FAST VARIATIONAL LEARNING IN STATE-SPACE GAUSSIAN PROCESS MODELS

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ABSTRACT

Gaussian process (GP) regression with 1D inputs can often be performed in linear time via a stochastic differential equation formulation. However, for non-Gaussian likelihoods, this reguires application of approximate inference methods which can make the implementation difficult, e.g., expectation propagation can be numerically unstable and variational inference can be computationally inefficient. In this paper, we propose a new method that removes such difficulties. Building upon an existing method called conjugate-computation variational inference, our approach enables linear-time inference via Kalman recursions while avoiding numerical instabilities and convergence issues. We provide an efficient JAX implementation which exploits just-in-time compilation and allows for fast automatic differentiation through large for-loops. Overall, our approach leads to fast and stable variational inference in state-space GP models that can be scaled to time series with millions of data points.

Index Terms— State-space models, variational inference, Gaussian processes, automatic differentiation

1. INTRODUCTION

Gaussian process (GP, [1]) models are non-parametric probabilistic tools shown to be effective in a variety of data analysis tasks. Their main drawback is $O(n^3)$ computational cost of inference, where n is the number of data examples. For a non-Gaussian likelihood, this becomes even more challenging due to the lack of a closed-form expression for the posterior. Developing low-cost algorithms is therefore essential to facilitate application of GPs to real-world problems.

Formulating a GP as a state-space model is one way to reduce the complexity of GP regression to O(n). For one-dimensional inputs, we can do so by using an equivalent stochastic differential equation (SDE) formulation [2] and extend to non-Gaussian problems by using state-of-the-art approximate inference methods [3], e.g., expectation propagation (EP, [1]). Doing so allows us to employ Kalman recursions which have O(n) computation and memory cost. Unfortunately, EP can suffer from numerical instability and convergence issues when the model exhibits highly nonlin-

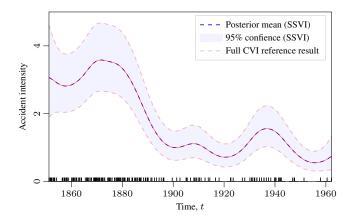


Fig. 1: Log-Gaussian Cox process applied to *coal mining accidents* data. Our proposed method, SSVI, recovers the same posterior with O(n) computation as the $O(n^3)$ CVI method.

ear behaviour. Variational inference (VI) is another popular choice which does not have such problems but it often requires $O(n^2)$ memory and cannot be conveniently implemented using Kalman recursions [4, 5]. Generally, even when Kalman recursions are used for such approximate inference methods, the practical implementation can be slow since it involves large for-loops, preventing the application of modern automatic differentiation techniques to optimise hyperparameters. Our goal in this paper is to remove such difficulties and enable fast learning.

We build upon a VI method called conjugate-computation variational inference (CVI, [6]). CVI converts non-Gaussian likelihoods to Gaussian ones, enabling the application of Kalman smoothing to perform inference with O(n) memory and computation cost. To handle large for-loops during hyperparameter learning, we provide an efficient JAX [7] implementation which employs just-in-time compilation and specifically avoids loop 'unrolling'. The resulting method, which we call State-Space VI (SSVI), enables fast learning on data containing more than a million points (see Fig. 2a). The updates of SSVI are identical to CVI (Fig. 1), and strikingly similar to EP, but do not suffer from numerical instability or convergence issues. Comparisons on real-world data demonstrate the efficiency of our method.

2. BACKGROUND

Gaussian processes form a non-parametric family of probability distributions on function spaces, and are completely characterized by a covariance function $\kappa(t,t'):\mathbb{R}\times\mathbb{R}\to\mathbb{R}$ and a mean function which we assume to be zero. Let $\{(t_i,y_i)\}_{i=1}^n$ denote a set of n input–output pairs, then GP models typically take the form

$$f(t) \sim \mathcal{GP}(0, \kappa(t, t')), \quad \mathbf{y} \mid \mathbf{f} \sim \prod_{i=1}^{n} p(y_i \mid f_i(t_i)), \quad (1)$$

which defines the prior for the latent function $f: \mathbb{R} \to \mathbb{R}$ and the likelihood model for y_i . For Gaussian likelihoods, the posterior distribution $p(\mathbf{f} \mid \mathbf{y})$ is Gaussian and can be obtained analytically, but this requires $O(n^3)$ computation in general. For non-Gaussian likelihoods, the computational overhead is even larger since the posterior is generally intractable and iterative approximate inference must be applied. Development of efficient, low-cost algorithms for GP models is an important area of research.

