Robust Sequential Online Prediction with Dynamic Ensemble of Multiple Models: A Concise Introduction

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Abstract—In this paper, I give a concise introduction to a generic theoretical framework termed Bayesian Dynamic Ensemble of Multiple Models (BDEMM), which is used for robust sequential online prediction with time series data. This framework has three major features: (1) it employs a model pool, rather than a single model, to capture possible statistical regularities underlying the data; (2) the model pool consists of multiple weighted candidate models, wherein the model weights are adapted online to capture possible temporal evolutions of the data; (3) the adaptation for the model weights follows Bayesian formalism. These features together define BDEMM. To make this introduction comprehensive, I describe BDEMM from five perspectives, namely the basic theories, its different forms of algorithmic implementations, its applications, its connections to related research, open resources for algorithm implementations, followed by a discussion of practical issues for applying it and some open problems that are worth further research.

Index Terms—Bayesian, dynamic ensemble of multiple models, robust, online prediction, sequential Monte Carlo, Gaussian process, time series, particle filter, Kalman filter, outliers, change points.

I. INTRODUCTION

In one of his most influential papers [1], Leo Breiman summarizes two cultures from the practice of statistical modeling. They are termed data modeling and algorithmic modeling. Following the former culture, people do data analysis based on a given stochastic data model, such as linear regression, logistic regression, and so on. Within the latter culture, the data generative process is assumed unknown, so there is no “given stochastic data model” available. The model to be deployed is given by an algorithm. Breiman encourages the community to pay more attention to the algorithmic modeling culture, claiming that commitments to the data modeling culture could lead to “irrelevant theory, questionable conclusions” [1].

In concept, the aforementioned two cultures can be taken as two extreme instances of a broad sense modeling culture, namely modeling by mixing the data with the prior knowledge of the modeler. In the context of the data modeling culture, the model is given by the modeler based on his (or her) prior knowledge. In the so-called algorithmic modeling culture, the model is yielded from running an algorithm, while the algorithm is surely designed by the modeler based on his (or her) prior knowledge. Hence the essential difference between the two cultures lies in the different ways in which the modeler’s prior knowledge is used. For the data modeling culture, such prior knowledge is used directly in specifying the “given stochastic data model”; for the algorithmic modeling culture, the prior knowledge is embedded in the algorithm used for building the model.

In addition to those two extreme instances, namely data modeling and algorithmic modeling, the broad sense modeling culture has other forms in its realizations, among which the BDEMM is the one to be introduced here. Specifically for BDEMM, a part of its model structure is given by the modeler, and the other part changes over time and is calculated out by an algorithm, which is developed based on Bayesian formalism.

BDEMM has three major features, which together define itself. These features are: (1) BDEMM employs a model pool, rather than a single model, to cover possible statistical regularities underlying the data; (2) the model pool consists of multiple weighted candidate models, whose weights are adapted online to capture possible temporal evolutions of the data; (3) the adaptation mechanism of the model weights follows Bayesian formalism.

The above features make BDEMM amenable to sequential online prediction (SOP) problems. Unlike offline prediction methods which build a model based on a static dataset, and then make predictions using this model, BDEMM considers data sequentially, with relevant weights of its member models being updated at each step. Using BDEMM, one does not need to build a model from scratch when new data items arrive, since its model updating procedure is conducted in an incremental manner, following Bayesian formalism. In contrast with offline methods that need to access the data items repeatedly, SOP methods like BDEMM only require one pass of the data items, thus all data items that have been accessed can be dropped to release the memory.

Recently, BDEMM has been used in different contexts, such as robust tracking of dynamic system states [2]–[7], dynamic multi-modal data fusion [8], Gaussian process based time-series online prediction [9], Bayesian optimization [10], and neural decoding for brain-computer interface [11]. Within each context, a robust state-of-the-art algorithm solution is derived based on BDEMM. Notwithstanding its success over those different application cases, there has yet been an article that can provide a comprehensive introduction to BDEMM. That motivates me to write this introductory article.

The contribution of this paper is that, for the first time, it provides a comprehensive introduction to BDEMM, including the basic theories, its different forms of algorithmic
implementations, its applications, its connections to related research, open resources for algorithm implementations, and a discussion of practical issues for applying it and open problems that are worth further research. See these contents in Sections II-VII respectively. The paper concludes in Section VIII.

II. THEORIES

In this section, I describe BDEMM from a theoretical perspective. Readers are expected to have a prerequisite knowledge background on Bayesian statistics, some classic references include [12]–[14]. To begin with, I give a concise review of Bayesian model averaging (BMA), as it acts as the theoretical basis of BDEMM. This can be given before Section II (Theories).

A. BMA: Bayesian Model Averaging

In the common practice of statistical modeling, one specifies a stochastic model \(M\) at first. This model stands for a hypothesis on how the data are generated. Given \(M\) with a fixed structure, the value of its parameter \(\theta\) is obtained by data fitting, which is formulated as an optimization task according to a prescribed criterion, such as maximum likelihood (ML), maximum a posterior (MAP), or minimum mean square error (MMSE). One can also adopt the Bayesian paradigm, in which a prior density is assigned on \(\theta\) and a likelihood function is used to characterize the likelihood of \(\theta\) given the data [12], [15]–[18]. The remaining task is to compute the posterior of \(\theta\), which is proportional to the product of the prior and the likelihood.

For many realistic cases, specifying a model with a fixed structure to describe the generative mechanism of the data is a somewhat arbitrary choice. The alternative choice is to consider multiple candidate models, \(M_1, M_2, \ldots, M_K\), together to handle the uncertainty at the model level [19]–[21].

Given a set of independent identically distributed (i.i.d.) data points \(y = (y_1, \ldots, y_n)\), where \(y_i \sim p(y_i|\theta_k)\), \(i = 1, \ldots, n\), according to \(M_k\), the probability of \(y\) given \(M_k\) can be computed as follows

\[
p_k(y) = \int_p p_k(y|\theta)p_k(\theta)d\theta, \tag{1}
\]

where \(p_k(\theta)\) and \(p_k(y|\theta)\) denote respectively the prior and the likelihood function defined in \(M_k\), \(k = 1, \ldots, K\). As is shown, \(\theta\) is marginalized out (integrated out) in Eqn.(1). So \(p_k(y)\) is also referred to as the marginal likelihood or model evidence in the context of Bayesian statistics.

