Mixture of robust Gaussian processes and its hard-cut EM algorithm with variational bounding approximation

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On the other hand, the Robust Gaussian processes (RGPs) [7–9] have been suggested to overcome the second problem. In conventional Gaussian processes, the noises are assumed to be also Gaussian. Under this assumption, the latent function can be integrated out analytically, and the marginal likelihood can be calculated explicitly. However, Gaussian distribution is not heavy-tailed, which means it is sensitive to outliers. In [8,9], student-t distribution or Laplace distribution is utilized to model the noise so that

the modified Gaussian process becomes robust. However, this robust Gaussian process becomes much more complicated than the conventional Gaussian process because its exact solving process of the parameters via Maximum likelihood (ML) is intractable. Therefore, certain approximate mechanisms should be adopted into the ML learning of the parameters such as Expectation Propagation (EP) [10], Laplace approximation [11], Variational Bayesian (VB) [12] and so on.

In practical applications, it is common that the data source is non-stationary, while there exist outliers at the same time, due to technical reasons or some factors beyond our control. Thus it is vital to develop a regression model that is not only able to model non-stationary data but also robust to outliers. In this paper, by combining the ideas of MGP and RGP together, we propose a novel model: Mixture of Robust Gaussian Processes (MRGP), which inherits the advantages of both MGP and RGP to solve the multi-model data and outlier-sensitive problems. Moreover, we design a hard-cut EM algorithm with variational bounding approximation for the parameter learning of MRGP. It is demonstrated by the experimental results on both synthetic and real-world datasets that our proposed MRGP model with the hard-cut EM algorithm is much more effective and robust than the competitive nonlinear regression models.

The contributions of this paper are summarized as follows:

- We establish a model that is both robust to outliers and able to model non-stationary data, which overcomes the problems of traditional Gaussian processes simultaneously.
- We develop an effective learning algorithm for the proposed model based on the variational bounding technique.
- We conduct extensive experiments on various datasets to compare common non-linear regression techniques in the presence of outliers.

The rest of this paper is organized as follows. In Section 2, we review related works on MGP, approximate inference in the training of GP, as well as the robust modeling. Then we introduce the GP and MGP models in Section 3. The MRGP model and its hard-cut EM algorithm are presented in Section 4. We summarize the experimental results on both synthetic and real-world datasets in Section 5. Finally, we conclude this paper in Section 6.

2. Related works

2.1. Mixture of Gaussian processes and learning algorithms

The mixture of experts (ME) was originally introduced in [2] with the idea that the final prediction result is a weighted summation of the prediction results obtained by certain local experts, and their weights are calculated by a gating function adaptively. Actually, this kind of ME architecture is discriminative, as shown in the left panel of Fig. 3. Tresp [4] adopted the idea of ME to the case of Gaussian processes and further introduced the mixture of Gaussian processes with the architecture in a similar way, as shown in the left panel of Fig. 4. The major difference between ME and MGP is that the samples of MGP are not independent but correlated, and the prediction is based on the correlation relationships between these samples. In the MGP model, both local experts and gating networks are Gaussian processes. So, we can utilize an MGP to model any general conditional probability density and address the input-dependent bandwidth problem of a stochastic process. The MGP model is further extended to the Dirichlet process based infinite mixture of Gaussian processes in [13].

From an alternative view of ME [3], the ME architecture can be fully generative and uses the posterior responsibilities from a mixture distribution as the gating network, as shown in the right panel of Fig. 3. Based on this architecture, an infinite mixture of Gaussian processes model [6] was also developed. In fact, the generative finite mixture of Gaussian processes has been investigated extensively in recent years [14–18], and the corresponding probabilistic graphical model is shown in Fig. 4. It is clear that the MGP model is generative in the sense that for each sample x_i, we assume there is a latent variable z_i such that (x_i, y_i) is generated from the z_i-th component.

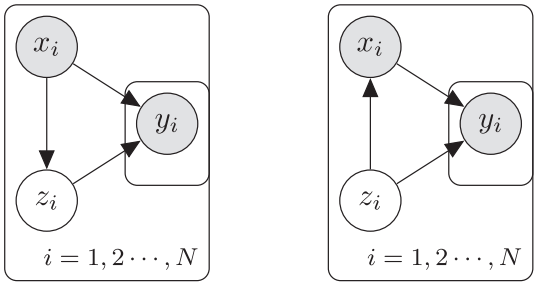


Fig. 3. Illustrations of two mixture of experts architectures. Here, x_i denotes i-th input, y_i denotes i-th output, and the latent variable z_i represents the expert index corresponding to i-th observation. **Left**: the discriminative mixture of experts model. **Right**: the generative mixture of experts model.

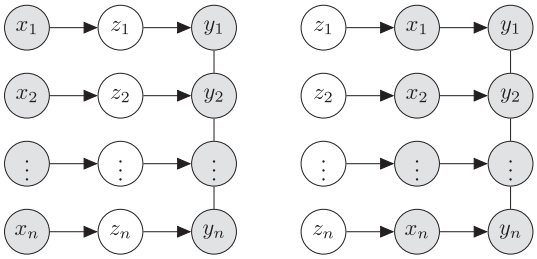


Fig. 4. Illustrations of two kinds of mixture of Gaussian processes. Note that the outputs $y_1, y_2, \cdots, y_n$ are no longer independent. Here, x_i denotes i-th input, y_i denotes i-th output, and the latent variable z_i represents the expert index corresponding to i-th sample. Note that the samples are not identically independently distributed in these models. **Left**: the discriminative mixture of Gaussian processes. **Right**: the generative mixture of Gaussian processes.

To date, there are three major approaches to parameter learning of the mixture model: EM algorithm [19,20], variational Bayesian inference [21], and MCMC [22]. As a stochastic simulation method, MCMC, or more precisely Gibbs sampling method [23] has been successfully applied in MGP [13,6]. However, its time consumption can be prohibitively large if you want to achieve accurate results on a large dataset. Variational Bayesian inference is efficient, but the conditional independent assumption sometimes leads to unsatisfactory results. Nevertheless, variational Bayesian inference has already been employed for the parameter learning of MGP [24,25]. The EM algorithm is a general framework for parameter estimation from incomplete data, which is both effective and efficient. When we use the EM algorithm to estimate the parameters of MGP, the main challenge is that there are exponentially many summations in the Q-function because the samples are not independent. To overcome this difficulty, several approximate EM methods have been proposed [14,26,15]. Certainly, it is a good way to combine these three methods to design new learning algorithms. For example, an MCMC-EM algorithm was already proposed to approximate the Q-function via MCMC sampling [17,18]. Moreover, the MCMC-EM algorithm can be extended to more general models such as the two-layer mixture of Gaussian processes [27] for functional data analysis.

2.2. Robust modeling and heavy-tailed distributions

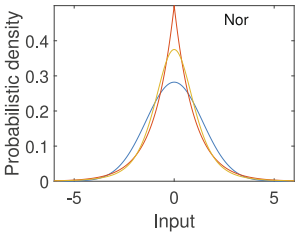
In regression analysis, there are probably outliers among the observations. Since they deviate far away from the normal observations or samples, they may influence the parameter learning as well as the prediction result strongly. As well-known, the common least square based methods are sensitive to outliers, and thus it is urgent to develop robust regression methods for outliers.

In fact, robust regression models have been investigated extensively, and one popular approach to robust modeling with outliers is to assume heavy-tailed distributions for the noises. In probability theory, heavy-tailed distributions are probability distributions whose tails are not exponentially attenuated. Intuitively, a distribution whose probabilistic density function has a heavier tail than the exponential distribution is heavy-tailed. According to this definition, student-t is heavy-tailed. Although Laplace distribution is not so heavy-tailed, it has a much heavier tail than Gaussian distribution. Actually, it has been used as the distribution of the noise in the least absolute deviation regression [28]. Moreover, student-t distribution and skew-t distribution have been adopted in the mixture-distribution models to enhance the robustness [29–31]. In Fig. 5, we sketch the probabilistic density functions of Gaussian distribution, Laplace distribution and student-t distribution with mean 0 and variance 2.