Fortunately, as discussed in [2], it is often possible to reformulate GP priors as state-space models which, for the Gaussian likelihoods, reduces the computation cost to O(n). Many widely used covariance functions admit this form exactly or approximately (e.g., the Matérn class, polynomial, noise, constant, squared-exponential, rational quadratic, periodic, and sums/products thereof). The general approach is to rewrite the GP as a linear time-invariant SDE, which has the general continuous-discrete (see [2], p. 200) form:

$$d\mathbf{f}(t) = \mathbf{F} \,\mathbf{f}(t) \,dt + \mathbf{L} \,d\boldsymbol{\beta}(t), \tag{2}$$

$$y_i \sim p(y_i \mid f_i = \mathbf{h}^\top \mathbf{f}(t_i)),$$
 (3)

where $\mathbf{f}(t) \in \mathbb{R}^d$ is the state and y_i is the measurement obtained at time instant t_i via the measurement vector $\mathbf{h} \in \mathbb{R}^d$. $\mathbf{F} \in \mathbb{R}^{d \times d}$ is the feedback matrix, and $\mathbf{L} \in \mathbb{R}^{d \times s}$ is the dispersion matrix. $\mathbf{G}(t) \in \mathbb{R}^s$ is the Brownian motion with diffusion matrix $\mathbf{Q} \in \mathbb{R}^{s \times s}$. For Gaussian likelihoods, inference then can be performed in O(n) by using Kalman recursions on the above model. This drastic reduction in computation makes the SDE approach an attractive alternative for inference in state-space GP models.

2.1. Issues with Learning in State-Space GP Models

For non-Gaussian likelihoods, Kalman recursions cannot be applied directly and an approximate inference method is required for tractability. Unfortunately, application of such methods brings new challenges. Methods such as expectation propagation (EP) provide a Gaussian approximation of the non-Gaussian likelihoods, which can then be used in Eq. (3) to perform inference with Kalman recursions [8]. Regrettably, EP suffers from numerical issues and is not guaranteed to converge. Methods such as variational inference (VI) do

not have these issues, but standard VI does not provide an EP-like Gaussian approximation of the non-Gaussian likelihood. Instead, a full-Gaussian approximation over $\mathbf{f}(t)$ is sought which requires storing a full $n \times n$ covariance matrix during optimization of the variational objective. It is possible to reparameterize the variational objective to reduce the number of parameters to O(n) [4, 9], but still a Kalman recursion algorithm cannot be directly applied to obtain a fast linear-time implementation. In general, these two types of methods suffer from different kinds of issues, making inference challenging.

A further issue is in the implementation of such methods. Despite the theoretical guarantee of linear time complexity, Kalman recursions involve large for-loops, making implementation in automatic differentiation frameworks problematic. Previous attempts to overcome this exploit the sparse structure in the precision matrices [10] or inducing points [11]. This typically requires a full reformulation of the model which can be unstable and difficult to implement. In this paper, we propose a new method that avoids these difficulties.

3. METHODS

We utilise conjugate-computation variational inference (CVI, [6]), forming our approximate inference problem in the variational setting by choosing a Gaussian approximate posterior $q(\mathbf{f}) = N(\mathbf{m}, \mathbf{V})$ whose natural parameters are $\boldsymbol{\lambda}^{(1)} = \mathbf{V}^{-1}\mathbf{m}$ and $\boldsymbol{\lambda}^{(2)} = -\frac{1}{2}\mathbf{V}^{-1}$. Variational inference aims to optimise $\boldsymbol{\lambda}$ to maximise a lower bound of model evidence $p(\mathbf{y})$:

$$\log p(\mathbf{y}) \ge \mathbb{E}_{q(\mathbf{f})} \left[\log \frac{p(\mathbf{y}, \mathbf{f})}{q(\mathbf{f})} \right] := \underline{\mathcal{L}}(\boldsymbol{\lambda}). \tag{4}$$

