Structured Recognition for Generative Models with Explaining Away

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Abstract

A key goal of unsupervised learning is to go beyond density estimation and sample generation to reveal the structure inherent within observed data. Such structure can be expressed in the pattern of interactions between explanatory latent variables captured through a probabilistic graphical model. Although the learning of structured graphical models has a long history, much recent work in unsupervised modelling has instead emphasised flexible deep-network-based generation, either transforming independent latent generators to model complex data or assuming that distinct observed variables are derived from different latent nodes. Here, we extend amortised variational inference to incorporate structured factors over multiple variables, able to capture the observation-induced posterior dependence between latents that results from "explaining away" and thus allow complex observations to depend on multiple nodes of a structured graph. We show that appropriately parametrised factors can be combined efficiently with variational message passing in rich graphical structures. We instantiate the framework in nonlinear Gaussian Process Factor Analysis, evaluating the structured recognition framework using synthetic data from known generative processes. We fit the GPFA model to high-dimensional neural spike data from the hippocampus of freely moving rodents, where the model successfully identifies latent signals that correlate with behavioural covariates.

1 Introduction

A central challenge of unsupervised learning is to identify and model patterns of statistical dependence in high-dimensional data. One approach to this challenge exploits latent-variable generative models, which capture the statistical structure of data through the modelled influence of the latent variables on observations, and through interactions between the latents themselves. Recent developments in deep learning have enabled deep generative models (DGM), with remarkable success in density estimation and high-fidelity image or text generation [1–5]. However, much of the DGM development has emphasised the expressiveness and accuracy of the latent-to-observation generative process, with the latents themselves often assumed independent *a priori*.

Variational learning requires inferring or approximating the posterior distribution of the latents conditioned on observations [6]. In a variational autoencoder [VAE; 1, 2], inference for a DGM is *amortised* by training a recognition network to return parameters of the variational posterior. The structured variational autoencoder [SVAE; 7] connects the DGM framework with richer models that include structured prior dependence amongst the latent variables. In an SVAE the structured latent prior is combined with a DGM link between each latent and a corresponding observation. Variational inference is amortised using recognition networks that return parameters of a factor associated with each link, which are combined with the structured prior to obtain the full posterior. However, in

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many generative models of interest, observations depend on more than one latent variable. Such interactions induce joint potentials in the likelihood, coupling latents in the posterior even if they are independent *a priori*, a phenomenon sometimes called "explaining away" [8]. To capture such observation-induced dependence in the DGM setting we develop the *structured recognition VAE* (SRVAE), where recognition potentials that incorporate joint factors induced by the observations are learnt in within a (structured) variational autoencoding framework.

We instantiate the SRVAE framework in contexts of both classical PGM and non-linear Gaussian process (GP) latent models. In the latter case, we bring together the GP-prior VAE [9, 10], and (sparse) Gaussian process factor analysis (GPFA) [11, 12] models, yielding a novel autoencoding model (SR-nlGPFA). Experiments show that SR-nlGPFA outperforms alternatives that lack structured amortisation. We apply SR-nlGPFA to data collected from a population of neurons in the hippocampal complex, and show that the unsupervised approach automatically captures dimensions underlying neural firing that reflect relevant behavioural correlates.

2 Background

2.1 Variational Inference and Structured Variational Autoencoders

Consider a general generative process with latent variables z and observations y,

$$z \sim p(z|\theta), \quad y \sim p(y|z;\gamma)\,,$$

where θ and γ are the parameters of the prior and conditional likelihood distributions, respectively (and we write $\Theta = \theta \cup \gamma$). We assume deterministic θ for simplicity, but distributions over θ (with conjugate hyperpriors) can be incorporated by variational Bayes (VB) [13]. The posterior distribution, $p(z|y,\Theta) \propto p(z|\theta)p(y|z,\gamma)$, is often analytically intractable. In such cases, a common approach is to seek an approximation $q(z)$ constrained to a tractable class $\mathcal{Q}$ by variational inference (VI); that is, by minimising the KL-divergence with respect to the true posterior distribution or, equivalently, maximising a variational free energy [6] $\mathcal{F}_{\text{VI}} = \big\langle \log p(y,z|\Theta) - \log q(z) \big\rangle_{q(z)}$:

$$q_{\text{VI}(\mathcal{Q})}(z|y,\Theta) = \operatorname*{argmin}_{q\in\mathcal{Q}} \mathbf{KL}[q(z)\|p(z|y,\Theta)] = \operatorname*{argmax}_{q\in\mathcal{Q}} \big\langle \log p(y,z|\Theta) - \log q(z) \big\rangle_{q(z)}\,. \tag{1}$$

In the variational autoencoder (VAE) architecture, the parametric optimisation of $q(z)$ implicit in (1) is amortised by a recognition network that takes as input the observed values y and returns parameters of q. The parameters of this recognition network are then trained jointly with the generative model by stochastic optimisation of the free energy [1, 2].

In both standard and amortised VI, the approximate distribution q is often constrained to factor over the latent variables, a so-called *mean-field* constraint. While tractable, such mean-field approximations may be too restrictive to capture the complexity of the true posterior [14, 15]. Many approaches have been proposed for improving the expressiveness of variational approximation [16–19]. Here we consider the structured VAE [SVAE; 7]. Unlike standard VAEs, the SVAE assumes the generative prior distribution to be specified by a structured probabilistic graphical model (PGM), $p(z|\theta) \propto \prod_{c\in C} \psi_c(z_c)$, where $\{\psi_c\}_{c\in C}$ correspond to C clique potentials. In addition, the amortised inference network outputs recognition factors, $r(z|y,\phi)$, that approximate the generative likelihood function rather than the full variational posterior. These recognition factors are combined with the structured prior distribution to obtain the amortised variational posterior,

$$q_{\text{SVAE}}(z|y,\Theta,\phi) = \operatorname*{argmax}_{q\propto r(z|y,\phi)p(z|\theta)} \sum_{y\in\mathcal{Y}} \left\langle \log\left(\frac{p(z|\theta)p(y|z,\gamma)}{q(z)}\right)\right\rangle_{q(z)} \propto r(z|y,\phi^*)p(z|\theta)\,, \tag{2}$$

where ϕ^* minimises the surrogate KL over the data observations $\mathcal{Y}$. Johnson et al. [7] considered recognition factors that are local (singleton) evidence potentials, chosen to be conjugate to $p(z|\theta)$. Nonetheless, the form of (2) does allow the dependency structure established by the prior distribution to be carried over to the variational posterior distribution. Further details of SVAE appear in Appendix A.

