Gray-box inference for structured Gaussian process models

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Abstract

We develop an automated variational inference method for Bayesian structured prediction problems with Gaussian process (GP) priors and linear-chain likelihoods. Our approach does not need to know the details of the structured likelihood model and can scale up to a large number of observations. Furthermore, we show that the required expected likelihood term and its gradients in the variational objective (ELBO) can be estimated efficiently by using expectations over very low-dimensional Gaussian distributions. Optimization of the ELBO is fully parallelizable over sequences and amenable to stochastic optimization, which we use along with control variate techniques and state-of-the-art incremental optimization to make our framework useful in practice. Results on a set of natural language processing tasks show that our method can be as good as (and sometimes better than) hard-coded approaches including SVM-struct and CRFs, and overcomes the scalability limitations of previous inference algorithms based on sampling. Overall, this is a fundamental step to developing automated inference methods for Bayesian structured prediction.

1 Introduction

Developing automated inference methods for complex probabilistic models has become arguably one of the most exciting areas of research in machine learning, with notable examples in the probabilistic programming community given by STAN (Hoffman and Gelman, 2014) and CHURCH (Goodman et al., 2008). One of the main challenges for these types of approaches is to formulate expressive probabilistic models and develop generic yet efficient inference methods for them. From a variational inference perspective, one particular approach that has addressed such a challenge is the black-box variational inference framework of Ranganath et al. (2014).

While the works of Hoffman and Gelman (2014) and Ranganath et al. (2014) have been successful with a wide range of priors and likelihoods, their direct application to models with Gaussian process (GP) priors is cumbersome, mainly due to the large number of highly coupled latent variables in such models. In this regard, very recent work has investigated automated inference methods for general likelihood models when the prior is given by a sparse Gaussian process (Hensman et al., 2015b; Dezfouli and Bonilla, 2015). While these advances have opened up opportunities for applying GP-based models well beyond regression and classification settings, they have focused on models with i.i.d observations and, therefore, are unsuitable for addressing the more challenging task of structured prediction.

Structured prediction refers to the problem where there are interdependencies between the outputs and it is necessary to model these dependencies explicitly. Common examples are found in natural language processing (NLP) tasks, computer vision and bioinformatics. By definition, observation models in these
problems are not i.i.d and standard learning frameworks have been extended to consider the constraints imposed by structured prediction tasks. Popular structured prediction frameworks are conditional random fields (CRFs; Lafferty et al., 2001), maximum margin Markov networks (Taskar et al., 2004) and structured support vector machines (SVM-struct, Tsochantaridis et al., 2005).

From a non-parametric Bayesian modeling perspective, in general, and from a GP modeling perspective, in particular, structured prediction problems present incredibly hard inference challenges because of the rapid explosion of the number of latent variables with the size of the problem. Furthermore, structured likelihood functions are usually very expensive to compute. In an attempt to build non-parametric Bayesian approaches to structured prediction, Bratières et al. (2015) have proposed a framework based on a CRF-type modeling approach with GPs, and use elliptical slice sampling (ESS; Murray et al., 2010) as part of their inference method. Unfortunately, although their method can be applied to linear chain structures in a generic way without considering the details of the likelihood model, it is not scalable as it involves sampling from the full GP prior.

In this paper we present an approach for automated inference in structured GP models with linear chain likelihoods that builds upon the structured GP model of Bratières et al. (2015) and the sparse variational frameworks of Hensman et al. (2015b) and Dezfouli and Bonilla (2015). In particular, we show that the model of Bratières et al. (2015) can be mapped onto a generalization of the automated inference framework of Dezfouli and Bonilla (2015). Unlike the work of Bratières et al. (2015), by introducing sparse GP priors in structured prediction models, our approach is scalable to a large number of observations. More importantly, this approach is also generic in that it does not need to know the details of the likelihood model in order to carry out posterior inference. Finally, we show that our inference method is statistically efficient as, despite having a Gaussian process prior over a large number of latent functions, it only requires expectations over low-dimensional Gaussian distributions in order to carry out posterior approximation.

Our experiments on a set of NLP tasks, including noun phrase identification, chunking, segmentation, and named entity recognition, show that our method can be as good as (and sometimes better than) hard-coded algorithms, including SVM-struct and CRFs, and overcomes the scalability limitations of previous inference algorithms based on sampling.

We refer to our approach as “gray-box” inference since, in principle, for general structured prediction problems it may require some human intervention. Nevertheless, when applied to fixed structures, our proposed inference method is entirely “black box”.

## 2 Gaussian process models for structured prediction

Here we are interested in structured prediction problems where we observe input-output pairs \( D = \{ (X^{(n)}, y^{(n)}) \}_{n=1}^{N_{\text{seq}}} \), where \( N_{\text{seq}} \) is the total number of observations, \( X^{(n)} \in \mathcal{X} \) is a descriptor of observation \( n \) and \( y^{(n)} \in \mathcal{Y} \) is a structured object such as a sequence, a tree, or a grid that reflects the interdependencies between its individual constituents. Our goal is that of, given a new input descriptor \( X^{(*)} \), predicting its corresponding structured labels \( y^{(*)} \), and more generally, a distribution over these labels.

A fairly general approach to address this problem with Gaussian process (GP) priors was proposed by Bratières et al. (2015) based on CRF-type models, where the distribution of the output given the input is defined in terms of cliques, i.e. sets of fully connected nodes. Such a distribution is given by:

\[
p(y|X, f) = \frac{\exp \left( \sum_c f(c, X_c, y_c) \right)}{\sum_{y' \in \mathcal{Y}} \exp \left( \sum_c f(c, X_c, y'_c) \right)},
\]

where \( X_c \) and \( y_c \) are tuples of nodes belonging to clique \( c \); \( f(c, X_c, y_c) \) is their corresponding latent variable; and \( f \) is the collection of all these latent variables, which are assumed to be drawn from a zero-mean GP prior with covariance function \( \kappa(\cdot, \cdot; \theta) \), with \( \theta \) being the hyperparameters. It is clear that such a model is a generalization of vanilla CRFs where the potentials are draws from a GP instead of being linear functions of the features.
2.1 Linear chain structures

In this paper we focus on linear chain structures where both the input and the output corresponding to datapoint \( n \) are linear chains of length \( T_n \), whose corresponding constituents stem from a common set. In other words, \( \mathbf{X}^{(n)} \) is a \( T_n \times D \) matrix of feature descriptors and \( \mathbf{y}^{(n)} \) is a sequence of \( T_n \) labels drawn from the same vocabulary \( \mathcal{V} \). In this case, in order to completely define the prior over the clique-dependent latent functions in Equation (1), it is necessary to specify covariance functions over the cliques. To this end, Bratières et al. (2015) propose a kernel that is non-zero only when two cliques are of the same type, i.e. both are unary cliques or both are pairwise cliques. Furthermore, these kernels are defined as:

\[
\kappa_u(t, x_t, y_t, (t', x'_t, y_t')) = \mathbb{1}[y_t = y_{t'}]\kappa(x_t, x'_t),
\]

(2)

\[
\kappa_{\text{bin}}((y_t, y_{t+1}), (y_{t'}, y_{t'+1})) = \mathbb{1}[y_t = y_{t'} \land y_{t+1} = y_{t'+1}],
\]

(3)

where \( \kappa_u \) is the covariance on unary functions and \( \kappa_{\text{bin}} \) is the covariance on pairwise functions. With a suitable ordering of these latent functions, we obtain a posterior covariance matrix that is block-diagonal, with the first \( |\mathcal{V}| \) blocks corresponding to the unary covariances, each of size \( T_n \); and the last block, corresponding to the pairwise covariances, being a diagonal (identity) matrix of size \( |\mathcal{V}|^2 \), where \( |\mathcal{V}| \) denotes the vocabulary size.

