A sequential prediction method of quasi-periodicity based on Gaussian process state space model

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***Abstract*—In this paper, we develop a sequential prediction method of quasi-periodicity based on Gaussian process state space model. We introduce a latent variable to represent the phase hidden in the quasi-periodic phenomenon. The proposed prediction method adopts the predictive distribution for the starting point of the next period. The hyperparameters of the Gaussian process can be inferred by using particle Markov Chain Monte Carlo method. By using basal body temperature data of 17 female subjects, we evaluated the performance of the proposed method in the prediction accuracy of menstrual cycle length. The results showed that the prediction accuracy was improved compared with the conventional calendar method in the case that the fluctuation of the cycle length within 5 days.**

I. Introduction

This study focuses on quasi-periodicity that appears in various natural phenomena. Quasi-periodicity means that the pattern obtained by observing the target system does not have a stationary period and that the period itself has fluctuations. We can observe quasi-periodic phenomena such as increase and decrease of population of living things [1], biological rhythm [2], atmosphere-ocean interaction such as El Nino phenomenon, Arctic oscillation, and climate change [3], sun black spots [4] and magnetic storm [5], etc. In addition, changes in basal body temperature of female correspond to circadian rhythm, which is one of the biological rhythms. We assume a situation where time-series data of quasi-periodic phenomena can be obtained sequentially, and consider to develop a method to predict the quasi-periodicity. Our aim is not to detect periodicity from time series data [6]–[11], but to predict the quasi-periods.

Predicting quasi-periods from observations of various phenomena brings many benefits to us, including the examples given below:

- Development of optimal dosage plan considering biological rhythm, active drug development with few side effects [2].
- Increase in crop yields due to improved weather forecast accuracy.
- Improvement of the accuracy of anomaly detection when the cycle deviates.
- Improvement of female's quality of life by predicting menstrual cycle length and ovulation period.

Therefore, development of a method to predict quasi-periods accurately is an important issue, and its demand is rising in recent years.

State Space Model (SSM) can be applied to model time series data which shows nonlinear variations. Several methods have also been proposed to model time-series data of quasi-periodic phenomena targeted by this study. In [12], a model is presented in which the observed values are represented by the sum of trigonometric functions, and their phase and amplitude follow the probability differential equation. The previous studies [13], [14] introduce a model that decomposes seasonal components of observation into a sum of several small parts representing a specific periodic variation, each of which also follows a second-order stochastic difference equation. However, in these models, the target of prediction was just an observation value, and prediction of the period itself was not considered. We consider that studies to estimate the period sequentially have been also conducted sufficiently.

In this study, we explicitly introduce the hidden phase in the quasi-periodic phenomena, and model both the phase and the observation with the Gaussian Process State Space Model (GP-SSM) [15]–[17]. GP-SSM is a class of SSM that the characteristics of nonlinearity and smoothness are represented via Gaussian process [18]. To express fluctuations of the phase hidden in the quasi-periodic phenomenon, we introduce the phase as a latent variable in this study. Furthermore, we estimate the phase sequentially from observation data obtained sequentially, and consider a method to predict the period with fluctuation, that is, the quasi-period. The feature of GP-SSM considered in this study is that the values of the state variable, hyperparameters of GP, and the joint posterior distribution of each function for SSM are estimated based on Particle Markov Chain Monte Carlo (Particle MCMC) [19]. To investigate the effectiveness of the proposed method, we conducted experiments for prediction of the next menstruation start date and evaluated the performance by the mean square error of prediction.

This paper is organized as follows: Section 2 describes modeling method and sequential prediction method based on GP-SSM. Section 3 describes the results of the prediction experiments and Section 4 discusses these results. Finally Section 5 summarizes the paper.

II. Modeling of quasi-periodic nonlinear phenomena

In modeling quasi-periodic nonlinear phenomena, we assume the existence of a potential phase for such phenom-

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ena [20]. The introduction of the phase makes it possible to quantitatively evaluate where the current observation is located in one cycle. Furthermore, we consider fluctuation of the phase as a probabilistic phenomenon and introduce phase as a latent variable (state variable) of the probabilistic model to express uncertainty. We apply SSM to mathematically describe the dynamic change of phase and time evolution, and formulate it using the phase as a state variable of SSM. In this study, we specifically target the basal body temperature and menstrual cycle length of female. Based on the formulation by SSM, the sequential prediction method of the next menstruation start date can be derived [20]. Furthermore, in this study, we propose an approach using GP-SSM.