2.2 Gaussian Process Factor Analysis

Gaussian Process Factor Analysis (GPFA) is a model used in neural data analysis to infer the dynamic latent structure underlying high-dimensional population spike trains [11]. Standard GPFA assumes

the following generative model:

$$\begin{aligned}
\text{latent functions: } & f^k(\cdot) \sim \mathcal{GP}\big(m_\theta^k(\cdot), \kappa_\theta^k(\cdot,\cdot)\big), \text{ for } k = 1, \dots, K\,, \\
\text{affine embeddings: } & h_n(\cdot) = \sum_{k=1}^{K} c_{nk} f^k(\cdot) + d_n, \text{ for } n = 1, \dots, N\,, \\
\text{observations: } & y_n(t) \sim p\big(y_n(t) | g(h_n(t))\big), \text{ for } t = 1, \dots, T\,,
\end{aligned} \tag{3}$$

where $m_\theta^k(\cdot)$ and $\kappa_\theta^k(\cdot,\cdot)$ parametrise the GP prior, c_{jk} and d_n define an affine mapping from the latent space to the observation space (or a transform of the observations for general likelihoods), and $g(\cdot)$ is a smooth scalar link function appropriate for the observation distribution. We take $m_\theta^k(\cdot) = 0$ unless stated otherwise. Correlations between observed neurons are captured by dependence on the common set of latents, while temporal correlations in the high-dimensional observations are modelled by the latent temporal correlations of the GPs. The PGM describing the GPFA generative model (with sparse variational approximation, see below) is shown in Fig 1a.

Although maximum-likelihood parameters for GPFA can be found using (variational) expectation-maximisation [20, 11] exact GP inference scales cubically in the number of observation times [21]. Sparse variational GP (svGP) inference based on auxilliary inducing points [22] reduces the time complexity of learning in GPFA [23], and also facilitates efficient extensions to (pointwise) non-conjugate likelihoods [12].

For $k = 1, \dots, K$, we introduce inducing values $\mathbf{u}_k$ representing the evaluations of the latent process f^k at M_k inducing locations, $\mathbf{z}_k$. For simplicity, we assume $M_1 = \cdots = M_K = M$ unless stated otherwise. The GPFA generative model (3) can be augmented to include these auxiliary variables:

$$p(\mathbf{u}_k|\mathbf{z}_k) = \mathcal{N}\big(\mathbf{0}, \mathbf{K}^k_{\mathbf{z}_k\mathbf{z}_k}\big), \quad p(f_k(\cdot)|\mathbf{u}_k) = \mathcal{GP}(\mathfrak{F}_k(\cdot)\mathbf{u}_k, \kappa_\theta^k(\cdot,\cdot) - \mathfrak{F}_k(\cdot)\mathbf{K}^k_{\mathbf{z}_k\mathbf{z}_k}\mathfrak{F}_k^T(\cdot)), \tag{4}$$

where $\mathfrak{F}_k(\cdot) = \kappa_\theta^k(\cdot, \mathbf{z}_k)(\mathbf{K}^k_{\mathbf{z}_k\mathbf{z}_k})^{-1}$ is the linear operator that maps $\mathbf{u}_k$ to $f_k(\cdot)$; $\kappa_\theta^k(\cdot, \mathbf{z}_k)$ is a vector-valued function with $\kappa_\theta^k(x; \mathbf{z}_k) = [\kappa_\theta^k(x, z_{k1}), \kappa_\theta^k(x, z_{k2}), \dots, \kappa_\theta^k(x, z_{kM_k})]$; and $\mathbf{K}^k_{\mathbf{z}_k\mathbf{z}_k}$ is the covariance matrix obtained by evaluation of the kernel function $\kappa_\theta^k(\cdot)$ at the inducing locations $\mathbf{z}_k$.

Introducing a variational distribution over the inducing points and the latent functions, and utilising the generative model (Fig 1a), the free energy of the sparse variational GPFA (svGPFA) can be expressed as following:

$$\mathcal{F}(\Theta, \mathbf{C}, \mathbf{d}, \mathbf{Z}, \phi) = \sum_{t=1}^{T} \left\langle \log \frac{p(\mathbf{y}_t|\mathbf{h}_t;\gamma)p(\mathbf{h}_t|\mathbf{f}_t;\mathbf{C},\mathbf{d})p(\mathbf{f}_t|\mathbf{U};\theta)p(\mathbf{U}|\mathbf{Z};\theta)}{q(\mathbf{f},\mathbf{U};\phi)} \right\rangle_{q(\mathbf{f},\mathbf{U};\phi)}. \tag{5}$$

where $\mathbf{C} = (c_{nk})_{nk} \in \mathbb{R}^{N\times K}$, $\mathbf{d} = (d_n)_n \in \mathbb{R}^n$, $\mathbf{U} = [\mathbf{u}_1, \dots, \mathbf{u}_K]^T \in \mathbb{R}^{K\times M}$, $\mathbf{Z} = [\mathbf{z}_1, \dots, \mathbf{z}_K]^T \in \mathbb{R}^{K\times M}$. The svGP approach constrains $q(\mathbf{f}, \mathbf{U}; \phi)$ to the form $q(\mathbf{U})p(\mathbf{f}|\mathbf{U}, \theta)$ with Gaussian $q(\mathbf{U})$ [22]. In the multi-GP case, the distribution is typically also taken to factorise over processes [23], $q(\mathbf{f}^{1:K}, \mathbf{u}_{1:K}) = \prod_{k=1}^{K} p(f^k|\mathbf{u}_k)q(\mathbf{u}_k)$, with $q(\mathbf{u}_k) = \mathcal{N}(\mathbf{m}_k, \mathbf{S}_k)$. Under these constraints on q, the svGPFA free energy simplifies to

$$\mathcal{F}_{\text{svGPFA}} = \sum_t \langle \log p(\mathbf{y}_t|\mathbf{h}_t)\rangle_{q(\mathbf{h}_t)} - \sum_{k=1}^{K} \mathbf{KL}[q(\mathbf{u}_k)\|p(\mathbf{u}_k|\mathbf{z}_k)]\,,$$

where $q(\mathbf{h}_t) = \int d\mathbf{U}\, p(\mathbf{h}_t|\mathbf{U})q(\mathbf{U})$ is itself a GP with mean and kernel functions given by

