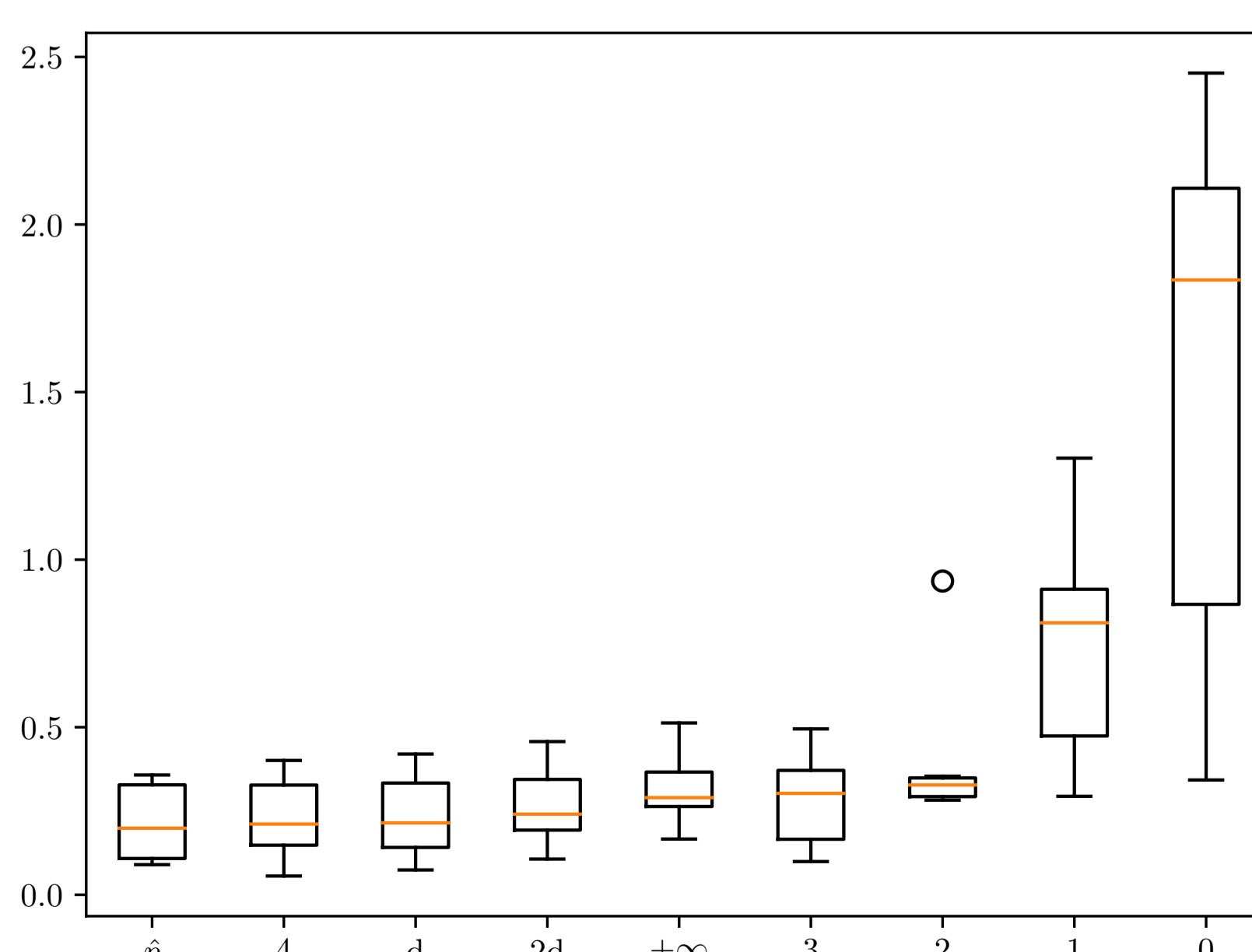


Fig. 2: Influence of the regularity on the loss for smooth problems.