CVI performs natural gradient ascent on the above lower bound. Natural gradients are a way of taking gradient steps that accounts for the informational geometry of the optimisation problem. CVI utilises the result from [4], which states that the variational posterior is a sum of the natural parameters of the prior, $\lambda_{\rm prior}^{(1)} = 0$ and $\lambda_{\rm prior}^{(2)} = \frac{1}{2} {\bf K}^{-1}$ and the approximated likelihood terms. CVI finds Gaussian approximations for the non-Gaussian likelihoods with natural parameters $\tilde{\lambda} = \{\tilde{\lambda}^{(1)}, \tilde{\lambda}^{(2)}\}$. The likelihood distribution becomes

$$p(y_i | f_i) \approx N(\tilde{y}_i | f_i, \tilde{\sigma}_i^2),$$
 (5)

where $\tilde{y}_i = \tilde{\lambda}_i^{(1)}/\tilde{\lambda}_i^{(2)}$ and $\tilde{\sigma}_i^2 = -1/(2\tilde{\lambda}_i^{(2)})$. Under this parametrisation, $\tilde{\lambda}$ are the free variational parameters to be optimised. We can think of performing variational inference in this setting as a series of GP regressions which provide the following approximate posterior:

$$q(\mathbf{f}) \propto \left[\prod_{i=1}^{n} N\left(\tilde{y}_{i} \mid f_{i}, \tilde{\sigma}_{i}^{2} \right) \right] N\left(\mathbf{f} \mid \mathbf{0}, \mathbf{K} \right).$$
 (6)

The likelihood parameters $\tilde{\lambda}$ are the local variational parameters necessary to compute the global posterior parameters λ .

We summarise the distributions and parametrisations in the following table.

Posterior approx	Prior	Likelihood approx
$\boldsymbol{\lambda}^{(1)} = \mathbf{V}^{-1}\mathbf{m}$	$oldsymbol{\lambda}_{ ext{prior}}^{(1)} = oldsymbol{0}$	$\tilde{\lambda}_i^{(1)} = f_i/\tilde{\sigma}_i^2$
$oldsymbol{\lambda}^{(2)} = -1/2 \mathbf{V}^{-1}$	$oldsymbol{\lambda}_{\mathrm{prior}}^{(2)} = -1/2\mathbf{K}^{-1}$	$\tilde{\lambda}_i^{(2)} = -1/2\tilde{\sigma}_i^2$

Key to the CVI method is that the natural gradient update can be elegantly computed using the derivatives of the expected log likelihood with respect to the mean parameters $\mu = \{\mathbf{m}, \mathbf{V} + \mathbf{m}\mathbf{m}^{\top}\}$ [6]. The two stage update of λ is then:

$$\tilde{\lambda}_{k+1} = (1 - \rho_k)\tilde{\lambda}_k + \rho_k \,\mathbf{g}(\lambda_k),\tag{7}$$

$$\lambda_{k+1} = \tilde{\lambda}_{k+1} + \lambda_{\text{prior}}, \tag{8}$$

where $\mathbf{g}(\boldsymbol{\lambda}_k) = \nabla_{\boldsymbol{\mu}} \mathbb{E}_q \left[\log p(\mathbf{y} \mid \mathbf{f}) \right] |_{\boldsymbol{\mu} = \boldsymbol{\mu}(\boldsymbol{\lambda}_k)}$, and ρ_k the step size. Essentially we can update the variational parameters $\tilde{\boldsymbol{\lambda}}$ using the derivatives of the likelihood terms with respect to parameters of our posterior. Combining local parameter updates and global conjugate regression steps avoid the need to directly optimise Eq. (4), which alleviates the performance issues with the optimal reduced parametrisation (cf. Sec. 2.1).

3.1. Evidence Lower Bound (ELBO) Derivation

Although the CVI method sidesteps direct computation of the ELBO for the variational parameter updates, it is still required for hyperparameter learning (*e.g.*, kernel length-scale and magnitude). We simplify Eq. (4) by using Eq. (6) to give

$$\underline{\mathcal{L}} = \mathbb{E}_{q(\mathbf{f})} \log \left[\frac{\prod_{i=1}^{n} p(y_i | f_i) \mathcal{Z}(\mathcal{GP}) N(\mathbf{f} | \mathbf{0}, \mathbf{K})}{\prod_{i=1}^{n} N(\tilde{y}_i | f_i, \tilde{\sigma}_i^2) N(\mathbf{f} | \mathbf{0}, \mathbf{K})} \right], \quad (9)$$

