We introduce a method for inferring and predicting latent states in the important and difficult case of state-space models where observations can only be simulated, and transition dynamics are unknown. In this setting, the likelihood of observations is not available and only synthetic observations can be generated from a black-box simulator. We propose a way of doing likelihood-free inference (LFI) of states and state prediction with a limited number of simulations. Our approach uses a multi-output Gaussian process for state inference, and a Bayesian Neural Network as a model of the transition dynamics for state prediction. We improve upon existing LFI methods for the inference task, while also accurately learning transition dynamics. The proposed method is necessary for modelling inverse problems in dynamical systems with computationally expensive simulations, as demonstrated in experiments with non-stationary user models.
but not to cases, where \(h_\theta\) is non-linear and cannot be sampled, and where the simulators are computationally expensive, as in system simulation experiments in meteorology [14, 15], simulation-based forecasting in cosmology [16, 17] or adaptive modelling of human behaviour [18, 19].

Current LFI methods for dynamical systems [20, 21] proceed by assuming some simplified form of transition dynamics in an SSM. However, unless the SSM is both linear and Gaussian, this approach leads to poor state value estimates. This issue has been addressed in a large and growing set of methods, including extended Kalman filters [22–24], GP-SSMs [25, 26], sequential Monte Carlo [27–30] and Bayes filtering [27, 31–33] methods in general. Unfortunately, when the latent states have the additional requirement of being valid simulator parameters, these methods need a tractable likelihood that is not available when the observation model is black-box. At the same time, recent works on LFI in SSMs have focused on more efficient sampling-based methods [34], generation of better matching statistics [35], and on establishing theoretical convergence guarantees [21, 36, 37]. Despite these advances, the problem of sample-efficient LFI in non-linear non-Gaussian SSMs remains unsolved.

In this paper, we introduce a method capable of likelihood-free state approximation and state prediction in discrete-time SSMs. We assume that the state transition model is unknown and can be non-linear, and that the number of samples from the observation model must be limited to be small, since simulations are computationally expensive. To solve the LFI problem in SSMs, we need to simultaneously estimate simulator parameters for observed measurements sample-efficiently, and the transition dynamics, which is required for state prediction. We propose a method, which uses a non-parametric multi-objective model for LFI of states, and a non-parametric model of transition dynamics for learning state transition dynamics. The contributions of the paper are:

- We solve the problem of state prediction in SSMs with unknown transition dynamics and limited simulation budget. We use samples from the LFI posterior approximations to accurately learn the state transition dynamics, as shown by comparisons with state-of-the-art SSM inference techniques.
- Focusing on problems where LFI has to be sample-efficient, we improve upon the current LFI methods for the state inference task by leveraging time-series information. This is done by using a multi-objective surrogate for the consecutive states and sampling from a transition dynamics model to determine where to run simulations next.
- We demonstrate that the proposed method is needed to tackle the crucial case of user modelling, where user models are non-stationary because user’s preferences and abilities change over time.

2 Background

For LFI of states, we follow the Bayesian optimization for LFI (BOLFI) approach [38], in which a Gaussian process (GP) surrogate is used for a discrepancy measure \(\delta\) (e.g. Euclidean distance) between an observed measurement \(x^*\) and synthetic observations \(x^{(i)}\). This approach assumes that if synthetic observations have a small discrepancy (smaller than a user-defined threshold \(\epsilon\)), they were produced by simulator parameters that could plausibly replicate the observed measurement. In this way, the posterior can be approximated as

\[
p(\theta|x^*) \propto F\left(\frac{\epsilon - \mu(\theta)}{\sqrt{\nu(\theta)} + \sigma^2}\right) p(\theta),
\]

where \(F(\cdot)\) is a Gaussian CDF with mean 0 and variance 1, \(\mu(\theta)\) and \(\nu(\theta)\) are the mean and standard deviation of the GP surrogate, and \(\sigma\) is a likelihood noise of the GP. Also note that the discrepancy \(\delta\) depends on \(x^*\) resulting in \(\mu(\theta)\), \(\nu(\theta)\) and \(\sigma\) depending on it as well, see Section 6.3 [38] for more details.
Figure 2: An overview of our approach, in which the $\tilde{\delta}$ surrogate is used for LFI and $\tilde{h}_\theta$ for the unknown transition dynamics. The $\tilde{\delta}_\theta$ models the corresponding discrepancies of several observations (green) inside a moving window (here, with the size of two), from which posteriors are extracted according to Equation (1). $\tilde{h}_\theta$ is trained with paired samples from posteriors of consecutive states (grey); its predictive samples are used as proposals (orange) for future simulations.

A main advantage of modelling the discrepancy with a GP is the uncertainty estimation. The GP predictive mean $\mu(\theta^{(i)})$ and variance $\nu(\theta^{(i)}):=k(\theta^{(i)},\theta^{(i)})$ are used to calculate the utility (e.g., Expected Improvement [39]) of sampling the objective function at the next candidate parameter value $\theta^{(i)}$. By maximizing this so-called acquisition function $A(\cdot)$ with respect to $\theta^{(i)}$, one chooses where to run simulations next. Because BOLFI actively chooses where to run simulations, its posterior approximation requires much fewer synthetic observations than other LFI methods. However, BOLFI was not designed for SSMs, and hence, does not make use of any temporal information that is typical for SSMs to improve the quality of inference.

An alternative approach to sample-efficient LFI is sequential neural estimation (SNE), which proceeds by learning the statistical relationship between observations and parameters directly through a neural network surrogate. This surrogate does not require retraining when the observation changes, which makes SNE methods especially suitable for series of inference tasks. The SNE neural network can be used as a surrogate for the posterior, likelihood or likelihood ratio, resulting in SNPE [40–42], SNLE [43], and SNRE [44, 45] methods respectively. These SNE methods address a more difficult problem than we do, of learning a model across all possible tasks. The price is that they require significantly more simulations than BOLFI, see Section 4.3 [46].

3 Likelihood-Free Inference in State-Space Models

In this section, we introduce a multi-objective approach to LFI in SSMs, which improves sample-efficiency of existing methods by using temporal information of SSMs while also learning the unknown transition dynamics. The main elements of the solution are presented in Figure 2. To estimate state values $\theta_i$, given $x_i$, we employ a multi-objective surrogate $\tilde{\delta}$ for discrepancies, and then extract the LFI posterior with (1). At the same time, we form pairs of consecutive posterior samples and train a non-parametric surrogate for the state transition $\tilde{h}_\theta$, whose predictive posterior proposes candidates for future simulations. We summarize our approach in Algorithm 1.