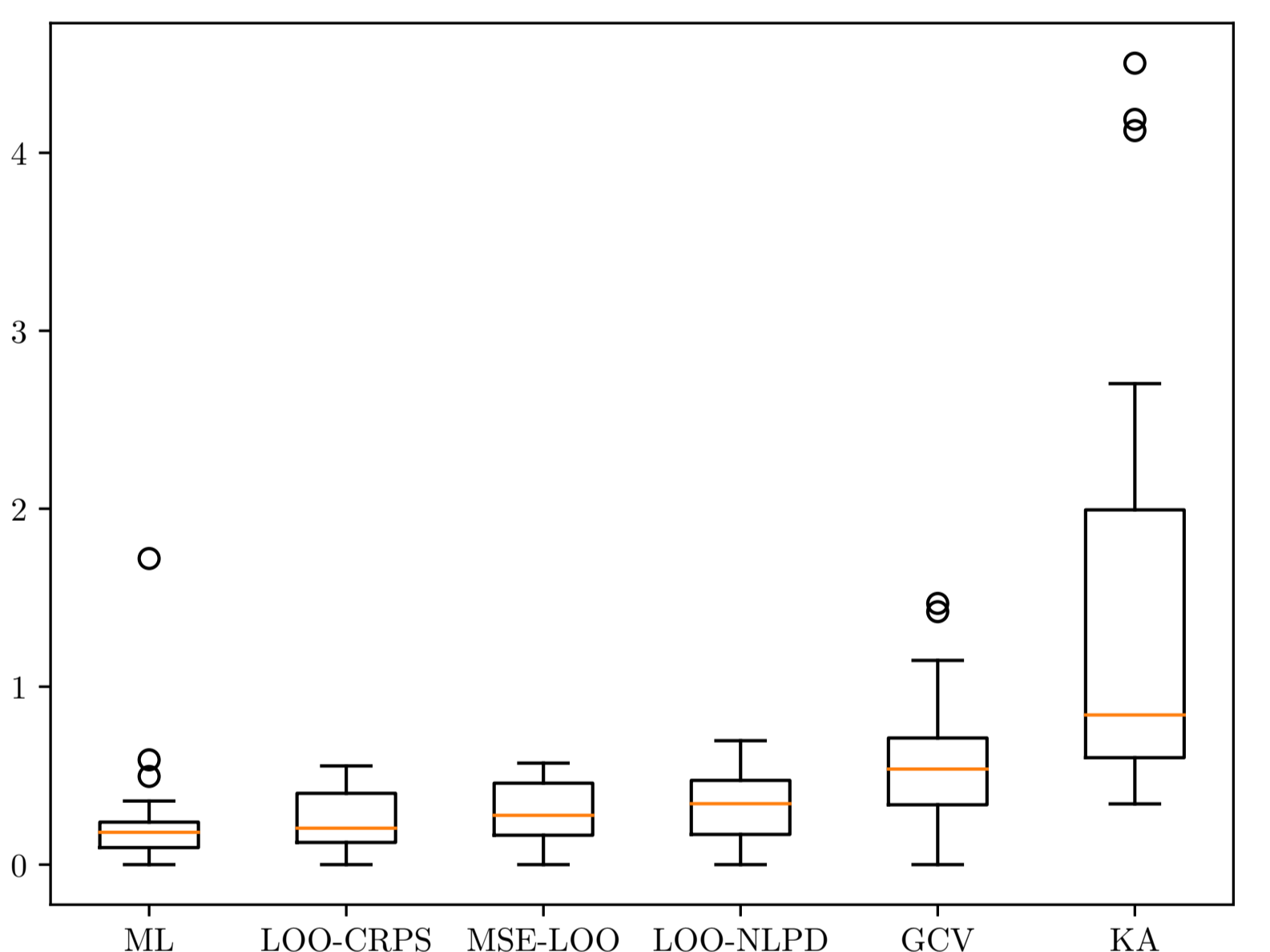


Fig. 3: Influence of the selection criteria on the MSPE.