where the log marginal likelihood of the approximate conjugate model is

$$\log \mathcal{Z}\left(\mathcal{GP}\right) = -\frac{1}{2}\log|\mathbf{K}_{\tilde{y}}| - \frac{1}{2}\tilde{\mathbf{y}}^{\top}\mathbf{K}_{\tilde{y}}^{-1}\tilde{\mathbf{y}} - \frac{n}{2}\log(2\pi)$$
(10)

for $\mathbf{K}_{\tilde{y}} := \mathbf{K} + \operatorname{diag}(\tilde{\sigma}^2)$. From Eq. (9), we get the complete expression for the ELBO:

$$= \sum_{i=1}^{n} \mathbb{E}_{q(\mathbf{f})} \log p(y_i | f_i) + \log \mathcal{Z}(\mathcal{GP})$$

$$\sum_{i=1}^{n} \begin{bmatrix} 1 & 1 \\ 1 & 1 \end{bmatrix} \begin{pmatrix} 1 & 1 \\ 1 & 1 \end{pmatrix}$$

$$-\sum_{i=1}^{n} \left[\frac{1}{2} \log \left(\frac{1}{2\pi \tilde{\sigma}_i^2} \right) - \frac{1}{2\tilde{\sigma}_i^2} \left(\left(\tilde{y}_i - m_i \right)^2 + v_i \right) \right]. \quad (11)$$

3.2. Proposed Method

Updating our variational parameters λ_{k+1} in Eq. (8) involves solving a GP regression problem, which scales as $O(n^3)$. We now show how we can perform the same calculations in O(n) using the Kalman filter and smoother, as well as demonstrating how the CVI updates can be used in the forward filter to initialise the variational parameters. We additionally discuss how the marginal likelihood approximation can be computed as an alternative to the ELBO for hyperparameter learning, and outline our efficient implementation in JAX.

3.3. Sequential CVI by Filtering and Smoothing

Certain LTI SDEs of the form in Eq. (2) have discrete-time solutions that can be computed in closed form and written:

$$\mathbf{f}_i = \mathbf{A}_{i-1}\mathbf{f}_{i-1} + \mathbf{q}_i, \qquad \mathbf{q}_{i-1} \sim \mathrm{N}(\mathbf{0}, \mathbf{Q}_{i-1}),$$
 (12)

where $\mathbf{f}_i = \mathbf{f}(t_i)$ and $\mathbf{A}_i = \exp(\mathbf{F}\Delta t_i)$ is the linear state transition matrix, for time step size $\Delta t_i = t_i - t_{i-1}$. \mathbf{Q}_i is the process noise covariance. For a Gaussian likelihood we can write the measurement model as a linear transformation of state vector with additive Gaussian noise:

$$y_i = \mathbf{h}^{\top} \mathbf{f}_i + \varepsilon_i, \qquad \varepsilon_i \sim \mathcal{N}(0, \sigma_i^2).$$
 (13)

 $\mathbf{h} \in \mathbb{R}^d$ is the measurement vector such that $f(t_i) = \mathbf{h}^{\top} \mathbf{f}_i$, which coincides with the GP model in Eq. (1). The exact solution to the model outlined above can be computed via the Kalman filter and Rauch-Tung-Striebel smoother (see [12]). For our non-Gaussian likelihood model, we must adjust the above to reflect our variational likelihood approximations,

$$\tilde{y}_i = \mathbf{h}^{\top} \mathbf{f}_i + \varepsilon_i, \qquad \varepsilon_i \sim \mathrm{N}(0, \tilde{\sigma}_i^2).$$
 (14)

We now derive our adjusted filtering and smoothing algorithms that explicitly incorporate the update steps of Eq. (7) and Eq. (8), as well as computing all required elements of Eq. (11): $\{m_i, v_i, \mathcal{Z}(\mathcal{GP}), \mathbb{E}_{q(\mathbf{f})} \log p(y_i | f_i)\}$.

