Variational Latent Gaussian Process for Recovering Single-Trial Dynamics from Population Spike Trains

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Abstract

A small number of common factors often explain most of the interdependence among simultaneously recorded neurons, a signature of underlying low-dimensional dynamics. We posit that simple neural coding and computation manifest as low-dimensional nonlinear dynamics implemented redundantly within a large population of neurons. Recovering the latent dynamics from observations can offer a deeper understanding of neural computation. We improve upon previously-proposed methods for recovering latent dynamics, which assume either an inappropriate observation model or linear dynamics. We propose a practical and efficient inference method for a generative model with explicit point process observations and an assumption of smooth nonlinear dynamics. We validate our method on both simulated data and population recording from primary visual cortex.

1 Introduction

Neural populations implement dynamics that produce robust behavior; however, our experimental observations of these dynamics are invariably indirect and partial. In classical analyses of neural spike trains, noisy responses are averaged over

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repeated trials that are presumably time-locked to a stereotypical computation process. However, neural dynamics are not necessarily time-locked nor precisely repeated from trial to trial; rather, many cognitive processes generate observable variations in the internal processes that manifest in behavior such as error trials, broad reaction time distributions, and change of mind [1-3]. In addition, it is difficult to disambiguate different possible neural implementations of computation from the average trajectory since they may only differ in their trial-to-trial variability [1,4]. Therefore, if we wish to understand how neural computation is implemented in neural populations, it is imperative that we recover these hidden dynamics from individual trials [5,6].

Advances in techniques for recording from larger subpopulations facilitate single-trial analysis, especially the inference of single-trial latent dynamics. Several statistical approaches have been developed for extracting latent dynamical trajectories that describe the activity observed populations [7-12]. For example, latent trajectories recovered from motor cortex suggest that these methods can provide insight to the coding and preparation of planned reaching behavior [13-15]. Latent dynamical trajectories also elucidate the low-dimensional noise structure of neural codes and computations [13,16,18].

Inference of latent dynamical trajectories is a dimensionality-reduction method for multi-variate time series, akin to Kalman smoothing or factor analysis [6]. Given a high-dimensional observation sequence, we aim to infer a shared, low-dimensional latent process that explains much of the variation in high-dimensional observations. A large class of methods assume an autoregressive linear dynamics model in the latent process due to its computational tractability [5,9,19], we refer to these as PLDS (Poisson Linear Dynamical System). Although the assumption of linear dynamics can help in smoothing, it can also be overly simplistic: interesting neural computations are naturally implemented as nonlinear dynamics, and evidence points to nonlinear dynamics in the brain in general. Therefore, we propose to relax this modeling assumption and impose a general Gaussian process prior to nonparametrically infer the latent dynamics, similar to the Gaussian process factor analysis (GPFA) method [7,20]. However, we differ from GPFA in that we use a point process observation model rather than a Gaussian observation model. A Gaussian observation model is often inappropriate for inference in the millisecond-range time scale. The price we pay is a non-conjugate prior and, consequently, approximate posterior inference [5]. We use a variational approximation [21] where we assume a Gaussian posterior process over the latents, and optimize a lower bound of the marginal likelihood for inference. Our algorithm, we call variational latent Gaussian process (vLGP) is fast and has better predictability compared to both GPFA and PLDS. We compare these algorithms on

\[^{1}\text{Code available online: https://github.com/catniplab/vLGP}\]
Figure 1: Generative model schematic for one neuron driven by two latent processes. Every neuron in the observed population are driven by the same set of latent processes. The inferred latent processes are more likely to be smooth, as assumed by the smooth Gaussian process prior. The point nonlinearity is fixed to be exponential $f(\cdot) = \exp(\cdot)$.

simulated systems with known latent processes, and apply to high-dimensional V1 data from anesthetized monkey.

2 Generative model

Suppose we simultaneously observe spike trains from $N$ neurons. Let $(y_{t,n})_{t=1,...,T}$ denote the spike count time-series from the $n$-th neuron for a small time bin. We assume the following parametric form of the conditional intensity function $\lambda^*(\cdot)$ for the point process likelihood [9, 22]:

$$\log p(y_{t,n} | x_t, h_{t,n}, \alpha_n, \beta_n) = y_{t,n} \log \lambda^*(t, n | h_{t,n}) - \lambda^*(t, n | h_{t,n}),$$

where $x_t$ is a latent process and $h_{t,n} = [1, y_{t-p,n}, y_{t-p+1,n}, \ldots, y_{t-1,n}]^T$ denotes the spike history vector [23, 24]. Each neuron is directly influenced by the observed self-history with weight $\beta_n$ and also driven by the common latent process with weight $\alpha_n$ (Fig. [1]). Neurons are conditionally independent otherwise: all trial-to-trial variability is attributed either to the latent process or individual point process noise (c.f., [18, 26, 27]).

