## Kriging for non-parametric ML estimation from regioncensored data

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## Abstract:

We consider a non-parametric density estimation problem with region-censored observations. The study is motivated by prevention of decompression sickness accidents through prediction of the amount of nitrogen bubbles produced during deep-sea diving. It relies on measurements of bubble grades – which reflect the peak gas volume in the diver's body – on a set of dives made by individuals in the population under analysis.

It is assumed that the instantaneous volume of gas  $B(\theta, P(\cdot), t)$  flowing through the right-ventricule of a diver characterised by a set of biophysical parameters  $\theta$  when executing dive profile  $P(\cdot)$  (a function of time) is well described by a known mathematical model [1]. Bubble grades,  $G \in \{0, \ldots, 4\}$ , are a strongly quantified version of peak gas volume (see Fig. 1):

$$G(\theta, P(.)) = i \Leftrightarrow \tau_i \le \max(B(\theta, P(\cdot), t)) < \tau_{i+1},$$

where  $\tau_0 = 0 < \tau_1 < \cdots < \tau_4 < \tau_5 = \infty$  is a set of thresholds assumed known.



Figure 1: Left: dive profile  $P(\cdot)$ . Right: model response (blue) and grade computation (threshold are shown in red). Observed grade is equal to 3 in this case.

We address determination of  $\hat{\pi}_{\theta}, \theta \in \Theta$ , the non-parametric Maximum Likelihood estimate (NPMLE) of the distribution of  $\theta$  in the population under study. Observation of grade G = i when executing  $P(\cdot)$  only indicates that  $\theta \in \mathcal{R}_i(P(\cdot)) = \{\theta \in \Theta : \tau_i \leq \max_t(B(\theta, P(\cdot), t)\} < \tau_{i+1}\}$  and thus we face a problem of density estimation from (region-)censored observations. For interval-censored observations it is known [3, 4] that  $\hat{\pi}_{\theta}$  is affected by several forms of indeterminacy, the major being that only the probability mass over the (finitely many) elements of a partition  $\mathcal{P}$  of the parameter space, determined by the set  $\mathcal{R}$  of observed regions  $\mathcal{R}_i(P(\cdot))$ , can be estimated. Moreover,  $\hat{\pi}_{\theta}$  is concentrated on a subset of the elements of  $\mathcal{P}$ , that can be found from the intersection graph of  $\mathcal{R}$ , see Fig. 2. These features carry over to censoring by regions of arbitrary geometry, as in our case, requiring only a slightly more complex determination of the support of  $\hat{\pi}_{\theta}$ .



Figure 2: Definition of  $\mathcal{P}$  for the observation of grades 1 and 3 for profile  $P_1$ , grade 2 for  $P_2$  and grade 1 for  $P_3$  ( $\theta \in \Theta \subset \mathbb{R}^2$ ). Left: observed regions and partition  $\mathcal{P}$  (the support of the  $\hat{\pi}_{\theta}$  is indicated in black). Right: intersection graph of  $\mathcal{R}$  (support of  $\hat{\pi}_{\theta}$  is determined by its cliques).

Central to the determination of the NPMLE is the identification of the regions  $\mathcal{R}_i(P(\cdot))$ , that must resort to numerical methods, requiring computation of the model response to  $P(\cdot)$  over a dense grid covering  $\Theta$ . In our case, we have 444 measures of grades along 48 different decompression profiles, rendering impractical direct use of the biophysical model. To overcome this problem, we rely on a set of kriged observation models, that predict the value of  $\max_t B(\theta, P(\cdot), t)$ , from the model response over a sparse  $(11 \times 11)$  grid. The response surface was estimated by simple kriging for an isotropic Mattern kernel using the package STK [2].

We present the NPML estimate of the probability mass of  $\pi_{\theta}$  over the elements of  $\mathcal{P}$ , which is based on a fast multiplicative algorithm [5]. We illustrate the pathological behaviour of this estimator, in particular its sensitivity to the detailed geometry of  $\mathcal{P}$ , and propose alternative (regularised) solutions that account for the entropy of the estimated distribution.

Our ultimate goal is to predict the distribution of grades for an arbitrary profile  $P(\cdot)$ :  $\hat{p}_P(i) = \hat{\pi}_{\theta}(\mathcal{R}_i(P(\cdot))) = \sum_{A \in \mathcal{P}} \hat{\pi}_{\theta}(A \cap \mathcal{R}_i(P(\cdot)))$ . These estimates are affected by two distinct uncertainties: (a) we do not know  $\hat{\pi}_{\theta}(A \cap \mathcal{R}_i(P(\cdot)))$  since  $\mathcal{R}_i(P(\cdot)) \notin \mathcal{P}$  for new profiles; (b) the identification of  $\mathcal{R}_i(P(\cdot))$  relies on kriging and is thus uncertain. We present upper and lower bounds on each  $\hat{p}_P(i)$  that take into account (a). Assessment of uncertainty source (b) concerns the determination of level sets based on kriging, as approached e.g. in [6] using the notions of Vorob'ev expectation and deviation and will be considered in the near future.

## References

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**Short biography** – After obtaining an engineer diploma (2008) and the master degree (2009), Y. Bennani worked in banking before starting a PhD thesis at Laboratory I3S (2012) on the estimation of the risk of decompression accidents among deep-sea divers. His thesis is conducted in the framework of contract DGA-DGCIS SAFE DIVE, a joint partnership between the company BF-Systèmes, Institut Langevin (ESPCI Paristech), and the laboratory I3S (UNS-CNRS).