A. Formulation by state space model

Let y_n be the temperature observed on the n-th day, and let θ_n be the phase of the n-th day. Suppose that the phase θ_n takes a value between 0 and 1. Moreover, it is assumed that the phase increases monotonically and that the phase is reset to 0 by taking $\theta_n = 1$ when the n-th day is the menstruation start date. Based on the above assumptions, the time evolution with uncertainty of the observed variable y_n and the state variable θ_n is described by the following equations:

$$\theta_n = (\theta_{n-1} + \epsilon_n) \mod 1, \ \ \epsilon_n \sim \mathrm{gamma}(\alpha, \beta) \quad (1)$$

$$y_n = g(\theta_n) + \sigma_n, \ \ \sigma_n \sim \mathcal{N}(0, \sigma^2) \quad (2)$$

$$g(\theta_n) = a_0 + \sum_{m=1}^{M} [a_m \cos(2m\pi\theta_n) + b_m \sin(2m\pi\theta_n)] \quad (3)$$

where $\mathrm{gamma}(\alpha, \beta)$ represents a gamma distribution with shape parameter α and scale parameter β. The parameters $\{\alpha, \beta, \sigma, a_0, a_1, \cdots, a_M, b_1, \cdots, b_M\}$ can be estimated by using the maximum likelihood method [20].

The increment of the phase added from the n day to the $(n + r)$-th day $(r \geq 1)$ is defined by the following formula.

$$\Delta(r \mid n) \stackrel{\mathrm{def}}{=} \theta_{n+r} - \theta_n \quad (4)$$

$$= \epsilon_n + \epsilon_{n+1} + \ldots + \epsilon_{n+r}, \quad (5)$$

where $\Delta(r \mid n)$ is also a random variable and follows $\mathrm{gamma}(r\alpha, \beta)$ because of the reproducibility of the gamma distribution. Assuming that the phase of the n-th day is θ_n, the increment of the phase required to reach the next menstruation start date is $1 - \theta_n$. The probability of the event that the next menstruation start date occurs at the $(n + r)$-th day is calculated by the following formula as the conditional cumulative distribution function $F(r \mid \theta_n)$ by the integral of the density function.

$$\begin{aligned} F(r \mid \theta_n) &\stackrel{\mathrm{def}}{=} P((\Delta(r \mid n) \geq 1 - \theta_n)) \\ &= \int_{1-\theta_n}^{\infty} \mathrm{gamma}(x; r\alpha, \beta)\, dx \\ &= 1 - G(1 - \theta_n; r\alpha, \beta) \end{aligned} \quad (6)$$

The cumulative distribution function of the above gamma distribution is represented by $G(\cdot; r\alpha, \beta)$. Based on the conditional cumulative distribution function, the conditional probability mass function $p(r \mid \theta_n)$ is calculated as

$$p(r \mid \theta_n) \stackrel{\mathrm{def}}{=} F(r \mid \theta_n) - F(r - 1 \mid \theta_n). \quad (7)$$

By combining the conditional probability mass function with the filter distribution $p(\theta_n \mid y_{1:n})$, the predictive distribution of the menstruation start date can obtained by

$$p(r \mid y_{1:n}) = \int p(r \mid \theta_n) p(\theta_n \mid y_{1:n})\, d\theta_n \quad (8)$$

Then, from $\hat{r}$ of the following equation giving the maximum value of the predictive distribution, the predicted value of the next menstruation start date starting from the n-th day is given as the $(n + \hat{r})$-th day.

$$\hat{r} = \arg\max_r p(r \mid y_{1:n}) \quad (9)$$

B. Formulation by Gaussian process state-space model

On the basis of the formulation described in the previous section, the basal body temperature can be modeled by GP-SSM:

$$f(\theta) \sim \mathcal{GP}_f\left(m_f(\theta), k_f(\theta, \theta'; \mathbf{\Theta}_f)\right) \quad (10)$$

$$\theta_n = (f(\theta_{n-1}) + \epsilon_n) \mod 1, \ \ \epsilon_n \sim \mathrm{gamma}(\alpha, \beta) \quad (11)$$

$$g(\theta) \sim \mathcal{GP}_g\left(m_g(\theta), k_g(\theta, \theta'; \mathbf{\Theta}_g)\right) \quad (12)$$

$$y_n = g(\theta_n) + \sigma_n, \ \ \sigma_n \sim \mathcal{N}(0, \sigma^2) \quad (13)$$

In this study, the mean function of the system model is given by $m_f(\theta) = \theta$. The mean function of the observation model is given by the Fourier series of order M:

$$m_g(\theta) = a_0 + \sum_{m=1}^{M} [a_m \cos(2\pi m\theta) + b_m \sin(2\pi m\theta)] \quad (14)$$

In this study, the coefficients a_m and b_m are estimated by using discrete Fourier transform.