The filtering distribution, $p(\mathbf{f}_i | \mathbf{y}_{1:i}) = N(\mathbf{f}_i | \mathbf{m}_i^f, \mathbf{P}_i^f)$, is computed in two stages. Firstly, the prediction step,

$$\mathbf{m}_{i}^{\mathrm{p}} = \mathbf{A}_{i} \mathbf{m}_{i-1}^{\mathrm{f}}, \qquad \mathbf{P}_{i}^{\mathrm{p}} = \mathbf{A}_{i} \mathbf{P}_{i-1}^{\mathrm{f}} \mathbf{A}_{i}^{\top} + \mathbf{Q}_{i},$$
 (15)

followed by the update step, in which we first compute the innovation mean (η_i) and variance (s_i) ,

$$\eta_i = \tilde{y}_i - \mathbf{h}^{\mathsf{T}} \mathbf{m}_i^{\mathsf{p}}, \qquad s_i = \mathbf{h}^{\mathsf{T}} \mathbf{P}_i^{\mathsf{p}} \mathbf{h} + \tilde{\sigma}_i^2.$$
 (16)

The log marginal likelihood of the Gaussian model, as required in Eq. (11), can now be evaluated from the above quantities: $\log \mathcal{Z}_i \left(\mathcal{GP}\right) = \sum_i^n \frac{1}{2} (\log 2\pi s_i + \eta_i^2/s_i)$. The updated filter mean and covariance are then

$$\mathbf{k}_{i} = \mathbf{P}_{i}^{\mathbf{p}} \mathbf{h} / s_{i},$$

$$\mathbf{m}_{i}^{\mathbf{f}} = \mathbf{m}_{i}^{\mathbf{p}} + \mathbf{k}_{i} \eta_{i}, \quad \mathbf{P}_{i}^{\mathbf{f}} = \mathbf{P}_{i}^{\mathbf{p}} - \mathbf{k}_{i} \mathbf{h}^{\mathsf{T}} \mathbf{P}_{i}^{\mathbf{p}}.$$
(17)

The marginal smoothing distribution is notated $p(\mathbf{f}_i | \mathbf{y}_{1:n}) = \mathrm{N}(\mathbf{f}_i | \mathbf{m}_i^{\mathrm{s}}, \mathbf{P}_i^{\mathrm{s}})$, and is computed through backward recursion of the following equations:

$$\mathbf{m}_{i}^{s} = \mathbf{m}_{i}^{f} + \mathbf{G}_{i} \left(\mathbf{m}_{i+1} - \mathbf{m}_{i+1}^{p} \right),$$
 (18)

$$\mathbf{P}_{i}^{s} = \mathbf{P}_{i}^{f} + \mathbf{G}_{i}(\mathbf{P}_{i+1} - \mathbf{P}_{i+1}^{p})\mathbf{G}_{i}^{\top}, \tag{19}$$

where $\mathbf{G}_i = \mathbf{P}_i^{\mathrm{f}} \mathbf{A}_{i+1}^{\mathrm{T}} [\mathbf{P}_{i+1}^{\mathrm{p}}]^{-1}$ is the smoother gain. The smoothing distribution gives the GP marginal posterior $q(f(t_i)) = \mathrm{N}(f(t_i) \mid m_i, v_i)$ where $m_i = \mathbf{h}^{\mathrm{T}} \mathbf{m}_i^{\mathrm{s}}$ and $v_i = \mathbf{h}^{\mathrm{T}} \mathbf{P}_i^{\mathrm{s}} \mathbf{h}$.

3.4. Variational Parameter Updates in the Filter/Smoother

The final required term in order to update $\tilde{\lambda}$ and compute the ELBO is the variational expectations, $\mathbb{E}_{q(\mathbf{f})} \log p \, (y_i \mid f_i)$, and their derivatives. Given we have just computed m_i and v_i , it is natural to perform this calculation in the smoother step. The derivatives with respect to the mean parameters $\mu_i = \{m_i, v_i + m_i^2\}$ directly provide the natural parameter update. Using the chain rule, we write down the following update rule at step k as a function of the source parameters m_i, v_i :

$$\mathcal{J}_i = \mathbb{E}_{N(f_i \mid m_i, v_i)} \left[\log p(y_i \mid f_i) \right], \tag{20}$$

$$\tilde{\lambda}_{i,k+1}^{(1)} = (1 - \rho_k)\tilde{\lambda}_{i,k}^{(1)} + \rho_k \left(\frac{\partial \mathcal{J}_i}{\partial m_i} - 2\frac{\partial \mathcal{J}_i}{\partial v_i} m_i\right), \quad (21)$$

$$\tilde{\lambda}_{i,k+1}^{(2)} = (1 - \rho_k)\tilde{\lambda}_{i,k}^{(2)} + \rho_k \frac{\partial \mathcal{J}_i}{\partial v_i}.$$
(22)