To carry out inference in this model, Bratières et al. (2015) propose a sampling scheme based on elliptical slice sampling (ess; Murray et al., 2010). In the following section, we show an equivalent formulation of this model that leverages the general class of models with i.i.d likelihoods presented by Nguyen and Bonilla (2014). Understanding structured GP models from such a perspective will allow us to generalize the results of Nguyen and Bonilla (2014); Dezfoli and Bonilla (2015) in order to develop an automated variational inference framework. The advantages of such a framework are that of (i) dealing with generic likelihood models; and (ii) enabling stochastic optimization techniques for scalability to large datasets.

3 Full Gaussian process priors and automated inference

Nguyen and Bonilla (2014) developed an automated variational inference framework for a class models with Gaussian process priors and generic i.i.d likelihoods. Although such an approach is an important step towards black-box inference with GP priors, assuming i.i.d observations is, by definition, unsuitable for structured models.

One way to generalize such an approach to structured models of the types described in §2.1 is to differentiate between GP priors over latent functions on unary nodes and GP priors over latent functions over pairwise nodes. More importantly, rather than considering i.i.d likelihoods over all observations, we assume likelihoods that factorize over sequences, while allowing for statistical dependences within a sequence. Therefore, our prior model for linear chain structures is given by:

\[
p(\mathbf{f}) = p(\mathbf{f}_u)p(\mathbf{f}_{\text{bin}}) = \prod_{j=1}^{|\mathcal{V}|} \mathcal{N}(\mathbf{f}_{u,j}; \mathbf{0}, \mathbf{K}_j) \mathcal{N}(\mathbf{f}_{\text{bin}}; \mathbf{0}, \mathbf{K}_{\text{bin}}),
\]

(4)

where \( \mathbf{f} \) is the vector of all latent function values of unary nodes \( \mathbf{f}_u \) and the function values of pairwise nodes \( \mathbf{f}_{\text{bin}} \). Accordingly, \( \mathbf{f}_{u,j} \) is the vector of unary functions of latent process \( j \), corresponding to the \( j \)th label in the vocabulary, which is drawn from a zero-mean GP with covariance function \( \kappa_j(\cdot, \theta_j) \). This covariance function, when evaluated at all the input pairs in \( \{\mathbf{X}^{(n)}\} \), induces the \( N \times N \) covariance matrix \( \mathbf{K}_j \), where \( N = \sum_{n=1}^N T_n \) is the total number of observations. Similarly, \( \mathbf{f}_{\text{bin}} \) is a zero-mean \( |\mathcal{V}|^2 \)-dimensional Gaussian random variable with covariance matrix given by \( \mathbf{K}_{\text{bin}} \). We note here that while the unary functions are draws from a GP indexed by \( \mathbf{X} \), the distribution over pairwise functions is a finite Gaussian (not indexed by \( \mathbf{X} \)).
Given the latent function values, our conditional likelihood is defined by:

\[ p(y|f) = \prod_{n=1}^{N_{\text{seq}}} p(y^{(n)}|f_n), \]

(5)

where, omitting the dependency on the input \( X \) for simplicity, each individual conditional likelihood term is computed using a valid likelihood function for sequential data such as that defined by the structured softmax function in Equation (1); \( y^{(n)} \) denotes the labels of sequence \( y^{(n)} \); and \( f_n \) is the corresponding vector of latent (unaries and pairwise) function values. We now have all the necessary definitions to state our first result.

**Theorem 1** The model class defined by the prior in Equation (4) and the likelihood in Equation (5) contains the structured GP model proposed by Bratières et al. (2015).

The proof of this is trivial and can be done by (i) setting all the covariance functions of the unary latent process \( (\kappa_j) \) to be the same; (ii) making \( K_{\text{bin}} = I \); and (iii) using the structured softmax function in Equation (1) as each of the individual terms \( p(y^{(n)}|f_n) \) in Equation (5). This yields exactly the same model as specified by Bratières et al. (2015), with prior covariance matrix with block-diagonal structure described in §2.1 above.

The practical consequences of the above theorem is that we can now leverage the results of Nguyen and Bonilla (2014) in order to develop a variational inference (vi) framework for structured GP models that can be carried out without knowing the details of the conditional likelihood. Furthermore, as we shall see in the next section, in order to deal with the intractable nonlinear expectations inherent to \( \text{vi} \), the proposed method only requires expectations over low-dimensional Gaussian distributions.

### 3.1 Automated variational inference

In this section we develop a method for estimating the posterior over the latent functions given the prior and likelihood models defined in Equations (4) and (5). Since the posterior is analytically intractable and the prior involves a large number of coupled latent variables, we resort to approximations given by variational inference (vi; Jordan et al., 1998). To this end, we start by defining our variational approximate posterior distribution:

\[ q(f) = q(f_u)q(f_{\text{bin}}), \quad \text{with} \]

(6)

\[ q(f_u) = \sum_{k=1}^{K} \pi_k q_k(f_u|b_k, \Sigma_k) = \sum_{k=1}^{K} \pi_k \prod_{j=1}^{\mathcal{V}} N(f_{u,j}; b_{kj}, \Sigma_{kj}) \quad \text{and} \]

(7)

\[ q(f_{\text{bin}}) = N(f_{\text{bin}}; m_{\text{bin}}, S_{\text{bin}}), \]

(8)

where \( q(f_u) \) and \( q(f_{\text{bin}}) \) are the approximate posteriors over the unary and pairwise nodes respectively; each \( q_k(f_{u,j}) = N(f_{u,j}; b_{kj}, \Sigma_{kj}) \) is a \( \mathcal{N} \)-dimensional full Gaussian distribution; and \( q(f_{\text{bin}}) \) is a \( |\mathcal{V}|^2 \)-dimensional Gaussian.

In order to estimate the parameters of the above distribution, variational inference entails the optimization of the so-called evidence lower bound (\( \mathcal{L}_{\text{elbo}} \)), which can be shown to be a lower bound of the true marginal likelihood, and is composed of a KL-divergence term (\( \mathcal{L}_{\text{kl}} \)), between the approximate posterior and the prior, and an expected log likelihood term (\( \mathcal{L}_{\text{ell}} \)):

\[ \mathcal{L}_{\text{elbo}} = -\text{KL}(q(f)||p(f)) + \langle \log p(y|f) \rangle_{q(f)}, \]

(9)

where the angular bracket notation \( \langle \cdot \rangle_q \) indicates an expectation over the distribution \( q \). Although the approximate posterior is an \( \mathcal{N} \)-dimensional distribution, the expected log likelihood term can be estimated efficiently using expectations over much lower-dimensional Gaussians.
Theorem 2 For the structured GP model defined in Equations (4) and (5), the expected log likelihood over the variational distribution defined in Equations (6) to (8) and its gradients can be estimated using expectations over \( T_n \)-dimensional Gaussians and \(|V|^2\)-dimensional Gaussians, where \( T_n \) is the length of each sequence and \(|V|\) is the vocabulary size.