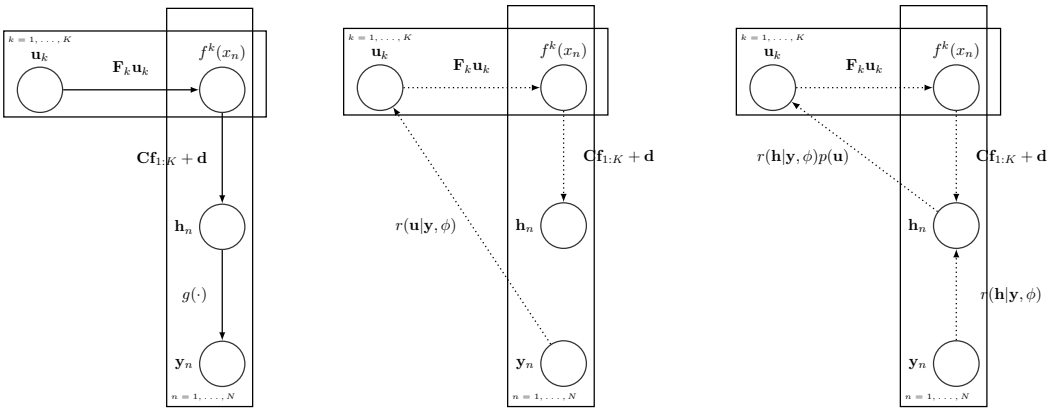
$$m_n^h(t) = \sum_{k=1}^{K} c_{nk}\mathfrak{F}_k(t)\mathbf{m}_k + d_n \text{ and } \nu_n^h(t,t') = \sum_{k=1}^{K} c_{nk}^2(\kappa_k(t,t') + \mathfrak{F}_k(t)(\mathbf{S}_k - \mathbf{K}_{\mathbf{z}_k\mathbf{z}_k})\mathfrak{F}_k(t')^T)\,.$$

Hence the computational cost for sparse variational GP inference reduces from $\mathcal{O}(T^3)$ down to $\mathcal{O}(M^3 + TM^2)$.

3 Structured Recognition and explaining away

3.1 Structured Recognition in VAEs

A general non-linear likelihood may induce additional latent dependency structure in the posterior beyond that of the prior (a simple illustrative example appears in Appendix C). Although the SVAE



(a) (b) (c)

Figure 1: **Graphical models for sparse variational GPFA models**. **(a)** Generative model of GPFA model with sparse inducing point approximation; **(b)** Standard GPFA inference with sparse amortised variational approximation (note that $\mathbf{C} = \mathbf{I}$ and $\mathbf{d} = \mathbf{0}$ for SGP-VAE [10]); **(c)** Structured recognition potential enables full-covariance variational inference in SR-nlGPFA model.

approach developed by Johnson et al. [7] composed amortised inference with a structured prior distribution, the recognition models these authors discussed all contributed amortised potentials that factored over latent variables. Such an approach cannot accurately model posteriors with dependence that differs from that of the prior PGM.

Here we adopt a recognition network that outputs structured factor potentials over the latents, providing amortised estimates of the additional dependencies induced by "explaining away". We denote the resulting model the *Structured Recognition VAE* (SRVAE). The SRVAE variational approximation takes the form

$$q_{\text{SRVAE}}(z|y, \theta, \phi) \propto \prod_{c \in C} \psi_c(z_c; \theta) \prod_{c \in C_r} \xi_c(z_c|y; \phi)\,, \tag{6}$$

where C_r is the set of recognition factors and the ξ_cs the associated factor potentials. We assume that the ξ_cs are chosen to be conjugate to the prior factors unless otherwise stated. Hence the analytical (approximate, if necessary) form of q_{SRVAE} can be computed with (variational) message passing. In the most general form, we could let $\xi(z|y; \phi)$ be a single joint factor potential over the complete set of latent variables.

The free energy objective takes the same form as the standard autoencoding free energy objective [1, 2], but with the structured amortised variational approximation, q_{SRVAE}, as the variational distribution.

$$\mathcal{F}_{\text{SRVAE}}(\Theta, \phi) = \langle \log p(z|\theta) + \log p(y|z, \gamma) - \log q_{\text{SRVAE}}(z|y, \phi, \theta) \rangle_{q_{\text{SRVAE}}(z|y,\phi,\theta)} \tag{7}$$

The training of the model follows standard VAE-style stochastic optimisation to update the parameters of the recognition and generative networks, as well as (optionally) the parameters of the prior PGM.

The following proposition supports the use of SRVAE framework (the proof appears in Appendix E).

Proposition 3.1. *The SRVAE objective function provides a tighter lower bound to the free energy than the SVAE objective function.*

$$\max_{q} \mathcal{F}_{VI(\mathcal{Q})}(\Theta, q) \geq \max_{\phi} \mathcal{F}_{SRVAE}(\Theta, \phi) \geq \max_{\phi} \mathcal{F}_{SVAE}(\Theta, \phi) \tag{8}$$

Below we describe two instantiations of the SRVAE framework, the first based on a latent Gaussian mixture model, and the second on a latent GPFA model, both with DGM outputs. Structured amortised inference facilitates scalable inference of the posterior latent distribution with full covariance structure, allowing more accurate learning than with factored recognition approaches. However, the SRVAE framework is more general-purposed, and can be combined with many different latent variable models. Further examples appear in Appendix E.