RBF kernels were applied to the kernel functions of the system model and the observation model.

$$k_f(\theta, \theta'; \mathbf{\Theta}_f) = s_f^2 \exp\left(-\frac{(\theta - \theta')^2}{2l_f}\right) \quad (15)$$

$$k_g(\theta, \theta'; \mathbf{\Theta}_g) = s_g^2 \exp\left(-\frac{(\theta - \theta')^2}{2l_g}\right) \quad (16)$$

where $\mathbf{\Theta}_f = \{s_f, l_f\}$, $\mathbf{\Theta}_g = \{s_g, l_g\}$ are the corresponding hyperparameters.

In the SSM formulation [20], the state transition function and the observation function were described by definite hyperparameters. The hyperparameters were determined by a grid search and Akaike Information Criterion (AIC) [21]. The observation function $g(\cdot)$ is the sum of trigonometric functions which approximates observation data. Linearity is assumed for the state transition function. In general, it is necessary to evaluate models with various possible functions, including

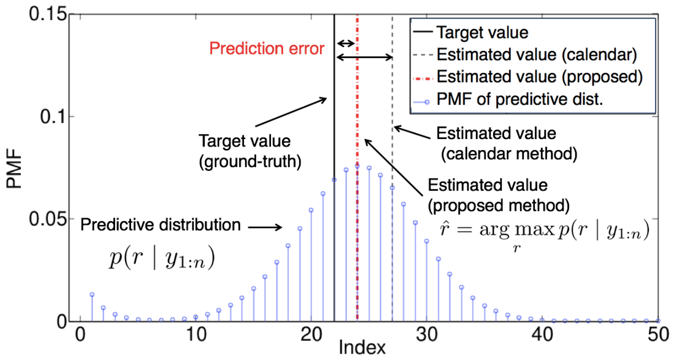


Fig. 1: Example of predictive distribution.

the number of terms of these trigonometric functions and the coefficients, and also necessary to select the final model based on a criterion. The proposed method does not require such model selection thanks to the characteristic of GP. We expect the proposed model will flexibly capture nonlinearity in various phenomena.

Given the observation $y_{1:n}$ up to the n-th day, according to the particle MCMC method, we can obtain the set of i.i.d.[1] samples $\{\theta_n^{(i)}\}_{i=1}^N$. The following empirical distribution can be calculated using these i.i.d. samples:

$$p_N(\theta_n \mid y_{1:n}) = \frac{1}{N}\sum_{i=1}^{N} \delta(\theta_n - \theta_n^{(i)}). \quad (17)$$

Since the above equation can be regarded as an approximation of the filter distribution $p(\theta_n \mid y_{1:n})$, plugging it into the right hand side of Eq. (8), we can calculate an approximation of the predicted distribution as Monte Carlo integration.

$$p(r \mid y_{1:n}) \simeq \frac{1}{N}\sum_{i=1}^{N} p(r \mid \theta_n^{(i)}) \quad (18)$$

Finally we can obtain the predicted value by Eq. (9).

The calculation of the prediction error of the next menstruation start date was performed as follows: First, the value of the predictive distribution is evaluated for each index r of the predictive distribution sequentially over all evaluation data. As shown in Fig. 1, the probability mass function of the predictive distribution can be obtained, and the predicted value is given from the index $\hat{r}$ which gives the maximum value. Figure 2 shows examples of sequential prediction and predictive distribution over days. A sequential prediction is performed by moving the entire distribution to the left. In the example shown, since the sequential prediction is close to the true prediction, the prediction error is reduced as a result. In Fig. 2 (d), we can see that the right tail of the prediction distribution is raised. This fact reflects the situation that the prediction for the next month is about to start.

III. Experimental Evaluation

To demonstrate the effectiveness of the proposed method, we conducted evaluation experiments about prediction of the next menstruation start date from female's basal body temperature data.

[1]Independent and Identically-Distributed.

TABLE I: Constraints imposed on the database to extract training/evaluation data and corresponding reduction rate.