Denoting the prior probability of \(M_k\) by \(Pr(M_k)\), one can get the posterior probability of \(M_k\) based on Bayes formula

\[
p(M_k|y) = \frac{Pr(M_k)p_k(y)}{\sum_{j=1}^{K}Pr(M_j)p_j(y)}, k = 1, \ldots, K. \tag{2}
\]

Denote by \(g \triangleq g(\theta)\) the target parameter to be predicted, where \(g\) is a function that maps \(\theta\) to \(x\). The idea of BMA is to take into account model uncertainty in predicting \(x\), as shown below [22], [23]

\[
\hat{x} = \sum_{k=1}^{K} \hat{x}_kw_k, \tag{3}
\]

where \(\hat{x}_k\) denotes the estimated or predicted value of \(x\) associated with \(M_k\) and \(w_k \triangleq p(M_k|y)\) the weight of \(M_k\) in making this estimation or prediction. In concept, BMA abandons selecting a model with a fixed structure for use by assigning probabilities on a set of candidate models:

\[
Pr\{M = M_k\} = w_k, k = 1, \ldots, K.
\]

For more details on BMA, especially its theoretical properties, readers are referred to [22], [23].

B. BDEMM: Bayesian Dynamic Ensemble of Multiple Models

In the setting of BMA, there is no time variable involved. It indicates that BMA is not capable of handling dynamic scenarios where the data evolve over time. The BDEMM framework provides an extension of BMA for dynamic systems in which the time variable plays a key role. Now the observations are denoted by \(y_{t}, t \in \mathbb{R}, t > 0\), where the subscript \(t\) is the discrete time index. The task is to predict \(x_t\) at each time step based on data that have been collected up to time \(t\), namely \(y_{1:t} \triangleq \{y_1, \ldots, y_t\}\). Corresponding to Eqn. (3), the BMA equation for predicting \(x_t\) becomes

\[
\hat{x}_t = \sum_{k=1}^{K} \hat{x}_{k,t}w_k, \tag{4}
\]

where \(w_{k,t} \triangleq p(M_k|y_{1:t})\) and \(\hat{x}_{k,t}\) denotes the predicted value of \(x_t\) given by \(M_k\).

BDEMM provides a generic solution to compute Eqn.(4) recursively. In the framework of BDEMM, each model component, say \(M_k\), is defined by a pair of state transition prior \(p_k(x_{t+1}|x_{t})\) and a likelihood function \(p_k(y_{t}|x_{t})\). Assume that \(p_k(x_{t-1}|y_{1:t-1})\) is available. The predictive distribution of \(x_t\) given by \(M_k\)

\[
p_k(x_t|y_{1:t-1}) = \int_{\chi} p_k(x_t|x_{t-1})p_k(x_{t-1}|y_{1:t-1})dx_{t-1}, \tag{5}
\]

where \(\chi\) denotes the value space of \(x\). Then the posterior distribution of \(x_t\) associated with \(M_k\) is

\[
p_k(x_t|y_{1:t}) = \frac{p_k(y_{1:t}|x_{t})p_k(x_{t}|y_{1:t-1})}{p(M_k|y_{1:t})}, \tag{6}
\]

where

\[
p(M_k|y_{1:t}) = \int_{\chi} p_k(y_{1:t}|x_{t})p_k(x_{t}|y_{1:t-1})dx_t \tag{7}
\]

is the marginal likelihood (normalizing constant) of \(M_k\). As is shown above, \(p_k(x_{t}|y_{1:t})\) may not be analytical. One can employ Monte Carlo methods, such as importance sampling [24], [25] and Markov Chain Monte Carlo (MCMC) [26], [27] to draw random samples from it, then get \(\hat{x}_{k,t}\) based on those samples, according to a criterion such as ML, MMSE or MAP.

In BDEMM, the recursive calculation of \(w_{k,t}\) involved in Eqn.(4) starts by specifying a Weight-Temporal-Transition
w_{k,t|t-1} \triangleq \Pr\{M_{\text{correct},t} = M_k|y_{1:t-1}\} = f(w_{1:K,t-1}).

Here $M_{\text{correct},t}$ denotes the correct model at time $t$, $w_{1:K,t-1} \triangleq \{w_{1,t-1},\ldots,w_{K,t-1}\}$. See subsection 11.C for possible choices of the WTT operator.

Given $w_{k,t|t-1}, k = 1,\ldots,K$, one can adopt the Bayesian theorem to get $w_{k,t}$, as shown below

\begin{equation}
  w_{k,t} = \frac{w_{k,t|t-1}p(M_k|y_{1:t})}{\sum_{j=1}^{K} w_{j,t|t-1}p(M_j|y_{1:t})}, k = 1,\ldots,K.
\end{equation}

To summarize, given $p_k(x_{t-1}|y_{1:t-1})$ and $w_{k,t-1}, k = 1,\ldots,K$, one can use Eqs. (5)-(9) to compute $p_k(x_t|y_{1:t})$ and $w_{k,t}, k = 1,\ldots,K$. For most cases, $p_k(x_t|y_{1:t})$ has no analytical form, while $\hat{x}_{k,t}$ can be obtained based on Monte Carlo samples drawn from $p_k(x_t|y_{1:t})$. Given $\hat{x}_{k,t}$ and $w_{k,t}, k = 1,\ldots,K, x_t$ is available through Eqn. (4).

Remark. BDEMM consists of a series of BMA phases that run sequentially. Between each neighboring pair of BMA phases, a WTT operation is performed, which generates the prior distribution of the correct model required for use in the latter BMA phase. As long as the WTT operation is appropriately specified, the BDEMM theory shares the same desirable theoretical properties of BMA. With aid of the WTT operator, BDEMM provides a way that allows BMA to work in dynamic settings. In another word, BDEMM can be regarded as a dynamic extension of the BMA theory.

C. WTT Operators

As mentioned above, BDEMM uses a WTT operation to give the predictive distribution of the correct model at each time instant. In what follows, I introduce five WTT operators that can be selected in practice.