In conventional Gaussian process analysis, the noise assumption of Gaussian distribution makes it tractable to get the exact ML solutions of the parameters, but the resulted model is very sensitive to outliers. As the noise assumption of heavy-tail distributions can make the model robust to outliers, Laplace distribution and student-t distribution have been adopted into the model of the Gaussian process to obtain a robust regression model [32,8,9]. However, none of these works extends such a robust modeling approach to the MGP model for the regression analysis of multi-modal or non-stationary temporal data.

2.3. Likelihood approximation methods in Gaussian processes

When the noises are assumed to be heavy-tail distributions, it is intractable to get the exact solutions of the parameters by maximizing the likelihood of the regression model on a given dataset. Therefore, we have to approximate the likelihood to make it tractable for finding the ML solution of the parameters as well as the corresponding inference. A comprehensive overview of approximate likelihood inference for Gaussian processes is summarized in [33]. Laplace likelihood approximation can be made with a second-order Taylor expansion of the posterior probability distribution around the posterior mode to construct a Gaussian approximation. Expectation propagation [10] can approximate each likelihood term with an un-normalized Gaussian, and iteratively update the parameters to match marginal moments. In [8], EP is employed to estimate the parameters in robust Gaussian processes with a student-t likelihood. KL-divergence minimization method can approximate the posterior by a Gaussian $\mathcal{N}(\mathbf{h},\mathbf{A})$, and determine the mean vector and covariance matrix, $\mathbf{h}$, $\mathbf{A}$, by minimizing the reverse KL-divergence between the exact and approximate posteriors. The variational bounding method can be considered as a special case of the KL-divergence minimization method which takes a variational lower bound instead of each likelihood term. By such a variational bound approximation, the intractable integral in each marginal likelihood is converted to a convex optimization problem based on Fenchel-Legendre duality [34]. In this paper, we will apply an optimization procedure to obtain a tighter lower bound of each marginal likelihood iteratively. A double-loop algorithm for variational bounding approximation is also proposed in [35,36] to solve the optimization problem in the majorization-minimization way [37].



The approximate likelihood approaches mentioned above have their advantages under different application scenarios, and there is no generally best one. We adopt the variational bounding method in this paper because it enjoys nice theoretical properties and guaranteed convergence [35,36].

2.4. Recent advances in Gaussian processes

Recently, Deep Gaussian processes (DGP) [38–40] has been an active topic in Gaussian process community. DGP can be seen as a deep extension of the Gaussian Processes Latent Variable Model (GP-LVM) [41]. Originally, GP-LVM was developed as a non-linear dimensional reduction technique. DGP is a generative model aiming at modeling high-dimensional data. This manuscript concerns the nonlinear regression problem, which is supervised, while dimensional-reduction and generative models are unsupervised.

Warped Gaussian processes (WGP) [42] attempts to model non-Gaussian processes by mapping the observations into a latent space. Compared with MGP model, this method resolves the problem that traditional GPs cannot model non-stationary data in a different way. Besides, robustness has not been taken into consideration in WGPs.

Various variational techniques have been developed for learning Gaussian processes in recent years, such as [43–46]. These techniques mainly target at making Gaussian processes scalable on large datasets. Scalability of Gaussian processes is also an important topic, which has also been discussed thoroughly in [47,48]. However, in this manuscript we concern about the robustness and non-stationarity.

3. Gaussian processes and mixture of Gaussian processes

3.1. Gaussian processes

The Gaussian process is one of the dominant models in non-parametric statistics for temporal data regression and classification. Recently, it has been adopted into the field of machine learning and applied widely for the learning and analysis of time series since Gaussian distributions involved in the process can be easily analyzed and processed. Mathematically, the Gaussian process model is defined as follows.

Suppose that there is a dataset $\mathcal{D}=\{(x_i,y_i)\}_{i=1}^N$ and we let $\mathbf{x}=[x_1,x_2,\cdots,x_N]^{\mathrm{T}}$, $\mathbf{y}=[y_1,y_2,\cdots,y_N]^{\mathrm{T}}$ for brevity. We say $\mathbf{y}$ is a Gaussian process with input $\mathbf{x}$ if they are linked by an underlying function f:

$$y_i=f(x_i)+\varepsilon_i,\ \forall i=1,2,\cdots,N,$$

where $f(x_i)$ is always subject to a Gaussian distribution and $\{\varepsilon_i\}_{i=1}^N$ are independent noises. Let $\mathbf{f}=[f(x_1),f(x_2),\cdots,f(x_N)]^{\mathrm{T}}$, the definition of Gaussian process is equivalent to say $\mathbf{f}|\mathbf{x}$ is a multivariate Gaussian random vector, *i.e.*, $\mathbf{f}|\mathbf{x}\sim\mathcal{N}(\boldsymbol{\mu},\mathbf{C})$. Usually, the mean $\boldsymbol{\mu}$ is

assumed to be zero for simplicity, while the covariance $\mathbf{C}$ is determined by $\mathbf{x}$. Given a covariance function $c(\cdot,\cdot;\boldsymbol{\theta})$ parameterized by $\boldsymbol{\theta}$, then $\mathbf{C}_{ij} = c(x_i, x_j; \boldsymbol{\theta})$.

and then get the final prediction result by

$$\hat{y} = \sum_{k=1}^{K} p(z_* = k)\hat{y}^{(k)},$$

where $\hat{y}^{(k)}$ is assumed to be the prediction result of the k-th Gaussian process at x_* given by Eq. (1).

4. The proposed mixture of robust Gaussian processes

4.1. Model formulation

Although the mixture of Gaussian processes is quite effective to model non-stationary temporal data which has a multi-model structure, it is still sensitive to outlier and thus not so robust in practical applications. In order to overcome this problem, we propose a mixture of robust Gaussian processes in which the noises of each component Gaussian process are assumed to be heavy-tail distributions instead of Gaussian ones. Here, we mainly consider Laplace noise and student-t noise. For a Laplace noise, the corresponding likelihood term takes the following form:

$$p(y_i|f_i;\gamma) = \frac{1}{2\gamma}\exp\left(-\frac{|y_i - f_i|}{\gamma}\right).$$

where γ is the dispersion parameter. For a student-t noise, the likelihood term is given by

$$p(y_i|f_i;\gamma) = \frac{\Gamma(\frac{\gamma+1}{2})}{\Gamma(\frac{\gamma}{2})}\frac{1}{\sqrt{\gamma\pi}}\left(1 + \frac{(y_i - f_i)^2}{\gamma}\right)^{-\frac{\gamma+1}{2}},$$

where $\Gamma(\cdot)$ is the Gamma function and γ is now the degree of freedom. The mixture of robust Gaussian processes can be defined in the same way as the mixture of Gaussian processes in Section 3.2 except that the probability density function of each noise is that of Laplace or student-t. Although the formal modification seems minor, it makes the analysis far more challenging because $\mathbf{y}_k|\mathbf{x}_k$ is no longer Gaussian. In fact, the marginal likelihood of the k-th component Gaussian process, i.e., the conditional probability of $\mathbf{y}_k$ with respect to $\mathbf{x}_k$, is

$$p(\mathbf{y}_k|\mathbf{x}_k;\theta_k,\gamma_k) = \int p(\mathbf{y}_k|\mathbf{f}_k;\gamma_k)p(\mathbf{f}_k|\mathbf{x}_k;\theta_k)\mathrm{d}\mathbf{f}_k. \tag{3}$$