3.1 Multi-Objective State Inference

As an extension to BOLFI, we employ a multi-objective surrogate model for the discrepancies $\delta_i$, thus considering multiple discrepancy objectives at the same time and leveraging information between consecutive states. More specifically, we pass discrepancy parameters of the consecutive states to the surrogate separately, but through the use of shared parameters of the multi-objective surrogate they become associated. This approach allows using a discrepancy model of the previous state to infer the current state value, instead of simply discarding it. Moreover, it allows having a much more flexible surrogate for LFI than the traditional GP used in BOLFI. These changes do not need any additional data.
We propose to train this model in an autoregressive fashion by forming a training set from paired sample points from 

\[ p(X_{t-1}, X_t) \]

While we gradually improve LFI posterior approximations 

\[ L \]

When we have a new observation, we simply need to recalculate the discrepancy values for all synthetic observations.

3.2 Learning State Transition Dynamics

When new observations present themselves and can be actively used throughout state inference for determining where to take the uncertainty associated with posterior approximations into account and be flexible enough to follow possibly non-linear transition dynamics.

\[ \text{Algorithm 1 Multi-Objective LFI with Transition Dynamics Model} \]

\[
\text{Input: observations } \{x_1, ..., x_T\}, \text{ observation simulator } g_\theta, \text{ moving window size } L, \text{ simulation budget } b_{\text{sim}}, \text{ prior } p(\theta); \\
\text{Output: state posterior approximation } P, \text{ transition dynamics model } h_\theta;
\]

set \( P = \emptyset \); initialize \( h_\theta \);
get initial simulations: \( x = g_\theta(\theta), \theta \sim p(\theta) \);
for \( t = L \) to \( T \) do
    calculate discrepancies \( \delta_t \) inside a moving window \( i = \{t - L...t\} \) for all simulations;
    train \( \delta_t \) on \( \{\theta, \delta_t\} \);
    extract posteriors \( p(\theta_i|x_i) \) with Equation (1);
    update \( h_\theta \) with pairs \( \{\theta_j^{(1:K)}, \theta_{j+1}^{(1:K)}\}_j \), where \( \theta_j^{(1:K)} \sim p(\theta_j|x_j) \);
    get \( b_{\text{sim}} \) new simulations \( \hat{x} = g_\theta(\theta), \theta \sim h_\theta(\theta_{t+1}|\theta_t) \);
    add to the set \( x \leftarrow \hat{x} \) and \( \theta \leftarrow \theta \);
end for

Once we have a trained surrogate for discrepancy objectives, we infer state posteriors \( p(\theta_t|x_t) \), similarly as in BOLFI.

There is an additional challenge for adapting multi-objective surrogates in SSMs, namely high computational cost associated with considering too many objectives. SSMs can potentially have hundreds of observations, and expanding the number of considered objectives may be detrimental for the performance of the surrogate. We avoid this problem by limiting the number of objectives the surrogate can have. Instead of considering all available time-steps as objectives, we propose to consider only \( L \) recent objectives by gradually including new objectives and discarding old ones that have little impact on current states. The size of this moving window depends on how rapidly the transition dynamics change. As the size \( L \) of the window grows, the model becomes less sensitive to the noise from the dynamics, at the cost of increased computations and decreased adaptability to the most recent state transitions. Overall, the moving window reduces the number of objectives \( L \) considered at a time, making multi-objective modelling for SSMs feasible.

In the Supplement, we further investigate the influence of the moving window size hyperparameter on state inference and prediction.

\[ p(\theta_{T+1}|x_T) = \int h_\theta(\theta_{T+1}|\theta_T)p(\theta_T|x_T)d\theta_T. \]
Figure 3: Graphical representation of the LMC. The discrepancy outputs $\delta_t^{(1:L)}$ are modelled as a linear combination of latent functions $u_q$. The model shares the same parameter values $\theta^{(1:L)}$ between all objectives.

This way, the state transition model $\hat{h}_\theta$ does not inform state posteriors directly, but only provides simulation candidates for the LFI surrogate. Ultimately, accumulating more simulations improves the discrepancy surrogate for the LFI of states and, by extension, quality of posterior samples, while higher-quality posterior samples allow more accurate learning of state transition dynamics.

3.3 Computational Complexity and Model Choices

The proposed multi-objective approach to LFI requires choosing surrogate models. Here, we present the model choices for our approach, followed by a resulting complexity analysis of the Algorithm 1.

Following the requirements for the surrogates from Sections 3.1 and 3.2, we chose a linear model of coregionalization (LMC) \cite{47} as a multi-objective surrogate for discrepancies and a Bayesian Neural Network (BNN) \cite{48,49} as a surrogate for state transition dynamics. LMC is one of the simplest multi-objective models that expresses each of its $L$ outputs $f_l$ as a linear combination $f_l(\theta^{(1:L)}) = \sum_{q=1}^{Q} a_{l,q} u_q$, as shown in Figure 3, where the $u_q \sim GP(0, k(\theta, \theta'))$ are latent GPs and the $a_{l,q}$ are linear coefficients that need to be solved. As regards BNN, it can be represented as an ensemble of neural networks, where each has its weights $w^{(h)}$ drawn from a shared, learnt probability distribution \cite{50} with $w^{(h)} \sim N(\mu^{(h)}, \log(1 + \rho^{(h)}))$, where $\rho^{(h)}$ and $\mu^{(h)}$ are the hyperparameters that require training.

Given the aforementioned model choices, the resulting computational complexity of the Algorithm 1 is dominated by three major stages: training of the multi-objective surrogate $\tilde{\delta}_\theta$, posterior extraction from discrepancy surrogates (Equation 1) and training of the transition dynamics model $\tilde{h}_\theta$. Starting with the cost of training $\tilde{\delta}_\theta$, it depends on the number of synthetic observations $I$, on the size of the moving window $L$ and on the user-specified number $M$ of inducing points \cite{51} for the LMC, resulting in the complexity $O(NLM^2)$, as opposed to $O(NM^2)$ by traditional GPs used in BOLFI. Moving on to the posterior extraction, this stage consists of finding the appropriate $\epsilon$, and then applying Equation 1, which is bounded by the complexity of calculating the variance of the surrogate for each of the $S_1$ samples from the prior, resulting in $O(LM^2S_1)$. Finally, if we apply variational inference \cite{52} to training of the transition dynamics model $\tilde{h}_\theta$, the computational cost is linear in the number $W$ of BNN parameters – $O(WKES_2)$, where $K$ is the overall amount of training data for $\tilde{h}_\theta$, $E$ is the number of epochs, and $S_2$ is the number of parameter samples from the posterior distribution that is required to get the distribution of outputs. Depending on the choice of hyperparameters, the computational complexity of the Algorithm 1 is bounded by either $O(NLM^2)$, $O(LM^2S_1)$ or $O(WKES_2)$. We provide recommendations for choosing these hyperparameters in the supplement.

4 Experiments

We assess the quality of our method for state inference and prediction tasks in a series of SSM experiments, where a simulator serves as the observation model $g_\theta$. In the experiments, our method uses the surrogate choices of LMC
and BNN, as was described in Section 3.3. We demonstrate that it can accurately learn state transition dynamics and improve upon existing LFI methods for the state inference task. Moreover, we investigate sample-efficiency of the proposed method and demonstrate its effectiveness in non-stationary user modelling case studies.