In the general case \mathcal{J}_i is intractable, and we employ Gauss–Hermite quadrature to compute this quantity and its derivatives numerically. Crucially, these parameter updates are not specific to the smoother, and can also be used in the first forward filtering pass as a novel way to initialise the variational parameters. Initialising the variational distribution to $N(\mathbf{0}, \infty)$ is standard practice, but by letting $m_i = \mathbf{h}^{\top} \mathbf{m}_i^f$ and $v_i = \mathbf{h}^{\top} \mathbf{P}_i^f \mathbf{h}$, *i.e.* using the marginal filtering distribution, and setting $\rho_k = 1$, we can utilise Eq. (20)–Eq. (22) to provide a much improved initialisation. In Sec. 4 we show how doing so results in superior convergence rates in practice.

This interpretation also shows that our CVI scheme can be seen as a new, general purpose nonlinear Kalman filter, whose nonlinear updates equate to a full natural gradient step in the evidence lower bound, and which reduces to the linear Kalman filter when the observation model is Gaussian.

3.5. Similarity to Expectation Propagation

It is worth noting that the parameter updates in Sec. 3.4 bear striking resemblance to the analogous updates used in filter-smoother version of expectation propagation [8], which can be written with $\mathcal{Z}_i = \log \mathbb{E}_{N(f_i \mid m_i, v_i)} [p(y_i \mid f_i)]$ as

$$\tilde{\lambda}_{i,\text{new}}^{(2)} = \frac{1}{2} \left(v_i + \frac{\partial \mathcal{Z}_i}{\partial v_i}^{-1} \right)^{-1}, \tag{23}$$

$$\tilde{\lambda}_{i,k+1}^{(1)} = (1 - \rho_k) \tilde{\lambda}_{i,k}^{(1)} + \rho_k \tilde{\lambda}_{i,\text{new}}^{(2)} \left(2 \frac{\partial \mathcal{Z}_i}{\partial v_i} \frac{\partial \mathcal{Z}_i}{\partial v_i}^{-1} - 2m_i \right), \quad (24)$$

$$\tilde{\lambda}_{i,k+1}^{(2)} = (1 - \rho_k)\tilde{\lambda}_{i,k}^{(2)} + \rho_k\tilde{\lambda}_{i,\text{new}}^{(2)}, \tag{25}$$

where m_i , v_i are now the parameters of the so called *cavity* distribution obtained by removing the likelihood from the marginal posterior: $v_i = ((\mathbf{h}^{\top} \mathbf{P}_i^{\mathrm{s}} \mathbf{h})^{-1} - \tilde{\lambda}_i^{(2)})^{-1}$ and $m_i = v_i((\mathbf{h}^{\top} \mathbf{P}_i^{\mathrm{s}} \mathbf{h})^{-1} \mathbf{h}^{\top} \mathbf{m}_i^{\mathrm{s}} - \tilde{\lambda}_i^{(1)})$.

3.6. Direct Marginal Likelihood Computation

In sequential models we also have available the marginal likelihood as an alternative to the ELBO as an optimisation objective for hyperparameter learning. The marginal likelihood can be written as a product of conditional terms,

$$p(\mathbf{y}) = p(y_1) p(y_2 \mid y_1) p(y_3 \mid \mathbf{y}_{1:2}) \prod_{i=4}^{n} p(y_i \mid \mathbf{y}_{1:i-1}). \quad (26)$$

Each term can be computed via numerical integration during the Kalman filter by noticing that,

$$p(y_i | \mathbf{y}_{1:i-1}) = \int p(y_i | \mathbf{f}_i, \mathbf{y}_{1:i-1}) p(\mathbf{f}_i | \mathbf{y}_{1:i-1}) d\mathbf{f}_i$$
$$= \int p(y_i | f_i = \mathbf{h}^{\top} \mathbf{f}_i) p(\mathbf{f}_i | \mathbf{y}_{1:i-1}) d\mathbf{f}_i. \quad (27)$$

The first component in the integral is the likelihood, and the second term is the filter prediction calculated in Eq. (15).