The main difficulty arises from the intractable integral in $p(\mathbf{y}_k|\mathbf{x}_k;\theta_k,\gamma_k)$. On one hand, in the M-step, the updating of $\{\theta_k,\gamma_k\}$ becomes difficult because $p(\mathbf{y}_k|\mathbf{x}_k;\theta_k,\gamma_k)$ does not have a closed-form expression. On the other hand, in the E-step, the allocation of z_i involves the calculation of $p(\mathbf{y}_i|x_i,\theta_k,\gamma_k)$ that is also intractable. Instead of calculating the marginal likelihood explicitly, we employ a variational bounding method to calculate the marginal likelihood approximately. Moreover, we need the posterior $\mathbf{f}_k$ of each component Gaussian process in the prediction stage. Since the noises are non-Gaussian, $[\mathbf{y}_k;f_*]$ is not Gaussian but $[\mathbf{f}_k;f_*]$ is still Gaussian and we can predict f_* by conditioning on $\mathbf{f}_k$. As we will see, this approximate marginal likelihood can lead to an approximate posterior at the same time.

4.2. Variational approximation of marginal likelihood

For ease of notation, we omit the subscript k in marginal likelihood and consider one single Gaussian process temporarily, since we learn each Gaussian process expert separately in the M-step. The variational bounding method introduced here has been used in large scale linear models [35], image processing [36] and Gaussian processes [50], but there are no complete derivations for the case of robust Gaussian processes to the best of our knowledge. For completeness, we give the strict derivations of the variational bounding approximation results for the marginal likelihood of robust Gaussian processes in detail, which are summarized in the following theorem.

Theorem 1. *Let $t(s;\gamma)$ be a super-Gaussian probabilistic density function centered at $0, g(x) = \log t(\sqrt{x})$ and $h(\lambda) = 2g^*(-1/(2\lambda))$ where g^* is the Fenchel-Legendre dual function of g. Furthermore, let*

$$\boldsymbol{\lambda} = \begin{bmatrix}\lambda_1\\ \lambda_2,\\ \vdots\\ \lambda_n\end{bmatrix},\ \boldsymbol{\Lambda} = \begin{bmatrix}\lambda_1 & 0 & \cdots & 0\\ 0 & \lambda_2 & \cdots & 0\\ \vdots & \vdots & \ddots & \vdots\\ 0 & 0 & \cdots & \lambda_n\end{bmatrix},\ h(\boldsymbol{\lambda}) = \sum_{i=1}^{n} h(\lambda_i),$$

we have the following theoretical results:

(a) *The marginal likelihood $p(\mathbf{y}|\mathbf{x};\theta,\gamma)$ takes the following variational form*

$$\begin{aligned} p(\mathbf{y}|\mathbf{x};\theta,\gamma) &= |\mathbf{C}|^{-1/2}\exp\left(-\tfrac{1}{2}\min_{\boldsymbol{\lambda}\geq 0,\mathbf{f}}\varphi(\boldsymbol{\lambda},\mathbf{f})\right),\\ \varphi(\boldsymbol{\lambda},\mathbf{f}) &= h(\boldsymbol{\lambda}) + \log|\mathbf{A}| + (\mathbf{y}-\mathbf{f})^{\mathrm{T}}\boldsymbol{\Lambda}^{-1}(\mathbf{y}-\mathbf{f}) + \mathbf{f}\mathbf{C}^{-1}\mathbf{f}. \end{aligned}$$

(b) *Given $\mathbf{v} = \nabla_{\lambda^{-1}}\log|\mathbf{A}| = \mathrm{diag}((\mathbf{C}^{-1}+\boldsymbol{\Lambda}^{-1})^{-1})$,*

$$\phi_{\mathbf{v}}(\boldsymbol{\lambda},\mathbf{f}) = \sum_{i=1}^{n}\frac{v_i + (y_i - f_i)^2}{\lambda_i} + h(\lambda_i) + \mathbf{f}\mathbf{C}^{-1}\mathbf{f} - g_1^*(\mathbf{v})$$

is an upper bound for $\varphi(\boldsymbol{\lambda},\mathbf{f})$.

(c) *$\phi_{\mathbf{v}}(\boldsymbol{\lambda},\mathbf{f})$ can be further optimized by the alternative minimization of $\boldsymbol{\lambda}$ and $\mathbf{f}$): the minimum of $\boldsymbol{\lambda}$ is $\lambda_i = -(2g\prime(v_i + (y_i - f_i)^2))^{-1}$ when $\mathbf{f}$ is fixed, while the minimum of $\mathbf{f}$ can be obtained by the gradient descent algorithm when $\boldsymbol{\lambda}$ is fixed.*

Proof. We prove the three results one by one. Since $t(s;\gamma)$ is a super-Gaussian [34] probabilistic density function (for example, Laplace distribution or Student-t distribution) centered at $0, \log t(s;\gamma)$ is symmetric and monotone decreasing with respect to s. Furthermore, $\sqrt{s} \to \log t(s;\gamma)$ is convex whenever $s \geqslant 0$, so $g(x) = \log t(\sqrt{x})$ is convex and monotone decreasing. According to Fenchel-Legendre duality, we have

$$g(x) = \sup_{w}(xw - g^*(w)),$$

where $g^*(w) = \sup_{x\geqslant 0}(xw - g(x))$ is the dual function of $g(x)$. Because $g(x)$ is decreasing, the domain of $g^*(w)$ must be $\mathbf{bR}_-$. Therefore, it is equivalent to have

$$g(x) = \sup_{w\leqslant 0}(xw - g^*(w)) = \sup_{w\geqslant 0}(-xw - g^*(-w)).$$

By taking $\lambda = 1/(2w), h(\lambda) = 2g^*(-1/(2\lambda))$, we have

$$\begin{aligned}\log t(s;\gamma) = g(s^2) &= \sup_{w\geqslant 0}\left(-\frac{s^2}{2\lambda} - g^*(-\frac{1}{2\lambda})\right)\\ &= \sup_{\lambda\geqslant 0}\left(-\frac{s^2}{2\lambda} - \frac{1}{2}h(\lambda)\right).\end{aligned} \tag{4}$$

Since $p(\mathbf{y}|\mathbf{f};\gamma) = \prod_{i=1}^{n}p(y_i|f_i;\gamma)$ is decomposable with respect to individual observations, we can consider each individual term separately. Putting $p(y_i|f_i;\gamma) = p(f_i - y_i|0;\gamma) = t(f_i - y_i)$ into Eq. (4), we obtain a variational representation of $\log p(y_i|f_i;\gamma)$ as follows:

$$\log p(y_i|f_i;\gamma) = \sup_{\lambda_i\geqslant 0}\left(-\frac{(y_i - f_i)^2}{2\lambda_i} - \frac{1}{2}h(\lambda_i)\right).$$

Consequently, we have

$$\log p(\mathbf{y}|\mathbf{f};\gamma) = \sup_{\boldsymbol{\lambda}\geqslant 0}\left(-\frac{1}{2}(\mathbf{y}-\mathbf{f})^{\mathrm{T}}\boldsymbol{\Lambda}^{-1}(\mathbf{y}-\mathbf{f}) - \frac{1}{2}h(\boldsymbol{\lambda})\right).$$