3.2 Structured Recognition with Latent Gaussian Mixture Model

We instantiate SRVAE with a classical latent variable model, the latent Gaussian mixture model (GMM) [24]. We assume the following generative process (Figure 5a):

$$\begin{aligned} z_t|\pi &\sim \text{Categorical}(z|\pi) \\ \mathbf{h}_t &\sim \mathcal{N}(\mathbf{h}|\boldsymbol{\mu}^{(z_t)}, \boldsymbol{\Sigma}^{(z_t)}) \\ \mathbf{y}_t|\mathbf{h}_t &\sim \mathcal{N}(\mathbf{y}|\boldsymbol{\mu}_{\text{NN}}(\mathbf{h}_t), \boldsymbol{\Sigma}_{\text{NN}}(\mathbf{h}_t)) \end{aligned} \tag{9}$$

This model was studied by Johnson et al. [7], using fully factorised recognition potentials, followed by variational message passing[VMP; 25] to obtain the GMM variational posterior (details can be found in Appendix A). However, the coupled conditional model, parametrised by a neural network, induces posterior correlations between the latent variables that do not exist *a priori*. Hence in order to implement the structured amortised inference, we assume a full covariance Gaussian recognition potential on $\mathbf{h}$, and the SRVAE-GMM variational approximation is computed with VMP given the recognition and prior factors.

3.3 Structured Recognition Variational Autoencoding Nonlinear GPFA

The GPFA model (3) incorporates a generalised-linear likelihood, with the link function $g(\cdot)$ acting separately on each affine embedding value h_n. We are now in a position to use the SAVAE framework to extend GPFA to include a DGM likelihood, greatly increasing the expressiveness of the generative model. Consider observations $\{(x_t, \mathbf{y}_t)\}_{t=1}^T$, defining $\mathbf{f}_t \in \mathbb{R}^K$ and $\mathbf{h}_t \in \mathbb{R}^N$ to be the corresponding vectors of latent process values and embeddings at x_t. In the generative model, we retain the affine mapping from $\mathbf{f}_t$ to $\mathbf{h}_t$, replacing the link function by a non-linear multivariate DGM: $\mathbf{y}_t \sim p(\mathbf{y}|g(\mathbf{h}_t, \gamma))$. Although the generative affine mapping could, in principle, be subsumed within the general deep network, the embeddings $\mathbf{h}_t$ will play a valuable role in parametrising structured amortised inference.

For amortised svGP inference, our goal is to define a variational distribution $q(\mathbf{U}|\mathbf{Y}, \phi)$. Ashman et al. [10] have considered a similar latent GP model called the SGP-VAE. There, the variational distribution over the latents was found by combining the prior GP distribution with an amortised approximation of the likelihood function factored over latent processes [22]:

$$q(\mathbf{F}, \mathbf{U}) = \prod_k p(\mathbf{f}_k|\mathbf{u}_k)q(\mathbf{u}_k), \text{ where } q(\mathbf{u}_k) \propto p(\mathbf{u}_k) \prod_t r(\mathbf{u}_k|\mathbf{y}_t, x_t, \mathbf{z}_k), \tag{10}$$

The graphical model for SGP-VAE inference is shown in Figure 1b, with $\mathbf{C} = \mathbf{I}$ and $\mathbf{d} = \mathbf{0}$. While this approach captures induced correlation amongst the inducing points, it fails to capture correlations *between* latent processes that arise in the posterior through "explaining away", potentially leading to sub-optimal inference and learning.

Our solution is to recast the output of the amortised inference to the likelihood of $\mathbf{h}$ rather than $\mathbf{U}$, and propose the following structured variational distribution.

$$q(\mathbf{F}, \mathbf{U}) = \left[\prod_k p(\mathbf{f}_k|\mathbf{u}_k)\right] q(\mathbf{U}), \text{ where } q(\mathbf{U}) \propto \int d\mathbf{h}\, p(\mathbf{U})p(\mathbf{H}|\mathbf{U}) \prod r(\mathbf{h}_t|\mathbf{y}_t) \tag{11}$$

where $r(\mathbf{h}_t|\mathbf{y}_t) = \mathcal{N}(\mathbf{h}|\mathbf{m}(\mathbf{y}_t;\phi), \boldsymbol{\psi}(\mathbf{y}_t;\phi)) = \mathcal{N}\big(\boldsymbol{\mu}_t^h, \boldsymbol{\Psi}_t^h\big)$, with $\boldsymbol{\Psi}_t^h$ diagonal, $\mathbf{F} = [\mathbf{f}(x_1), \ldots, \mathbf{f}(x_T)]^T$, $\mathbf{H} = [\mathbf{h}(x_1), \ldots, \mathbf{h}(x_T)]$. Given the linear-Gaussian relationship between $\mathbf{U}$ and $\mathbf{h}$ (Fig 1a), the integral in (11) can be computed in closed form. Furthermore, even though the recognition potential on $\mathbf{h}$, $r(\mathbf{h}|\mathbf{y}_t)$, is assumed to be fully factorised over the dimensions of each $\mathbf{h}_t$, the variational distribution on $\mathbf{U}$ includes coupling between latent processes induced by the affine mixing coefficients. Hence $q(\mathbf{U})$ captures the correlations both between the latent processes and through time (through combination with the GP prior under the structured autoencoding formulation).

Specifically, given the general expression of the GPFA generative model and the sparse approximation with inducing points, the linear Gaussian relationship between $\mathbf{h}$ and $\mathbf{U}$ at any x is given by

$$p(\mathbf{h}|\mathbf{U}, x) = \mathcal{N}\big(\mathbf{C}\mathfrak{F}(x)\mathbf{U} + \mathbf{d}, \mathbf{C}(\mathbf{K}_x - \mathfrak{F}(x)\mathbf{K}_\mathbf{U}\mathfrak{F}(x)^T)\mathbf{C}^T\big), \tag{12}$$

where

$$\mathfrak{F}(x) = \begin{bmatrix} \mathfrak{F}_1(x) & & \\ & \ddots & \\ & & \mathfrak{F}_K(x) \end{bmatrix}, \quad \mathbf{K}_\mathbf{U} = \begin{bmatrix} \mathbf{K}_{\mathbf{z}_1\mathbf{z}_1} & & \\ & \ddots & \\ & & \mathbf{K}_{\mathbf{z}_K\mathbf{z}_K} \end{bmatrix}$$