3.7. Efficient Hyperparameter Learning with JAX

The sequential formulation of GP models is an extremely efficient approach to inference. However, a problem arises in the machine learning context, where it is desirable to optimise the model hyperparameters via gradient-based methods using automatic differentiation. Most automatic differentiation libraries work by 'tracing' a computational graph. This involves passing arbitrary values through the supplied functions and constructing a list of the necessary operations and their derivatives. Functions involving large for-loops (such as a Kalman filter) result in massive computational graphs that involve large compilation overheads, memory usage and runtime. For this reason, most machine learning approaches to temporal GPs either use finite differences [3], which are slow when the number of parameters is large, or reformulate the model entirely to exploit linear algebra tricks applicable to sparse precision matrices [10].

We utilise the following novel capabilities of the increasingly popular differential programming Python framework, JAX [7]: (i) we avoid 'unrolling' of for-loops, i.e. instead of building a large graph of repeated operations, a smaller graph is recursively called, reducing the compilation overhead and memory. (ii) we just-in-time (JIT) compile the for-loops, to avoid the cost of graph retracing. This results in an overhead setup cost on the first function call (this effect is seen in Fig. 2a), but means that every subsequent call only involves reuse of the static graph, which is very efficient. (iii) JAX also allows for the use of accelerated linear algebra (XLA) to speed up the underlying filtering/smoothing operations. Combined, the above implementation details result in an extremely fast method that scales to millions of data points. Fig. 2a shows that one training iteration for a one-dimensional GP with one million data points takes approximately 20 s.

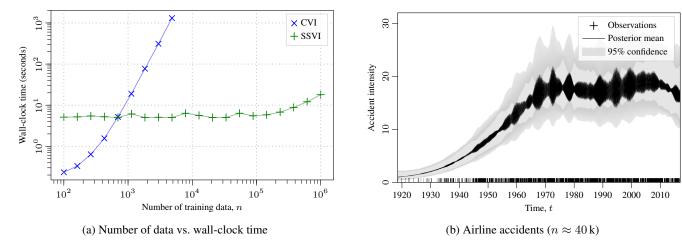


Fig. 2: (a) Empirical wall-clock times (averages over 5 runs) for taking ten variational steps and evaluating the ELBO and its gradient for hyperparameter learning in a simulated GP classification task. CVI is implemented in GPflow 2 and shows cubic computational cost in n. SSVI delivers the same result in linear time. The set-up cost (\sim 6 s) in SSVI is dominating up to 10^5 , whereafter the scaling is linear (subsequent iteration steps do not suffer from the setup time). (b) The posterior for the *airline accidents* intensity modelling task with a slow trend and multiple periodic kernels for day-of-week and time-of-year effects.

4. EXPERIMENTS

Initial experiments show that SSVI is an efficient inference method for fitting large non-Gaussian time series models. We show that the SSVI posterior is equal to CVI one, as expected. Furthermore, on large datasets our method performs comparably to EP in terms of test performance and convergence speed. In addition to choosing the ELBO as a training objective we also use the marginal likelihood and compare their performance. The practical computational complexity is also shown, by running a wall-clock test on a simple GP classification task. All experiments were performed using a MacBook pro with a 2.4 GHz Intel core i5 processor and 16 Gb RAM.

4.1. Comparison to Full-CVI

Fig. 2a shows the computation times for CVI (implemented in GPflow 2) vs. SSVI on a GP classification example where both return the same solution. The data were simulated from $y_i \sim \text{Bern}(f_i)$, where $f(t) = 6\sin(\frac{\pi t}{10})/\pi\frac{t}{10}+1$ and a Matérn-5/2 GP prior was used. The number of observations n was varied from 100 data points to one million. The chart shows the linear computational complexity in n of SSVI versus the cubic complexity for CVI, noting that SSVI's setup cost dominates until around n=1,000. It should be noted that subsequent iterations do not include the setup cost, making optimisation very fast.