The vector $x_t$ denotes the $L$-dimensional latent process at time $t$. The vector $\beta_n$ consists of the weights of the spike history and a time-independent bias term of the log firing rate for each neuron, and $h_{t,n}$ is a vector of length $(1 + p)$ containing the dummy value 1 for the bias and $p$ time-step spike self-history. This

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2It is straightforward to add external covariates similar to the self-history in this point process regression [25].
parametrization assumes that at most \( p \) bins in the past influence the current intensity.

Under conditional independence, the joint distribution (data likelihood) of \( N \) spike trains is given by,

\[
p(y_{1,...,T,1,...,N} | x_{1,...,T}, \alpha_{1,...,N}, \beta_{1,...,N}) = \prod_{t=1}^{T} \prod_{n=1}^{N} p(y_{t,n} | x_t, h_{t,n}, \alpha_n, \beta_n). \tag{2}
\]

Note that this model is not identifiable (see later sections for further discussions):

\[\alpha_T^T x_t = (\alpha_n^T C)(C^{-1} x_t) = \alpha'_T x'_t \]

where \( C \) is an arbitrary \( L \times L \) invertible matrix. Also, the mean of latent process \( x \) can be traded off with the bias term in \( \beta \).

Our assumptions about the latent process—namely the smoothness over time in this paper—are encoded in the prior distribution over the latent process. We use the popular Gaussian process (GP) framework [28] for flexible prior design of each dimension \( x_l(t) \) independently:

\[x_l(t) \sim \mathcal{GP}(\mu_l, \kappa_l) \tag{3}\]

where \( \mu_l(t) \), and \( \kappa_l(t, s) \) are mean and covariance functions, respectively. When time is discretized, the GP prior reduces to a multi-variate Gaussian distribution over the latent time series. We use the following form:

\[p(x_l) = \mathcal{N}(x_l | 0, K_l), \quad l = 1, \ldots, L. \tag{4}\]

For the analyses in this manuscript, we choose the squared exponential covariance function [28] for general smoothness over time,

\[\text{cov}(x_{t,l}, x_{s,l}) = \sigma_l^2 \exp(-\omega_l(t - s)^2). \tag{5}\]

where \( \sigma_l \) and \( \omega_l \) are hyperparameters corresponding to the magnitude and inverse length scale of the latent process, respectively.

### 3 Variational inference

Our goal is to infer the posterior distribution over the latent process and fit the model parameters given the observed data. By Bayes’ theorem, the posterior distribution of the latent process is,

\[p(x_{1:L} | y_{1:N}) = \frac{p(y_{1:N} | x_{1:L}) p(x_{1:L})}{p(y_{1:N})}, \tag{6}\]

However, unlike in GPFA, the posterior under a point process likelihood and Gaussian process prior does not have an analytical form [5]. Consequently, we
must turn to an approximate inference technique. We employ variational inference, which aims to find an approximate distribution \( q(x) \) of the intractable true posterior \( p(x \mid y) \). We can introduce this approximate posterior into the likelihood by re-writing it as,

\[
\log p(y_{1 \ldots N}) = E_q \left[ \log p(y_{1 \ldots N}, x_{1 \ldots L}) \right] = E_q \left[ \log \frac{p(y_{1 \ldots N}, x_{1 \ldots L})}{q(x_{1 \ldots L})} \cdot \frac{q(x_{1 \ldots L})}{p(x_{1 \ldots L} \mid y_{1 \ldots N})} \right] = E_q \left[ \log \frac{q(x_{1 \ldots L})}{p(x_{1 \ldots L} \mid y_{1 \ldots N})} \right] + E_q \left[ \log p(x_{1 \ldots L} \mid y_{1 \ldots N}) \right]
\]  

(7)

where \( E_q \) denotes an expectation over \( q(x) \), and \( D_{KL}(q \parallel p) \) is the Kullback-Leibler divergence, which measures the difference in the true posterior and its variational approximation. Since \( D_{KL}(q \parallel p) \) is non-negative, \( \mathcal{L}(q) \) is the lower bound for the marginal likelihood. Finding an approximate posterior \( q \) close to the true posterior by minimizing the Kullback-Leibler divergence is equivalent to maximizing the lower bound \( \mathcal{L}(q) \).

We further assume the \( q \) distribution factorizes into Gaussian distributions with respect to each dimension of the latent process, so that

\[
q(x_{1 \ldots L}) = \prod_{l=1}^{L} \mathcal{N}(x_l \mid \mu_l, \Sigma_l).
\]

(9)