with $\mathbf{K}_x = \text{diag}[\kappa_\theta^k(x,x)]$. Combining this result with the fully factorised recognition potential on $\mathbf{h}$ at x_t (11), we obtain the structured variational distribution on $\mathbf{U}$:

$$q(\mathbf{U}) = \mathcal{N}(\mathbf{m}_\mathbf{U}, \mathbf{S}_\mathbf{U}) \propto p(\mathbf{U}) \prod_t \mathcal{N}(\mathbf{C}\mathfrak{F}(x_t)\mathbf{U}|\boldsymbol{\mu}_t^h, \boldsymbol{\Psi}_t^h), \text{ with} \tag{13}$$

$$\mathbf{S}_\mathbf{U}^{-1} = \mathbf{K}_\mathbf{U}^{-1} + \sum_t \mathfrak{F}(x_t)^T \mathbf{C}^T (\boldsymbol{\Psi}_t^h)^{-1} \mathbf{C}\mathbf{F}(x_t), \quad \mathbf{m}_\mathbf{U} = \mathbf{S}_\mathbf{U}\left(\sum_t \mathfrak{F}(x_t)^T \mathbf{C}^T (\boldsymbol{\Psi}_t^h)^{-1}(\boldsymbol{\mu}_t^h - \mathbf{d})\right).$$

This variational posterior on $\mathbf{U}$ leads to a corresponding posterior on $\mathbf{h}$ at each x:

$$q(\mathbf{h}(x)) \propto p(\mathbf{h}|\mathbf{U})q(\mathbf{U}) = \mathcal{N}\big(\mathbf{C}\mathfrak{F}(x)\mathbf{m}_\mathbf{U} + \mathbf{d}, \mathbf{C}(\mathbf{K}_n + \mathfrak{F}(x)(\mathbf{S}_\mathbf{U} - \mathbf{K}_\mathbf{U})\mathfrak{F}(x)^T)\mathbf{C}^T)\big).$$

and we write $q(\mathbf{h}(x_t)) = \mathcal{N}\big(\mathbf{m}_t^h, \mathbf{S}_t^h\big)$. Then the complete (reparametrised) Monte Carlo estimate of the free energy objective given a mini-batch of data, $\{(x_b, \mathbf{y}_b)\}_{b=1}^B$, takes the following expression.

$$\mathcal{F}(\theta, \gamma, \phi, \mathbf{C}, \mathbf{d}, \mathbf{Z}) = \sum_{b=1}^B \frac{1}{S} \sum_{s=1}^S \log p(\mathbf{y}_b|\mathbf{m}_b^h + \mathbf{L}_b^h \epsilon_s) - \mathbf{KL}[q(\mathbf{U})\|p(\mathbf{U})] \tag{13}$$

where $\epsilon_s \sim \mathcal{N}(\mathbf{0}, \mathbf{I})$, θ is the set of kernel parameters, $\mathbf{L}_b^h$ is the lower-triangular Cholesky component of $\mathbf{S}_b^h$ such that $\mathbf{S}_b^h = \mathbf{L}_b^h(\mathbf{L}_b^h)^T$.

We note that we have retained the scalability of amortised inference by choosing an amortised diagonal-Gaussian potential on $\mathbf{h}$. However, the linear-Gaussian relationship between the inducing points $\mathbf{U}$ and $\mathbf{h}(x)$ (12) leads to a full-covariance variational Gaussian approximation for $\mathbf{U}$, allowing amortised inference to capture the observation-induced posterior correlations between latent processes (commonly referred to as the "explaining away" effect). Thus, the retention of the affine GPFA mapping introduces a key extenstion to SGP-VAE. We will refer to the new model as *structured recognition non-linear GPFA* (SR-nlGPFA). The generative model corresponds to that of svGPFA (Figure 1a) but with the nonlinearity $g(\cdot)$ generalised to a flexible form modelled by a neural network. The complete inference procedure for SR-nlGPFA is graphically illustrated in Figure 1c.

The implicit computation of the variational distribution over $\mathbf{U}$ given the recognition potentials on $\mathbf{h}$ also makes it possible to carry out svGP inference with changed inducing locations (13). This is particularly useful in situations that require inference over test datasets of different durations to those seen in training. In particular, it may be possible to learn an amortised inference network using short sub-sequences drawn from a longer dataset, and then infer a posterior over latent GPs for the complete data sequence efficiently by optimising the placement of inducing points along its full length. See further details on the free-form svGP inference step in Appendix F.2.

4 Related work

Structured Deep Generative Models. Ample literature has studied the inclusion of latent graphical structures into DGM [26, 27, 7, 28–30]. The prominent work by Johnson et al. [7] proposed structured autoencoding, where the recognition network outputs conjugate local (singleton) evidence potentials on the latent variables, which is combined with the prior PGM to yield the variational approximation of the latent posterior. Hence the variational distribution incorporates both the factored structure in the prior PGM and the flexibility induced by the neural network-based recognition potential. In another closely related work, Lin et al. [28] proposed structured inference network, which approximates the variational distribution as the combination of the recognition potential and a separate structured latent distribution independent of the prior, the independent structured latent distribution can have non-conjugate factors to improve the expressiveness of the model. Our model builds on and generalises the structured autoencoding framework. Instead of local evidence potentials, the recognition network outputs structured (potentially different from the structure of the prior PGM) recognition potentials on the latent variables, increasing the flexibility of variational approximation, and capturing the additional posterior factor potentials induced by the generative likelihood that does not exist *a priori*.

svGPFA and Extensions. High-dimensional time-series data, such as population neural firing pattern, usually lie on a low-dimensional manifold that can be characterised by the small number of dynamical covariates that fully explain the temporal correlation exhibited in the observations. Extraction of the latent covariates is particularly essential in analysing neural data, where the set of

