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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 with the lowest expected log marginal likelihood, or equivalently, minimal $\frac{1}{2} K_{\theta}^{-1} + \log(\det(K_{\theta}))$,

    \[ L(\theta) = \frac{1}{2} \sum_{i=1}^{n} \log(N(\mathbf{y}_i, \mathbf{K}_{\theta}^{-1})), \]

    where $K_{\theta}$ is the covariance matrix of $\mathbf{Y}$ at points $X = (x_1, \ldots, x_d)$ for parameters $\theta$ and $x = (x_1, \ldots, x_d) \mathbf{I}^T$ denotes the values of $f$ at $X$.

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 $S: \mathcal{P} \times \mathbb{R} \rightarrow \mathbb{R}$ where $\mathcal{P}$ is a class of probability distributions, with $S(P, x)$ representing a loss for observing $x$ while predicting $P$.

- Given a scoring rule $S$ the corresponding LOO criterion is

    \[ L_{\text{LOO}}(\theta) = \frac{1}{2} \sum_{i=1}^{n} S(N(\mathbf{y}_i, \mathbf{K}_{\theta}^{-1})), x_i), \]

    where $N(\mathbf{y}_i, \mathbf{K}_{\theta}^{-1})$ denotes LOO predictive distributions.

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 $k(x, y) \rightarrow f(x)(y)$

5 Numerical study

We use a set of 36 problems:

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

- Mystery ($d = 2$)

- 94-dimensional Rosenbrock and 504-dimensional polynomials in $d = 5$.

- 500-dimensional polynomial, 1000-dimensional polynomial, 1500-dimensional polynomials.

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].

References