We then obtain

\[
\mathcal{L}(q) = \sum_{t=1}^{T} \sum_{n=1}^{N} E_q \left[ \log p(y_{t,n} \mid x_t, h_{t,n}, \alpha_n, \beta_n) \right] - \sum_{l=1}^{L} E_q \left[ \log \frac{q(x_{1 \ldots L} \mid \mu_t, \Sigma_t)}{p(x_{1 \ldots L} \mid y_{1 \ldots N})} \right]
\]

\[
= \sum_{t=1}^{T} \sum_{n=1}^{N} [y_{t,n} (\alpha_n^\top \mu_t + \beta_n^\top h_{t,n}) - \exp(\alpha_n^\top \mu_t + \beta_n^\top h_{t,n} + \frac{1}{2} \alpha_n^\top \Sigma_t \alpha_n)]
\]

\[
- \frac{1}{2} \sum_{l=1}^{L} [\mu_l^\top K_l^{-1} \mu_l + \text{tr}(K_l^{-1} \Sigma_t) - \log \det(K_l^{-1} \Sigma_t) - T].
\]

(10)

where \( T \) is the number of total time steps, and each temporal slice \( \mu_t \) is a vector of posterior means of the \( L \) latent variables at time \( t \). Each temporal slice \( \Sigma_t \) is a diagonal matrix whose diagonal contains the variances of the \( L \) latent variables at time \( t \).

Variational inference for the entire posterior over latents, parameters, and hyperparameters all be formulated in terms of maximizing \( \mathcal{L}(q) \). We sequentially

\( ^3 \mathcal{L}(q) \) is often called the Evidence Lower BOund (ELBO).
update all parameters coordinate-wise; each conditional update turns out to be a convex-optimization problem except for hyperparameters as explained below. The algorithm is summarized in Algorithm 1.

Our algorithm scales linearly in space \(O(Ts)\) and time \(O(Tr^2L)\) per iteration (for a fixed hyperparameter) where \(s = \max(rL, pN)\) thanks to the rank-\(r\) incomplete Cholesky factor of the prior covariance matrix. For comparison, time complexity of GPFA is \(O(T^3L^3)\), and that of PLDS is \(O(T(L^3 + LN))\).

3.1 Posterior over the latent process

The variational distribution \(q_l\) is assumed to be Gaussian and thus determined only by its mean \(\mu_l\) and covariance \(\Sigma_l\). The optimal solution is therefore obtained by

\[
\mu^*_{1...L}, \Sigma^*_{1...L} = \arg \max_{\mu_{1...L}, \Sigma_{1...L}} \mathcal{L}(q),
\]

while holding other parameters and hyperparameters fixed.

Denote the expected firing rate of neuron \(n\) at time \(t\) by \(\lambda_{t,n}\),

\[
\lambda_{t,n} = \mathbb{E}_q[\lambda^*(t, n \mid h_{t,n})] = \exp \left( \beta_n^\top h_{t,n} + \alpha_n^\top \mu_t + \frac{1}{2} \alpha_n^\top \Sigma_t \alpha_n \right).
\]

The optimal \(\mu_l\) can be obtained by the Newton-Raphson method. The gradient and Hessian are given as

\[
\nabla_{\mu_l} \mathcal{L} = \sum_{t,n} (y_{t,n} - \lambda_{t,n})a^*_{n,l} e_t - K^{-1}_l \mu_l,
\]

\[
\nabla^2_{\mu_l} \mathcal{L} = -\sum_{t,n} \lambda_{t,n} a^2_{n,l} e_t e_t^\top - K^{-1}_l.
\]

where \(e_t\) is a vector of length \(T\) with value 1 at \(t\) and zero elsewhere. Note that the Hessian is negative definite, and hence this is a convex optimization given the other arguments and \(\lambda_{t,n}\). In each iteration, the update is

\[
\mu^{new}_l = \mu^{old}_l - (\nabla^2_{\mu_l} \mathcal{L})^{-1}(\nabla_{\mu_l} \mathcal{L}).
\]

If we set the derivative w.r.t. \(\Sigma_l\) to 0,

\[
\nabla_{\Sigma_l} \mathcal{L} = -\sum_{t,n} \lambda_{t,n} a^2_{n,l} e_t e_t^\top - \frac{1}{2} K^{-1}_l + \frac{1}{2} \Sigma^{-1}_l = 0,
\]

we obtain the optimal covariance,

\[
\Sigma_l = \left( K^{-1}_l + \sum_{t,n} \lambda_{t,n} a^2_{n,l} e_t e_t^\top \right)^{-1}
\]
Algorithm 1 Pseudocode for variational inference