The proof is constructive and can be found in the supplementary material. Here we state the final result on how to compute these estimates:

\[
\mathcal{L}_{\text{ell}} = \sum_{n=1}^{N_{\text{eq}}} \sum_{k=1}^{K} \pi_k \left( \log p(y^{(n)}|f_n) \right)_{q_k(f^{(n)}_n)q(f_{\text{bin}})}, 
\]

\[
\nabla \lambda_{\text{ell}}^{(k,n)} \mathcal{L}_{\text{ell}} = \left( \nabla \lambda_{\text{ell}}^{(k,n)} \log q_k(f^{(n)}_u) \log p(y^{(n)}|f_n) \right)_{q_k(f^{(n)}_n)q(f_{\text{bin}})}, 
\]

\[
\nabla \lambda_{\text{bin}}^{(k,n)} \mathcal{L}_{\text{ell}} = \left( \nabla \lambda_{\text{bin}} \log q(f_{\text{bin}}) \log p(y^{(n)}|f_n) \right)_{q_k(f^{(n)}_n)q(f_{\text{bin}})}, 
\]

where \( q_k(f^{(n)}_n) \) is a \((T_n \times |V|)\)-dimensional Gaussian with block-diagonal covariance \( \Sigma_{k(n)} \), each block of size \( T_n \times T_n \). Therefore, we can estimate the above term by sampling from \( T_n \)-dimensional Gaussians independently. Furthermore, \( q(f_{\text{bin}}) \) is a \(|V|^2\)-dimensional Gaussian, which can also be sampled independently. In practice, we can assume that the covariance of \( q(f_{\text{bin}}) \) is diagonal and we only sample from univariate Gaussians for the pairwise functions.

It is important to emphasize the practical consequences of Theorem 2. Although we have a fully correlated prior and a fully correlated approximate posterior over \( N = \sum_{n=1}^{N_{\text{eq}}} T_n \) unary function values, yielding full \( N \)-dimensional covariances, we have shown that for these classes of models we can estimate \( \mathcal{L}_{\text{ell}} \) by only using expectations over \( T_n \)-dimensional Gaussians. We refer to this result as that of statistical efficiency of the inference algorithm.

Nevertheless, even when having only one latent function and using a single Gaussian approximation \((K = 1)\), optimization of the \( \mathcal{L}_{\text{elbo}} \) in Equation (9) is completely impractical for any realistic dataset concerned with structured prediction problems, due to its high memory requirements \( \mathcal{O}(N^3) \) and time complexity \( \mathcal{O}(N^3) \). In the following section we will use a sparse GP approach within our variational framework in order to develop a practical algorithm for structured prediction.

4 Sparse Approximation

In this section we describe a scalable approach to inference in the structured GP model defined in §3 by introducing the so-called sparse GP approximations (Quinonero-Candela and Rasmussen, 2005) into our variational framework. Variational approaches to sparse GP models were developed by Titsias (2009) for Gaussian i.i.d likelihoods, then made scalable to large datasets and generalized to non-Gaussian (i.i.d) likelihoods by Hensman et al. (2015a, b); Dezfouli and Bonilla (2015). The main idea of such approaches is to introduce a set of \( M \) inducing variables \( \{u_j\}_{j=1}^{M} \) for each latent process, which lie in the same space as \( \{f_j\} \) and are drawn from the same GP prior. These inducing variables are the latent function values of their corresponding set of inducing inputs \( \{Z_j\} \). Subsequently, we redefine our prior in terms of these inducing inputs/variables.

In our structured GP model, only the unary latent functions are drawn from GPs indexed by \( \mathbf{X} \). Hence we assume a GP prior over the inducing variables and a conditional prior over the unary latent functions, which both factorize over the latent processes, yielding the joint distribution over unary functions, pairwise functions and inducing variables given by:

\[
p(f, u) = p(u)p(f_u|u)p(f_{\text{bin}}), \text{ with } p(f_u|u) = \prod_{j=1}^{|V|} N(f_{u,j}; \tilde{\mu}_j, \tilde{K}_j) \text{ and } p(u) = \prod_{j=1}^{|V|} p(u_j),
\]
with the prior over the pairwise functions defined as before, i.e. \( p(f_{\text{bin}}) = \mathcal{N}(f_{\text{bin}}; \mathbf{0}, \mathbf{K}_{\text{bin}}) \), and the means and covariances of the conditional distributions over the unary functions are given by:

\[
\hat{\mu}_j = \mathbf{A}_j \mathbf{u}_j \quad \text{and} \quad \hat{\mathbf{K}}_j = \kappa_j(\mathbf{X}, \mathbf{X}) - \mathbf{A}_j \kappa_j(\mathbf{Z}_j, \mathbf{X}), \quad \text{with} \quad \mathbf{A}_j = \kappa(\mathbf{X}, \mathbf{Z}_j) \kappa_j(\mathbf{Z}_j, \mathbf{Z}_j)^{-1}. \tag{14}
\]

By keeping an explicit representation of the inducing variables, our goal is to estimate the joint posterior over the unary functions, pairwise functions and inducing variables given the observed data. To this end, we assume that our variational approximate posterior is given by:

\[
q(f, \mathbf{u}|\mathbf{\lambda}) = p(f_{\text{bin}}|\mathbf{u}) q(\mathbf{u}|\mathbf{\lambda}_u) q(f_{\text{bin}}|\mathbf{\lambda}_{\text{bin}}), \tag{15}
\]

where \( \mathbf{\lambda} = \{ \mathbf{\lambda}_u, \mathbf{\lambda}_{\text{bin}} \} \) are the variational parameters; \( p(f_{\text{bin}}|\mathbf{u}) \) is defined in Equation (13); \( q(f_{\text{bin}}|\mathbf{\lambda}_{\text{bin}}) \) is defined as in Equation (8), i.e. a Gaussian with parameters \( \mathbf{\lambda}_{\text{bin}} = \{ \mathbf{m}_{\text{bin}}, \mathbf{S}_{\text{bin}} \} \); and

\[
q(\mathbf{u}|\mathbf{\lambda}_u) = \sum_{k=1}^{K} \pi_k q_k(\mathbf{u}|\mathbf{m}_k, \mathbf{S}_k) = \sum_{k=1}^{K} \prod_{j=1}^{|\mathcal{V}|} \mathcal{N}(\mathbf{u}_j; \mathbf{m}_{kj}, \mathbf{S}_{kj}), \tag{16}
\]

with \( \mathbf{\lambda}_u = \{ \pi_k, \mathbf{m}_k, \mathbf{S}_k \} \) and \( \mathbf{m}_{kj}, \mathbf{S}_{kj} \) denoting the posterior mean and covariance of the inducing variables corresponding to mixture component \( k \) and latent function \( j \).