4.1 Experimental setup

We simulated time series of observations based on single sampled trajectories from true transition dynamics of five SSMs, as described in Section 4.2. Our goal was to estimate the simulator parameters that likely produced these observations, and learn the model of transition dynamics for state prediction based on the sampled trajectory.

For the state inference task, we compare the quality of state estimates by our approach against other LFI methods: BOLFI [38], SNPE [40], SNLE [43], SNRE [44]. We use a fixed simulation budget for all these methods, with 20 simulations to initialize the models, and then with 2 additional simulations for each new time-step. For the SNE approaches (SNPE, SNLE, SNRE), we provided all simulations at once, since that is their intended mode of operation. As for the prediction task, we sampled trajectories from the transition model and evaluated them against trajectories from the true dynamics. We performed these experiments in SSMs with simulators that have tractable likelihoods, providing the ground-truth likelihoods to the state-of-the-art SSM inference methods GP-SSM [26, 53] and PR-SSM [54], while our method was still doing LFI. For all methods in the prediction task, we provided 50 observations, and then sampled trajectories that had the same length of 50 time-steps.

We also compared two variants of our method that differ only in the way the next simulations are sampled: LMC-BLR, where samples were taken from Bayesian linear regression (BLR) models that linearized the transition dynamics along 50 observed time-steps; and LMC-qEHVI, where a popular acquisition function for multitask BO, q-expected hypervolume improvement (qEHVI) [55], was used to provide samples. The role of these variants was to evaluate how the choice of the future simulations impacts the quality of state inference and prediction.

All models were assessed in terms of the root-mean-square error (RMSE) between the state estimates and their ground-truths. The experiments were repeated 30 times with different random seeds. Additional details on implementation of the methods and all code for replicating the experiments are provided in the Supplement.

4.2 The State-Space Models

In this section, we present two case studies with non-stationary user models and three SSMs with tractable likelihoods. In user modelling experiments, we simulated behavioural data from humans that completed a certain task in two different experiments, described in Sections 4.2.1 and 4.2.2. During the first task, the user searched for a target on a display and the search time was measured. For the second task, the user evaluated dataset embeddings for a classification problem, and the evaluation score was used as behavioural data. Our task in the experiments was to track the changing parameters of user models and learn their dynamics.

In addition to non-stationary user models, we also experimented with three models with tractable likelihoods, common in SSM literature: linear Gaussian (LG), non-linear non-Gaussian (NN) and stochastic volatility (SV) models. In the LG model, the state transition dynamics and observation model are both linear, with high observational noise. The NN model is a popular non-linear SSM [56], where each observation has two unique solutions. Lastly, we used the SV model [57], which is used for predicting volatility of asset prices in stock markets [58, 59]. The dimensionality of states in these models ranges from one to three. We provide full descriptions of these SSMs in the Supplement.

4.2.1 UMAP Parameterization

With the first non-stationary user model, we infer uniform manifold approximation and projection (UMAP) [60] parameters that best satisfy human subject’s needs. We assume that the subject uses UMAP to generate low-dimensional data representations for a classification task, and that their preferences change with time. Specifically, in the beginning, the subject does not have any prior knowledge of the dataset, so data exploration takes the priority. As they become more familiar with the data, the priority gradually shifts from exploration to maximizing classification accuracy of their model. Our hypothesis is that by modelling the change in subject’s preferences, we can anticipate the preferences and propose good UMAP parameter candidates faster to the human user.

For this experiment, the subject’s needs are simulated by an evaluation function that takes the embedding of the handwritten digit dataset [61] as an input and assigns a corresponding preference score. The evaluation function is based on the weighted sum of the density based cluster validity (DBCV) score \(U_i^{(i)}\) [62] and the c-support vector classification (SVC) [63, 64] accuracy \(P_i^{(i)}\). By regulating the weight \(w_t\), one can prioritize data exploration \(U_i^{(i)}\) or maximization of a classification accuracy \(P_i^{(i)}\) with...
\[ \delta_t^{(i)} = (1 - w_t) U_t^{(i)} + w_t \mathcal{D}_t^{(i)}, \quad w_t = \frac{1}{1 + e^{-0.1(t-25)}}. \]  

We assume the subject cannot explicitly specify the ideal embedding, and hence the SSM observations \( x_t \) are latent. But since the subject has the ability to evaluate embeddings with the preference score, we model the preference score \( \delta_t^{(i)} \) directly as an objective. The goal is to infer the state values \( \theta = \{ \theta_d, \theta_{dist}, \theta_n \} \) of the UMAP parameters: the dimension of the target reduced space \( \theta_d \), an algorithmic parameter \( \theta_{dist} \) that controls how densely the points packed, and the neighbourhood size \( \theta_n \) to use for local metric approximation. In summary, the UMAP algorithm serves as an observation model and the transition dynamics are unknown, but implicitly regulated through (3). We use uniform priors for states throughout the experiments:

\[
\begin{align*}
\theta_d &\sim \text{Unif}(1, 64) \in \mathbb{Z} \\
\theta_{dist} &\sim \text{Unif}(0, 0.99) \in \mathbb{R} \\
\theta_n &\sim \text{Unif}(2, 200) \in \mathbb{Z}.
\end{align*}
\]

Details on the implementation of the UMAP algorithm and preference score are in the Supplement.

### 4.2.2 Eye Movement Control For Gaze-Based Selection

For the second non-stationary user model, we infer properties of human gaze in a series of simulated eye movement control trials [65, 66]. In these trials, the user model of the human searches for a target on a 2D screen by performing eye movements (saccades), based on its beliefs about the target location and information from peripheral vision. When the gaze location matches the location on the screen, the task is considered complete and a new target appears. As the human subject performs more tasks, they get weary, which results in an increasing latency between saccades \( \theta_l \). We believe that modelling the dynamics of eye movement latency will allow robust inference of the individual characteristics that are independent of weariness.