1: procedure vLGP(y_{1...T}, h_{1...T,1...N}, \sigma^2_{1...L}, \omega_{1...L}, tol)
2: \begin{align*}
G_l &= \text{ichol}(\sigma^2_l, \omega_l), \quad l = 1 \ldots L \quad \triangleright \text{construct incomplete Cholesky decomposition [29]} \\
\end{align*}
3: Initialize \(\alpha_n\) and \(\mu_l\) by factor analysis
4: \(\beta_n \leftarrow (h_{1...T,n}^T h_{1...T,n})^{-1} h_{1...T,n}^T y_{1...T}, \quad n = 1 \ldots N \quad \triangleright \text{linear regression}
5: \text{while true do}
6: \quad \text{for } l \leftarrow 1 \ldots L \text{ do}
7: \quad \quad \lambda_{l,n} \leftarrow \alpha_n^T \mu_l + \beta_n^T h_{l,n} + \frac{1}{2} \alpha_n^T \Sigma_n \alpha_n, \quad t = 1 \ldots T, \quad n = 1 \ldots N
8: \quad \quad u_l \leftarrow G_l G_l^T (y - \lambda) \alpha_l - \mu_l^{old}
9: \quad \quad B_l \leftarrow G_l^T \text{diag}(W_l) G_l
10: \quad \quad \mu_l^{new} \leftarrow \mu_l^{old} + [I_T - G_l G_l^T W_l + G_l B_l (I_l + B_l)^{-1} G_l^T W_l] u_l \quad \triangleright \text{Newton-step for } \mu
11: \quad \quad \mu_l^{new} \leftarrow (\mu_l^{new} - \bar{\mu}_l^{new}) \quad \triangleright \text{constrain } \mu
12: \quad \quad \text{end for}
13: \quad \text{for } n \leftarrow 1 \ldots N \text{ do}
14: \quad \quad \lambda_{l,n} \leftarrow \alpha_n^T \mu_l + \beta_n^T h_{l,n} + \frac{1}{2} \alpha_n^T \Sigma_n \alpha_n, \quad t = 1 \ldots T, \quad n = 1 \ldots N
15: \quad \quad \alpha_n^{new} \leftarrow \alpha_n^{old} + [(\mu + V \circ \alpha_n^{old})^T \text{diag}(\lambda_n)] (\mu + V \circ \alpha_n^{old}) + \text{diag}(V^T \lambda_n)^{-1} [\mu^T y_n - (\mu + V \circ \alpha_n^{old})^T \lambda_n] \quad \triangleright \text{Newton-step for } \alpha
16: \quad \quad \beta_n^{new} \leftarrow \beta_n^{old} + [h_n^T \text{diag}(\lambda_n) h_n]^{-1} h_n^T (y_n - \lambda_n) \quad \triangleright \text{Newton-step for } \beta
17: \quad \quad \text{end for}
18: \quad \quad \alpha_l^{new} \leftarrow \alpha_l^{new} / \|\alpha_l^{new}\|, \quad l = 1 \ldots L \quad \triangleright \text{constrain } \alpha
19: \quad \quad W \leftarrow \lambda \alpha_l^{2T} \quad \triangleright \text{update diagonals of } W
20: \quad \quad B_l \leftarrow G_l^T \text{diag}(W_l) G_l, \quad l = 1 \ldots L
21: \quad \quad V_{1...T,l} \leftarrow [G_l \circ (G_l - G_l B_l + G_l B_l (I_l + B_l)^{-1} B_l)] 1, \quad l = 1 \ldots L
22: \quad \text{Optimize } \sigma_t, \quad l = 1 \ldots L \text{ with line search every } k \text{ iterations}
23: \quad \text{Optimize } \omega_l, \quad l = 1 \ldots L \text{ with line search every } k \text{ iterations}
24: \quad \text{if } |L(q)^{new} - L(q)^{old}| < tol * |L(q)^{old}| \text{ then}
25: \quad \quad \text{break}
26: \quad \text{end if}
27: \quad \quad \mu_{l,1...L}^{old} \leftarrow \mu_{l,1...N}^{new}, \quad \alpha_{l,1...N}^{old} \leftarrow \alpha_{l,1...N}^{new}, \quad \beta_{l,1...N}^{old} \leftarrow \beta_{l,1...N}^{new}
28: \quad \text{end while}
29: \text{end procedure}
\[ W_l = \sum_{t,n} \lambda_{t,n} a_{n,l}^2 e_t e_t^T \] is a diagonal matrix. Therefore, there is no need for optimization of the covariance. This simple form of variational posterior covariance has been noted before \[30\]. Also note that \( \nabla_\mu^2 \mathcal{L} = -\Sigma^{-1}_l \).

There is a redundancy between the bias term in \( \beta \) and the mean \( \mu \). During optimization, we constrain the latent mean \( \mu \) by zero-centering, and normalize the loading \( \alpha \) by its max-norm latent-wise.

The prior covariance matrix \( K_l \) is large \((T \times T)\) and is often severely ill-conditioned. We only keep a truncated incomplete Cholesky factor \( G \) \[29\] of size \( T \times r \) where \( r \) is the rank of the resulting approximation,

\[ K_l \approx G_l G_l^T, \] (19)

which provides both a compact representation and numerical stability. Now, we derive key quantities that are necessary for a memory-efficient and numerically stable implementation. For convenience and without ambiguity, we omit the subscript \( l \) of all vectors and matrices below. By the matrix inversion lemma \[28\], we have

\[ \Sigma = (K^{-1} + W)^{-1} = K - K(W^{-1} + K)^{-1}K. \] (20)

and applying the lemma again

\[ (W^{-1} + K)^{-1} = W -WG(I + B)^{-1}G^TW, \] (21)

where \( B = G^TWG \). We obtain two useful identities as a result:

\[ \Sigma = GG^T - GBG^T + GB(I + B)^{-1}BG^T, \] (22)

\[ K^{-1}\Sigma = I - WGG^T + WG(I_k + B)^{-1}BG^T. \] (23)