### 4.1 Evidence lower bound

The KL term in the evidence lower bound now considers a KL divergence between the joint approximate posterior in Equation (15) and the joint prior in Equation (13). Because of the structure of the approximate posterior, it is easy to show that the term \( p(f_{\text{bin}}|\mathbf{u}) \) vanishes from the KL, yielding an objective function that is composed of a KL between the distributions over the inducing variables; a KL between the distributions over the pairwise functions; and the expected log likelihood over the joint approximate posterior:

\[
\mathcal{L}_{\text{elbo}}(\mathbf{\lambda}) = -\text{KL}(q(\mathbf{u})||p(\mathbf{u})) - \text{KL}(q(f_{\text{bin}})||p(f_{\text{bin}})) + \sum_{n=1}^{N_{\text{seq}}} \log p(\mathbf{y}^{(n)}|f_{n, \cdot}) \right)_{q(f, \mathbf{u}|\mathbf{\lambda})}, \tag{17}
\]

where \( \text{KL}(q(f_{\text{bin}})||p(f_{\text{bin}})) \) is a straightforward KL divergence between two Gaussians and \( \text{KL}(q(\mathbf{u})||p(\mathbf{u})) \) is a KL divergence between a Mixture-of-Gaussians and a Gaussian, which we bound using Jensen’s inequality. The expressions for these terms are given in the supplementary material.

Let us now consider the expected log likelihood term in Equation (17), which is an expectation of the conditional likelihood over the joint posterior \( q(f, \mathbf{u}|\mathbf{\lambda}) \). The following result tells us that, as in the full (non-sparse) case, these expectations can still be estimated efficiently by using expectations over low-dimensional Gaussians.

**Theorem 3** The expected log likelihood term in Equation (17), with a generic structured conditional likelihood \( p(\mathbf{y}^{(n)}|f_{n, \cdot}) \) and variational distribution \( q(f, \mathbf{u}|\mathbf{\lambda}) \) defined in Equation (13), and its gradients can be estimated using expectations over \( T_n \)-dimensional Gaussians and \( |\mathcal{V}|^2 \)-dimensional Gaussians, where \( T_n \) is the length of each sequence and \( |\mathcal{V}| \) is the vocabulary size.

As in the full (non-sparse) case, the proof is constructive and can be found in the supplementary material. This means that, in the sparse case, the expected log likelihood and its gradients can also be computed using Equations (10) to (12), where the means and covariances of each \( q_{k(n)}(f_{n}^{(n)}) \) are determined by the means and covariances of the posterior over the inducing variables. Thus, as before, \( q_{k(n)}(f_{n}^{(n)}) \) is a \( (T_n \times |\mathcal{V}|) \)-dimensional Gaussian with block-diagonal structure, where each of the \( j = 1, \ldots, |\mathcal{V}| \) blocks has mean and covariance given by:

\[
\mathbf{b}_{kj(n)} = \mathbf{A}_{jn} \mathbf{m}_{kj}, \quad \Sigma_{kj(n)} = \hat{\mathbf{K}}_{kj}^{(n)} + \mathbf{A}_{jn} \mathbf{S}_{kj} \mathbf{A}_{jn}^T, \tag{18}
\]

\[
\mathbf{A}_{jn} \overset{\text{def}}{=} \kappa(\mathbf{X}_n, \mathbf{Z}_j) \kappa_j(\mathbf{Z}_j, \mathbf{Z}_j)^{-1} \quad \text{and} \quad \hat{\mathbf{K}}_{kj}^{(n)} \overset{\text{def}}{=} \kappa_j(\mathbf{X}_n, \mathbf{X}_n) - \mathbf{A}_{jn} \kappa_j(\mathbf{Z}_j, \mathbf{X}_n), \tag{19}
\]

where, as mentioned in §2.1, \( \mathbf{X}^{(n)} \) is the \( T_n \times D \) matrix of feature descriptors corresponding to sequence \( n \).
4.2 Expectation estimates

In order to estimate the expectations in Equations (10) to (12), we use a simple Monte Carlo approach where we draw samples from our approximate distributions and compute the empirical expectations. For example, for the $L_{\text{cell}}$ we have:

$$
\hat{L}_{\text{cell}} = \frac{1}{S} \sum_{n=1}^{N_{\text{seq}}} \sum_{k=1}^{K} \sum_{i=1}^{S} \log p(y^{(n)}|\mathbf{f}_{u^{(k,i)}}, \mathbf{f}_{\text{bin}}^{(i)}),
$$

with $\mathbf{f}_{u^{(k,i)}} \sim \mathcal{N}(\mathbf{b}_{k(n)}, \Sigma_{k(n)})$ and $\mathbf{f}_{\text{bin}}^{(i)} \sim \mathcal{N}(\mathbf{m}_{\text{bin}}, \mathbf{S}_{\text{bin}})$, for $i = 1, \ldots, S$, where $S$ is the number of samples used, and each of the individual blocks of $\mathbf{b}_{k(n)}$ and $\Sigma_{k(n)}$ are given in Equation (18). We use a similar approach for estimating the gradients of the $L_{\text{cell}}$ and they are given in the supplementary material.

5 Learning

We learn the parameters of our model, i.e. the parameters of our approximate variational posterior well as the hyperparameters $\{\lambda, \theta\}$ through gradient-based optimization of the variational objective ($L_{\text{elbo}}$). One of the main advantages of our method is the decomposition of the $L_{\text{cell}}$ in Equation (20) and its gradients as a sum of expectations of the individual likelihood terms for each sequence. This result enables us to use parallel computation and stochastic optimization in order to make our algorithms useful in practice.

Therefore, we consider batch optimization for small-scale problems (exploiting parallel computation) and stochastic optimization techniques for larger problems. Nevertheless, from a statistical perspective, learning in both settings is still hard due to the noise introduced by the empirical expectations (in both the batch and the stochastic setting) and the noisy gradients when using stochastic learning frameworks such as stochastic gradient descend (SGD). In order to address these issues, we use variance reduction techniques such as control variates in the batch case. In the stochastic setting, in addition to standard control variates used in sampling methods and some stochastic variational frameworks (Ranganath et al., 2014), we use the recently developed SAGA method for optimization. We describe in section 5.1 why these two approaches, standard control variates and SAGA, are complementary and should improve learning in our method.

Computational complexity The time-complexity of our stochastic optimization is dominated by the computation of the posterior’s entropy, Gaussian sampling, and running the forward-backward algorithm, which yields an overall cost of $O(M^3 + T_n^3 + ST_n |V|^2)$. The space complexity is dominated by storing inducing-point covariances, which is $O(M^2)$. To put this in the perspective of other available methods, the existing Bayesian structured model with ess sampling (Bratières et al., 2015) has time and memory complexity of $O(|N|^3)$ and $O(|N|^2)$ respectively, where $N$ is the total number of observations (e.g. words). CRF’s time and space complexity with stochastic optimization depends on the feature dimensionality, i.e. it is $O(D)$. The actual running time of CRF also depends on the cost of model selection via a cross-validation procedure. ess sampling makes the method of Bratières et al. (2015) completely unfeasible for large datasets and CRF has high running times for problems with high dimensions and many hyperparameters. Our work aims to make Bayesian structured prediction practical for large datasets, while being able to use infinite-dimensional feature spaces as well as sidestepping a costly cross-validation procedure.