1) Operator I: A straightforward choice of the WTT operation is to set

\begin{equation}
  w_{k,t|t-1} = w_{k,t-1}, k = 1,\ldots,K.
\end{equation}

This setting assumes that the model switching process is totally guided by the observations, other than any prior knowledge of the modeler. When BDEMM is used to select one correct model from a number of candidate ones to describe a static dataset whose data items arrive sequentially, then this operator is preferable for use to the others, which shall be introduced in what follows.

2) Operator II: Another simple WTT operation is to let

\begin{equation}
  w_{k,t|t-1} = C_k, k = 1,\ldots,K,
\end{equation}

where $C_k, k = 1,\ldots,K$ are constants specified by the modeler, satisfying $\sum_{k=1}^{K} C_k = 1$. This operator assumes that the model switching process can be fully characterized by the prior knowledge encoded by $C_k, k = 1,\ldots,K$. This operator is suitable for use in cases where the time-series observations cannot provide any clue for inferring the model switching law.

3) Operator III: The third WTT operator to be introduced assumes that the transition of the correct model follows a Markov model defined by a $K$ by $K$ mode transition matrix (MTM). An example of the MTM is given as follows

\begin{equation}
  T = \begin{pmatrix}
  0.9 & 0.1 \\
  0.1 & 0.9 \\
  \vdots & \vdots \\
  0.1 & 0.1 \\
  \end{pmatrix}_K.
\end{equation}

Denote the $(i,j)$th element of $T$ by $T_{ij}$. The value of $T_{ij}$ represents the probability of the event that the correct model changes from $M_i$ to $M_j$, i.e., $k = 1,\ldots,K, j = 1,\ldots,K$, in one time step. The specification of $T$ shown in Eqn. (12) corresponds to an assumption that the correct model changes infrequently (with probability 10% per time instance). Given $T$, the WTT operation defined by Eqn. (8) translates into

\begin{equation}
  w_{k,t|t-1} = \sum_{i=1}^{K} w_{i,t-1}T_{ik}, k = 1,\ldots,K.
\end{equation}

In contrast with operator II which is data-independent, this operator is data-dependent. The prior probability of a model at time $t$ relates closely to its posterior probability at time $t-1$, whose value depends on the data item received at time $t-1$.

4) Operator IV: As is shown above, the setup of a matrix like Eqn. (12) requires one to set values for $K^2$ elements. Usually, there is little information available for doing so. It is preferable to specify the MTM using a forgetting mechanism, which only requires to specify one value for a hyper-parameter termed forgetting factor. The basic idea of forgetting goes back to [28].

Denote the forgetting factor by $\alpha$, $0 < \alpha < 1$. Given $\alpha$, the WTT operation is defined to be

\begin{equation}
  w_{k,t|t-1} = \frac{w_{k,t-1}^{\alpha}}{\sum_{i=1}^{K} w_{i,t-1}^{\alpha}}, k = 1,\ldots,K.
\end{equation}

Such forgetting based method has been commonly used in the BDEMM framework. An empirical guideline for setting the value of $\alpha$ is to make it slightly below 1, corresponding to an assumption that the model transition process is smooth. This operator is preferable to operator III for cases where one is aware of that the model switching law is Markov, but does not have enough prior knowledge to specify an appropriate MTM.

5) Operator V: The last WTT operator assumes that the model-switching law can be described or approximated by a Pólya urn process, as proposed in [30]. Specifically, it sets

\begin{equation}
  w_{k,t|t-1} = \frac{\beta_k + \sum_{\tau=1}^{t-1} w_{k,\tau}}{\sum_{j=1}^{K} (\beta_j + \sum_{\tau=1}^{t-1} w_{j,\tau})}, k = 1,\ldots,K,
\end{equation}

where $\beta_k \in \mathbb{N}$ is a positive integer for $k = 1,\ldots,K$ preset by the modeler. According to Eqn. (15), the probability of switching to a particular model at one time instant depends on all weights this model has been previously received. It is shown that, by so doing, the Markovian switching assumption is broken, and a long-term memory for the correct model can be employed to improve the performance for some application cases [30]. This operator is better than the others for cases
where the model switching process is not Markovian but has a long-term memory structure that can be approximately characterized by a Pólya urn process.

D. Importance Sampling for Marginal Likelihood Estimation

To make the BDEMM framework work in practice, a crucial computing issue, namely the calculation of the marginal likelihood, i.e., Eqn. (7), should be addressed. The stochastic integral in Eqn. (7) may have an analytical solution for some special cases, in which the prior and the likelihood function are conjugate, while for most realistic cases, no such analytical solution is available. BDEMM employs importance sampling to seek an approximation of the marginal likelihood.

Here we use $\pi(x)$ to denote the product of the prior and the likelihood, which is proportional to the posterior associated with our target model $M$. The importance sampling method starts by specifying a proposal distribution $q(x)$ that is absolutely continuous with respect to $\pi(x)$. Given $q(x)$, the marginal likelihood of $M$ is shown to be

$$l(M) = E_q \left[ \frac{\pi(x)}{q(x)} \right],$$  \hspace{1cm} (16)

where $E_q$ denotes the expectation operation with respect to distribution $q$. Given a set of i.i.d. random samples $x^1, \ldots, x^N$ drawn from $q$, an unbiased and consistent Monte Carlo estimate of the marginal likelihood is

$$\hat{l}(M) = \frac{1}{N} \sum_{i=1}^{N} \frac{\pi(x^i)}{q(x^i)},$$  \hspace{1cm} (17)

where $\frac{\pi(x^i)}{q(x^i)} \triangleq \hat{w}^i$ is termed the importance weight.

The efficiency of the above estimator depends on the choice of the proposal $q$ [33]. A straightforward choice is to set $q$ as the prior. Then the estimator becomes the average of the samples’ likelihoods, as the prior cancels out in the numerator and denominator. An empirical guideline for designing $q$ is to make it approximate the posterior as much as possible in the shape [32]. Following this guideline, some adaptive importance sampling (AIS) methods have been proposed, which design $q$ iteratively in a data-driven manner [32], [34], [35]. When the posterior is highly multimodal, the annealing strategy can be embedded in AIS, which leads to the adaptive annealed importance sampling (AAIS) algorithm [36].