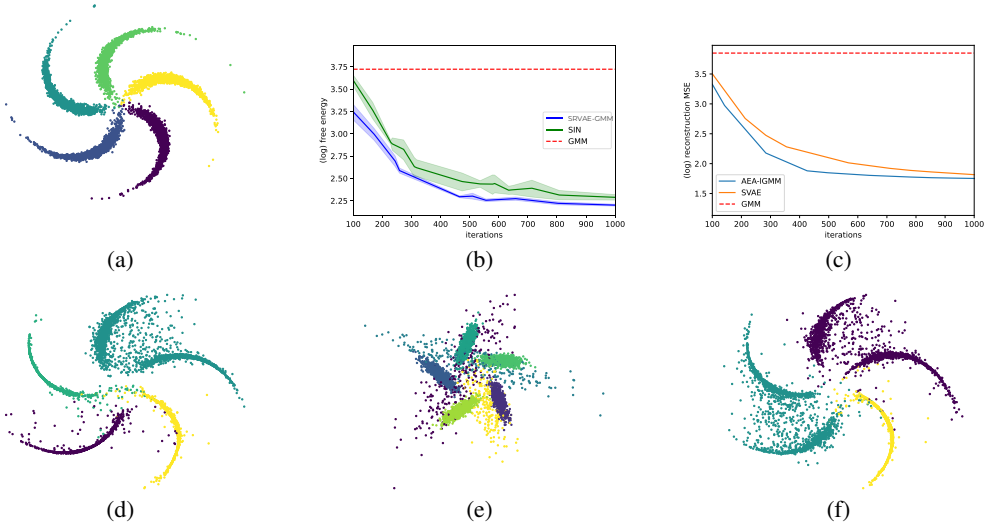


Figure 2: **Empirical Evaluations on Pinwheel Dataset.** (a) Sampled data from the pinwheel dataset; Training curves of the (b) variational free energy objective and (c) testing reconstruction MSE through out training (all in log-scale); Sampled data given trained model of (d) SRVAE-GMM; (e) variational GMM; (f) SIN-GMM [28]. All evaluations are based on the averages over 5 random seeds.

external measurable variables and internal mental states are potentially entangled and go through a highly non-linear process to influence the neuronal firing. Hence latent variable models such as GPFA are usually adopted for extracting the relevant latent covariates that contains non-trivial temporal correlations [11, 31, 12]. Recent advances have proposed sparse variational inference and methods for dealing with non-conjugate likelihood function to promote the scalability and applicability of GPFA models [23, 12, 32]. There also exists prior works of combining DGM (e.g., VAEs) with GP latents [9, 33, 10]. However, SR-nlGPFA differs from all prior GPFA models in two ways. Firstly, SR-nlGPFA yields a fully non-linear generalisation of GPFA generative models, replacing the pointwise non-linearity with a neural network. Secondly, SR-nlGPFA employs a recognition network to perform amortised svGP inference on the inducing points, whilst incorporating the structures inherent in the GPFA generative model to facilitate scalable variational Gaussian approximation with full covariance matrices. The closest related model to SR-nlGPFA is SGP-VAE [10], which similarly incorporates the latent temporal dynamics into posterior inference through the latent GP prior under the SVAE formulation. However, since SGP-VAE directly imposes a mean-field recognition potential on the inducing points, it i) cannot capture the posterior correlations between the latent processes; ii) does not allow additional svGP inference step with changed inducing locations.

5 Results

Here we empirically examine the performance of SRVAE-GMM and SR-nlGPFA, and compare to relevant baselines on various synthetic and real datasets. Empirical results on the instantiations of the SAVAE framework with other latent variable models can be found in Appendix F[1].

5.1 Experiments with SRVAE-GMM

To assess the empirical performance of structured amortisation in latent-GMM, we evaluate SRVAE-GMM on the classical pinwheel dataset (Figure 2a) [7]. We compare SRVAE-GMM with the structured inference network [SIN; 28], which is a more flexible instantiation of the SVAE framework. From Figure 2, we observe that SAVAE-GMM outperforms SIN-GMM in terms of the training variational free energy, reconstruction mean-squared error, and generation fidelity. Hence the empirical improvement acts as the proof-of-concept for our theoretical claims that the proposed structured amortisation captures the "explaining away" posterior factors, leading to better training and stronger generation.

[1]Python implementation can be found at `https://github.com/changmin-yu/structured-recognition-neurips-2022`

Methods	**synthetic dataset**	**EEG datset**	**Population spike dataset**
SR-nlGPFA	$\mathbf{0.31 \pm 0.02}$	$\mathbf{0.27 \pm 0.05}$	$\mathbf{0.47 \pm 0.18}$
SGP-VAE [10]	0.36 ± 0.05	0.35 ± 0.05	0.55 ± 0.19
Vanilla-VAE [1, 2]	1.05 ± 0.02	0.57 ± 0.09	3.19 ± 1.98
SVAE-LDS [7]	0.933 ± 0.02	3.04 ± 0.38	2.52 ± 1.31

Table 1: Quantitative comparison of performance between SR-nlGPFA and baseline models on synthetic dataset, EEG dataset and population spiking dataset (Section 5.2.2) with respect to standarised mean squared error (SMSE) on test dataset. All evaluations are averaged over 5 seeds.

5.2 Experiments with SAVAE-svGPFA

5.2.1 Synthetic and EEG Dataset

We firstly empirically evaluate whether SR-nlGPFA outperforms methods that do not capture the intra-latent posterior correlation. We use a synthetic dataset and a small-scale EEG dataset for comparison. Note that we assume Squared Exponential (SE) kernel, $\kappa(x, x') = \lambda \exp(-\frac{||x-x'||^2}{\tau^2})$, unless stated otherwise, where λ and τ are the scale and length-scale parameters, respectively.

Baselines Our main baseline model is SGP-VAE [10], which we introduce and provide discussions relative to SR-nlGPFA in Section 3.3 and 4, respectively. For completeness, we additional compare against a vanilla VAE with fully factorised Gaussian variational distribution [1, 2], and SVAE with linear dynamical system (SVAE-LDS) latent prior [7]. All models are implemented with the same recognition and generative network architectures (see Appendix G for implementation details).