5.1 Variance reduction techniques

Our goal is to approximate an expectation of a function $g(f)$ over the random variable $f$ that follows a distribution $q(f)$, i.e. $\mathbb{E}_q[g(f)]$ via Monte Carlo samples. The simplest way to reduce the variance of the empirical estimator $\hat{g}$ is to subtract from $g(f)$ another function $h(f)$ that is highly correlated with $g(f)$. That is, the function $\hat{g}(f) := g(f) - \hat{a}h(f)$ will have the same expectation as $g(f)$ i.e. $\mathbb{E}_q[\hat{g}] = \mathbb{E}_q[g]$, provided that $\mathbb{E}_q[h] = 0$. More importantly, as the variance of the new function is $\text{Var}[\hat{g}] = \text{Var}[g] + \hat{a}^2\text{Var}[h] - 2\hat{a}\text{Cov}[g, h]$.

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1We note that, in general, to ensure unbiasedness, $\mathbb{E}_q[h]$, if easily and efficiently computable, can be subtracted from $h$ to form an estimator $\hat{g} := g - h + \mathbb{E}_q[h]$. 

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Table 1: Mean error rates and standard deviations in brackets on small-scale experiments using 5-fold cross-validation. The average number of observed words \( N \) on these problems range from 942 to 3740. SVM corresponds to structured support vector machines; CRF to conditional random fields; GP-ESS corresponds to GPSTRUCT with ESS for inference (Bratières et al., 2015); GP-VAR-B and GP-VAR-S correspond to our method with batch optimization and stochastic optimization respectively; and GP-VAR-P corresponds to our method with stochastic optimization using a piecewise pseudo-likelihood.

| Dataset     | SVM    | CRF    | GP-ESS | GP-VAR-B | GP-VAR-S | GP-VAR-P |
|-------------|--------|--------|--------|----------|----------|----------|
| BASE NP     | 5.91 (0.44) | 5.92 (0.23) | 4.81 (0.47) | 5.17 (0.41) | 5.27 (0.24) | 5.37 (0.33) |
| CHUNKING    | 9.79 (0.97) | 8.29 (0.77) | 8.77 (1.08) | 8.76 (1.09) | 10.02 (0.41) | 9.58 (0.87) |
| SEGMENTATION| 16.21 (2.21) | 14.94 (5.65) | 14.88 (1.80) | 15.61 (1.90) | 14.97 (1.38) | 15.16 (1.57) |
| JAPANESE NE | 5.64 (0.82) | 5.11 (0.66) | 5.83 (0.83) | 5.23 (0.68) | 4.99 (0.41) | 4.80 (0.65) |

6 Experiments

For comparison purposes, we used the same benchmark dataset suite as that used by Bratières et al. (2015), which targets several standard NLP problems and is part of the CRF++ toolbox\(^2\). This includes noun phrase identification (BASE NP); chunking, i.e. shallow parsing labels sentence constituents (CHUNKING); identification of word segments in sequences of Chinese ideograms (SEGMENTATION); and Japanese named entity recognition (JAPANESE NE). As we will see, on these tasks our approach is on par with competitive benchmarks which, unlike our method, exploit the structure of the likelihood.

For more details of these datasets and the experimental set-up for reproducibility of the results see the supplementary material.
6.1 Small-scale experiments

Table 1 shows the error rates on the small experiments across the different datasets considered. Overall, we observe that our method in batch mode (GP-VAR-B) is consistently better than SVM and compares favorably with CRF. When compared to GP-ESS, both versions of our method, the batch and the stochastic, also have similar performance with the notable exception of GP-VAR-S on CHUNKING. However, we do note that GP-VAR-S has the smallest standard deviation among all compared methods over all datasets. We credit this desirable property to the usage of doubly controlled variates (SAGA + standard control variates), as well as to the conservative learning rates chosen for these tests. From these results we can conclude that, despite not knowing the details of the conditional likelihood, our method is very competitive with other methods that exploit this knowledge and has similar performance to GP-ESS.

6.1.1 Accelerating inference with a piecewise pseudo-likelihood

In order to demonstrate the flexibility of our approach, we also tested the performance of our framework when the true likelihood is approximated by a piecewise pseudo-likelihood (Sutton and McCallum, 2007) that only takes in consideration the local interactions within a single factor between the variables in our model. We emphasize that this change did not require any modification to our inference engine and we simply used this pseudo-likelihood as a drop-in replacement for the exact likelihood. As we can see from the results in Table 1 (GP-VAR-P), the performance of our model under this regime is comparable to the one for GP-VAR-S. Furthermore, every step of stochastic optimization ran roughly twice as fast in GP-VAR-P as in GP-VAR-S, which made up for the fact that for a linear-chain structure the computation time of forward-backward is quadratic in the label cardinality while for the piecewise pseudo-likelihood the cost is linear. Such an approach might be considered for extending our framework to models such as grids or skip-chains, for which the evaluation of the true structured likelihood would be intractable. Alternatively, a structured mean field approximation using tractable approximating families of sub-graphs (linear chains, for instance) might be used for the same purpose.

6.2 Larger-scale experiments

Here we report the results on an experiment that used the largest dataset in our benchmark suite (BASE NP). For this dataset we used a five-fold cross-validation setting and $N_{seq} = 500$ training sequences. This amounts to roughly 11,611 words on average. For testing we used the remaining (323) sequences. In this setting GP-ESS is completely impractical. We compare the results of our model with CRF, which from our previous experiment was the most competitive baseline. Unlike the small experiments where the regularization parameter was learned through cross-validation, because of the large execution times, here we report the error rates for two values of this parameter $\lambda_{reg} \in \{0.1, 1\}$, where we obtained 5.13% and 4.50% respectively. Our model (GP-VAR-S) attained an error rate of 5.14%, which is comparable to CRF’s performance. As in the small experiments, we conclude that our model, despite not knowing the details of the likelihood, it performs on par with methods that were hard-coded for these types of likelihoods. See the supplementary material for more analysis.

7 Related work

Recent advances in sparse GP models for regression (Titsias, 2009; Hensman et al., 2013) have allowed the applicability of such models to very large datasets, opening opportunities for the extension of these ideas to classification and to problems with generic i.i.d likelihoods (Hensman et al., 2015a; Nguyen and Bonilla, 2014; Dezfouli and Bonilla, 2015; Hensman et al., 2015b). However, none of these approaches is actually applicable to structured prediction problems, which inherently deal with non-i.i.d likelihoods.

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2This was developed by Taku Kudo and can be found at https://taku910.github.io/crffpp/.
Twin Gaussian processes (Bo and Sminchisescu, 2010) address structured continuous-output problems by forcing input kernels to be similar to output kernels. In contrast, here we deal with the harder problem of structured discrete-output problems, where one usually requires computing expensive likelihoods during training. The structured continuous-output problem is somewhat related to the area of multi-output regression with GPs for which, unlike discrete structured prediction with GPs, the literature is relatively mature (Álvarez et al., 2010; Álvarez and Lawrence, 2011, 2009; Bonilla et al., 2008).