The subject needs several moves to reach the target because the actions and observations are corrupted with two noise sources: the ocular motor noise \( \theta_{om} \) and the spatial noise of peripheral vision \( \theta_s \). The quantitative values for these two variables vary for each individual, while the saccade latency \( \theta_l \) varies between different trial instances. We assess the performance of the subject based on total time \( x \in \mathbb{R} \) it took for the gaze to reach the target,

\[ x_t = \sum_e (2.7 A_e^{(e)} + \theta_{l,t}), \quad \theta_{l,t} = 12 \log(t + 1) + 37. \]

Here, the \( x_t \) are SSM observations, \( \theta = \{ \theta_{om}, \theta_s, \theta_l \} \) are state values that need to be inferred, \( A_e^{(e)} \) is the saccade amplitude, and \( e \) is the saccade index. The increase of the latency \( \theta_l \) serves as state transition dynamics \( h_l \) that needs to be modelled for prediction, while eye movement control task environment is considered as an observation model \( g_\theta \). To produce behavioural data, ground truth values of 0.01 and 0.09 for \( \theta_{om} \) and \( \theta_s \) respectively were used in the observation model. Finally, we calculate a Euclidean distance directly applied to \( x \) as a discrepancy and use the following priors for the states:

\[
\begin{align*}
\theta_{om} &\sim \text{Unif}(0, 0.2) \in \mathbb{R} \\
\theta_s &\sim \text{Unif}(0, 0.2) \in \mathbb{R} \\
\theta_l &\sim \text{Unif}(30, 60) \in \mathbb{R}.
\end{align*}
\]

The user model was implemented with reinforcement learning by [67]. More details on implementation can be found in the Supplement.

### 4.3 Results and Analysis

The results for the inference and prediction tasks are presented in Tables 1 and 2 respectively. The lower the RMSE, the better is the quality of estimation. In the inference task, LMC-based methods clearly outperformed BOLFI and SNE approaches. This indicates that considering multiple objectives at the same time was beneficial for the state
Table 1: Comparison of LFI methods (rows) in different SSMs (columns) for the state inference task. The performance was measured with 95% confidence interval (CI) of the RMSE between estimated vs ground truth state values for 50 time-steps. The best results in each column are highlighted in bold.

| Methods   | LG    | NN    | SV    | UMAP   | Gaze   |
|-----------|-------|-------|-------|--------|--------|
| LMC-BNN   | 1.77 ± 0.12 | 6.92 ± 0.51 | 16.14 ± 3.27 | **58.24 ± 3.62** | 58.7 ± 5.4 |
| LMC-BLR   | **1.3 ± 0.1** | **6.86 ± 0.54** | **13.15 ± 3.25** | 59.19 ± 3.31 | 60.6 ± 5.8 |
| LMC-qEHVI | 1.5 ± 0.1 | 7.03 ± 0.55 | 24.4 ± 2.5 | 64.96 ± 3.72 | **56.9 ± 4.5** |
| BOLFI     | 1.55 ± 0.15 | 7 ± 0.6 | 27.35 ± 3.45 | 84.31 ± 3.54 | 73.45 ± 5.75 |
| SNPE      | 7.15 ± 0.65 | 18.2 ± 0.93 | 77.4 ± 3.1 | 74.13 ± 3.21 | 68.1 ± 7.8 |
| SNLE      | 6 ± 0.5 | 10.35 ± 0.64 | 54.25 ± 2.45 | 71.45 ± 3.44 | 77.25 ± 4.05 |
| SNRE      | 10.4 ± 1.7 | 17.93 ± 1.34 | 57.15 ± 2.35 | 75.85 ± 1.26 | 80.75 ± 1.35 |

Table 2: Comparison of transition dynamics models (rows) in different SSMs (columns). The performance was measured with 95% CI of the RMSE between sampled vs ground truth trajectories of length 50. The best results in each column are highlighted in bold.

| Methods   | LG    | NN    | SV    | UMAP   | Gaze   |
|-----------|-------|-------|-------|--------|--------|
| LMC-BNN   | 210 ± 4 | 148 ± 2 | 117 ± 21 | **1394 ± 27** | **1365 ± 3** |
| LMC-BLR   | 64 ± 7 | 154 ± 4 | **100 ± 37** | 1409 ± 49 | 1372 ± 3 |
| GP-SSM    | 284 ± 71 | 2204 ± 111 | 3206 ± 1175 | - | - |
| PR-SSM    | 253 ± 68 | 610 ± 510 | 1378 ± 740 | - | - |

Table 3: Time comparison of LFI methods (rows) in different SSMs (columns) for training 50 time-steps. The running time is shown in minutes along with 95% CI. The best results in each column are highlighted in bold.

| Methods   | LG    | NN    | SV    | UMAP   | Gaze   |
|-----------|-------|-------|-------|--------|--------|
| LMC-BNN   | 87.6 ± 2.6 | 79.2 ± 1 | 81 ± 2.9 | 171.2 ± 5 | 408 ± 8 |
| LMC-BLR   | 82.1 ± 5.5 | 48.2 ± 0.8 | 93.5 ± 4 | 149.4 ± 4.5 | 442.5 ± 8.8 |
| LMC-qEHVI | 25.5 ± 1.5 | 23.9 ± 0.5 | 24.7 ± 0.7 | **116 ± 4.6** | **347.2 ± 7.3** |
| BOLFI     | 1.1 ± 0 | 1 ± 0 | 1.7 ± 0.1 | 129.3 ± 11.7 | 369.5 ± 16.5 |
| SNPE      | **0.1 ± 0** | **0.1 ± 0** | **0.4 ± 0** | **0.4 ± 0** | **0.4 ± 0** |
| SNLE      | 119.4 ± 2.9 | 137.3 ± 5.8 | 355.3 ± 23.1 | 582.7 ± 23.8 | 1003.4 ± 92.4 |
| SNRE      | 34 ± 1.5 | 35.4 ± 0.3 | 110.2 ± 6.1 | 309.6 ± 8.6 | 446.4 ± 14 |

Figure 4: The performance of LFI methods for the state inference tasks with various simulation budgets in two non-stationary user modelling experiments. The box plots were computed from 30 repetitions with different random seeds. The horizontal line on box plots shows the median, the bar shows upper and lower quartiles, and the whiskers indicate the rest of the quartiles. The diamond points indicate outliers.
inference, and that the model actually leverages information from consecutive states without hindering the performance. Additionally, it can be seen that all LMC-based variants performed differently, which can be only attributed to how the next simulations were chosen, since the surrogate was exactly the same in all three methods. As the results show, having BNN as a model for state transition was beneficial for experiments with non-stationary user models, while having BLR was more preferable for the simpler models. This suggests that BLR is expressive enough to replicate simple transitions, but struggles with more complex ones, for which BNN was more suitable.

The comparisons with GP-SSMs and PR-SSMs for learning transition dynamics show that our method learns the accurate dynamics or, at least, relative to the SSM method baselines. The SSMs methods showed worse results than BLR and BNN approaches. This can be explained by the lack of observations for learning state transitions by the SSM methods, which also explains the high variance in the sampled trajectories from these methods. As for comparisons between BLR and BNN, BLR performs better only in LG and SV models, while BNN performs better in more complex case studies. Moreover, it should be noted that trajectory sampling from BLR is possible only by retaining all local linearizations of the dynamics, which is a far more limiting approach than having one single model. Therefore, BNN is a more preferable transition dynamics model.