With this representation, we further have $p(\mathbf{y}|\mathbf{x};\boldsymbol{\theta},\gamma)$:

$$\begin{aligned} p(\mathbf{y}|\mathbf{x};\boldsymbol{\theta},\gamma) &= \int p(\mathbf{y}|\mathbf{f};\gamma)p(\mathbf{f}|\mathbf{x};\boldsymbol{\theta})\mathrm{d}\mathbf{f} \\ &= \int \exp\left(\log p(\mathbf{y}|\mathbf{f};\gamma)\right)\mathcal{N}(\mathbf{f}|0,\mathbf{C})\mathrm{d}\mathbf{f} \\ &= \max_{\boldsymbol{\lambda}\geqslant 0}\exp\left(-\tfrac{1}{2}h(\boldsymbol{\lambda})\right)\int \exp\left(-\tfrac{1}{2}(\mathbf{y}-\mathbf{f})\boldsymbol{\Lambda}^{-1}(\mathbf{y}-\mathbf{f})\right)\mathcal{N}(\mathbf{f}|0,\mathbf{C})\mathrm{d}\mathbf{f}. \end{aligned} \tag{5}$$

The term inside the integral is actually a lower bound of the posterior of $\mathbf{f}$. By completing the squares, we can find out that the approximate posterior of $\mathbf{f}$ given observations $\mathbf{x},\mathbf{y}$ and parameter $\boldsymbol{\lambda}$ is Gaussian $\mathcal{N}(\mathbf{h},\mathbf{A}^{-1})$ where

$$\mathbf{A} = \boldsymbol{\Lambda}^{-1} + \mathbf{C}^{-1}, \mathbf{h} = \mathbf{A}^{-1}\boldsymbol{\Lambda}^{-1}\mathbf{y}. \tag{6}$$

The integral in Eq. (5) can be calculated explicitly, but we seek a variational form for further purpose. Given $\mathbf{h}$ and $\mathbf{A}$ defined above, we have

$$\begin{aligned} &\frac{\exp\left(-\frac{1}{2}(\mathbf{y}-\mathbf{f})\boldsymbol{\Lambda}^{-1}(\mathbf{y}-\mathbf{f})\right)\mathcal{N}(\mathbf{f}|0,\mathbf{C})}{\int \exp\left(-\frac{1}{2}(\mathbf{y}-\mathbf{f})\boldsymbol{\Lambda}^{-1}(\mathbf{y}-\mathbf{f})\right)\mathcal{N}(\mathbf{f}|0,\mathbf{C})\mathrm{d}\mathbf{f}} \\ &= \frac{|\mathbf{A}|^{1/2}}{(2\pi)^{n/2}}\exp\left(-\frac{1}{2}(\mathbf{f}-\mathbf{h})^{\mathrm{T}}\mathbf{A}(\mathbf{f}-\mathbf{h})\right). \end{aligned}$$

Taking maximum with respect to $\mathbf{f}$, we further have

$$\begin{aligned} &\int \exp\left(-\tfrac{1}{2}(\mathbf{y}-\mathbf{f})\boldsymbol{\Lambda}^{-1}(\mathbf{y}-\mathbf{f})\right)\mathcal{N}(\mathbf{f}|0,\mathbf{C})\mathrm{d}\mathbf{f} \\ &= \tfrac{(2\pi)^{n/2}}{|\mathbf{A}|^{1/2}}\max_{\mathbf{f}}\exp\left(-\tfrac{1}{2}(\mathbf{y}-\mathbf{f})\boldsymbol{\Lambda}^{-1}(\mathbf{y}-\mathbf{f})\right)\mathcal{N}(\mathbf{f}|0,\mathbf{C}) \\ &= \tfrac{1}{|\mathbf{AC}|^{1/2}}\max_{\mathbf{f}}\exp\left(-\tfrac{1}{2}(\mathbf{y}-\mathbf{f})\boldsymbol{\Lambda}^{-1}(\mathbf{y}-\mathbf{f}) - \tfrac{1}{2}\mathbf{f}^{\mathrm{T}}\mathbf{C}^{-1}\mathbf{f}\right). \end{aligned} \tag{7}$$

By combining Eq. (5) and (7), we can rewrite $p(\mathbf{y}|\mathbf{x};\boldsymbol{\theta},\gamma)$ into a variational form with respect to $\mathbf{f}$ and $\boldsymbol{\lambda}$ as

$$\begin{aligned} p(\mathbf{y}|\mathbf{x};\boldsymbol{\theta},\gamma) &= |\mathbf{C}|^{-1/2}\exp\left(-\tfrac{1}{2}\min_{\boldsymbol{\lambda}\geqslant 0,\mathbf{f}}\varphi(\boldsymbol{\lambda},\mathbf{f})\right), \\ \varphi(\boldsymbol{\lambda},\mathbf{f}) &= h(\boldsymbol{\lambda}) + \log|\mathbf{A}| + (\mathbf{y}-\mathbf{f})^{\mathrm{T}}\boldsymbol{\Lambda}^{-1}(\mathbf{y}-\mathbf{f}) + \mathbf{f}\mathbf{C}^{-1}\mathbf{f}. \end{aligned}$$

This proves part (a) of Theorem 1.

It follows from (a) that the problem of calculating marginal likelihood $p(\mathbf{y}|\mathbf{x};\boldsymbol{\theta},\gamma)$ boils down to solve the optimization problem $\min_{\boldsymbol{\lambda}\geqslant 0,\mathbf{f}}\varphi(\boldsymbol{\lambda},\mathbf{f})$. The main difficulty lies in the term $\log|\mathbf{A}|$ that depends on $\boldsymbol{\lambda}$. We use a majorization-minimization method to tackle this problem. As shown in [36], let $\boldsymbol{\lambda}^{-1} = [\lambda_1^{-1},\lambda_2^{-2},\cdots,\lambda_n^{-1}]^{\mathrm{T}}$, then $\boldsymbol{\lambda}^{-1}\to -\log|\mathbf{A}|$ is a convex function. Again by Fenchel-Legendre transformation, we obtain $\log|\mathbf{A}| = \min_{\mathbf{v}\geqslant 0}\left(\mathbf{v}^{\mathrm{T}}\boldsymbol{\lambda}^{-1} - g_1^*(\mathbf{v})\right)$, where g_1^* is the dual function. For a fixed $\boldsymbol{\lambda}^{-1}$, the equality holds when

$$\mathbf{v} = \nabla_{\boldsymbol{\lambda}^{-1}}\log|\mathbf{A}| = \mathrm{diag}((\mathbf{C}^{-1}+\boldsymbol{\Lambda}^{-1})^{-1}). \tag{8}$$

For a general $\mathbf{v}\geqslant 0, \log|\mathbf{A}| \leqslant \mathbf{v}^{\mathrm{T}}\boldsymbol{\lambda}^{-1} - g_1^*(\mathbf{v})$, and we thus have

$$\begin{aligned} \phi_{\mathbf{v}}(\boldsymbol{\lambda},\mathbf{f}) &= \mathbf{v}^{\mathrm{T}}\boldsymbol{\lambda}^{-1} - g_1^*(\mathbf{v}) + h(\boldsymbol{\lambda}) + (\mathbf{y}-\mathbf{f})^{\mathrm{T}}\boldsymbol{\Lambda}^{-1}(\mathbf{y}-\mathbf{f}) + \mathbf{f}\mathbf{C}^{-1}\mathbf{f} \\ &= \sum_{i=1}^{n}\tfrac{v_i+(y_i-f_i)^2}{\lambda_i} + h(\lambda_i) + \mathbf{f}\mathbf{C}^{-1}\mathbf{f} - g_1^*(\mathbf{v}), \end{aligned}$$

which is an upper bound of $\varphi(\boldsymbol{\lambda},\mathbf{f})$. This proves part (b) of Theorem 1.