The experiment in Fig. 1 uses the coal mining disaster dataset [8] that contains dates for 191 explosions that killed ten or more men in Britain between 1851–1962. We use a log-Gaussian Cox process, which is an inhomogeneous Poisson process (approximated with a Poisson likelihood for 200 equal-time interval bins). We use a Matérn-5/2 GP prior with

likelihood model $p(\mathbf{y} \mid \mathbf{f}) \approx \prod_{i=1}^n \operatorname{Poisson}(y_i \mid \exp(f(\hat{t}_i)))$, where \hat{t}_i is the bin coordinate and y_i the number of disasters in the bin. Given a small data size we can use CVI and SSVI and compare the posterior mean and variances for both methods after training for 500 iterations using the Adam optimizer. The plot shows negligible difference between the methods.

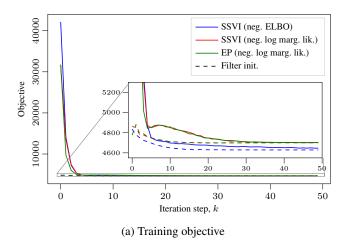
4.2. Large-scale log-Gaussian Cox Process Modelling

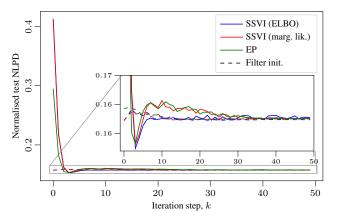
We now examine the efficacy of the presented SSVI method as a practical machine learning algorithm on a large time series dataset consisting of 1210 dates of commercial airline accidents between 1919–2017 [3]. In applying a log-Gaussian Cox process it is necessary to use a bin-width of one day in order to capture the fast varying behaviour (weekly, monthly, and yearly trends), which results in n=35,959 observations.

The GP prior contains two components representing long and medium term trends and two representing quasi-periodic behaviour: $\kappa(t,t') = \kappa(t,t')_{\text{Mat.}^5/2}^{\text{long}} + \kappa(t,t')_{\text{Mat.}^5/2}^{\text{med.}} + \kappa(t,t')_{\text{Cos}}^{\text{3 months}} \kappa(t,t')_{\text{Mat.}^5/2} + \kappa(t,t')_{\text{Cos}}^{\text{1 week}} \kappa(t,t')_{\text{Mat.}^5/2}$. We approximate the process with a Poisson likelihood, as above.

Fig. 3 shows a comparison of the training objective and test performance for various algorithmic choices. The natural gradient parameter updates ensure that SSVI converges almost as quickly as EP (which is usually posed as a fast-converging alternative to VI). Fig. 3b suggests that using the ELBO as a training objective can result in slower convergence than the marginal likelihood, in terms of test performance.

As discussed in Sec. 3.4, the interpretation of SSVI as a general nonlinear Kalman filter enables us to treat the first filtering pass as an opportunity to *initialise* the variational parameters. Doing so provides a much improved starting point





(b) Test negative log predictive density (NLPD)

Fig. 3: Training objective and test performance for various algorithmic choices in the airline accidents modelling task, using 10-fold cross validation (mean values shown). The natural gradient parameter updates ensure that SSVI/CVI converges almost as quickly as EP, and convergence can be further sped up by using the filtering (forward) pass for initialization (dashed lines).

for the optimisation, and results in far superior convergence, as shown by the dashed lines in Fig. 3.

5. CONCLUSION

We have shown how to efficiently employ variational inference in temporal GP models with non-conjugate likelihood models. The method SSVI is a linear-time algorithm that builds on CVI, and is also applicable to more general discrete and continuous-discrete state-space models. We derive the closed-form expressions for efficient evaluation of the variational update step and evidence lower bound (ELBO) by Kalman filtering and smoothing. Furthermore, we proposed an initialization technique for the variational parameters that leverage the forward filter, which showed clear practical benefits. We also demonstrated how to efficiently learn the model hyperparameters using JAX, which allows for automatic differentiation through the state-space model—something that has previously been difficult in major ML frameworks.

In our experimental validation, we empirically recovered a posterior that matches standard CVI, and demonstrated the benefits of linear-time inference on a large benchmarking problem with around 40 thousand data points. We conclude that JAX shows promise in making auto-differentiation part of the ML toolchain even in sequential models. Codes for this paper are available at http://github.com/AaltoML/kalman-jax.

Author contributions PEC and AS had the original idea after discussions with MEK. WJW and PEC implemented the method and ran the experiments. PEC wrote the first draft of the paper, after which all authors contributed to writing.

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