The empirical time costs for running the LFI methods are shown in Table 3. It can be seen that the SNPE method was the fastest for the computationally cheap simulators (of SSMs with tractable likelihoods), while the LMC-qEHVI required the least amount of time for the non-stationary user models. This is expected, since the SNEs learn the model only once, and then simply use it for all observations, which is suitable for the computationally cheap simulations with simple LFI solutions. However, for the non-stationary user models, where there are no closed-form likelihoods available, learning a single model actually requires much more time. To summarize, the LMC variants are clearly preferable for the computationally heavy simulators, which dominate the cost of training a transition dynamics model and a multi-objective surrogate.

Finally, Figure 4 shows how the performance of the LFI models changes with different simulation budgets: 2, 5, and 10 simulations per each time-step. As expected, in general, all methods improved their performance with increased budgets. However, there is little difference in how these methods compare with respect to each other. This indicates that the results are not sensitive to the precise simulation budget.

In all experiments, we attribute the success of the proposed LMC-BNN method to a more flexible multi-output surrogate, and a more efficient way of choosing simulation candidates. The LMC allows multi-fidelity modelling and leveraging information from multiple consecutive time-steps, unlike standard GPs. At the same time, samples from the transition model provide better candidates for simulations than the alternatives. The flexible surrogate along with adaptive acquisition make our method particularly suitable for online settings, where only a handful of samples are allowed per time-step.

5 Discussion

We proposed an approach for state inference and prediction in the challenging SSM setting, where the transition dynamics are unknown and observations can only be simulated. Importantly, our model of transition dynamics was obtained with few simulations, making it suitable for cases with computationally expensive simulators. This is important because typically sample-efficient LFI approaches discard any temporal information from observed time-series, and cannot do state prediction, which is necessary for choosing the next simulations when simulation budget is limited. We proposed a solution for both these challenges: we use a multi-objective surrogate model for the discrepancy measure between observed and synthetic data, which connects the consecutive states through shared parameters, and we train an additional surrogate for state transitions with samples from LFI state posteriors. Additionally, our method does not restrict the family of admissible solutions for the state transitions to be linear or Gaussian, unlike existing LFI methods for SSMs [34, 37], making it more widely applicable.

Although our method uses a more flexible surrogate for LFI, we demonstrated that it requires neither additional data nor significantly more training time than traditionally used GP surrogates. We reached the sample-efficiency goal by sharing synthetic observations across all discrepancy objectives, allowing the method to use the same simulations an indefinite amount of times. As for the decreased training time, we proposed a moving window approach that allowed the surrogate to focus only on a few recent SSM time-steps at a time. In conclusion, having a more flexible surrogate improved state inference and provided better samples from state posteriors for learning the unknown dynamics.

The main limitation of our approach is that the proposed transition dynamics model does not account for long-term state dependencies. Our state transition surrogate considers only the most recent state as an input, assuming the Markov property, and therefore cannot forecast far into the future. The resulting predictions have very low variance and have a
tendency to converge to similar values, which can be explained by training only on a single trajectory. This limits our method to cases where observations are highly informative.

Acknowledgements

This work was supported by the Academy of Finland (Flagship programme: Finnish Center for Artificial Intelligence FCAI; grants 328400, 319264, 292334) and UKRI Turing AI World-Leading Researcher Fellowship EP/W002973/1. HP was also supported by European Research Council grant 742158 (SCARABEE, Scalable inference algorithms for Bayesian evolutionary epidemiology). Computational resources were provided by the Aalto Science-IT Project.

Code Availability

All code is available through https://github.com/alexaushev/LFI-in-SSMs-with-Unknown-Dynamics

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We summarize the performance of our multi-objective LFI approach with various moving window lengths in Tables 4, where the surrogate struggles with modelling a lot of objectives. At the same time, these performance losses with LMC-BNNs, with more objectives, the transition dynamics model gets samples from more frequently updated state posterior approximations, since each objective stays longer inside a moving window and their corresponding posteriors are updated every time the window moves. This is beneficial for simple transition dynamics where the multi-objective surrogate maintains a good fit with high number of objectives (e.g. LG, NN), but not for the SV case, where the surrogate struggles with modelling a lot of objectives. At the same time, these performance losses with LMC-BNNs, with more objectives, the transition dynamics model gets samples from more frequently updated state posterior approximations, since each objective stays longer inside a moving window and their corresponding posteriors are updated every time the window moves. This is beneficial for simple transition dynamics where the multi-objective surrogate maintains a good fit with high number of objectives (e.g. LG, NN), but not for the SV case, where the surrogate struggles with modelling a lot of objectives. The next acquisition method, LMC-qEHVI, is not impacted by the quality of the extracted posteriors. Instead, it prioritizes optimization of objectives inside the moving window without taking into the account future states. Specifically, it works only when future objectives are very similar to the current ones, and completely fails when transition dynamics have erratic behaviour (as in SV, UMAP and Gaze). Lastly, the BLR acquisition linearizes the transition dynamics locally and when this locality increases by including more objectives, the considered locality becomes less and less linear. As a result, increasing the moving window size hinders the performance of the LMC-BLR in all cases. In conclusion, small window size for all three methods is preferable.

Table 4: Comparison of LFI methods (rows) in different SSMs (columns) for the state inference task with different moving window lengths (a number in parentheses). The performance was measured with 95% confidence interval (CI) of the RMSE between estimated vs ground truth state values for 50 time-steps. The best results in each column are highlighted in bold.

| Methods     | LG     | NN     | SV     | UMAP   | Gaze   |
|-------------|--------|--------|--------|--------|--------|
| LMC-BNN (2) | 1.77 ± 0.12 | 6.92 ± 0.51 | 16.14 ± 3.27 | 58.24 ± 3.62 | 58.7 ± 5.4 |
| LMC-BNN (3) | 1.78 ± 0.12 | 6.95 ± 0.53 | 15.86 ± 2.6 | 56.99 ± 2.68 | 59.45 ± 5.02 |
| LMC-BNN (5) | 1.76 ± 0.11 | **6.84 ± 0.49** | 17.6 ± 2.69 | 58.89 ± 2.9 | 60.26 ± 5.31 |
| LMC-BLR (2) | **1.3 ± 0.1** | 6.86 ± 0.54 | 13.15 ± 3.25 | 59.19 ± 3.31 | 60.6 ± 5.8 |
| LMC-BLR (3) | 1.76 ± 0.13 | 6.84 ± 0.65 | **12.14 ± 2.46** | 61.68 ± 4.22 | 60.49 ± 5.01 |
| LMC-BLR (5) | 1.8 ± 0.16 | 7.12 ± 0.54 | 12.83 ± 2.78 | 61.8 ± 5 | 60.35 ± 5.29 |
| LMC-qEHVI (2) | 1.5 ± 0.1 | 7.03 ± 0.55 | 24.4 ± 2.5 | 64.96 ± 3.72 | **56.9 ± 4.5** |
| LMC-qEHVI (3) | 1.47 ± 0.1 | 7.37 ± 0.53 | 26.02 ± 2.5 | 68.75 ± 4.13 | 61.68 ± 4.85 |
| LMC-qEHVI (5) | 1.41 ± 0.07 | 6.92 ± 0.64 | 26.64 ± 2.7 | 67.42 ± 2.92 | 60.76 ± 4.74 |