Condition	Reduction rate
Days of non-registered $\leq$ 3.	92.0%
Date skip is up to 2 days	96.7%
Average menstrual cycle length less than 60 days	1.4%
Average menstrual cycle length is more than 15 days	13.5%
Minimum menstrual cycle length less than 15 days	80.4%

A. Experimental Condition

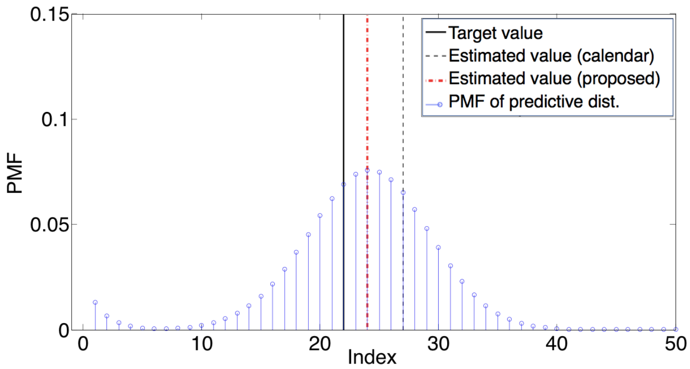
1) Dataset: QOL Corporation (Ueda, Japan) maintains the database which contains the daily body temperature data of each subject. The body temperature and menstruation onset data was collected via a website called *Ran's story*, which is a website that allows registered users to upload their self-reported daily BBT and days of menstruation onset to QOL Corporation's data servers. All users of Ran's story agree to the use of their data for academic research. If the number of registered data is tiny, e.g., less than one month, it is difficult to evaluate the prediction method because sufficient amounts of data cannot be secured for inference and evaluation. Although the inference algorithm for the proposed method is based on particle MCMC, it is also challenging to perform model inference for a large number of subjects even if using parallel computing. Therefore, to secure sufficient data for inference and evaluation, we selected subjects whose number of body temperature registrations was one year or more. The reduction rate for the entire database at this time was 76.7%.

Furthermore, the number of subjects was reduced by imposing the conditions shown in Table I. The reason for imposing the restriction is to guarantee the continuity of the observation as much as possible. The reason for the high reduction rate of the minimum menstrual cycle includes those due to date jumps. Finally, we selected body temperature data from 17 subjects for 30-44 years. Those met all these conditions. In this experiment, we used continuous half-year data for inference and another consecutive half-year data for evaluation. They did not overlap each other.

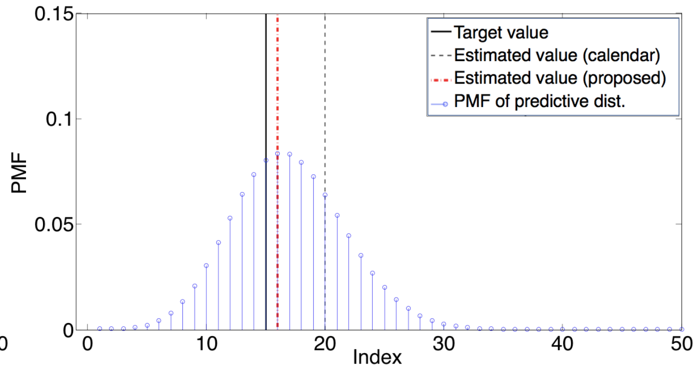
2) Settings of parameters: Based on the result of the preliminary experiment, the number of MCMC iterations was set to 15,000. The number of particles was set to 10,000 for both inference and prediction. The variance of the Gaussian distribution of Eq.(13) was set by preliminary experiments to $\sigma^2 = 0.2$, and the initial value of the state variable was 0.0. For the observation, the order M of the Fourier series was set to 3.

Parameters of the gamma distribution of Eq.(11) were estimated by the Particle MCMC method. In the experiment, α was sampled from the uniform distribution $[1.1, 1, 000]$ and β was calculated by using the following constraint

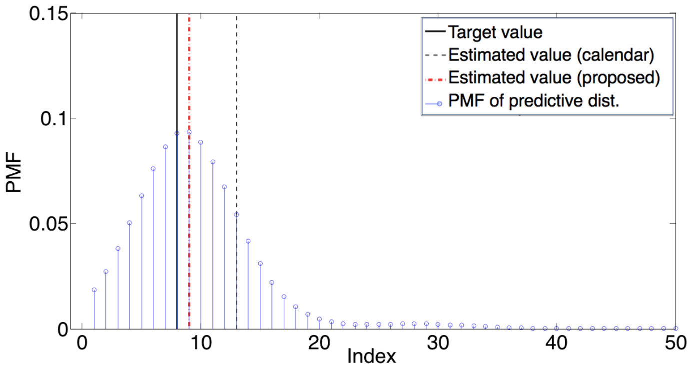
$$\alpha\beta = \frac{1}{\overline{T}}, \quad (19)$$