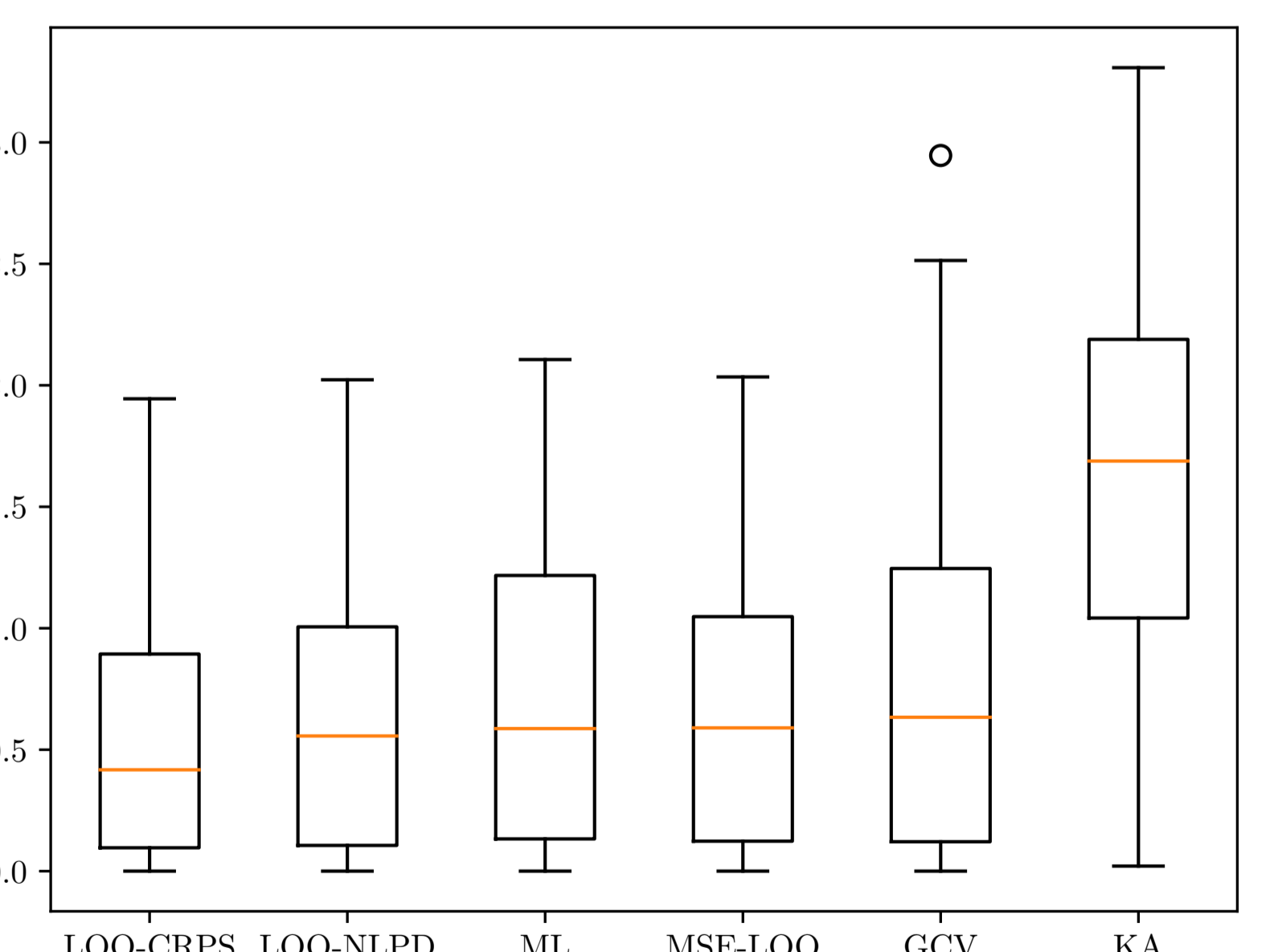


Fig. 4: Influence of the selection criteria on the interval score.

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