III. ALGORITHMS

Here I introduce three major types of algorithms developed underlying the BDEMM framework. The forms of these algorithms depend on the model structures, i.e., the structures of the state transition prior and the likelihood function. If they are both Gaussian, then Kalman filtering (KF) is most suitable for computing Eqns. (5)-(7) [37], [38]. For cases that involve nonlinear and/or non-Gaussian, the Sequential Monte Carlo (SMC) methodology is often adopted to provide an approximate estimation of the true answer [39], [40]. Except for the KF- and SMC-based BDEMM, I will also describe an algorithm termed instantaneous TEmporal structure Learning (INTEL) [9], which can be regarded as a Gaussian process time series (GPTS) model based implementation of the BDEMM theory. Each algorithm introduced here can select one WTT operator from those described in subsection III-C for use.

A. KF-based BDEMM

Assume that the state transition prior and the likelihood function at time instance $t$ given by $M_k$ are $\mathcal{N}(A_kx_{t-1}, Q_k)$ and $\mathcal{N}(B_kx_t, R_k)$, respectively, where $\mathcal{N}(\mu, \Sigma)$ denotes a Gaussian distribution with mean $\mu$ and covariance $\Sigma$. Suppose that $p_k(x_t|y_{1:t-1}) = \mathcal{N}(\hat{x}_{k,t-1}, \Sigma_{k,t-1})$, $k = 1, \ldots, K$, is available. Then Eqn. (5) translates into [37], [38]

$$p_k(x_t|y_{1:t-1}) = \mathcal{N}(\hat{x}_{k,t-1}, P_{k,t|t-1}),$$  \hspace{1cm} (18)

where $\hat{x}_{k,t-1} = A_k\hat{x}_{k,t-1}, P_{k,t|t-1} = A_k\Sigma_{k,t-1}A^T_k + Q_k, A^T$ denotes the transposition of $A$. Then Eqn. (6), which is used to compute the posterior distribution of $x_t$ associated with $M_k$, translates to be [37], [38]

$$p_k(x_t|y_{1:t}) = \mathcal{N}(\hat{x}_{k,t}, \hat{Z}_t, P_{k,t|t}),$$  \hspace{1cm} (19)

where $G_{k,t} = P_{k,t|t-1}B_k^T\Sigma_{k,t}^{-1}, \hat{Z}_t = y_t - B_k\hat{x}_{k,t}, A^{-1} \Sigma_{k,t} = B_kP_{k,t|t-1}B_k^T + R_k, P_{k,t|t} = P_{k,t|t-1} - G_{k,t}B_kP_{k,t|t-1}$. Since $p_k(x_t|y_{1:t-1})$ and the likelihood function are both Gaussian in the above setting, the marginal likelihood specified by Eqn. (7) becomes an integral of the product of two Gaussians, which can be solved numerically.

Given one WTT operator described in subsection III-C one can calculate $w_{k,t|t-1}$ via Eqn. (8), and then get $w_{k,t}$ via Eqn. (9). Then the set of $w_{k,t}, k = 1, \ldots, K$ is then used to calculate an average mean and covariance to be used in the next time step. In this way, the Gaussian mixture $\sum_{k=1}^{K} w_{k,t}p_k(x_t|y_{1:t})$ is approximated by one Gaussian, which is then used to initialize the $K$ Gaussian components for the next time step. Note that, if most of the Gaussian components in the mixture distribution have negligibly small weights, then the mixture distribution can be adequately approximated by a single Gaussian, otherwise, serious approximation error may appear. Here the major concern for approximating the Gaussian mixture with a single Gaussian is computational. By so doing, we preclude the number of Gaussian components in the posterior to exponentially grow over time.

B. SMC-based BDEMM

SMC employs a set of weighted samples to approximate a series of target distributions. Compared with KF, SMC does not restrict the model to be linear Gaussian. Assume that the posterior distribution of $x_{t-1}$ is approximated by a weighted sample set $\{x_{t-1}^i, w_{k,t-1}^i\}_{i=1}^{N}$, where $N$ denotes the sample size. That says

$$p_k(x_{t-1}|y_{1:t-1}) \approx \sum_{i=1}^{N} w_{k,t-1}^i \delta(x_{t-1} - x_{t-1}^i),$$  \hspace{1cm} (20)

where $\delta(x)$ takes value 1 if $x = 0$ and 0 otherwise. Now, let see how to obtain $w_{k,t}$ and $\{x_{t-1}^i, w_{k,t-1}^i\}_{i=1}^{N}$, which will be used for approximating $p(x_{1:t}|y_{1:t})$, based on $\{x_{t-1}^i, u_{t-1}^i\}_{i=1}^{N}$ and $w_{k,t-1}, k = 1, \ldots, K$. 

Given \( \{x_{i-1}^t, u_{i-1}^t\}_{i=1}^N \) and \( p_k(\mathbf{x}_t | \mathbf{x}_{t-1}) \), one can generate a new sample set \( \{x_{k,t}^i, u_{k,t}^i\}_{i=1}^N \), in which \( x_{k,t}^i \) is drawn from \( p_k(\mathbf{x}_t | \mathbf{x}_{t-1}) \). This new sample set approximates \( p_k(\mathbf{x}_t | \mathbf{y}_{1:t-1}) \) as below

\[
p_k(\mathbf{x}_t | \mathbf{y}_{1:t-1}) \approx \sum_{i=1}^N u_{i-1}^i \delta(\mathbf{x}_t - x_{k,t}^i). \tag{21}
\]

Following the importance sampling theory \cite{25}, we update the sample weight as below

\[
\bar{u}_{k,t}^i = \frac{u_{i-1}^i p_k(\mathbf{y}_t | x_{k,t}^i)}{\sum_{j=1}^N \bar{u}_{k,t}^j}, \quad i = 1, \ldots, N, \tag{22}
\]

\[
u_{k,t}^i = \frac{\bar{u}_{k,t}^i}{\sum_{j=1}^N \bar{u}_{k,t}^j}, \quad i = 1, \ldots, N, \tag{23}
\]

then the updated sample set \( \{x_{k,t}^i, u_{k,t}^i\}_{i=1}^N \) constitutes a Monte Carlo approximation to \( p_k(\mathbf{x}_t | \mathbf{y}_{1:t}) \) as below

\[
p_k(\mathbf{x}_t | \mathbf{y}_{1:t}) \approx \sum_{i=1}^N u_{k,t}^i \delta(\mathbf{x}_t - x_{k,t}^i). \tag{24}
\]

and \( \hat{x}_{k,t} \) can be computed based on the sample set \( \{x_{k,t}^i, u_{k,t}^i\}_{i=1}^N \) according to a prescribed criterion, such as ML, MAP or MMSE.