With (22) and (23), we can avoid large matrices in above equations such as,

\[ \text{tr}[K^{-1}\Sigma] = T - \text{tr}[B] + \text{tr}[B(I + B)^{-1}B], \] (24)

\[ \log \det[K^{-1}\Sigma] = \log \det[I - B + B(I + B)^{-1}B], \] (25)

\[ \text{diag}(\Sigma) = [G \circ (G - GB + GB(I_k + B)^{-1}B)]1, \] (26)

\[ \Sigma \nabla_\mu \mathcal{L} = (I - GG^TW + GB(I_k + B)^{-1}G^TW)u, \] (27)

where \( 1 \) is the all-ones vector, and \( u = GG^T(y - \lambda)\alpha_l - \mu \). In addition, by the one-to-one correspondence between \( W \) and \( \Sigma \), we use the diagonal of \( W \) as a representation of \( \Sigma \) in the algorithm.
3.2 Weights

Denote the temporal slices of $\Sigma_l$’s by $T \times L$ matrix $V$. The optimal weights $\alpha_n$ and $\beta_n$ given the posterior over the latents can be obtained by the Newton-Raphson method with the following derivatives and Hessians,

$$
\nabla_{\alpha_n} L = \mu^\top (y_n - \lambda_n) - \text{diag}(V^\top \lambda_n) \alpha_n, \\
\nabla^2_{\alpha_n} L = - (\mu + V \circ 1a_n^\top) \text{diag}(\lambda_n)(\mu + V \circ 1a_n^\top) - \text{diag}(V^\top \lambda_n),
$$

and

$$
\nabla_{\beta_n} L = h_n^\top (y_n - \lambda_n), \\
\nabla^2_{\beta_n} L = - h_n^\top \text{diag} (\lambda_n) h_n.
$$

The updating rules are

$$
\alpha_n^{\text{new}} = \alpha_n^{\text{old}} - (\nabla^2_{\alpha_n} L)^{-1} \nabla_{\alpha_n} L, \\
\beta_n^{\text{new}} = \beta_n^{\text{old}} - (\nabla^2_{\beta_n} L)^{-1} \nabla_{\beta_n} L.
$$

Once again, both Hessians are negative definite, and hence in the territory of convex optimization.

3.3 Hyperparameters

For the squared-exponential covariance kernel, we rewrite the kernel matrix as,

$$
K_l = \sigma^2_l C_l = \sigma^2_l \exp(-\omega_l D), \quad l = 1 \ldots L.
$$

where $C_l$ is the correlation matrix and $D$ is the matrix of squared distances of each time pair. Hyperparameters $\sigma^2_l$ and $\omega_l$ corresponds to prior variance and inverse length-scale, and once again we maximize (10) given the parameters and posterior.

Taking derivative w.r.t. $\sigma^2_l$, we have

$$
\frac{\partial L}{\partial \sigma^2_l} = - \frac{1}{2} \left[ -\sigma^{-4}_l \mu_l^\top C_l^{-1} \mu_l - \sigma^{-4}_l \text{tr}(C_l^{-1} \Sigma_l) + T \sigma^{-2}_l \right].
$$

Setting (35) to 0, $\sigma^2_l$ can be obtained by

$$
\sigma^2_l = \frac{1}{T} \left[ \mu_l^\top C_l^{-1} \mu_l + \text{tr}(C_l^{-1} \Sigma_l) \right].
$$

Note that $\omega_l$ must be positive. So we take the derivative w.r.t. $\log \omega_l$ instead

$$
\frac{\partial L}{\partial \log \omega_l} = \text{tr} \left( \frac{\partial L}{\partial K_l} \frac{\partial K_l}{\partial \log \omega_l} \right).
$$
\[
\frac{\partial L}{\partial K_l} = \frac{1}{2} \left( K_l^{-1} \mu_l \mu_l^\top K_l^{-1} + K_l^{-1} \Sigma_l K_l^{-1} - K_l^{-1} \right)
\]

(38)

\[
\frac{\partial K_l}{\partial \log \omega_l} = K_l \circ \log C_l
\]

(39)

where \( \circ \) is the Hadamard product. The optimal value can be found by common gradient algorithms or line search for each latent independently.

The above derivation of the hyperparameter optimization technique assumes a fixed posterior and parameters. Thus it requires complete prior covariance matrices and explicit posterior covariance matrices rather than low-rank decompositions. In order to avoid numerical singularity, we add a small quantity to the diagonal of prior covariance matrices. It would be extremely costly to use these complete covariance matrices for long, consecutive time series. Therefore, we randomly sample many shorter temporal segments of the consecutive posterior for fast computation [7]. One hyperparameter iteration is performed every fixed number of iterations of posterior and parameter optimization. We constrain the each hyperparameter to be updated at most by a factor of 5 on each iteration.