We further employ the double loop optimization method to optimize $\varphi(\boldsymbol{\lambda},\mathbf{f})$, *i.e.*, to get a tighter bound instead. In the inner loop, we minimize the upper bound $\varphi_{\mathbf{v}}(\boldsymbol{\lambda},\mathbf{f})$ given $\mathbf{v}$. While in the outer loop, we update current $\mathbf{v}$ to achieve tighter bounds. In the inner loop there are two variables, and we solve this optimization problem with the two variables alternatively. For the $\boldsymbol{\lambda}$ part, according to the definition of $h(\lambda_i)$, it is easy to get

$$\begin{aligned} \min_{\lambda_i\geqslant 0}\tfrac{v_i+(y_i-f_i)^2}{\lambda_i} + h(\lambda_i) &= \min_{\lambda_i\geqslant 0}\left(2\tfrac{v_i+(y_i-f_i)^2}{2\lambda_i} + 2g^*\left(-\tfrac{1}{2\lambda_i}\right)\right) \\ &= -2\max_{\lambda_i\geqslant 0}\left(-\tfrac{v_i+(y_i-f_i)^2}{2\lambda_i} - g^*(-2\lambda_i)\right) \\ &= -2g(v_i+(y_i-f_i)^2) = -2\log t\left(\sqrt{v_i+(y_i-f_i)^2}\right) \\ &= -2\log p\left(y_i|\sqrt{v_i+(y_i-f_i)^2}+y_i;\gamma\right). \end{aligned}$$

At first glance, this result is a little surprising since we do not need to know the explicit form of h. By the optimal condition, when f_i is fixed, the optimal value is obtain when $\lambda_i = -(2g'(v_i+(y_i-f_i)^2))^{-1}$. After updating $\boldsymbol{\lambda}$, the objective function becomes

$$\mathbf{f}^{\mathrm{T}}\mathbf{C}^{-1}\mathbf{f} - 2\sum_{i=1}^{n}\log p\left(y_i|\sqrt{v_i+(y_i-f_i)^2}+y_i;\gamma\right),$$

which can be easily solved using the gradient descent algorithm. This process is very similar to finding the posterior mode of $\mathbf{f}$, the only difference here is the likelihood term is smoothed by $\mathbf{v}$.

To calculate approximate marginal likelihood $p(\mathbf{y}|\mathbf{x};\boldsymbol{\theta},\gamma)$ according to Theorem 1 in practice, we begin to iteratively update $\boldsymbol{\lambda}$ and $\mathbf{f}$ in the inner loop until convergence. Then, we turn to the outer loop and update $\mathbf{v}$ according to Eq. (8) to get a new upper bound for $\varphi(\boldsymbol{\lambda},\mathbf{f})$. The entire optimization process is guaranteed to converge due to the convexity [35,36]. After the process has converged, we also obtain an approximation for the posterior of $\mathbf{f}$ given $\mathbf{y}$ as indicated in Eq. (6). The approximate marginal likelihood in Theorem 1 involves optimization procedure and has no explicit formula, so it is still intractable to calculate gradients with respect to $\boldsymbol{\theta}$ and γ. However, part (c) of Theorem 1 gives an $\mathbf{f}$, which is an estimation of latent function values without noises. Therefore we can approximate the gradients by taking derivates of the surrogate log-likelihood:

$$-\frac{1}{2}\log|\mathbf{C}| - \frac{1}{2}\mathbf{f}^{\mathrm{T}}\mathbf{C}^{-1}\mathbf{f} + \sum_{i=1}^{n}\log t(y_i-f_i;\gamma).$$

4.3. The hard-cut EM algorithm

We further establish the hard-cut EM algorithm for mixtures of

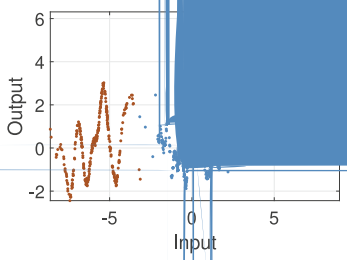
given in Section 4.2 in the EM algorithm. With the hard-cut version of $\mathbf{z}$, let $\mathscr{I}_k = \{i|z_i = k\}$, then the Q-function is given by

$$Q(\boldsymbol{\Theta}) = \sum_{k=1}^{K}\sum_{i\in\mathscr{I}_k}(\log\pi_k + \log p(x_i;\mu_k,\sigma_k)) + \sum_{k=1}^{K}\log p(\mathbf{y}_k|\mathbf{x}_k;\boldsymbol{\theta}_k,\gamma_k).$$

The M-step aims to maximize $Q(\boldsymbol{\Theta})$ with respect to all the parameters. For $\{\pi_k, \mu_k,$

Table 1
Parameters of basic datasets $\mathscr{S}_1$.

Dataset	π_k	μ_k	σ_k^2	$\boldsymbol{\theta}_k$
$\mathscr{S}_1$	/3	−6	1.5	[2.00, 3.33, 0.10]
		0	1.5	[0.75, 10.00, 0.10]
		6	1.5	[1.50, 1.25, 0.10]
$\mathscr{S}_7$		−12	1.5	[2.00, 3.33, 0.10]
		−6	1.5	[0.75, 10.00, 0.10]
		0	1.5	[1.50, 1.25, 0.10]
		6	1.5	[0.50, 2.50, 0.10]
		12	1.5	[1.50, 5.00, 0.10]



(f) FNN: Feedforward neural network with three hidden layers containing 10, 10, 5 units, respectively.

For the fairest, we adopt the "two-stage" versions of GP, MGP, SVM, and FNN. That is, we firstly use a common outlier detection method to remove possible outliers from the training set, and then perform the corresponding algorithms on the improved training set.

Our proposed methods are the MRGP models with Laplace noises and Student-t noises through the parameter learning of the hard-cut EM algorithm, being referred to as MRGP (Laplace) and MRGP (Student-t), respectively. For all the MGP methods, the number of Gaussian processes is set to be the number of actual Gaussian processes in the dataset, *i.e.*, 3 for $\mathscr{S}_1 - \mathscr{S}_6$ and 5 for $\mathscr{S}_7 - \mathscr{S}_{12}$. The implementation is based on the GPML toolbox [50], and all experiments are conducted on a personal computer [Intel(R) Core(TM) i7-6700HQ CPU 2.60 GHz, 8G RAM].

We begin to fix outlier level v to be 2, and vary outlier ratio in $\{0.05, 0.10, 0.15\}$. For each dataset, we add outliers to the training set with low, medium and high ratios, then we test the prediction performances of all the methods. The performance is measured by Rooted Mean Square Error (RMSE), which is defined as

$$\text{RMSE} = \sqrt{\frac{1}{M}\sum_{j=1}^{M}(\hat{y}_j - \tilde{y}_j)^2},$$

where M is the size of test set, $\{\tilde{y}_j\}_{j=1}^{M}$ are ground-truth values, while $\{\hat{y}_j\}_{j=1}^{M}$ are the predicted results. Since the final results of the algorithms depend on the initializations of $\{z_i\}_{i=1}^{N}$ and $\{\boldsymbol{\theta}_k, \gamma_k\}_{k=1}^{K}$, different runs may lead to different results due to randomness. Therefore, we repeat the experiments for 10 times, and the average RMSEs of all the methods are listed in Table 2. To investigate the effect of the outlier level, we then fix the outlier ratio η to be 0.10, and vary outlier level v in $\{1.5, 2.5\}$. The average RMSEs of all the methods in this situation are listed in Table 3.