Given \( w_{k,t-1} \), one can select one WTT operator (see subsection II-C) for use to get \( w_{k,t+1} \), \( k = 1, \ldots, K \). Substituting Eqn. (21) into Eqn. (7), one obtains a Monte Carlo estimate of the marginal likelihood as follows

\[
p(\mathcal{M}_k | \mathbf{y}_{1:t}) \approx \sum_{i=1}^N u_{i-1}^i p_k(\mathbf{y}_t | x_{k,t}^i), \quad k = 1, \ldots, K. \tag{25}
\]

Then, substituting \( w_{k,t+1} \) and Eqn. (25) into Eqn. (9), one obtains \( \hat{\mathcal{S}}_k \), \( k = 1, \ldots, K \). Finally, the estimate of \( \hat{x}_i \) is available using Eqn. (4).

Based on the BDEMM setting, the posterior has a mixture form as follows

\[
p(\mathbf{x}_t | \mathbf{y}_{1:t}) = \sum_{k=1}^K w_{k,t} p_k(\mathbf{x}_t | \mathbf{y}_{1:t}). \tag{26}
\]

Substituting Eqn. (24) into the above equation, then one gets a Monte Carlo approximation to the posterior:

\[
p(\mathbf{x}_t | \mathbf{y}_{1:t}) \approx \sum_{k=1}^K \sum_{i=1}^N w_{k,t} u_{k,t}^i \delta(\mathbf{x}_t - x_{k,t}^i). \tag{27}
\]

To get rid of particle degeneracy \cite{41}, a resampling procedure is performed to draw a set of equally weighted samples from the augmented sample set

\[
\mathbf{D} \triangleq \{ \{x_{1,t}^i, u_{1,t}^i\}_{i=1}^N, \ldots, \{x_{K,t}^i, u_{K,t}^i\}_{i=1}^N \},
\]

which is used to approximate \( p(\mathbf{x}_t | \mathbf{y}_{1:t}) \) in Eqn. (27). Let reexpress \( \mathbf{D} \) as \( \mathbf{D} \triangleq \{ x_{j}^i, \bar{u}_j^i \}_{j=1}^{NK} \) for brevity in nomenclature. The resampling procedure consists of the following operations, which finally yield an equally weighted sample set \( \{x_{n,t}^i, 1/N\}_{n=1}^N \):

- For \( \forall n \in \{1, \ldots, N\} \):
  1) Draw a random sample \( v \) from the uniform distribution \( \mathcal{U}(0, 1) \).
  2) Find an index \( j \) that satisfies \( \sum_{i=1}^j \bar{u}_j^i \leq v \leq \sum_{i=1}^{j+1} \bar{u}_j^i \).
  3) Set \( x_{n,t}^i = \bar{x}_i^j \).

Readers are referred to \cite{42} for more details of resampling procedures popularly used in SMC.

The updated sample set \( \{x_{1}, 1/N\}_{1=1}^N \) and model weights \( w_{k,t}, k = 1, \ldots, K \) will be used in the algorithm iteration for the following time instance \( t + 1 \).

Note that the above procedure stands for a generic version of the implementation of SMC-based BDEMM. For some specific cases, the implementation can be simplified. For example, there exist cases wherein all models share the same state transition prior, e.g., in \cite{7, 8}. Then we only need to generate one renewed sample set \( \{x_{k,t}^i\}_{i=1}^N \) for approximating the posterior and estimating the marginal likelihood for each model, since this sample set can be shared for all models. Then the required overload of memory and computations can be reduced remarkably.

### C. The INTEL Algorithm

The INTEL algorithm \cite{9} combines the idea of GPTS modeling and BDEMM. It employs multiple weighted GPTS models together. The model weights are updated in the same way as shown in Eqns. (8), (9), while the model averaging operation is performed in terms of predictive distributions instead of point predictions. Specifically, each GPTS model yields a predictive Gaussian distribution of \( x_t \). Then a weighted generalization of the product of experts (POE) operation is used for combining those Gaussian distributions to generate the final prediction. In the setting of INTEL, the object to be predicted at time instance \( t \), namely \( x_t \), is the upcoming data point of the next time instance, i.e., \( y_{t+1} \).

Thanks to the elegant theoretical properties of Gaussian process (GP) (see details in \cite{43}), for each GPTS model, say \( M_k \), one can bypass the definition of the state transition prior and the likelihood function to compute its marginal likelihood \( p(M_k | \mathbf{y}_{1:t}) \) directly and analytically. Specifically, the GPTS model assumes that the observation \( y_t \) is Gaussian distributed as follows

\[
y_t = f(t) + \eta_t, \tag{28}
\]

where \( f \sim \mathcal{GP}(\mu, k_{\theta}), \eta_t \sim \mathcal{N}(0, \sigma_{\eta}^2) \). \( \mathcal{GP}(\mu, k_{\theta}) \) represents a GP with a mean function \( \mu(\cdot) \) and a covariance kernel function \( k_{\theta}(\cdot, \cdot) \) parameterized with \( \theta \). Then, given a historical dataset \( \{t, y\} \) wherein \( t = \{t - \tau + 1, \ldots, t\} \), \( y = \{y_{t-\tau+1}, \ldots, y_t\} \), one can derive that the predictive distribution of \( y_{t+1} \) is Gaussian with analytically solvable mean and variance. Here \( \tau \) denotes the length of the time window considered.

The basic idea underlying the INTEL algorithm is to employ multiple GPTS models together, each making use of a set of hyper-parameter values to capture one type of temporal structures of the data. Denote \( p_k(y_{t+1}) \) as the predictive distribution of \( y_{t+1} \) yielded by \( M_k \). The final predictive distribution given by the INTEL algorithm is

\[
p(y_{t+1}) \propto \Pi_{k=1}^K (p_k(y_{t+1}))^{w_{k,t+1}}, \tag{29}
\]
where $\omega_{t+1|t}$ is given by the WTT operation, see subsection IIC. Note that $p(y_{t+1})$ is also Gaussian with analytical solvable mean and variance. For more details on INTEL, readers are referred to [9].