4 Results

We apply our inference algorithm to two simulated systems and one real dataset. We compare our method (vLGP) against GPFA and PLDS.

4.1 Evaluation

We use a leave-one-neuron-out prediction likelihood to compare models. For each dataset comprising of several trials, we choose one of the trials as test trial and the others as training trials. First, the weights and posterior are inferred from the training trials. Next, we leave one neuron out of the test trial and make inference on the posterior by the remaining neurons with the weights estimated from the training trials. Then the spike train of the left-out neuron are predicted by the model given the weights estimated from the training trials and the posterior inferred from the test trial. We do this procedure on each neuron of one trial and each trial of one sample. Finally we obtain the prediction of all spike trains in the sample.

For simulated datasets, we know the true latent process that generates observations. Since latent space is only identifiable up to affine transformation, we quantify using the angle between subspaces [10] [19].
4.2 Simulation

We simulate two datasets: one with deterministic nonlinear dynamics, and one with linear dynamics and model-mismatched nonlinear observation. Each dataset consists of 5 samples and each sample contains 10 trials from 50 neurons which last for 1 sec. We choose a bin size of 1 ms.

In the first dataset, the latent dynamics are sampled from the standard Lorenz
system with the time step of 0.0015. The system is defined by the equations,

\[
\begin{align*}
    x_1' &= \sigma(x_2 - x_1), \\
    x_2' &= x_1(\rho - x_3) - x_2, \\
    x_3' &= x_1 x_2 - \beta x_3.
\end{align*}
\] (40)

Spike trains are simulated by (1) with 10 ms suppressive history filter given the latent dynamics.

In the second dataset, Poisson spike trains are simulated from a 3-dimensional linear dynamical system (LDS) defined as

\[
\begin{align*}
    y_{t,n} | x_t & \sim \text{Poisson}(\log(1 + \exp(c_n^\top x_t + d_n))) \\
    x_0 & \sim \mathcal{N}(\mu_0, Q_0) \\
    x_{t+1} | x_t & \sim \mathcal{N}(Ax_t + b_t, Q).
\end{align*}
\] (41)

Figure 2 shows one trial from each dataset and corresponding inferred posterior mean latent processes. The posterior means are rotated toward the true latent subspace. The PLDS inference (blue) looks the farthest away from the true Lorenz latent relatively but much closer to the LDS latent because the true latent meets its assumption. However, PLDS inference lacks of smoothness. The GPFA inference (green) is better than PLDS for Lorenz latent but shows deviations from the true LDS latent. The smoothness is kept in the inference. The inference of our model (red) are very close to the true latent in both cases along the time while being smooth at the same time.

The angle between two subspaces of the posterior and true latent dynamics gives a measure of the goodness of the posterior. If the angle is small, the two spaces are nearly linearly dependent which indicates that the posterior recovers more information about the underlying trajectory. For one sample, we compute the angle between the posterior and true latent after concatenate all the trials. Since the models do not assume continuity between trials and impose constrains on the posterior mean, the concatenation is performed before computing the angle. Note that the GPFA cuts the trials into small segments for estimating the loading matrix and bias. Thus such rotations become infeasible while the algorithm is running. We then use the raw concatenated posterior mean to compute the angle of each iteration and use the rotated one for the final result. Thus declines happened at the final iteration in the figures. However, those declines are relatively small so the angles are still meaningful for comparison. The resulting angle is an overall measure of the whole sample.

Figure 3 shows the angle between the posterior mean and true latent versus running time (log scale). The figures shows our model (vLGP) resulted in overall smaller angles than the PLDS and GPFA for almost all samples of both datasets.
(a) Subspace angle (Lorenz)  
(b) Subspace angle (LDS)

Figure 3: Performance comparison on simulated datasets. (a,b) Convergence speed of each algorithm in terms of inferred subspace angle between the true generative latent time series and the inferred mean posterior. GPFA is the fastest, and PLDS converges very slowly. vLGP achieves the smallest subspace angle, yet an order of magnitude faster than PLDS. The origin of time is shifted to 1 for convenience.

after the algorithms end. PLDS uses nuclear norm penalized rate estimation as initialization. The angles from PLDS stayed near the initial value through the optimization which implies this initialization is close to the optimal value under the criterion of PLDS. Both the GPFA and our model use factor analysis as initialization. It is obvious that our model makes much improvement to the result of factor analysis in terms of the angle between subspaces.