Synthetic Dataset We generate from the GPFA generative model (Eq. 3), with $g(\cdot) = \sigma(\Phi(\cdot))$, where $\Phi(\cdot)$ represents the functional mapping through a fixed, randomly-initialised 2-layer MLP with ReLU hidden non-linearity, and $\sigma(\cdot)$ is the sigmoid function.

EEG Dataset We follow the experimental procedure as described in Requeima et al. [34], and consider an EEG measurement dataset spanning 1 second at $256Hz$ frequency when images are shown to the patients [35]. Each datapoint consists of the voltage readings from 7 electrodes positioned on the patient's scalp. We assume all data are observed, contrary to the settings in [34, 10] (we include results and further discussion on partial observability in appendix F.2).

Given the evaluation comparison in Table 1, we see that comparing to all selected baseline models, SR-nlGPFA achieves stronger performance on both the synthetic and EEG dataset, with respect to both the SMSE and NLL metric (see Table 4 for the NLL comparison). Hence the empirical results provide evidence for the advantages of the inclusion of structured amortised inference for capturing the additional posterior correlations that do not exist *a priori*. Moreover, the computational complexity of SR-nlGPFA is on the same order as SGP-VAE (see appendix F.2).

5.2.2 Population Neuronal Firing Data

It is well-known that the hippocampal CA1 place cells and medial Entorhinal Cortex (mEC) grid cells are spatially modulated [36, 37], and previous work has also established speed and directional modulation of CA1 and mEC neurons [38–40]. Moreover, there are often non-trivial correlations between the behavioural covariates. For instance, one might reasonably expect correlation between speed and spatial location as an animal runs fastest in the central area of the environment and slower near the boundaries. Neither svGPFA or SGP-VAE can capture the posterior correlations between latent variables given their mean-field assumptions, whereas SR-nlGPFA, given its free-form variational approximation with full covariance structure, is able to capture arbitrary correlation between the latents whilst utilising the same mutually independent GP priors, and hence is an ideal model for unsupervised learning of the latent structure that correctly reflect the behavioural covariates underlying the neural firing pattern.

We use the single-cell spiking data of neurons in the hippocampal CA1 and mEC regions of rats recorded during exploration in a Z-shaped track reporte by [41]. The dataset contains 28 experiment sessions, each spanning 10 minutes. Exemplary neural firing patterns of the population are shown in Figure 11. Note that due to the nature of the task, we can interpret the spatial location of the rat being standard and "unfolded" distances along the track ("unfolded" meaning the sign of the distance value is dependent on the direction of movement). Other considered behavioural correlates are speed, direction of movement (inbound v.s. outbound), and head-direction.

We again use the same generative model in Eq. 3, but with Poisson observation likelihood.

$$\mathbf{y}(x) = \prod_{d=1}^{D} \text{Poisson}(y_d(x)|\lambda_{\text{NN}}(\mathbf{h}(x))_d) \tag{14}$$

where x represents discretised timepoints, D is the number of recorded neurons, $\lambda_{\text{NN}}(\cdot)$ represents the neural-network mapping from the GPFA features, $\mathbf{h}$, to the rate of Poisson-distributed firing counts for each neuron over contiguous $100ms$ bins.

We apply SR-nlGPFA and SGP-VAE to the dataset, In Table 4 we show that SR-nlGPFA quantitatively outperforms SGP-VAE (and other baselines) with respect to SMSE of prediction.

Having trained the model, and given the nth observation, $(x_n, \mathbf{y}_n)$, we could immediately compute the variational posterior latent distribution over the latent processes.

$$q(\mathbf{f}_n) \propto p(\mathbf{f}|\mathbf{U})q(\mathbf{U}) = \mathcal{N}(\mathbf{m}_n^f, \mathbf{S}_n^f), \quad \mathbf{m}_n^f = \mathbf{F}(x_n)\mathbf{m}_{\mathbf{U}}, \quad \mathbf{S}_n^f = \mathbf{K}_n + \mathbf{F}(x_n)(\mathbf{S}_{\mathbf{U}} - \mathbf{K}_{\mathbf{U}})\mathbf{F}(x_n)^T$$

where $q(\mathbf{U})$ is computed as described in Section 3.3 (13). Note that due to computational constraints and the stochastic mini-batch nature of the training process, the number of inducing points is much smaller than the total number of observations (64 v.s. 6000 in this case), hence causing temporal chunking artifacts in the posterior estimation. As discussed in Section 3.3, we note that SR-nlGPFA can alleviate the temporal chunking with an additional svGP inference step over a much larger time window (i.e., increasing the number of inducing points) with the weights of the recognition network fixed at the final state of the training process (see further discussion in Section F.3.2).

We perform the two-dimensional Canonical Correlation Analysis (CCA) between the variational posterior means and the behavioural correlates over the entire trajectory [42]. Here we choose one session for in-depth investigation and mostly show the qualitative predictions and comparison, more qualitative and quantitative results across sessions can be found in Appendix F.3.2.

The heatmap of the correlation coefficients between the canonical correlates of the posterior means ($CCX\{1, 2\}$) and each of the behavioural correlates is shown in Figure 3a. We observe an overall pattern of high-correlations, indicating the low-dimensional manifold parametrised by the conjunctive set of behavioural correlates can be accurately captured by the posterior latent variables learned with SR-nlGPFA solely from neural spikes.

In order to verify that the learned latent structure indeed contains decodable information with respect to the behavioural covariates, we extract the direction-modulated neurons predicted by the trained model (details in appendix F.3.2). In Figure 3b, we compare the direction-modulation of the model-predicted neurons against that of the rest of the neurons, where the direction-modulation is defined as the correlation between raw single-cell spike counts and the direction values. We observe that the model-predicted direction-modulated neurons exhibits significantly greater direction-modulation than the other neurons (p-value=5.56×10^{-4}) [43]. For the neuron with the strongest predicted direction-modulation, we show the firing profiles of the neuron when the animal is travelling along both directions, we observe from Figure 3c that the predicted neuron indeed has different firing fields corresponding to different travel direction, exhibiting clear direction-modulation [43]. Similar comparison holds for spatial and speed modulations as well, indicating SR-nlGPFA is able to, in a purely unsupervised fashion, learn the latent space that contains linearly decodable information of the behavioural covariates associated with individual neuronal firing, even for neurons whose firings exhibit conjunctive coding mechanism.