IV. APPLICATIONS

In this section, I describe a number of classical applications of BDEMM that indicate its versatility.

A. Robust Tracking of Dynamic System States

1) Robust SMC methods: SMC methods, also known as particle filters (PFs), have dominated the field of nonlinear non-Gaussian state filtering, while their performance degrades rapidly when outliers appear temporarily in the measurements, due to sudden changes in the environment, e.g., the appearance of sensor faults. Such outliers have to be handled appropriately to avoid divergence. To this end, a robust PF (RPF) algorithm is proposed in [7], which is a type of SMC-based BDEMM method. The idea is to add a nominal Gaussian noise model as well as two heavy-tailed Student’s t noise models into the model pool, to take into account both regular observations and observations contaminated by outliers. Thanks to the dynamic model re-weighting mechanism given by BDEMM, when regular observations arrive, the nominal model becomes prevailing; while, once an outlier arrives, then the one heavy-tailed Student’s t model will be evoked and then dominate the filtering process. Therefore the influence of the outlier on the filtering performance is mitigated automatically.

The BDEMM type robust SMC methods indeed have found wide applications in different contexts [2], [3], [5], [6], [45]. For instance, a research team from German Aerospace Center and Karlsruhe Institute of Technology adapt the aforementioned RPF method to track a high-speed moving train using earth magnetic field distortion data [2]. A strong positive experimental result is reported, which shows that RPF is robust against periodic noise introduced by currents in the overhead line and distortions caused by passing trains or outdated values in the map of the magnetic field along the railway tracks. With aid of RPF, an overall performance corresponding to a root-mean-square-error (RMSE) below five meters is achieved with only the earth magnetic field distortion data. This performance is comparable to that obtained with the global navigation satellite system (GNSS).

In [5], a BDEMM-type SMC method is used for tracking the instantaneous frequency (IF) of a non-stationary signal. For that problem, the difficulty lies in the requirement to estimate the IF accurately online, while the IF may vary over time irregularly. In the BDEMM-type SMC method proposed there, six plausible IF evolution models are considered together. Then the BDEMM theory is adopted to deal with the uncertainty on which is the best one to use at each time instance. In that context, those candidate models have different state-transition priors but share the same nonlinear likelihood function. The proposed algorithm adopts a forgetting based WTT operator, and achieves a remarkable performance consistently over differing cases.

In [6], an SMC-based BDEMM type method is presented for tracking a moving object in a low-resolution video stream. In that case, two candidate models are used, corresponding to the color feature and the texture feature of the object to be tracked. They share the same state-transition prior that captures the temporal correlation in the sequence of frame images. The difference of the candidate models lies in the likelihood function since they use different features and each feature defines one specific likelihood function. The BDEMM theory allows one feature to take a larger effect when the other feature changes abruptly due to e.g., occlusion, the appearance of confusing colors. The proposed algorithm is shown to have a remarkable performance in terms of robustness, expressivity, and comprehensibility.

2) Robust KF: In [4], the authors consider how to accurately predict the output strip thickness online for a cold rolling mill. For that problem, several physically motivated models are available, but it is uncertain which is the correct one for use. A Markov chain model, specified in terms of forgetting, is used to characterize the temporal transition of the correct model. The resulting method, termed dynamic model averaging (DMA) there, is a kind of KF-based BDEMM in spirit. It is shown that DMA is better than the best physical model and that when the best model is included in the model pool, DMA converges to it quickly.

B. Dynamic Multi-Modal Data Fusion

Based on a model uncertainty perspective, a type of SMC-based BDEMM algorithm is proposed for robust multi-modal data fusion (RMMDF) in dynamic systems [8]. Such an RMMDF approach employs a set of candidate models, each representing a hypothesis on which modality (modalities) fails (fail). Once a modality failure happens, the RMMDF approach will down-weight the candidate models associated with the failing modality (or modalities) promptly, while simultaneously up-weighting the other candidate models, a property given by the underlying Bayesian formulation of BDEMM.

C. Robust GPTS based Online Prediction

For time-series online prediction, the presence of outliers and/or change points is one of the major obstacles to be bypassed, especially when the temporal structure of the data evolves over time. A robust online prediction algorithm is proposed in [9], which embeds multiple GPTS models into the BDEMM framework, each model characterizing one type of the temporal structure. The major part of the resulting algorithm, namely INTEL, is briefly introduced in subsection III-C. The robustness of that algorithm is demonstrated by extensive experimental results based on real data. See details in [2].

D. Bayesian Optimization

An INTEL type BDEMM algorithm, termed accelerated Bayesian Optimization (ABO), is proposed to address the following question: how to make use of low-fidelity (LF) data to accelerate a searching process that aims to find the
global optimum of a black-box objective function that is highly expensive to evaluate [10]. ABO works by dynamically weighting two candidate models, an LF GP model, and a high-fidelity (HF) GP model, similarly to INTEL. The weight of the LF GP model takes a larger value at the initial searching phase, as less HF data are available during that period. As more and more HF data are sampled and provided to update the HF GP model, the LF GP model is down-weighted gradually following Bayesian formalism. ABO thus provides an elegant way to harness LF data to accelerate the searching process of BO without compromise in searching quality.

E. Neural Decoding for Brain-Computer Interfaces

A non-stationary neural decoding approach termed dynamic ensemble modeling (DyEnsemble) is proposed for intracortical brain-computer interfaces (iBCIs) [11]. In contrast with other commonly used neural decoders, which assume a static mapping relationship from the neural signals to the motor intention, DyEnsemble allows such mapping relationship to vary over time by employing diverse measurement models that are dynamically weighted. It is shown that DyEnsemble is capable of remarkably alleviating the decoding performance degradation caused by noises, missing neural data, or changes in brain activities due to neuroplasticity. The decoding process of DyEnsemble is an SMC-based BDEMM procedure in spirit. Compared with other BDEMM methods, DyEnsemble is featured by its candidate model generation strategy, which is inspired by the dropout operation originally developed in [46].