In Table 1, we use predicted firing rates and spikes in the corresponding time bins as the mean and observation to compute the prediction log-likelihood (PLL) as a measure of prediction performance (the higher the better). The PLL of one trial is given as

$$PLL = \frac{\left[\sum_{t,n}(y_{y,n} \log(\lambda_{t,(-n)}) - \lambda_{t,(-n)})\right] - \left[\sum_{t,n}(y_{y,n} \log(\bar{y}) - \bar{y})\right]}{(# \text{ of spikes}) \log(2)},$$  

(42)

where $\lambda_{t,(-n)}$ is the leave-neuron-out prediction to the firing rate of neuron $n$ at time $t$, and $\bar{y}$ is the population mean. Both PLDS and our model assume exponential link. GPFA assumes a Gaussian likelihood, it is incompatible to compare directly. Since GPFA is applied to the square root of spike count to stabilize marginal variance, we use square link function to transform the predicted observation and compute the point process likelihood. However, square link often shows detrimental effects due to large negative predictions, therefore we also use a linear rectifier which is better behaved. Denote the linear predictor by $\eta$ omitting
the neuron, time and model. The prediction is given as

\[
\lambda = \begin{cases} 
\eta^2 & \text{GPFA (square link)} \\
\log(1 + \exp(500\eta))/500 & \text{GPFA (rectifier link)} \\
\exp(\eta + \frac{1}{2}\alpha^TV\alpha) & \text{PLDS and vLGP}
\end{cases}
\]  

(43)

Table 1: Predictive log-likelihood (PLL)

| Dataset | Sample | PLDS | GPFA (square) | GPFA (rectifier) | vLGP |
|---------|--------|------|---------------|------------------|------|
| Lorenz  | 1      | 0.41 | -4.63         | -0.22            | 0.58 |
|         | 2      | 0.50 | -5.30         | -0.52            | 0.74 |
|         | 3      | 0.50 | -5.60         | -0.68            | 0.74 |
|         | 4      | 0.51 | -5.97         | -0.83            | 0.76 |
|         | 5      | 0.44 | -5.80         | -0.78            | 0.66 |
| LDS     | 1      | 0.79 | -2.86         | 0.72             | 0.83 |
|         | 2      | 0.94 | -2.37         | 0.87             | 0.98 |
|         | 3      | 0.99 | -2.24         | 0.91             | 1.03 |
|         | 4      | 0.97 | -2.28         | 0.92             | 1.01 |
|         | 5      | 0.97 | -2.24         | 0.91             | 1.01 |
| V1      | N=63   | 0.81 | -2.90         | 0.97             | 0.99 |
|         | N=148  | 1.28 | -2.45         | 1.29             | 1.35 |

4.3 V1 population recording

We apply our method to a large scale recording to validate that it picks up meaningful signals, and investigate the population-wide trial-to-trial variability structure. We use the dataset [31] where 72 different equally spaced directional drifting gratings were presented to an anesthetized monkey for 50 trials each (array-5, 148 simultaneously recorded single units). We use 63 V1 neurons by only considering neurons with tuning curves that could be well approximated ($R^2 \geq 0.75$) by bimodal circular Gaussian functions (the sum of two von Mises functions with different preferred orientations, amplitudes and bandwidths) according to [31]. We do not include the stimulus drive in the model, in hopes that the inferred latent processes would encode the stimulus. We used bin size of 1 ms.

We use 4-fold cross-validation to determine the number of latents. A 15-dimensional model is fitted to a subsample composed of the first trial of each direction at first. In each fold, we use its estimated parameter to infer the latent process from another subsample composed of the second trial of each direction. The inference is made by leaving a quarter of neurons out, and we predict the spike trains of the left-out neurons given the first $k$ ($k = 1 \ldots 15$) orthogonalized
latent process corresponding to $k$-dimension. Finally we choose 5 as the dimension where the predictive log-likelihood reaches the top.

We re-fit a 5-dimensional vLGP model using the subsample of the first trials. To quantify how much the model explains, we report pseudo-$R^2$ defined as

$$R^2 = 1 - \frac{LL_{\text{null}} - LL_{\text{model}}}{LL_{\text{saturated}} - LL_{\text{null}}} \quad (44)$$

where $LL_{\text{null}}$ refers to the log-likelihood of population mean firing rate model (single parameter). The pseudo-$R^2$ our model (vLGP with 5D latents) is 20.88%. This model explains with shared variability through the latents, and heterogeneity of baseline firing of individual neurons. For a baseline model with only per neuron noise component (and no shared latent), the pseudo-$R^2$ is 6.77%.

Table 1 shows the PLLs based on two subsets. The first one is 4 trials ($0^\circ$, $90^\circ$, $180^\circ$, $270^\circ$) of the subset of 63 neurons with 5-dimensional latent process. The second one is 10 trials (5 trials of $0^\circ$ and 5 trials of $90^\circ$) of all 148 neurons with 4-dimensional latent process.