The original structured Gaussian process model, (gpstruct, Bratières et al., 2015) uses Markov Chain Monte Carlo (MCMC) sampling as the inference method and is not equipped with sparsification techniques that are crucial for scaling to large data. Bratières et al. (2014) have explored a distributed version of gpstruct based on the pseudo-likelihood approximation (Besag, 1975) where several weak learners are trained on subsets of gpstruct’s latent variables and bootstrap data. However, within each weak learner, inference is still done via MCMC. A variational alternative for gpstruct inference (Srijith et al., 2014) is also available. However, it relies on pseudo-likelihood approximations and was only evaluated on small-scale problems. Unlike this work, our approach can deal with both pseudo-likelihoods and generic (linear-chain) structured likelihoods, and we rely on our sparse approximation procedure and our automated variational inference technique – rather than on bootstrap aggregation – to achieve good performance on larger datasets.

8 Conclusion & discussion

We have presented a Bayesian structured prediction model with GP priors and linear-chain likelihoods. We have developed an automated variational inference algorithm that is statistically efficient in that only requires expectations over very low-dimensional Gaussians in order to estimate the expected likelihood term in the variational objective. We have exploited these types of theoretical insights as well as practical statistical and optimization tricks to make our inference framework scalable and effective. Our model generalizes recent advances in CRFs (Koltun, 2011) by allowing general positive definite kernels defining their energy functions and opens new directions for combining deep learning with structure models (Zheng et al., 2015).

As mentioned in the introduction, for general structured prediction problems one may need to set up the configuration of the latent functions (e.g. the unary and pairwise functions in the linear-chain case). Thus, the process of developing an inference procedure for a different structure (e.g. when going from linear chains to skip-chains) requires some human intervention. Nevertheless, when applied to fixed structures our approach is entirely “black box” with respect to the choice of likelihood, inasmuch as different likelihoods can be used without any manual change to the inference engine.

Furthermore, we have already seen in our small-scale experiments a possible way to extend our method to more general structured likelihoods, where the exact likelihood is replaced by a piecewise pseudo-likelihood. Such an approach might be considered for using our framework in models such as grids or skip-chains, for which the evaluation of the true structured likelihood would be intractable. The performance of our small-scale experiments in which the true likelihood was approximated by its pseudo-likelihood was very encouraging and we leave a more in-depth investigation of the efficacy of this approach for future work. We also leave to future work the challenging task of automating the very procedure that turns a structured specification into a likelihood-agnostic inference procedure.

Overall, we believe our approach is a fundamental step to developing automated inference methods for general structured prediction problems.

Supplementary Material

A Proof of Theorem 2

Here we proof the result that we can estimate the expected log likelihood and its gradients using expectations over low-dimensional Gaussians.
A.1 Estimation of $L_{\text{ell}}$ in the full (non-sparse) model

For the $L_{\text{ell}}$ we have that:

\[
L_{\text{ell}} = \sum_{n=1}^{N_{\text{seq}}} \log p(y^{(n)}|f_n^{(n)}) \bigg|_{q(f_u^{(n)})q(f_{\text{bin}})}
\]

\[
= \sum_{n=1}^{N_{\text{seq}}} \int_{f_{\text{bin}}} \int_{f_u^{(n)}} q(f_u^{(n)}) q(f_{\text{bin}}) \log p(y^{(n)}|f_n^{(n)}) \, df_u^{(n)} df_{\text{bin}}
\]

\[
= \sum_{n=1}^{N_{\text{seq}}} \int_{f_{\text{bin}}} \int_{f_u^{(n)}} q(f_u^{(n)}) q(f_{\text{bin}}) \log p(y^{(n)}|f_n^{(n)}) \, df_u^{(n)} df_{\text{bin}}
\]

\[
= \sum_{n=1}^{N_{\text{seq}}} \left( \log p(y^{(n)}|f_n^{(n)}) \right)_{q(f_u^{(n)})q(f_{\text{bin}})}
\]

where $q_k(n)(f_u^{(n)})$ is a $(T_n \times |V|)$-dimensional Gaussian with block-diagonal covariance $\Sigma_k(n)$, each block of size $T_n \times T_n$. Therefore, we can estimate the above term by sampling from $T_n$-dimensional Gaussians independently. Furthermore, $q(f_{\text{bin}})$ is a $|V|^2$-dimensional Gaussian, which can also be sampled independently. In practice, we can assume that the covariance of $q(f_{\text{bin}})$ is diagonal and we only sample from unary Gaussians for the pairwise functions.

A.2 Gradients

Taking the gradients of the $k$th term for the $n$th sequence in the $L_{\text{ell}}$:

\[
L_{\text{ell}}^{(k,n)} = \left( \log p(y^{(n)}|f_n^{(n)}) \right)_{q_k(n)(f_u^{(n)})q(f_{\text{bin}})}
\]

\[
= \int_{f_{\text{bin}}} \int_{f_u^{(n)}} q_k(n)(f_u^{(n)}) q(f_{\text{bin}}) \log p(y^{(n)}|f_n^{(n)}) \, df_u^{(n)} df_{\text{bin}}
\]

\[
\nabla \lambda_k^x L_{\text{ell}}^{(k,n)} = \int_{f_{\text{bin}}} \int_{f_u^{(n)}} q_k(n)(f_u^{(n)}) q(f_{\text{bin}}) \nabla \lambda_k^x \log q_k(n)(f_u^{(n)}) \log p(y^{(n)}|f_n^{(n)}) \, df_u^{(n)} df_{\text{bin}}
\]

\[
= \left( \nabla \lambda_k^x \log q_k(n)(f_u^{(n)}) \log p(y^{(n)}|f_n^{(n)}) \right)_{q_k(n)(f_u^{(n)})q(f_{\text{bin}})}
\]

where we have used the fact that $\nabla_x f(x) = f(x) \nabla_x \log f(x)$ for any nonnegative function $f(x)$. Similarly, the gradients of the parameters of the distribution over binary functions can be estimated using:

\[
\nabla \lambda_{\text{bin}} L_{\text{ell}}^{(k,n)} = \left( \nabla \lambda_{\text{bin}} \log q(f_{\text{bin}}) \log p(y^{(n)}|f_n^{(n)}) \right)_{q_k(n)(f_u^{(n)})q(f_{\text{bin}})}
\]

B KL terms in the sparse model

The KL term ($L_{kl}$) in the variational objective ($L_{\text{elbo}}$) is composed of a KL divergence between the approximate posteriors and the priors over the inducing variables and pairwise functions:

\[
L_{kl} = -KL(q(u)||p(u)) -KL(q(f_{\text{bin}})||p(f_{\text{bin}}))
\]