F. A Toy Experiment

Here I present a toy experiment to showcase the basic features and advantages of BDEMM. Let consider a time-series experiment presented in [47]. The hidden state \( x \) underlying the time-series observations \( y \) evolves over time according to

\[
x_{t+1} = 1 + \sin(0.04\pi \times (t + 1)) + 0.5x_t + u_t, \quad (30)
\]

where \( u_t \) is a Gamma(3,2) distributed random noise item. The observation at time \( t \) relates to \( x_t \) in a way as follows

\[
y_t = \begin{cases} 
0.2x_t^2 + u_t, & t \leq 30 \\
0.2x_t - 2 + u_t, & t > 30
\end{cases} \quad (31)
\]

where \( u_t \) denotes the observation noise. The goal is to track the hidden state \( x_t \) in real-time based on noisy observations \( y_{1:t}, \ t = 1, \ldots, 60 \). In the original experiment presented in [47], \( n_t \) is assumed to be drawn from a known zero-mean Gaussian distribution. Let consider a more challenging case here, in which the distribution of \( n_t \) is time varying. Following [7], assume that \( n_t \) is drawn randomly from a uniform distribution between 40 and 50 for time steps \( t = 7, 8, 9, 20, 37, 38, 39, 50 \). At the other time steps, it is drawn from a known zero-mean Gaussian distribution. In the experiment, the algorithm agent is not aware of when the distribution of the observation noise deviates from the known zero-mean Gaussian and what distribution it follows when it deviates from the known zero-mean Gaussian.

I adapt the BDEMM based robust SMC algorithm presented in subsection [V-A1] to deal with the above task. It employs two member models, one corresponds to the hypothesis that \( n_t \) is zero-mean Gaussian distributed, and the other assumes that \( n_t \) is uniformly distributed between \(-50 \) and \( 50 \). I compare this robust SMC algorithm to the traditional single-model based SMC method. I consider two versions of the traditional SMC methods, one models \( n_t \) to be zero-mean Gaussian distributed, and the other models it to be uniformly distributed between \(-50 \) and \( 50 \).

Each algorithm is run 30 times independently. Table I presents their performances in terms of the mean square error (MSE). As is shown, BDEMM outperforms the others significantly. The posterior probabilities of the member models averaged over those 30 independent runs are plotted in Figure 1. As is shown, when the observation noise deviates from the default Gaussian distribution at time steps \( t = 7, 8, 9, 20, 37, 38, 39, 50 \), the posterior probability of the 2nd model is quickly increased by the algorithm agent. That means the algorithm agent can accurately detect the appearance of the abnormalities in the observations and quickly select the right model to be the dominated one.

| TABLE I | MEAN AND VARIANCE OF THE MSE CALCULATED OVER 30 INDEPENDENT RUNS FOR EACH ALGORITHM |
|---------|-----------------------------------------------|
|         | mean   | var    |
| BDEMM   | 0.58675 | 0.016263 |
| SMC I   | 0.61869 | 0.025482 |
| SMC II  | 0.65352 | 0.032834 |

Fig. 1. Averaged posterior probability of the member models outputted by the BDEMM based robust SMC method.

V. CONNECTIONS TO RELATED RESEARCH

From a modeling perspective, BDEMM is in concept closely related to the Markov switching system (MSS) or jump Markov system (JMS) model, which dates back to [48], [49]. There are a large number of variants or extensions of MSS, such as the conditional dynamic linear models [50], dynamic...
linear models with Markov switching [51], the interacting multiple model (IMM) [52], [53], state-space model with regime-switching [54], to name just a few. In such MSS type models, a set of continuous latent processes, usually formulated by state-space models, together with a discrete-time, discrete-state Markov model that captures the unobserved switching process of the prevailing model, are used for describing the generative process of the observations. The hierarchical structure of MSS allows it to capture many practical aspects of time series, such as outliers, nonlinearities, sudden maneuvers in target tracking, heteroscedasticity. However, most of existing works that adopt MSS use linear Gaussian model components, with a few exceptions in e.g. [55], [56]. That says, conditional on that the prevailing model is known, then the generative process of the observation is assumed to be linear Gaussian.

In contrast, BDEMM is more general and more expressive in at least two aspects. First, BDEMM allows the model structure to be either state-space or GPTS. Further, it allows each model component to be either linear Gaussian or nonlinear non-Gaussian. Second, BDEMM is more flexible in expressing the model switching process. It allows the prevailing model to be unchanged, corresponding to WTT Operator I, or to be switched over time, corresponding to WTT Operators II-V. Further, it allows different kinds of model switchings, such as the independent switching, the Markov type switching, the forgetting mechanism based switching, and the Pólya urn process based switching, corresponding to WTT Operators II, III, IV, and V, respectively.

From the algorithmic perspective, the KF-based BDEMM algorithm is equivalent to KF methods applied to the MSS type models, such as the IMM KF [57]. There are two major issues that deserve special attentions when applying them to address practical problems. The first is the gross approximation of a Gaussian mixture form posterior distribution by a single Gaussian component at each time step. This can be improved by using a parsimonious mixture with a fixed number of Gaussian components to approximate the posterior. The second issue is that the conditional linear system assumption underlying such methods is hard to hold in practice. One can replace the routine KF with the extended KF method to deal with conditional nonlinear systems, as proposed in [58]. A more general solution to address nonlinear non-Gaussian issues is of course via SMC methods. By extending the KF-based BDEMM algorithm with SMC, We get the SMC-based BDEMM algorithm.

The SMC-based BDEMM algorithm has straightforward connections to SMC approaches for MSS, which add the mode (regime) variable into the state vector, and then apply SMC to this augmented state [59], [60]. For the latter, numerical problems are likely to appear when one mode’s probability is very low, and then only few alive particles are assigned to it. An IMM based PF algorithm is proposed in [61], which resolves the above issue, while it always approximates the posterior using a finite Gaussian mixture, thus may lose accuracy due to the approximation error that can be accumulated over time. In contrast, the SMC-based BDEMM algorithm has neither the aforementioned numerical problem nor the limitation caused by the finite Gaussian mixture approximation. Recently, the particle Gibbs sampling [30] and variational inference [62] methods have also been introduced into the regime-shifting state space models. These works can be regarded as alternative implementations or algorithmic extensions of the BDEMM framework.