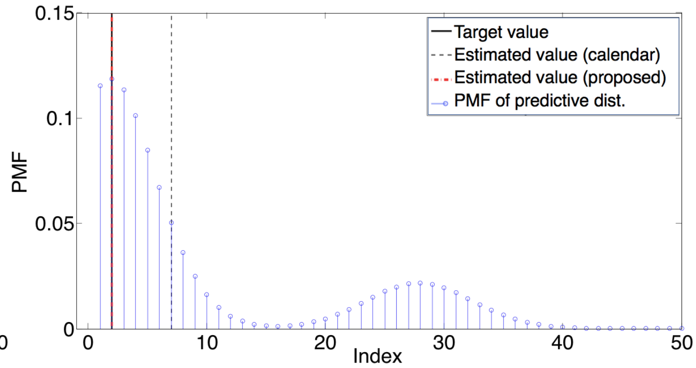
(a) 23 days before next menstruation



(b) 16 days before next menstruation



(c) 9 days before next menstruation



(d) 2 days before next menstruation

Fig. 2: Example of sequential prediction.

where $\overline{T}$ is the averaged menstrual cycle length for each subject. By imposing the above constraint, we can expect that the phase reset occurs at $\overline{T}$ intervals on average. This is because the mean of gamma distribution is given by $\alpha\beta$ and the expectation can be calculated when we calculate a sequence of phase values from $n = 1$ to $n = \overline{T}$ by using Eq.(11) as follows:

$$E[\theta] = E\left[\theta_0 + \sum_{i=1}^{\overline{T}} \epsilon_i\right] = \sum_{i=1}^{\overline{T}} E[\epsilon_i] = \sum_{i=1}^{\overline{T}} \alpha\beta \quad (20)$$

$$= \overline{T} \cdot \frac{1}{\overline{T}} = 1 \equiv 0 \pmod 1, \quad (21)$$

where $\theta_0 = 0$.

For estimation of GP, we set prior distributions for hyper-parameters of GP as follows: $s_f \sim [1.0 \times 10^{-3}, 3.0]$, $l_f \sim [1.0 \times 10^{-3}, 1.0 \times 10^{3}]$ for k_f and $s_g \sim [1.0 \times 10^{-3}, 5.0]$, $l_g \sim [1.0 \times 10^{-3}, 1.0 \times 10^{3}]$ for k_g.

3) Comparative methods: We adopted two methods for comparison:

- **Method 1**: T_{av} days after the previous menstruation start date is used as the prediction of the next menstruation, where T_{av} is the average menstrual cycle length calculated the evaluation data for each subject.
- **Method 2**: 29 days after the last menstrual period. In fact, calculated from 37,148 menstrual cycles of 3,997 subjects, the mode was 29 days.

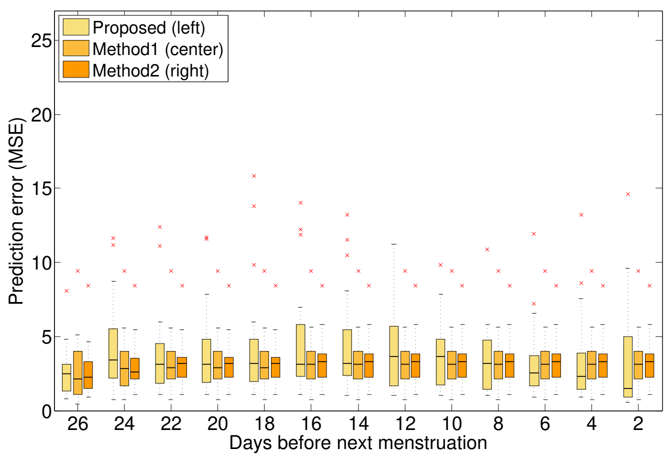


Fig. 3: Box plot of prediction error.

B. Experimental results

Box plots of the prediction error are shown in Fig 3. The horizontal axis shows how many days ago the forecast was made from the menstruation start date of each month. That is, the right side of the figure shows the prediction error when approaching the next day of the menstruation start date. The vertical axis is the mean squared error (MSE), which is

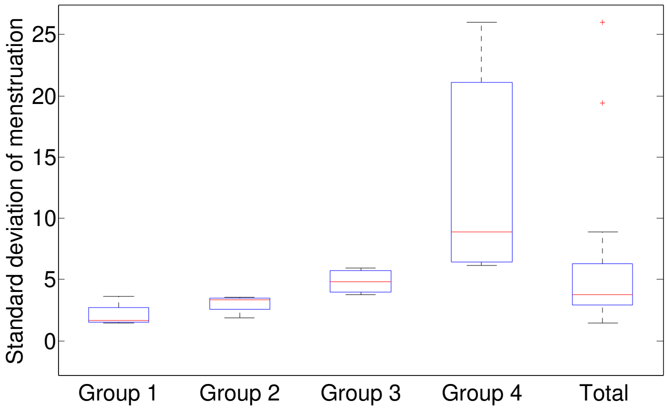


Fig. 4: Box plot of standard deviation of menstruation cycle for each group where “Total” means all subjects.

the prediction error that is summed up and averaged at each predicted time point. In the figure, the average values of the prediction errors for **Method 1** and **Method 2** are also plotted. From figure 3, we could not find significant improvement viewed over the whole subjects. In the next section, we will consider this result and the cause.