Table 5: Comparison of transition dynamics models (rows) in different SSMs (columns) with different moving window lengths (a number in parentheses). The performance was measured with 95% CI of the RMSE between sampled vs ground truth trajectories of length 50. The best results in each column are highlighted in bold.

| Methods     | LG     | NN     | SV     | UMAP   | Gaze   |
|-------------|--------|--------|--------|--------|--------|
| LMC-BNN (2) | 210 ± 4 | 148 ± 2 | 117 ± 21 | 1394 ± 27 | 1365 ± 3 |
| LMC-BNN (3) | 209 ± 3 | 147 ± 2 | 123 ± 25 | 1408 ± 28 | 1367 ± 2 |
| LMC-BNN (5) | 208 ± 3 | **147 ± 1** | 134 ± 27 | 1416 ± 36 | 1366 ± 2 |
| LMC-BLR (2) | **64 ± 7** | 154 ± 4 | 100 ± 37 | 1409 ± 49 | 1372 ± 3 |
| LMC-BLR (3) | 197 ± 6 | 153 ± 4 | **79 ± 22** | **1387 ± 56** | 1367.2 |
| LMC-BLR (5) | 197 ± 5 | 150 ± 2 | 84 ± 22 | 1404 ± 67 | 1370 ± 5 |

A Moving Window Experiments

We summarize the performance of our multi-objective LFI approach with various moving window lengths in Tables 4 and 5, where the moving window size is shown in parentheses after the method’s name. The main finding of these experiments is that including only two objectives inside the moving window is sufficient to get the most performance benefits, while having more objectives leads to increased computation time and inconsistent performance results. The increase in computation (Table 6) is evident from the complexity analysis in Section 3.3, as it makes the multi-objective surrogate training time to grow linearly. As for the inconsistent performance, the results become worse when transition dynamics have a rapid change rate, which makes the consequent objectives dissimilar and, hence, multi-objective modelling more difficult. For example, LMC-BNN and LMC-qEHVI improved for the LG and NN cases (see Tables 4 and 5), which had mostly smooth trajectories, but struggled with the SV case, which had occasional erratic transitions, as shown in Figure 5. These results indicate that one should choose the moving window size according to the transition dynamics’ change rate, which is difficult to determine when dynamics are unknown. Therefore, because any supposed improvements of having bigger moving windows are small and computationally more costly, when dealing with unknown dynamics we recommend setting moving window size to two objectives.

It is also noteworthy to mention how different acquisition methods are impacted by having additional objectives. Starting with LMC-BNNs, with more objectives, the transition dynamics model gets samples from more frequently updated state posterior approximations, since each objective stays longer inside a moving window and their corresponding posteriors are updated every time the window moves. This is beneficial for simple transition dynamics where the multi-objective surrogate maintains a good fit with high number of objectives (e.g. LG, NN), but not for the SV case, where the surrogate struggles with modelling a lot of objectives. At the same time, these performance losses and gains remain negligible. The next acquisition method, LMC-qEHVI, is not impacted by the quality of the extracted posteriors. Instead, it prioritizes optimization of objectives inside the moving window without taking into the account future states. Specifically, it works only when future objectives are very similar to the current ones, and completely fails when transition dynamics have erratic behaviour (as in SV, UMAP and Gaze). Lastly, the BLR acquisition linearizes the transition dynamics locally and when this locality increases by including more objectives, the considered locality becomes less and less linear. As a result, increasing the moving window size hinders the performance of the LMC-BLR in all cases. In conclusion, small window size for all three methods is preferable.
Table 6: Time comparison of LFI methods (rows) in different SSMs (columns) with different moving window lengths (a number in parentheses) for training 50 time-steps. The running time is shown in minutes along with 95% CI. The best results in each column are highlighted in bold.

| Methods       | LG    | NN    | SV   | UMAP  | Gaze  |
|---------------|-------|-------|------|-------|-------|
| LMC-BNN (2)   | 87.6 ± 2.6 | 79.2 ± 1 | 81 ± 2.9 | 171.2 ± 5 | 408 ± 8 |
| LMC-BNN (3)   | 105.8 ± 5.8 | 96.8 ± 2 | 84.9 ± 5.7 | 201.4 ± 6.2 | 457.9 ± 6.4 |
| LMC-BNN (5)   | 93.8 ± 2.2 | 97.3 ± 2.1 | 102.4 ± 3.6 | 198.2 ± 6.1 | 434.4 ± 8.1 |
| LMC-BLR (2)   | 82.1 ± 5.5 | 48.2 ± 0.8 | 93.5 ± 4 | 149.4 ± 4.5 | 442.5 ± 8.8 |
| LMC-BLR (3)   | 82.9 ± 1.6 | 58.5 ± 4.1 | 112.2 ± 1.4 | 189.5 ± 7.5 | 496.7 ± 13.2 |
| LMC-BLR (5)   | 64 ± 1.8 | 62.8 ± 2.7 | 111.6 ± 2.2 | 190.3 ± 6.4 | 513.5 ± 11.5 |
| LMC-qEHVI (2) | 25.5 ± 1.5 | 23.9 ± 0.5 | 24.7 ± 0.7 | 116 ± 4.6 | 347.2 ± 7.3 |
| LMC-qEHVI (3) | 24.7 ± 1.5 | 27.7 ± 0.9 | 25.4 ± 1 | 159 ± 6 | 340.2 ± 7.1 |
| LMC-qEHVI (5) | 28.6 ± 0.8 | 41.3 ± 18.3 | 31.7 ± 0.4 | 141.6 ± 7.6 | 394.5 ± 10.1 |

B The State-Space Models with Tractable Likelihoods

In this section, we present details on the three SSMs with tractable likelihoods that were used to assess the quality of state transition models in the experiments. For all three SSMs, we define transition dynamics and an observation model along with priors for LFI. As observations, we used datasets of 10 points, and their mean and standard deviation as summary statistics. The objective in Bayesian Optimization (BO) was the logarithm of Euclidean distance between the observed and simulated summary statistics.

**Linear Gaussian (LG).** In the LG model, state transition dynamics (Figure 5a) and an observation model are both linear

\[
\theta_t = 0.95 \times \theta_{t-1} + v_t, \quad x_t = \theta_t + w_t, \tag{11}
\]

with added Gaussian noise \(v_t \sim \mathcal{N}(0, 1^2)\) and \(w_t \sim \mathcal{N}(0, 10^2)\). The initial state value for the transition dynamics is \(\theta_0 = 100\). The prior for the state values is \(\theta \sim \text{Unif}(0, 15) \in \mathbb{R}\).