![Figure 4: Single trial spike trains and inferred latent. The visual stimulus was only on for the first half of the trial. The left two columns are the spike trains and respective inferred latent of 2 trials of $0^\circ$. The right ones are 2 trials of $90^\circ$.](image)

Although the parameters are estimated from a subsample, we can use them to infer the latent process of all trials of all 72 directions. Figure 4 shows inferred latent processes for two trials for two directions. We rotate the inferred latent process by the singular value decomposition. (The detail will be given later.) Variational posterior distribution over the latents are shown for each trial. During the second half of the trial when the stimulus was off, and the firing rate was lower, the uncertainty in the latent processes increases. There are visible trial-to-trial variability in the spike trains which is reflected in the variations of latents.
First we investigate how the “signal” is captured by the latent processes. We average the inferred latent processes over 50 trials with identical spatiotemporal stimuli (Fig. 5). Since the stimuli are time-locked, corresponding average latent trajectory should reveal the time-locked population fluctuations driven by visual input. We concatenate the average latent processes along the dimension of time. Then we orthogonalize it by SVD. The dimensions of orthogonalized one are ordered by the respective singular values. The latent process of a single trial is also rotated to the same subspace.

Furthermore, we visualized the trajectories in 3D (see supplementary online video\(^4\)) that show how signal and noise are dynamically encoded in the state space. Figure 6 shows the projection of average latent process corresponding to each orientation to the first 3 principal components. The projection topologically preserves the orientation tuning in the V1 population. We see torus like encoding of two circular variables, orientation and temporal phase of oscillation (see online video).

To see if our model captures the noise correlation structure through the latents as one would predict from recent studies of cortical population activity \[18,26,27\], we calculated pairwise correlations between all neurons during the off-stimulus period (1400–2560 ms, no signal, “spontaneous activity”). The lower half in Figure 7a shows the correlation of real spike trains of all orientations in descending order by the population neuron-wise firing rates. The correlation from the model shows similar structure to the real one but slightly underestimated as seen in Figure 7b. Proposed model explains 39% of the total power in noise-correlation: \[\| C_{\text{model}} - C_{\text{raw}} \|_F / \| C_{\text{raw}} \|_F = 0.61\] where \(C\) is the zero-diagonal correlation matrix w.r.t. its subscript and \(\| \cdot \|_F\) is the Frobenius norm.

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\(^4\) https://www.youtube.com/watch?v=CrY5AfNH1ik
Figure 6: 3D projection of mean latent trajectories given each orientation. We plot the first three singular vectors of the inferred latent corresponding to the signal interval (0–1400 ms) colored by orientation. The colored circles are cycle averages that visualize the temporal phase of oscillation per direction, and form an approximate torus. The black circle visualizes the circular orientation that goes through the center of the torus. The left side shows 0–180° and the right side shows 180–360°.

Figure 7: Noise-correlation during the off-stimulus period (1400–2560 ms). (a) The lower triangular part is the correlation coefficient between true spike trains of all trials and all orientations, while the upper triangular part is from model-predicted ones. The diagonal is omitted. The neurons are in descending order by their respective global firing rates during off-stimulus period. (b) Histogram of true and predicted correlation coefficients between neurons (1400–2560 ms).
These results show that vLGP is capable of capturing both the signal—repeated over multiple trials—and noise—population fluctuation not time locked to other task variables—present in the cortical spike trains.

5 Discussion

We propose vLGP, a method that recovers low-dimensional latent dynamics from high-dimensional time series. Latent state-space inference methods are different from methods that only recover the average dynamics time-locked to an external observation \[14, 32\] and requires trial averaging. By inferring latent dynamics from each trial, it provides a flexible framework for studying internal processes that are not time-locked. Higher-order processes such as decision-making, attention, and memory recall are well suited to be analyzed via recovered latent trajectories. It can perform dimensionality reduction on a single trial basis and allows decomposition of neural signals into a small number of temporal signals and their relative contribution to the population signal.

We compare our method to two widely used latent state space modeling tools in neuroscience, GPFA \[7\] and PLDS \[9\]. Unlike GPFA, vLGP allows a generalized linear model observation which is suitable for a wide class of point process observations. Moreover, vLGP is faster than PLDS which assumes a Poisson process observation given the latent trajectory, yet it shows superior performance in capturing the spatio-temporal structures in the neural data to both PLDS and GPFA.

To test its validity in real electrophysiological recordings, we used V1 population recording driven by fixed stimulus as a litmus test for vLGP. We showed that our inferred latents contain meaningful information about the external stimuli, encoding both orientation and temporal modulation.

We only considered smoothness encoded in the GP prior in this manuscript, but a plethora of GP kernels are available \[28, 33\]. For example, to capture prior assumptions about periodicity in some of the latent processes, we can use spectral kernels \[34\]. This can be particularly useful for capturing internal neural oscillations \[35\]. In addition, it is straightforward to incorporate additional covariates such as external stimuli \[25\] or local field potential \[36\] to vLGP.

The proposed method has potential application in many areas, and it will be particularly useful in discovering how specific neural computations are implemented as neural dynamics. We are working on applying this method and its extensions to sensorimotor decision-making process where the normative model guides what is being computed, but it is unclear as to how the neural system implements it.
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