IV. Discussion

From the results shown in the figure 3, the prediction error is large at two days before the next menstruation start date, so the subjects were classified into the following four groups in order of increasing error from group 1 based on this prediction error.

- Group 1: Prediction error less than 25 percentile (# of subjects = 4)
- Group 2: Prediction error 25 percentile or more and less than 50 percentile (# of subjects = 4)
- Group 3: Prediction error 50 percentile or more and less than 75 percentile (# of subjects = 4)
- Group 4: Prediction error 75th percentile or more (# of subjects = 5)

To grasp the relationship between prediction error and the menstrual cycle length, we calculated the standard deviation of the menstrual cycle length for each group. The result is shown in figure4. Clearly, in group 1 and 2, the variation was small with a small prediction error. Conversely, in group 3 and 4, the variation was considerable with a significant prediction error. For those two groups, it is suggested that the proposed method could not absorb a fluctuation of the cycle and therefore could not predict the period accurately.

Fig.5 shows the re-aggregation of the results in Fig.3 for each group. For Group 1, about one-fourth of the whole subjects, the reduction of prediction error was obtained by using the proposed method. However, enough improvement was not obtained for group 3 and 4. In the formulation of the proposed method, the phase is reset to 0 according to the menstruation start date. Therefore, the prediction error is affected by the variation of menstrual cycle length, especially for those two groups. From Fig.5, it can be observed that the standard deviation of the menstrual cycle length is about 5 days in group 3 and about 10 days in group 4. For those two groups, the proposed method could not absorb the fluctuations of the cycle and could not predict the cycle accurately.

Observing the estimated state transition function, the trend was organized as follows:

- Group 1: The state transition function is linear with little change from the initial value.
- Group 2 and 3: Although it is a monotonically increasing function, the gradient is not steep compared to the group 1, and the gradient itself tends to decrease gradually. The phase is reset before the value reaches 1.
- Group 4: There are some things that decrease rather than increase the phase.