The GPTS-based BDEMM, namely the INTEL algorithm [9], shows the potential of BDEMM to address non-state-space models. Before the appearance of INTEL, most of GPTS based algorithms resort to a complex model structure to capture possible regime shifts in the future observations [44], [63]–[66], e.g., a student’s t based observation model [67] or a non-stationary kernel function [68], which then leads to the absence of an analytical inference solution. The BDEMM framework provides a way to get rid of using any complex model structure by employing a set of simple, analytically solvable models, which renders the resulting INTEL method to own a rich modeling capacity to cover complex temporal structures as well as a much higher computational efficiency.

Finally but not least, BDEMM has a connection to forecasting theories and techniques, which have been widely used in operations, economics and finance, energy industry, environmental research such as forecasting of climate change. See [68] for an encyclopedic review of the forecasting models, methods, and applications. In concept, forecasting is a broader concept that covers different types of predictions, e.g., temporal and spatial predictions. BDEMM can be treated as a specific type of forecasting technique applicable for robust sequential online prediction based on the time series type data.

VI. Open Resources

Here I introduce some open resources for implementing the BDEMM-type algorithms.

Currently, RPF and RMMDF, as presented in subsections IV-A1 and IV-B, have open-sourced codes released at [https://github.com/robinlau1981/dmapf] and [https://github.com/robinlau1981/fusion].

As presented in Section III importance sampling plays a key role in estimating marginal likelihoods of models. AAIS is an advanced importance sampling method featured by its powerful capability for multimodal posterior exploration [59]. A Matlab code of AAIS is available at [https://github.com/robinlau1981/AAIS]. Codes to implement another AIS algorithm, termed layered AIS [69], can be found at [http://www.lucamartino.altervista.org/Code.LAIS_non_iterative.pdf].

For SMC, I recommend Matlab codes of Nando de Freitas, which are available at [http://www.cs.ubc.ca/~nando/software/upf_demos.tar.gz].

Nicolas Chopin shares an SMC python library at [https://nc chopin.github.io/software] which implements differing versions of SMC described in [70].

For GP, a resource pool that consists of a large volume of software, papers, books, and events can be found at [http://www.gaussianprocess.org/].
VII. DISCUSSIONS

In this section, I discuss practical issues that may be encountered when applying the BDEMM framework. I also point out open problems that are worth further research.

A. Advanced WTT Operators

The WTT operator plays a key role in the BDEMM framework. It is this operator that connects the sequentially performed BMA operations. It determines the prior probabilities of each candidate model at each time instant. The current BDEMM framework encompass five WTT operators for choice, as shown in subsection III-C Each operator corresponds to a prior assumption of the model switching law. In the current BDEMM framework, it is the modeler who determines beforehand which operator to use for the current task, while how to select an appropriate WTT operator for use remains unaddressed. Besides, despite that the existing operators can cover most realistic cases, one may encounter new cases for which no existing operator is suitable. It is thus desirable to develop an adaptive approach to do the operator selection, or even to design an appropriate operator online.

B. How to Build up the Candidate Models?

As described above, one major feature of BDEMM is the use of a set of candidate models. A natural question is how to build up such models beforehand.

In some cases, the candidate models can be already known beforehand, see e.g. in [4], [5], where each model corresponds to a physical hypothesis.

In more general cases, one may only have a nominal model beforehand, which will be used by default. For example, in most application scenarios of the KF algorithm, the measurement noise model is fixed to be a zero-mean Gaussian with a fix valued variance. The modeler can a priori know that there may be outliers appearing at some time instances. Then the modeler can build up another candidate model via adjusting the nominal one by e.g., enlarging its variance value or modifying its form to be heavy-tailed student’s t, as proposed in [7].

There are also cases in which what the modeler has beforehand is some historical data, not a nominal model. For such cases, if there is no domain knowledge for use, then one can use a data-driven approach to build up the candidate models. For instance, in [71], each candidate model corresponds to a specific segmentation of the historical data. The parameter values of each candidate model is set via a Bayesian optimization procedure that maximizes the log-likelihood of the data within this segmentation. If there is some domain knowledge for use, then the modeler can combine the data and the domain knowledge to build up the candidate models. For example, one can build up a nominal model at first by fitting it to the historical data, then build up other candidate models by parameter perturbations on the nominal model based on the domain knowledge. For instance, both the DyEnsemble method [11] and the INTEL algorithm [9] adopt the perturbation strategy. The difference lies in that the former uses a stochastic perturbation inspired by the dropout operation originally developed in the context of deep artificial neural networks [46], while the latter performs a deterministic perturbation.

There are three recognized Bayesian perspectives for quantification of model uncertainty, which are known as M-closed, M-complete, and M-open [72]. The M-closed perspective assumes that the correct model is among the candidate models under consideration, while in the other two perspectives, the correct model is outside of the candidate model pool. As a dynamic extension of BMA, BDEMM follows the M-closed perspective. In theory, the classical BMA theory is no longer applicable for the M-complete and M-open frameworks [73], [74]. An open question for BDEMM is thus how to generalize it to be applicable for the M-complete and M-open frameworks.

C. More Advanced Inference Algorithms

For most of current algorithms developed within the BDEMM framework, standard versions of KF and SMC are used as the major inference engine. It is interesting to investigate approaches to combine other type inference methods, e.g., variational inference [62], [75], [76], particle flow [77], approximate Bayesian computation [78]–[80], with BDEMM, to yield more advanced inference algorithms for robust online prediction with non-stationary time series data.

VIII. CONCLUSIONS

As a dynamic extension of the BMA theory, BDEMM has found a wide range of successful applications in sequential online prediction problems. However, there has yet been an article in the literature that can give a full introduction to BDEMM. For the first time, this paper gives a concise while comprehensive introduction to BDEMM, including the related basic theories, its algorithmic implementations, its applications in different contexts, its connections to related research, open resources to implement it, and a discussion of practical issues for applying it, and several open problems that are worth further research. This paper provides a parsimonious information accumulation and organization for BDEMM, instead of an exhaustive literature review, as the aim is to let readers learn about it comprehensively, quickly and conveniently. Hopefully this effort can make the paper more readable, then stimulate more theoretical or applied research on BDEMM.

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