**Non-linear non-Gaussian (NN).** The NN model is a popular non-linear SSM [56], where the transition dynamics (Figure 5b) and observation model are

\[
\theta_{h,t} = \frac{\theta_{h,t-1}}{2} + 25 \frac{\theta_{h,t-1}}{2} \frac{\theta_{h,t-1}}{2} + 8 \cos(1.2t) + v_t, \quad x_t = \theta_{h,t}^2 + w_t, \tag{12}
\]

with added Gaussian noise \(v_t \sim \mathcal{N}(0, 10)\) and \(w_t \sim \mathcal{N}(0, 10)\). The initial state value for the noise standard deviation \(\theta_{h,0}\) is 0 with the prior \(\theta_h \sim \text{Unif}(-30, 30) \in \mathbb{R}\).

**Stochastic volatility (SV)** models are widely used for predicting volatility of asset prices [58] [59]. Here, we use the model by [57] that specifies transition dynamics (Figure 5c) of volatility \(\theta_v\), as

\[
\theta_{v,t+1} = (z_t - z_{t+1} + \sum_{j=1}^{k} e_j), \quad z_{t+1} = \exp(-\lambda)z_t + \sum_{j=1}^{k} \exp(-\lambda(t + 1 - c_j))e_j, \tag{13}
\]

with \(e_{1:k} \sim \text{Unif}(t, t + 1), e_{1:k} \sim \text{Expon}(0.5/0.25^2)\) and \(\lambda = 0.01\). The random increases of volatility are regulated by the Poisson distributed variable \(k \sim \text{Poisson}(0.5\lambda^2/0.25^2)\). The observation model for the log-return of an asset \(x_t \in \mathbb{R}\) follows

\[
x_t = \theta_{\mu} + \theta_{\nu}x_{t} + (\theta_{\nu}^{0.5} + 10^{-5})e_t, \tag{14}
\]

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Figure 5: Transition trajectories (different colours) of states (y-axis) sampled from three SSM transition dynamics across 50 time-steps (x-axis) with different random seeds. The complexity of the dynamics gradually increases in SSMs, starting with the smooth LG (a) dynamics, where the difference between consecutive states is very small, followed by NN (b) with more erratic behaviour, and finishing with the SV model (c), whose dynamics has occasional drastic changes of state values.

where $\varepsilon_t \sim \mathcal{N}(0, 1); \theta_\mu = 0$ and $\theta_\beta = 0$ remain the same, while the volatility $\theta_v$ follows the transition dynamics, starting with the initial value for the volatility $\theta_{v,0}$ of 1. We set the following priors for LFI of state values: $\theta_\mu \sim \text{Unif}(-2, 2) \in \mathbb{R}, \theta_\beta \sim \text{Unif}(-5, 5) \in \mathbb{R}, \theta_v \sim \text{Unif}(0, 3) \in \mathbb{R}$.

C Technical Details

C.1 Eye Movement Control for Gaze-Based Selection

An observation model in the gaze selection experiment is a simulated environment, where a human-subject is modelled through a reinforcement learning agent. In this environment, the agent searches for a target on a 2D display, where the target location, actions, observations, and beliefs of the agent are represented by two coordinates $\{c_1, c_2\}, c_1, c_2 \in [-1, 1]$ on the display. At each episode of the environment $e$, the agent receives noisy observations of the target $o_e = \mathcal{N}(q, \theta_s \times E(e))$ and moves the gaze to a new location $a_e = \mathcal{N}(PPO(o_e, \theta_{om} \times A(e)))$. The beliefs $b_e$ about the target location $q$ are updated according to

$$b_{e+1} = \frac{\sigma^2_{(o,e+1)} o_{e+1} + \sigma^2_{(b,e)} b_e}{\sigma^2_{(o,e+1)} + \sigma^2_{(b,e)}}, \quad \sigma_{(b,e+1)} = \sqrt{\frac{\sigma^2_{(o,e+1)} \sigma^2_{(b,e)}}{\sigma^2_{(o,e+1)} + \sigma^2_{(b,e)}}}.$$  \hspace{1cm} (15)

where $\sigma_{(o,e)}$ and $\sigma_{(b,e)}$ are observation and belief uncertainties respectively, $A(e)$ is the amplitude, and $E(e)$ is the eccentricity of the saccade at the episode $e$. The user model was trained on 10 000 episodes using the Proximal Policy.
Optimization (PPO) algorithm [68], provided by the Stable Baselines3 library [69]. We used default parameters, a multilayer perceptron policy and a clipping parameter set to 0.15. The environment was implemented by Chen et al. [67] in Python with the Open AI gym framework [70].

### C.2 UMAP Parameterization

In the UMAP parameterization model, the ground truth for state values is not available, because the human-subject cannot specify the ideal embeddings. Therefore, we approximate the ground truth by using ABC with rejection sampling. Usually, this requires running millions of simulations for each time-step, but we make use of the weighted form of the preference score that allows us to use the same simulations across all time-steps.

The embeddings for the UMAP parameterization model were computed for the handwritten digit dataset [61]. The preference score was computed as a weighted sum between the relative validity $U(t)$ and the classification accuracy $P(t)$ on the validation set. The relative validity $U(t)$ is an approximation of the Density Based Cluster Validity (DBCV) score [62], which is often used as a quality measure of clustering. Intuitively, it shows how separable all the clusters are. We use the HDBSCAN* package [72] and the HDBSCAN Boruvka KDTree [73] algorithm to cluster the points of the embeddings. We set the smallest size grouping to 60, the density parameter of clusters to 10 and leave the rest parameters to their default values. The classification accuracy $P(t)$ was calculated for the C-Support Vector Classifier (SVC) [63, 64] with the Scikit-learn package [74] and default parameters.

The embeddings for the UMAP parameterization model were computed for the handwritten digit dataset [61]. The dataset was randomly split on the training and validation sets, resulting in 1198 and 599 8x8 pixel images of digits in 10 digit classes. The UMAP algorithm was implemented with the UMAP-learn package [75].

### C.3 Implementation Details of Methods

LFI methods from Sections C.3.1-C.3.3 were integrated in the Engine for Likelihood-Free Inference (ELFI) [76] for application and further development.

#### C.3.1 BOLFI

**GP surrogate.** The implementation for the GP surrogate was provided by the GPy package [77]. It was initiated with zero mean function, and with the following priors for the RBF kernel lengthscale $l$, its variance $\sigma^2$, and the variance of the bias term $\sigma^2_b$:

$$l \sim \text{Gamma}\left(\frac{\theta_{\text{max}} - \theta_{\text{min}}}{3}, 1\right), \quad \sigma^2 \sim \text{Gamma}\left(\frac{\max(\delta(i))^2}{9}, 1\right), \quad \sigma^2_b \sim \text{Gamma}\left(\frac{\max(\delta(i))^2}{36}, 1\right).$$  \hspace{1cm} (16)

where $\theta_{\text{min}}, \theta_{\text{max}}$ are the lower and upper bounds for $\theta(i)$, $(\theta(i), \delta(i))$ are initial training points, and 1 is an all-ones vector. The GP was minimized by using the SCG optimizer [78] on the GP negative log-likelihood with a maximum number of iterations of 50. All inputs $\theta(i)$ for the GP were centred and normalized.