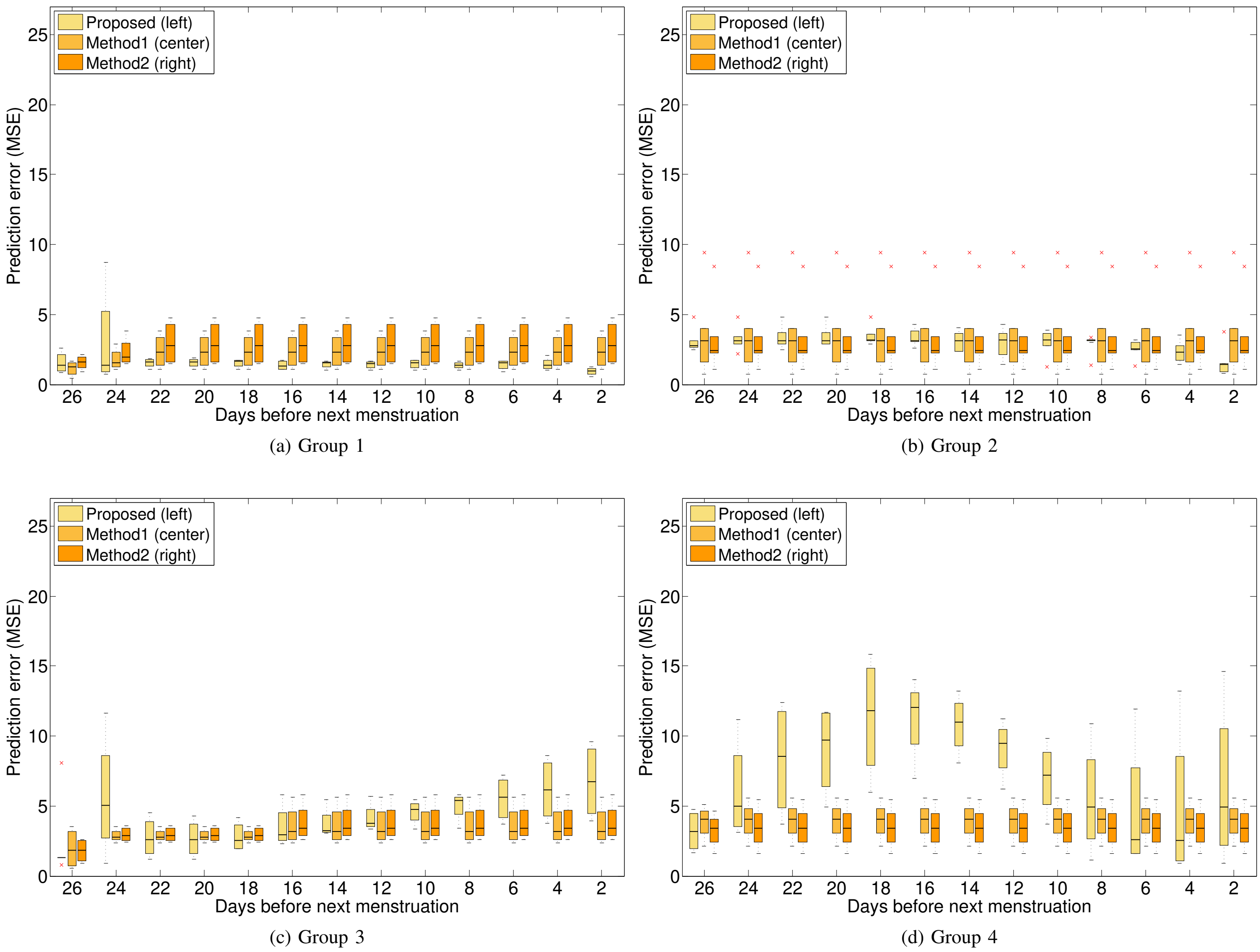
Figures 6(a) to 6(d) show the experimental results of representative subjects extracted from each group as examples. Each plot shows (i) average prediction error of menstruation start date, (ii) sequential prediction value of menstruation start date, and (iii) estimated mean function. For (ii), the estimated values at each time step are shown as “Ground truth” and “Proposed” (estimated value obtained by the proposed method). In group 2 and 3, the prediction error tended to increase gradually as the next menstruation start date approached. This is because the entire predictive distribution gradually stagnates at the same location as the phase increase gradually decreases. For subjects in group 4 whose phase decreased, the prediction error increased significantly because the whole predictive distribution was move in reverse direction.

In summary, the proposed method cannot cope with large fluctuation of cycle length. However, in the case that the fluctuation is within 5 days, the proposed method can predict the cycle length.

V. Conclusions and Future Works

In this study, we have modeled quasi-periodic non-linear phenomena by Gaussian process state-space model (GP-SSM) and developed a method to predict quasi-periodicity sequentially. Assuming the existence of a phase hidden in the phenomena, we have introduced it as a latent variable. State space model describes the time evolution of state uncertainty. Furthermore, GP-SSM considered in this study has been derived by expressing the state transition function and observation function in the state space model based on GP. Model parameters can be estimated based on the particle MCMC method. The quasi-periodic sequential prediction method is formulated by approximating the predicted distribution at the start of the next cycle.

Compared with the method of predicting the next menstruation date as 29 days after the last menstruation (i.e., a calendar calculation method), we confirmed that the proposed method improved the prediction accuracy. As for menstrual cycle, we should consider that trends may differ from generation to generation, so more robust prediction will be possible by classifying data by age and performing model estimation on each. Introducing a prior knowledge according to the characteristics of the body temperature data and menstrual



(a) Group 1

(b) Group 2

(c) Group 3

(d) Group 4

Fig. 5: Box plot of prediction error for each group.

cycle length will be useful. For instance, to capture variations of the cycle length, we can introduce a mixture of distributions which represent standard and non-standard menstrual cycles. We also consider that the prediction accuracy will be further improved if statistical information such as the mode value of the cycle from about 4,000 people of the QOL database, is incorporated into the formulation of the model effectively.