We plot $CCX\{1, 2\}$ against the spatial location (Figure 3d), where we observe clear clustered latent structure with respect to the direction of movement, indicating the latent dimensions learned by SR-nlGPFA exhibit disentanglement of direction from spatial location given simple linear projection, despite the conjunctive coding mechanism exhibited in the CA1 neurons. Comparing to the same plot with SGP-VAE (Figure 14b), we observe that the corresponding latent space does not yield the similar disentangled representation, hence qualitatively indicating the superiority of SR-nlGPFA.

Figure 3e shows the temporal evolution of the latent CCs for SR-nlGPFA and SGP-VAE, as well as the spatial location of the rat. We observe that $CCX1$ and $CCX2$ of SR-nlGPFA consistently track the dynamics of the distance (with perfect phase alignment and half-cycle offset, respectively), whereas neither $CCX1$ or $CCX2$ of SGP-VAE could accurately reflect the distance. Moreover, given the additional svGP inference step over the entire trajectory (with increased number of inducing points), latent signals of SR-nlGPFA exhibit significantly greater smoothness than that of SGP-VAE.

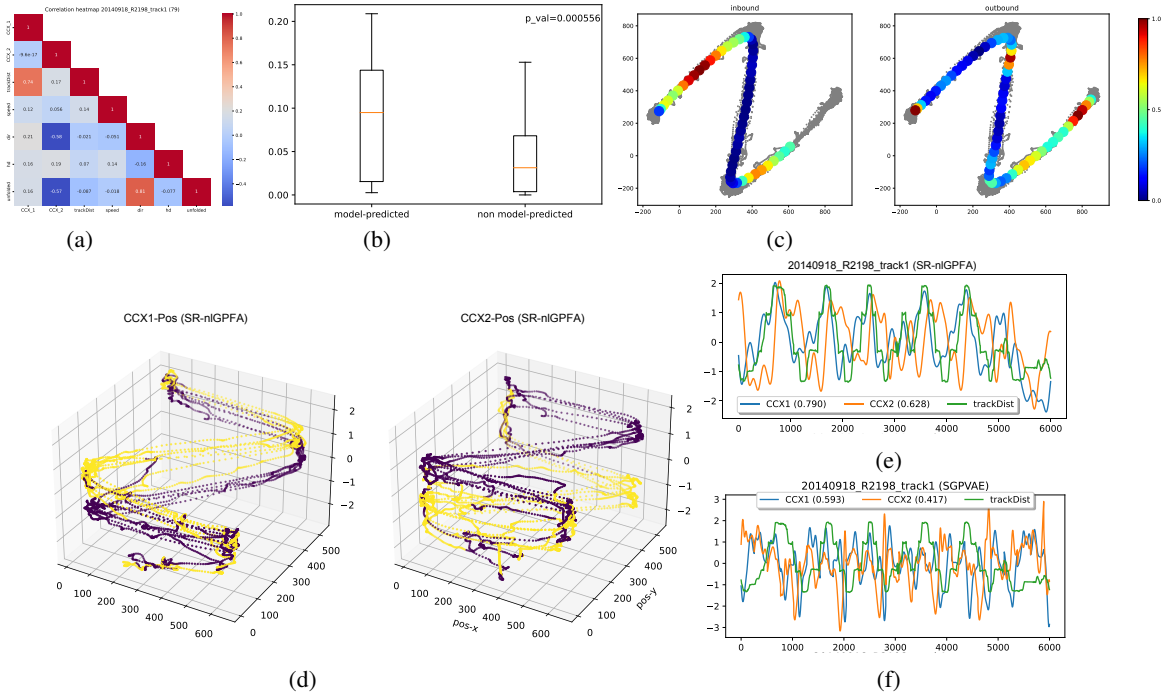


Figure 3: **Analysis of SR-nlGPFA posterior latent structure**. **(a)** Heatmap of the correlation between the CCs and the behavioural covariates for the selected session; **(b)** Directional-modulation comparison between the model-predicted direction-modulated neurons against other neurons; **(c)** Exemplary firing fields of the model-predicted direction-modulated neuron during inbound v.s. outbound movements; **(d)** Plot of $CCX\{1,2\}$ of SR-nlGPFA posterior latents against spatial location, color indicates direction of movement (yellow: inbound, magenta: outbound); **(e-f)** Temporal evolution of (standardised values of) $CCX\{1,2\}$ and spatial location for SR-nlGPFA and SGP-VAE.

6 Discussion

In this paper, we proposed structured amortised inference, which can be viewed as a strict generalisation of the SVAE framework [7], where our model allows structured amortised factor potentials to capture the posterior correlations induced by the "explaining away" effect. The SRVAE framework yields a strictly tighter bound on the log-likelihood than the SVAE free energy objective.

We introduce SR-nlGPFA, a combination of the proposed SRVAE framework with GPFA latents, where scalable free-form variational Gaussian approximation can be achieved. SR-nlGPFA supports a fully non-linear, non-conjugate extension to standard GPFA [11, 23, 12], which is particularly well-suited to settings where posterior inference must be scaled to additional data. We show that SR-nlGPFA outperforms the baseline on all presented tasks, both quantitatively and qualitatively. Studying population spiking data of hippocampal neurons, we show that SR-nlGPFA is able to identify latent signals that exhibit strong correlation with the behavioural covariates that are well-known to be conjunctively encoded by the recorded neurons, but without direct access to these covariates. While here we focused on temporal correlation exhibited in time-series data, we note that the sparse amortised variational approximation presented here can also be straightforwardly applied to other GP-latent models, such as GP-LVM [44, 45]. We note that here we only looked at spiking data, which could in principle be combined with the inferred latent processes by applying our model to EEG or calcium imaging data recorded during the same session, possibly with different likelihoods functions. Such joint analysis of latent structures given different recordings within the same session could potentially facilitate new findings with respect to, e.g., replay, phase coding, etc.

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   (a) Do the main claims made in the abstract and introduction accurately reflect the paper's contributions and scope? [Yes]
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