From these two tables, we have the following significant observations. First, all the robust models obtain better results than conventional Gaussian process based models, which demonstrates that Laplace or Student-t noises improve the robustness of the regression model. Second, two-stage methods usually achieve lower RMSEs in comparison with the original methods, but in certain cases, the process of removing outliers makes the results worse. One possible explanation is that it is very difficult to identify which samples are outliers, and thus the outlier detection algorithm is likely to falsely remove non-outliers or fail to identify outliers. Third, the adoption of a mixture structure usually improves the performance of the regression model because MGP is more flexible than GP. However, GP outperforms MGP occasionally, the reason is that in the learning process, each component has fewer samples and it is more easily to be affected by extreme out-

Table 2
The average RMSEs of our MRGP and competitive regression methods on 12 synthetic datasets over 10 trials, where the outlier level v is fixed to be 2 and the outlier ratio η varies in $\{0.05, 0.10, 0.15\}$, and the best results are in bold.

Outlier ratio	Method	$\mathscr{S}_1$	$\mathscr{S}_2$	$\mathscr{S}_3$	$\mathscr{S}_4$	$\mathscr{S}_5$	$\mathscr{S}_6$	$\mathscr{S}_7$	$\mathscr{S}_8$	$\mathscr{S}_9$	$\mathscr{S}_{10}$	$\mathscr{S}_{11}$	$\mathscr{S}_{12}$
Low ($\eta = 0.05$)	GP	0.5400	0.4520	0.4493	0.5846	0.4924	0.6082	0.5362	0.7158	0.3761	0.5596	0.5992	0.6276
	GP (TS)	0.5352	0.3326	0.3664	1.1176	0.3421	0.4792	0.8739	0.4638	0.2924	0.5734	0.3223	0.4397
	SVM	0.6340	0.5723	0.6128	0.8040	0.5132	0.7262	0.6830	1.0649	0.8271	0.9303	0.9521	0.9675
	SVM (TS)	0.6192	0.7468	0.6329	0.9790	0.5597	0.9149	0.7302	1.1217	0.7871	0.9526	0.8941	1.2704
	FNN	0.7206	0.7867	0.9111	0.9280	0.8937	1.0610	0.7764	1.0618	0.8158	0.9775	0.7570	1.0105
	FNN (TS)	0.6789	0.5527	0.5610	0.8304	0.4839	0.5518	0.7351	0.8649	0.5026	0.8682	1.0765	0.4729
	RGP (Laplace)	0.2951	0.3232	0.3511	0.3196	0.3409	0.4682	0.2842	0.4228	0.2573	0.3576	0.2232	0.4124
	RGP (Student-t)	0.2673	0.3404	0.3416	0.3175	0.4300	0.4944	0.3128	0.4479	0.2231	0.3732	0.2203	0.3696
	MGP	0.4256	0.4291	0.5794	0.5251	0.3841	0.5765	0.4980	0.8658	0.3597	0.5148	0.6279	0.5949
	MGP (TS)	0.5082	0.3050	0.2618	0.9272	0.2378	0.3934	0.4747	0.4019	0.2844	0.3960	0.2344	0.3426
	MRGP (Laplace)	**0.2337**	0.3067	0.2749	0.2254	0.1983	0.3638	0.2639	0.3806	0.2259	0.2873	0.1907	**0.3180**
	MRGP (Student-t)	0.2423	**0.3042**	**0.2579**	**0.2175**	**0.1913**	**0.3521**	**0.2448**	**0.3346**	**0.1716**	**0.2839**	**0.1843**	0.3498
Medium ($\eta = 0.10$)	GP	0.7016	0.6503	0.6376	0.7378	0.5475	0.7241	0.4490	0.6233	0.4854	0.6545	0.5435	0.6198
	GP (TS)	0.3921	0.4050	0.4421	1.1092	0.9433	0.5273	0.7827	0.5054	0.3799	0.5747	0.3236	0.4574
	SVM	0.5497	0.6017	0.6469	0.7451	0.5128	0.8483	0.6839	1.0515	0.8651	0.9253	0.9332	1.2003
	SVM (TS)	0.6559	0.7621	0.6909	0.9613	0.6052	0.8823	0.7979	1.0965	0.7544	0.9060	0.9030	1.0341
	FNN	0.7998	0.8114	0.9290	1.0415	0.9035	1.0000	0.6563	1.0923	0.8244	0.9356	1.0852	1.0427
	FNN (TS)	0.5656	0.8313	0.4430	1.2403	0.6054	0.5850	0.3775	1.3183	0.8635	0.6244	0.5952	1.1725
	RGP (Laplace)	0.2706	0.3657	0.3815	0.3620	0.3551	0.4985	0.3066	0.4280	0.3028	0.4442	0.2491	0.4260
	RGP (Student-t)	0.2772	0.3483	0.3810	0.3322	0.4151	0.5076	0.3081	0.4983	0.2797	0.3729	0.2510	0.3718
	MGP	0.6027	0.6286	0.5859	0.7606	0.5319	0.6762	0.4662	0.5556	0.5236	0.7324	0.5124	0.6475
	MGP (TS)	0.3319	0.3633	0.3734	1.0008	0.4990	0.4814	0.3042	0.3754	0.3088	0.3588	0.3394	0.4319
	MRGP (Laplace)	**0.2345**	0.3318	0.2847	0.3005	0.2256	0.3876	0.2679	0.3565	0.2276	0.3295	0.2275	0.3517
	MRGP (Student-t)	0.2386	**0.3066**	**0.2487**	**0.2206**	**0.1905**	**0.3519**	**0.2557**	**0.3334**	**0.1756**	**0.2856**	**0.1816**	**0.3483**
High ($\eta = 0.15$)	GP	0.7638	0.7572	0.6772	0.5284	0.6902	0.7660	0.6386	0.9249	0.6012	0.6628	0.6867	0.7110
	GP (TS)	0.6405	0.4680	0.5191	0.9625	0.4749	0.5387	0.4655	0.5018	0.4118	0.5728	0.4870	0.5194
	SVM	0.6512	0.7286	0.6013	0.7446	0.5717	0.9725	0.6919	1.0509	0.7539	0.9679	0.9028	0.8428
	SVM (TS)	0.6774	0.5645	0.6914	1.0055	0.5044	0.7471	0.7239	1.0886	0.7939	0.9586	0.9126	1.0185
	FNN	0.7828	1.0117	1.0115	0.9070	0.8758	0.8234	0.8956	1.2199	0.7831	1.0207	1.1145	1.3124
	FNN (TS)	0.6940	0.8043	1.3943	0.9322	0.6360	0.5590	0.4354	1.0600	0.7791	0.7547	0.6825	0.7442
	RGP (Laplace)	0.4906	0.4616	0.4324	0.3582	0.5282	0.5017	0.3732	0.4730	0.3446	0.5010	0.3987	0.4406
	RGP (Student-t)	0.3534	0.3631	0.3600	0.3154	0.4480	0.5281	0.2961	0.4591	0.2516	0.3972	0.2571	0.4034
	MGP	0.8257	0.7689	0.6554	0.7423	0.6015	0.7788	0.6346	0.9758	0.6540	0.6620	0.7462	0.7363
	MGP (TS)	0.6007	0.4221	0.8251	0.8401	0.4597	0.4720	0.3438	0.4039	0.3982	0.6399	0.6649	0.4876
	MRGP (Laplace)	0.2844	0.3947	0.3573	0.3532	0.2459	0.4042	0.3034	**0.3751**	0.2480	0.4402	0.3555	**0.3943**
	MRGP (Student-t)	**0.2412**	**0.3192**	**0.2664**	**0.2130**	**0.3526**	**0.3531**	**0.2504**	0.3815	**0.1733**	**0.3892**	**0.1814**	0.4388

Table 3
The average RMSEs of our MRGP and competitive regression methods on 12 synthetic datasets over 10 trials, where the outlier level v is fixed to be 0.10 and the outlier ratio η varies in $\{1.5, 2.5\}$, and the best results are in bold.