**LCBSC acquisition.** The BOLFI implementation uses LCBSC [39] as an acquisition function, which chooses points that minimize the lower confidence bound (LCB)

$$\text{LCB}(x) = \mu(x) - \beta_t^{1/2} \sigma(x), \quad \beta_t = 2\log(t^{2d+2} / 3\delta),$$  \hspace{1cm} (17)

where $\beta_t$ is the confidence parameter, $\delta = 0.1$ is the inverse exploration rate and $d$ is an input dimension.

**Posterior sampling.** The BOLFI posterior was obtained by weighting the prior samples and using corresponding unnormalized likelihoods as weights

$$p(x^*|\theta) \propto F\left(\frac{\epsilon - \mu(\theta)}{\sqrt{\nu(\theta) + \sigma^2}}\right),$$  \hspace{1cm} (18)
with $F(\cdot)$ being a Gaussian CDF with the mean 0 and the variance 1, and where $\epsilon$ is the minimum of the GP surrogate mean function $\mu(\cdot)$ obtained by using the L-BFGS-B optimizer \[80\] with a maximum number of iterations of 1000.

### C.3.2 Muti-Objective LFI

**LMC surrogate.** The LMC model was implemented in BoTorch \[81\]. Its latent GPs were initialized with linear mean functions $\mu(x) = kx + b$, and RBF kernels. The lengthscales of the kernels were parameterized in log scale, and initialized with 0 along with the constant $b$ of the mean function. For the RBF kernel, ARD was also enabled to assign separate lengthscales for each input dimension. GP latents were also initialized with 50 inducing points uniformly sampled inside the input bounds for each latent GP. The LMC training used Adam optimizer from the tensor computation package PyTorch \[82\] with a learning rate of 0.1 to minimize the variational evidence lower bound (ELBO). The optimized parameters included LMC coefficients, inducing points locations, and hyperparameters for the mean functions and kernels. We used the default training step size and 1000 epochs for training. All inputs for the LMC were centred and normalized.

**qEHVI acquisition.** The qEHVI acquisition function used a Quasi-MC sampler \[83\] with scrambled Sobol sequences \[84\] and a sample size of 128. The reference point that was used for calculating the hypervolume for each objective was set to -5. The acquisition points were acquired sequentially using successive conditioning \[85\] with a maximum number of restarts of 20, a batch size limit of 10, and a maximum number of iterations for the optimizer of 200.

**Bayesian neural network (BNN)** \[50\] was built from stacked Bayesian layers implemented in torch zoo (BLiTZ) \[49\]. We used an architecture with 2 hidden layers, where each layer had 256 nodes. During the training process, stochastic gradient descent \[86\] was used with a learning rate of 0.001 for minimizing the ELBO loss with squared L2 norm. The total gradient norm was clipped in order to prevent exploding gradients at a value of 5.0, and z-score passing was used to assign separate lengthscales for each input dimension. The training data was updated each time the moving window moved.

**Bayesian linear regression (BLR)** is defined as $\theta_{t+1} = \theta_t^T \beta + \epsilon$, where $\epsilon \sim N(0, \sigma^2 I)$. The hyperparameters $\sigma \in \mathbb{R}$ and $\beta \in \mathbb{R}^{m \times m}$ were inferred with maximum likelihood estimation (MLE) \[87\] of

$$
p(\theta_{t+1}|\theta_t) \propto \frac{1}{\sigma} \exp\left[\frac{-(\theta_{t+1} - \theta_t \beta)^T(\theta_{t+1} - \theta_t \beta)}{2\sigma^2}\right]. \tag{19}
$$

The BLR model was implemented with the probabilistic programming package, PyMC3 \[88\] that used 100 random samples from three latest inference steps. The pairs $(\theta_{t-1}, \theta_t)$ and $(\theta_{t-2}, \theta_{t-1})$ pairs were used as inputs for training, and the normal distribution was chosen as a prior family of the BLR parameters. The model was fitted by using the No-U-Turn Sampler (NUTS) \[89\] with two chains of 2000 samples, 2000 tuning iterations, and a target acceptance rate of 0.85.

**Posterior sampling.** Similar to BOLFI, the posterior was sampled by using an importance-weighted resampling. Because the main model was implemented in PyTorch, we used the Adam optimizer to learn the threshold $\epsilon$. It used a learning rate of $10^{-4}$ and 100 optimizing iterations. The optimization started at the parameter point that produced a synthetic observation with the smallest discrepancy.

### C.3.3 Sequential Neural Estimators

All three SNEs (SNPE, SNLE and SNRE) and their corresponding surrogate models were implemented in the simulation-based inference \[90\] and PyTorch \[82\] packages with default parameters. In all three methods, Adam optimizer with the learning rate of $5 \times 10^{-4}$ and the training batch size of 50 in 20 epochs were used for training the surrogate. The total gradient norm was clipped in order to prevent exploding gradients at a value of 5.0, and z-score passing was used for surrogate model inputs and outputs.

For SNPE \[42\] and SNLE \[43\], the masked autoregressive flow (MAF) surrogate was used for approximating the posterior $p(\theta|x)$ and likelihood, $p(x|\theta)$ respectively. The MAF consisted of 5 transformations with 50 hidden features in each of 2 blocks. Each autoregressive transformation had tanh activation along with batch normalization. In contrast, SNRE \[44\] approximates the ratio $p(\theta, x) / p(\theta|x)$, where a residual network \[91\] is used as a classifier trained to approximate likelihood ratios. The goal of the classifier is to predict which of the $(\theta, x)$ pairs was sampled from $p(\theta, x)$ and which from $p(\theta)p(x)$. The residual network had 50 hidden features in 2 residual blocks with 10 $(\theta, x)$ pairs to use for classification.
C.3.4 Recurrent State-Space Models with GP Transitions

In the experiments, we used two variants of recurrent state-space models with GP transitions: GP-SSM with a variationally coupled dynamics and trajectories, in which the variational inference scheme for GP transition dynamics is used [53], and probabilistic recurrent state-space model PR-SSM [54], which uses doubly stochastic variational inference for efficient incorporation of latent state temporal correlations. Both methods were implemented in the GPT package [53]. The GPs were using Matern32 kernels with linear mean functions, along with 50 randomly sampled inducing points. The number of latent dimensions was set equal to the number of simulator parameters of the observation model. The ELBO loss was calculated from 10 posterior samples and optimized with Adam using a learning rate of 0.001 in 3000 iterations.