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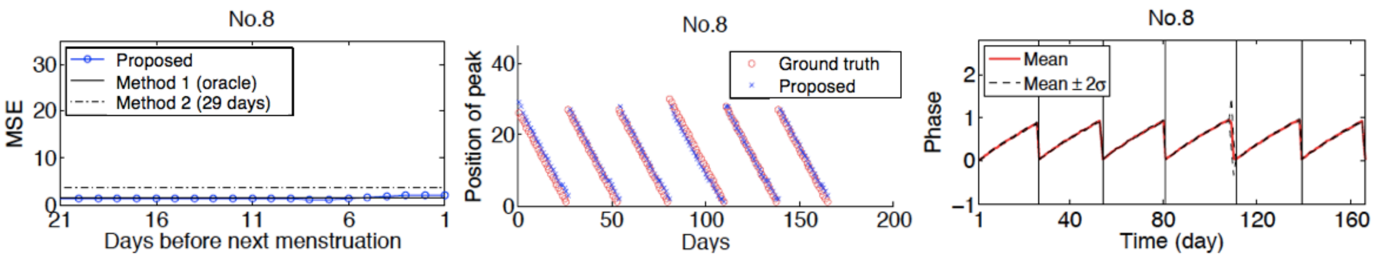
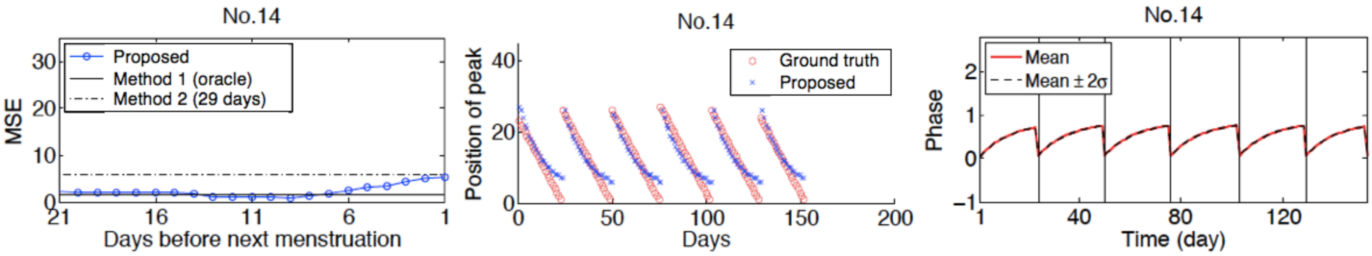
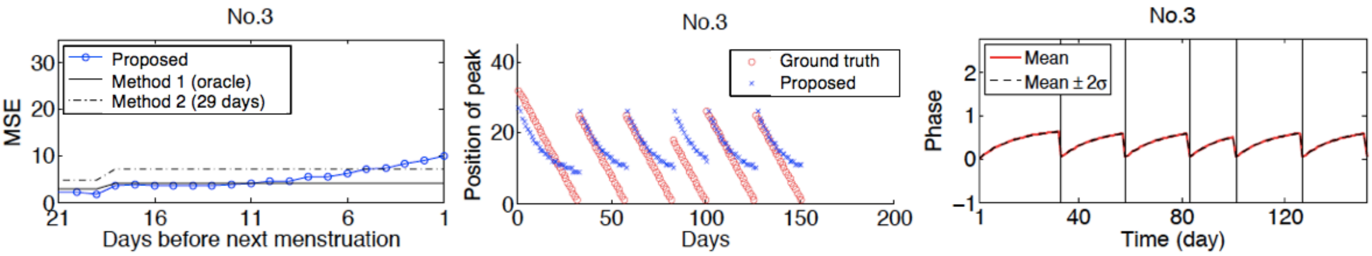


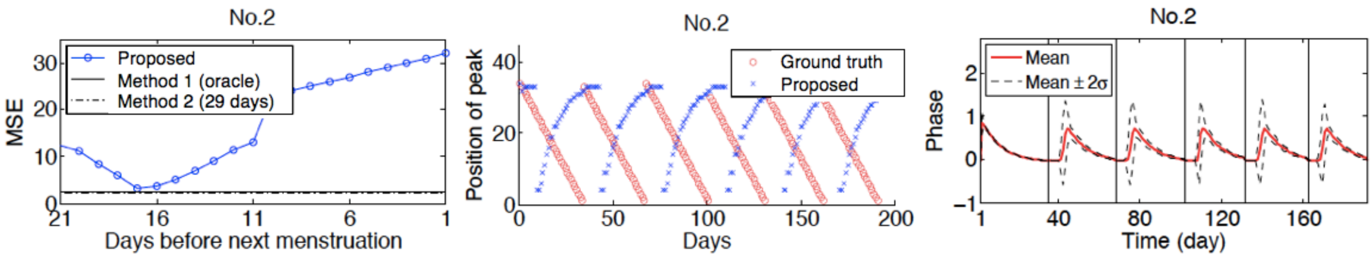
(a) Subject belonging to Group 1



(b) Subject belonging to Group 2



(c) Subject belonging to Group 3



(d) Subject belonging to Group 1

Fig. 6: Box plot of prediction error for each group.

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