Outlier level	Method	$\mathscr{S}_1$	$\mathscr{S}_2$	$\mathscr{S}_3$	$\mathscr{S}_4$	$\mathscr{S}_5$	$\mathscr{S}_6$	$\mathscr{S}_7$	$\mathscr{S}_8$	$\mathscr{S}_9$	$\mathscr{S}_{10}$	$\mathscr{S}_{11}$	$\mathscr{S}_{12}$
Low ($v = 1.5$)	GP	0.5815	0.9124	0.5052	0.7265	0.5381	0.6693	0.5401	0.5714	0.4223	0.5323	0.4586	0.6529
	GP (TS)	0.3554	0.4678	0.4806	1.1282	0.4302	0.9689	0.9045	0.5263	0.3263	0.5163	0.4693	0.4512
	SVM	0.5843	0.7907	0.6400	0.8825	0.5117	0.8211	0.6768	1.0485	0.8682	0.9242	0.7092	1.0971
	SVM (TS)	0.6052	0.7901	0.6600	1.0219	0.5726	0.9329	0.7735	1.0686	0.8484	0.9251	0.9031	1.2059
	FNN	0.7795	1.0624	1.0836	0.8211	0.8548	1.0864	0.8595	0.8541	0.9031	0.9287	1.0611	0.9513
	FNN (TS)	0.6085	0.6892	0.8602	0.8547	0.5002	0.6120	0.5915	1.1037	0.7963	0.9556	1.1165	0.7909
	RGP (Laplace)	0.2772	0.3752	0.3822	0.3329	0.3503	0.4865	0.3332	0.4338	0.2727	0.3532	0.2407	0.4248
	RGP (Student-t)	0.3470	0.3427	0.3780	0.3242	0.4209	0.4951	0.2969	0.4253	0.2226	0.3621	0.2427	0.3807
	MGP	0.4734	0.8827	0.5617	0.6385	0.3800	0.6549	0.4887	0.5394	0.3870	0.5980	0.4386	0.6850
	MGP (TS)	0.3577	0.4963	0.5293	1.0362	0.3679	1.1550	0.6118	0.4723	0.2817	0.4068	0.4312	0.4815
	MRGP (Laplace)	0.2454	0.3295	0.3000	0.2994	0.2096	0.3960	0.2641	0.3738	0.2011	0.3012	0.2265	0.3562
	MRGP (Student-t)	**0.2308**	**0.3069**	**0.2486**	**0.2182**	**0.1911**	**0.3568**	**0.2530**	**0.3366**	**0.1738**	**0.2889**	**0.1766**	**0.3521**
High ($v = 2.5$)	GP	0.8333	0.8952	0.6695	0.9217	0.7114	0.8344	0.6561	0.9250	0.5149	0.7747	0.6471	0.7967
	GP (TS)	0.3935	0.3776	0.4518	1.1000	0.3655	0.6355	0.8009	0.4960	0.3593	0.6713	0.3841	0.5105
	SVM	0.5737	0.6755	0.6331	0.8132	0.5771	0.7490	0.6864	1.0585	0.8207	0.8996	0.8179	1.1225
	SVM (TS)	0.5372	0.7552	0.5887	0.9769	0.5172	0.9883	0.8181	1.1089	0.8510	0.9610	0.8921	1.0987
	FNN	1.3731	0.8585	1.0517	1.0505	0.9015	2.8179	0.7714	1.2513	0.8520	0.8899	0.9924	1.2133
	FNN (TS)	0.5754	0.8092	1.0313	1.0387	0.5670	0.7117	0.6830	1.0960	0.8531	0.6736	1.1491	0.8296
	RGP (Laplace)	0.2702	0.3658	0.3746	0.4047	0.5446	0.4743	0.3438	0.4437	0.3086	0.4154	0.2936	0.4544
	RGP (Student-t)	0.3427	0.3486	0.4267	0.3153	0.2953	0.5094	0.2962	0.4442	0.2380	0.3867	0.2554	0.4213
	MGP	0.7807	0.9288	0.7934	0.9149	0.7557	0.8304	0.6083	1.1960	0.7060	0.8164	0.7260	0.6668
	MGP (TS)	0.3843	0.3946	0.3859	0.9135	0.2755	0.6007	0.3322	0.3667	0.3149	0.7110	0.3192	0.4317
	MRGP (Laplace)	**0.2200**	0.3391	0.2865	0.3684	0.3670	0.3947	0.3311	0.3903	0.2251	0.3505	0.2504	**0.3585**
	MRGP (Student-t)	0.2528	**0.3108**	**0.2502**	**0.2229**	**0.1908**	**0.3515**	**0.3193**	**0.3358**	**0.1735**	**0.2841**	**0.1768**	0.3640

liers. Finally, our proposed methods obtain the best results in almost all cases, which demonstrates the effectiveness of the proposed models. We can observe that MRGP (Student-t) outperforms MRGP (Laplace) almost all, but there are a few cases that MRGP (Laplace) outperforms MRGP (Student-t). Therefore, we can not conclude which model is generally better, and this may depend

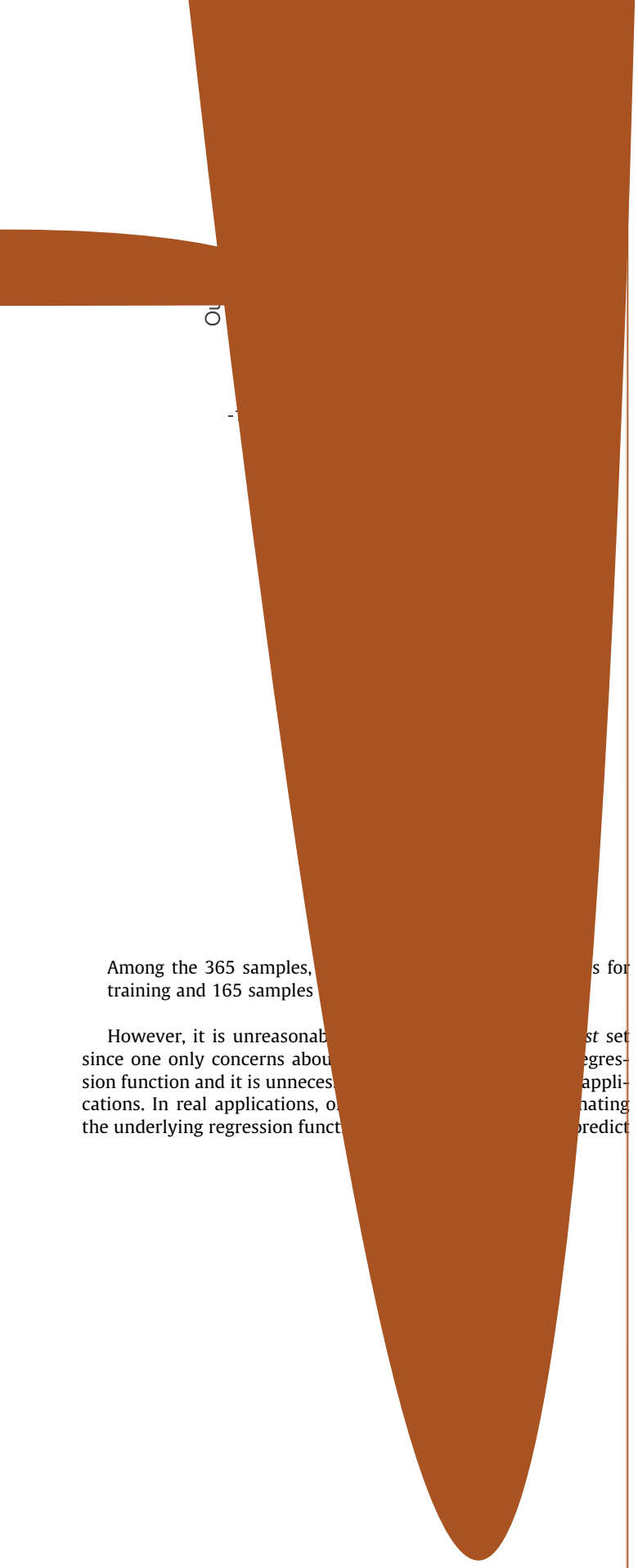
on the dataset. Empirically, we find out that when the outlier ratio is relatively low, MRGP (Laplace) and MRGP (Student-t) lead to similar results, but as the outlier ratio increases, MRGP(Student-t) generally becomes better than MRGP (Laplace).

