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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
  \[
  L = \sum_{i=1}^{n} -\log p(X_i | \theta),
  \]
  where \(X_i\) is the covariance matrix of \(X\) at points \(X_i = (x_1, \ldots, x_{d})\) for parameters \(\theta\) and \(z = (z_1, \ldots, z_d)^T\) denotes the values of \(f\) at \(X_i\).

2 Cross-validation

Leave-one-out (LOO) [5] 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
  \[
  L_S^\text{LOO}(\theta) = \sum_{i=1}^{n} S(N(X_{-i} | \theta), f(X_i | \theta)),
  \]
  where \(N(X_{-i} | \theta), f(X_i | \theta))\) denotes LOO predictive distributions.

In this work we consider the following scoring rules [4]:
- \(S_{\text{MSPE}}(P, z) = (1 - \text{MSPE}) = 1 - \frac{\text{MSPE}}{\text{MSPE}_{\text{best}}},\)
- \(S_{\text{CRPS}}(P, z) = (1 - \text{CRPS}) = 1 - \frac{\text{CRPS}}{\text{CRPS}_{\text{best}}},\)
- \(S_{\text{MSE}-\text{LOO}}(P, z) = (1 - \text{MSE}) = 1 - \frac{\text{MSE}}{\text{MSE}_{\text{best}}},\)
- \(S_{\text{LOO-CRPS}}(P, z) = (1 - \text{LOO-CRPS}) = 1 - \frac{\text{LOO-CRPS}}{\text{LOO-CRPS}_{\text{best}}},\)
- \(S_{\text{LOO-MSPE}}(P, z) = (1 - \text{LOO-MSPE}) = 1 - \frac{\text{LOO-MSPE}}{\text{LOO-MSPE}_{\text{best}}},\)
- \(S_{\text{LOO-NLPD}}(P, z) = (1 - \text{LOO-NLPD}) = 1 - \frac{\text{LOO-NLPD}}{\text{LOO-NLPD}_{\text{best}}},\)
- \(S_{\text{LOO-BOR}}(P, z) = (1 - \text{LOO-BOR}) = 1 - \frac{\text{LOO-BOR}}{\text{LOO-BOR}_{\text{best}}},\)

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 \(K_0\) with the data.
- Can also be seen as a similarity between \(K_0\) and the covariance matrix obtained from the kernel \((x, y) \rightarrow f(x)(y)\).

5 Numerical study

We use a set of 36 problems:
- Goldstein-Price \((d \in \{1, 2\})\)
- Mystery \((d = 2)\)
- Time 829 \((k \in \{0, 1, 2\}, d \in \{2, 5\})\)
- Rotated Rosenbrock \((d \in \{2, 5\})\)
- Borobocho \((d = 8)\)

with space-filling designs \(X_0\) with \{1std, 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 \(\nu\) of a Matérn covariance function, by setting \(\nu \in \{0, 1, 2, 3, 4, 6, 2d, d + \infty\}\) or automatically selecting its value using the selection criteria.
- We present averaged results through repetitions (using random \(X_0\) for instance).

An example

- Procedure ML, LOO-MSPE, LOO-NLPD and LOO-CRPS give similar accuracies.
- The influence of \(\nu\) on the accuracy is strong.

Influence of the set of selection criteria

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

<table>
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<th>MSPE</th>
<th>ML</th>
<th>LOO-MSPE</th>
<th>LOO-NLPD</th>
<th>LOO-CRPS</th>
<th>GA</th>
<th>GCV</th>
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<td>2.00</td>
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<td>1.00</td>
<td>0.74</td>
</tr>
</tbody>
</table>

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

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

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

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

References


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