(31)
where, as the approximate posterior and the prior over the pairwise functions are Gaussian, the KL over pairwise functions can be computed analytically:

\[
L_{\text{kl}}^{\text{bin}} = -\text{KL}(q(f_{\text{bin}})||p(f_{\text{bin}})) = \text{KL}(\mathcal{N}(f_{\text{bin}}; m_{\text{bin}}, S_{\text{bin}})||\mathcal{N}(f_{\text{bin}}; 0, K_{\text{bin}})) \\
= -\frac{1}{2} (\log |K_{\text{bin}}| - \log |S_{\text{bin}}| + m_{\text{bin}}^T K_{\text{bin}}^{-1} m_{\text{bin}} + \text{tr} K_{\text{bin}}^{-1} S_{\text{bin}} - |\mathcal{V}|).
\]  

(32)

For the distributions over the unary functions we need to compute a KL divergence between a mixture of Gaussians and a Gaussian. For this we consider the decomposition of the KL divergence as follows:

\[
L_{\text{kl}}^u = -\text{KL}(q(u)||p(u)) = \mathbb{E}_q[-\log q(u)] + \mathbb{E}_q[\log p(u)],
\]

(33)

where the entropy term \( \mathcal{L}_{\text{ent}} \) can be lower bounded using Jensen’s inequality:

\[
\mathcal{L}_{\text{ent}} \geq -\sum_{k=1}^K \pi_k \log \sum_{\ell=1}^K \pi_{\ell} \mathcal{N}(m_k; m_{\ell}, S_k + S_{\ell}) \overset{\text{def}}{=} \hat{\mathcal{L}}_{\text{ent}}.
\]

(35)

and the negative cross-entropy term \( \mathcal{L}_{\text{cross}} \) can be computed exactly:

\[
\mathcal{L}_{\text{cross}} = -\frac{1}{2} \sum_{k=1}^K \pi_k \sum_{j=1}^{|\mathcal{V}|} \left[ M \log 2\pi + \log |\kappa(Z_j, Z_j)| + m_{kj}^T \kappa(Z_j, Z_j)^{-1} m_{kj} + \text{tr} \kappa(Z_j, Z_j)^{-1} S_{kj} \right].
\]

(36)

### C Proof of Theorem 3

To prove Theorem 3 we will express the expected log likelihood term in the same form as that given in Equation (25), showing that the resulting \( q_k(n)(f_k^{(n)}) \) is also a \( (T_n \times |\mathcal{V}|) \)-dimensional Gaussian with block-diagonal covariance, having \( |\mathcal{V}| \) blocks each of dimensions \( T_n \times T_n \). We start by taking the given \( \mathcal{L}_{\text{cell}} \), where the expectations are over the joint posterior \( q(f, u|\lambda) = p(f|u)q(u)q(f_{\text{bin}}) \):

\[
\mathcal{L}_{\text{cell}} = \left\langle \sum_{n=1}^{N_{\text{seq}}} \log p(y^{(n)}|f_n) \right\rangle_{p(f_n|u)q(u)q(f_{\text{bin}})}
\]

(37)

\[
= \int_f \log p(y|f) \int_u q(u)p(f|u)du q(f_{\text{bin}})df,
\]

(38)

where our approximating distribution is:

\[
q(f) = q(f_{\lambda})q(f_{\text{bin}})
\]

(39)

\[
q(f_{\lambda}) = \int_u q(u)p(f_{\lambda}|u)du,
\]

(40)

which can be computed analytically:

\[
q(f_{\lambda}) = \sum_{k=1}^K \pi_k q_k(f_{\lambda}) = \sum_{k=1}^K \pi_k \prod_{j=1}^{|\mathcal{V}|} \mathcal{N}(f_{\lambda,j}; b_{kj}, \Sigma_{kj})
\]

(41)

\[
b_{kj} = A_j m_{kj}
\]

(42)

\[
\Sigma_{kj} = \bar{K}_j + A_j S_{kj} A_j^T.
\]

(43)
We note in Equation (41) that $q_k(f_u)$ has a block diagonal structure, which implies that we have the same expression for the $L_{\text{ell}}$ as in Equation (25). Therefore, we obtain analogous estimates:

$$L_{\text{ell}} = \sum_{n=1}^{N_{mn}} \sum_{k=1}^{K} \pi_k \left\langle \log p(y^{(n)}|f_u^{(n)}) \right\rangle \frac{q_k(f_u^{(n)})}{q(f_u^{(n)})} ,$$

Here, as before, $q_k(f_u^{(n)})$ is a $(T_n \times |V|)$–dimensional Gaussian with block-diagonal covariance $\Sigma_k$, each block of size $T_n \times T_n$. The main difference in this (sparse) case is that $b_k$ and $\Sigma_k$ are constrained by the expressions in Equations (42) and (43). Hence, the proof for the gradients follows the same derivation as in §A.2 above.

D Gradients of $L_{\text{elbo}}$ for sparse model

Here we give the gradients of the variational objective wrt the parameters for the variational distributions over the inducing variables, pairwise functions and hyper-parameters.

D.1 Inducing variables

D.1.1 KL term

As the structured likelihood does not affect the KL divergence term, the gradients corresponding to this term are similar to those in the non-structured case (Dezfouli and Bonilla, 2015). Let $K_{zz}$ be the block-diagonal covariance with $|V|$ blocks $\kappa(Z_j, Z_j), j = 1, \ldots, Q$. Additionally, lets assume the following definitions:

$$C_{kl} \overset{\text{def}}{=} S_k + S_\ell,$$

$$N_{k\ell} \overset{\text{def}}{=} N(m_k; m_\ell, C_{kl}),$$

$$z_k \overset{\text{def}}{=} \sum_{\ell=1}^{K} \pi_\ell N_{k\ell}.$$ 

The gradients of $L_{\text{kl}}$ wrt the posterior mean and posterior covariance for component $k$ are:

$$\nabla_{m_k} L_{\text{cross}} = -\pi_k K_{zz}^{-1} m_k,$$

$$\nabla_{S_k} L_{\text{cross}} = -\frac{1}{2} \pi_k K_{zz}^{-1},$$

$$\nabla_{\pi_k} L_{\text{cross}} = -\frac{1}{2} |V| \sum_{j=1}^{Q} [M \log 2\pi + \log |\kappa(Z_j, Z_j)| + m_k^T \kappa(Z_j, Z_j)^{-1} m_k + \text{tr} \, \kappa(Z_j, Z_j)^{-1} S_{kj}],$$

where we note that we compute $K_{zz}^{-1}$ by inverting the corresponding blocks $\kappa(Z_j, Z_j)$ independently. The gradients of the entropy term wrt the variational parameters are:

$$\nabla_{m_k} \hat{L}_{\text{ent}} = \pi_k \sum_{\ell=1}^{K} \pi_\ell \left( N_{k\ell}/z_k + N_{k\ell}/z_\ell \right) C_{kl}^{-1} (m_k - m_\ell),$$

$$\nabla_{S_k} \hat{L}_{\text{ent}} = \frac{1}{2} \pi_k \sum_{\ell=1}^{K} \pi_\ell \left( N_{k\ell}/z_k + N_{k\ell}/z_\ell \right) [C_{kl}^{-1} - C_{kl}^{-1} (m_k - m_\ell) (m_k - m_\ell)^T C_{kl}^{-1}],$$

$$\nabla_{\pi_k} \hat{L}_{\text{ent}} = -\log z_k - \sum_{\ell=1}^{K} \pi_\ell N_{k\ell}/z_\ell.$$
D.1.2 Expected log likelihood term