The hard-cut EM algorithm is an approximation of the original EM algorithm. Specifically, in the E-step, the posterior distributions of latent variables $\{z_i\}_{i=1}^N$ are approximated by deterministic hard-cut allocations. Such an approximation may cause errors in the learning process. We evaluate the quality of approximation empirically. Since the original EM algorithm for MGP consists of exponentially many summation terms and is prohibitively time-consuming, it is intractable to run the original EM algorithm and compare the performances with the results of the hard-cut EM algorithm. Nevertheless, we can calculate the Classification Accuracy Rates (CARs) to validate the effectiveness of the hard-cut EM algorithm. In synthetic datasets, we have the ground-truth component labels, so we can compare the estimated component labels $\{\hat{z}_i\}_{i=1}^N$ by hard-cut EM algorithm with the ground-truth labels $\{z_i\}_{i=1}^N$. Formally, the CAR is defined as

$$\text{CAR} = \max_{\xi \in \Pi_K} \frac{1}{N} \sum_{i=1}^{N} \mathbf{bI}(z_i = \xi(\hat{z_i})).$$

Here, Π_K denotes the set of K-permutations, and the permutation ξ is employed to account for the label switching problem. Intuitively, CAR measures how well we cluster the observations into correct components. The results are shown in Table 4. Since MGP is also learned by the hard-cit EM algorithm, we also include the CARs of MGP for comparison. From this table, we find that in terms of CARs, the hard-cut EM algorithm based MGP and MRGP methods perform well on all the synthetic datasets, under all settings. This observation demonstrates that the hard-cut EM algorithm is effective and the quality of approximation is satisfying. We also find the CARs are relatively high on $\mathscr{S}_5, \mathscr{S}_{11}$ and relatively low on $\mathscr{S}_6, \mathscr{S}_{12}$. This observation coincides with the fact that $\mathscr{S}_5, \mathscr{S}_{11}$ are mildly overlapped thus easier to cluster the samples, while $\mathscr{S}_6, \mathscr{S}_{12}$ are heavily overlapped thus harder to cluster the observations correctly. Besides, we find that on $\mathscr{S}_6$ and $\mathscr{S}_{12}$, the classification accuracy rates of MGP drop significantly ($97.0\% \rightarrow 95.3\%$ and $98.2\% \rightarrow 96.8\%$) as we increase the outlier ratio and outlier level from $\eta = 0.05, v = 2.0$ to $\eta = 0.10, v = 2.5$. On the other hand, the classification accuracy rates of MRGP (Laplace) and MRGP (Student-t) are not sensitive to the outlier ratios and outlier levels. This further demonstrates that MRGP models are more robust than the MGP model.

For further comparison, the posterior curves of these methods



Among the 365 samples, s for training and 165 samples

However, it is unreasonab *st* set since one only concerns abou egression function and it is unneces applications. In real applications, o nating the underlying regression funct predict

outliers. Including outliers in the test set will introduce bias in the evaluation metrics. In practice, we first use Grubbs's outlier detection method to detect the outliers of the *test* set and then move them into the training set.

We compare our proposed methods with GP, SVM, FNN, RGP (Laplace), RGP (Student-t) and MGP(hard-cut) as in experiments on synthetic datasets. For the mixture models, since we do not know the correct number of components a prior, we set the num-

ber of components in $\{2, 3, 4, 5\}$ respectively. For each dataset, we run each method for 10 times, and list the average RMSE (together with standard deviations) and running time in Table 5. From this table, we can find out MRGP (Laplace) and MRGP (Student-t) outperform the other methods on the prediction performance. Specifically, on Boston housing dataset MRGP (Student-t) with $K = 2$ achieves the lowest RMSE, and MRGP (Laplace) with $K = 3$ obtains the best results on Electricity and Weather datasets. This indicates both MRGP (Laplace) and MRGP (Student-t) have their own advantages and it is generally difficult to determine which model is more suitable for the task in hand. The choice of K is also subtle. From Table 5, we can see K influence the prediction performances severely. The choice of K also depends on the dataset. On Electricity and Weather datasets, 2 components are far from enough to fit the data, while too many components ($i.e.$,$K = 5$) also lead to large errors due to over-fitting. On the Boston housing dataset, increasing K almost always leads to larger errors. One possible explanation is the inputs lie in a 13-dimensional space, but we only have 250 training samples. Therefore, dividing these samples to several components will cause difficulty for learning in each individual component since the samples are too sparse in the 13-dimensional space. We can observe that the proper number of components for different mixture models are almost the same: $K = 2$ for Boston housing dataset and $K = 3$ for Electricity and Weather dataset. Thus, how to set K relies heavily on the dataset rather than the mixture model. Finally, we can also find out that our proposed methods are much more time-consuming than the other methods because. Therefore, the proposed methods may not be well-suited for real-time tasks.

6. Conclusion and discussion

We have established the mixture of robust Gaussian processes (MRGP) by adopting Laplace or student-t noises with heavy-tailed property into Gaussian processes. In such a way, the MRGP model has the ability to model non-stationary temporal data effectively and also to be insensitive to outliers. The hard-cut EM algorithm is further developed for the MRGP model with the help of the variational bounding method to make the marginal likelihood of the robust Gaussian process be tractable in the ML solving process. It is demonstrated by the experimental results on both synthetic and real-world datasets that our proposed MRGP methods are much more effective and robust than the competitive nonlinear regression models.

How to set the number of components adaptively in real applications is an interesting direction. We can further develop automated model selection methods for the mixture of robust Gaussian processes. In fact, split-and-merge EM algorithm [53,54], rival penalized EM algorithm [55], reversible jump MCMC [56,57], entropy penalty [58–60] and Bayesian Ying-Yang (BYY) harmony learning [61–65] have been shown to be effective for the automated mode selection on mixture models. However, these methods are not so easy to apply to the mixture of Gaussian processes since the samples are not independent and highly correlated. A synchronously balancing criterion [66] has been proposed for model selection of MGP, but its penalty coefficient is still difficult to determine. The automatic model selection for the mixture of robust Gaussian processes is certainly a potential future direction. It is also promising to reduce the computational cost by introducing inducing points to our proposed model. Using inducing points [47,67,43] in Gaussian processes can improve the computational complexity significantly, and the extension to a mixture of Gaussian processes has been studied in [16]. However, sparse Gaussian processes usually have lower prediction accuracy, and how to balance the trade-off between performance and computational time generally depends on the particular task in hand. The extensions of the proposed model to classification task [33] or state-space model [68–70] is also promising. Finally, further incorporating domain-specific priors in the model [71] is a potential direction.

CRediT authorship contribution statement

Tao Li: Conceptualization, Investigation, Methodology, Software, Validation, Visualization, Writing - original draft. **Di Wu:** Conceptualization, Formal Analysis, Investigation, Methodology, Writing - review & editing. **Jinwen Ma:** Conceptualization, Formal Analysis, Funding acquisition, Investigation, Methodology, Project administration, Resources, Supervision, Writing - review & editing.

Declaration of Competing Interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

Acknowledgment

This work was supported by the National Key R&D Program of China (2018YFC0808305).

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