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Gaussian process model selection for computer experiments

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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

$$L^2(K_\theta) + 4\det(K_\theta),$$

where $K_\theta$ is the covariance matrix of $x$ at points $X_0 = (x_1, \ldots, x_d)$ for parameters $\theta$ and $z = (z_1, \ldots, z_d)^T$ denotes the values of $f$ at $X_0$.

2 Cross-validation

Leave-one-out (LOO) [4] 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 $S : (\mathbb{P}, R) \to R$ where $\mathbb{P}$ 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

$$L^2(S)(\theta) = \sum_{i=1}^n S(N(X_0, \theta), z_i),$$

where $N(X_0, \theta)$ denotes LOO predictive distributions.

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

- $S_{\text{Logit}}(P, z) = \log(|d_{\text{Logit}}(P)|)$.
- $S_{\text{Sipix}}(P, z) = -\log(Sipix)$, with $P$ the pdf of $P$.
- $S_{\text{Sipix}}(P, z) = \|F - X_0 \|_{L_2(R^d)}$, with $P$ 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 $(\xi, \lambda) \to f(x)(y)$.

5 Numerical study

We use a set of 36 problems

- Goldstein-Price (of \{1, 2\})
- Mystery (of \{2\})

Influence of the selection criteria

We compare the selection procedures with automatically selected $\alpha$.

Fig. 1: Inflence of the selection criteria on the MSPE.

Fig. 2: Inflence of the selection criteria on the NLPD.

Fig. 3: Inflence of the selection criteria on the CRPS.

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

References


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