Retaking the gradients in the full model In Equations (29), we have that:

\[
\nabla \lambda^u_k \mathcal{L}_{\text{ell}}^{(k,n)} = \left( \nabla \lambda^u_k \log q_k(n)(f_u^{(n)}) \log p(y^{(n)} | f_u) \right) \left( q_k(n)(f_u^{(n)}) q(f_u) \right),
\]

where the variational parameters \( \lambda^u_k \) are the posterior means and covariances (\( \{m_{kj}\} \) and \( \{S_{kj}\} \)) of the inducing variables. As given in Equation (41), \( q_k(f_u) \) factorizes over the latent process \( (j = 1, \ldots, |V|) \), so do the marginals \( q_k(n)(f_u^{(n)}) \), hence:

\[
\nabla \lambda^u_k \log q_k(n)(f_u^{(n)}) = \nabla \lambda^u_k \sum_{j=1}^{|V|} \log N(f_{uj}; b_{kj(n)}, \Sigma_{kj(n)}),
\]

where each of the distributions in Equation (54) is a \( T_n \)-dimensional Gaussian. Let us assume the following definitions:

\[
X_n \quad \text{all feature vectors corresponding to sequence } n
\]

\[
A_{jn} \overset{\text{def}}{=} \kappa(X_n, Z_j)\kappa(\Sigma_{j}, Z_j)^{-1}
\]

\[
\tilde{K}^{(n)}_j \overset{\text{def}}{=} \kappa_j(X_n, X_n) - A_{jn} \kappa_j(\Sigma_{j}, X_n), \quad \text{therefore:}
\]

\[
b_{kj} = A_{jn} m_{kj},
\]

\[
\Sigma_{kj(n)} = \tilde{K}^{(n)}_j + A_{jn} S_{kj} A_{jn}^T.
\]

Hence, the gradients of \( \log q_k(f_u) \) wrt the variational parameters of the unary posterior distributions over the inducing points are:

\[
\nabla_{m_{kj}} \log q_k(n)(f_u^{(n)}) = A_{jn}^T \Sigma_{kj(n)}^{-1} \left( f_{uj} - b_{kj(n)} \right),
\]

\[
\nabla_{S_{kj}} \log q_k(n)(f_u^{(n)}) = \frac{1}{2} A_{jn}^T \left[ \Sigma_{kj(n)}^{-1} \left( f_{uj} - b_{kj(n)} \right) \left( f_{uj} - b_{kj(n)} \right)^T \Sigma_{kj(n)}^{-1} - \Sigma_{kj(n)}^{-1} \right] A_{jn}
\]

Therefore, the gradients of \( \mathcal{L}_{\text{ell}} \) wrt the parameters of the distributions over unary functions are:

\[
\nabla_{m_{kj}} \mathcal{L}_{\text{ell}} = \frac{\pi_{k}}{S} \kappa(Z_j, Z_j)^{-1} \sum_{n=1}^{N_{\text{seq}}} \kappa(Z_j, X_n) \Sigma_{kj(n)}^{-1} \sum_{i=1}^{S} \left( f_{uj}^{(k,i)} - b_{kj(n)} \right) \log p(y^{(n)} | f_{uj}^{(k,i)}), f_{uj}^{(i)}),
\]

\[
\nabla_{S_{kj}} \mathcal{L}_{\text{ell}} = \frac{\pi_{k}}{2S} \sum_{n=1}^{N_{\text{seq}}} A_{jn}^T \left( \sum_{i=1}^{S} \left[ \Sigma_{kj(n)}^{-1} \left( f_{uj}^{(k,i)} - b_{kj(n)} \right) \left( f_{uj}^{(k,i)} - b_{kj(n)} \right)^T \Sigma_{kj(n)}^{-1} - \Sigma_{kj(n)}^{-1} \right] \right) A_{jn}
\]

D.1.3 Pairwise functions

The gradients of the \( \mathcal{L}_{\text{kl}}^{\text{bin}} \) wrt the parameters of the posterior over pairwise functions are given by:

\[
\nabla_{m_{bin}} \mathcal{L}_{\text{kl}}^{\text{bin}} = -K_{\text{bin}}^{-1} m_{bin}
\]

\[
\nabla_{S_{bin}} \mathcal{L}_{\text{kl}}^{\text{bin}} = \frac{1}{2} \left( S_{\text{bin}}^{-1} - K_{\text{bin}}^{-1} \right)
\]

The gradients of the \( \mathcal{L}_{\text{ell}} \) wrt the parameters of the posterior over pairwise functions are given by:

\[
\nabla_{m_{bin}} \mathcal{L}_{\text{ell}} = \frac{1}{S} \sum_{n=1}^{N_{\text{seq}}} \sum_{k=1}^{K} \pi_{k} \sum_{i=1}^{S} S_{\text{bin}}^{-1} \left( f_{bin}^{(i)} - m_{bin} \right) \log p(y^{(n)} | f_{uj}^{(k,i)}), f_{uj}^{(i)}
\]

\[
\nabla_{S_{bin}} \mathcal{L}_{\text{ell}} = \frac{1}{2S} \sum_{n=1}^{N_{\text{seq}}} \sum_{k=1}^{K} \pi_{k} \sum_{i=1}^{S} \left( S_{\text{bin}}^{-1} \left( f_{bin}^{(i)} - m_{bin} \right) \right) \log p(y^{(n)} | f_{uj}^{(k,i)}), f_{uj}^{(i)}
\]

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Table 2: Datasets used in our experiments. For each dataset we see the number of categories (or vocabulary |V|), the number of features (D), the number of training sequences used in the small experiments (N_{seq small}), and the average (across folds) number of training words for the small experiments (\bar{N}).

| Dataset      | |V| | D   | N_{seq small} | \bar{N} small |
|--------------|---|---|-----|---------------|---------------|
| BASE NP      | 3 | 6,438 | 150 | 3739.8        |
| CHUNKING     | 14 | 29,764 | 50  | 1155.8        |
| SEGMENTATION | 2 | 1,386 | 20  | 942           |
| JAPANESE NE  | 17 | 102,799 | 50 | 1315.4        |

E Experiments

E.1 Experimental set-up

Details of the benchmarks used in our experiments can be seen in Table 2. For the experiments with batch optimization, we optimized the three sets of parameters separately in a global loop (variational parameters for unary nodes, variational parameters for pairwise nodes, and hyper-parameters). In each global iteration, each set of parameters were optimized while keeping the rest of the parameters fixed. Variational parameters for unary nodes were optimized for 50 iterations, variational parameters for pairwise nodes were optimized for 10 iterations, and hyper-parameters were updated for 5 iterations. We used L-BFGS algorithm for optimizing each set of parameters, and parameters were optimized for a maximum of 5 1/2 hours, or until the convergence, whichever comes first. Convergence was detected when the objective function in two consecutive global iterations was less than 1e-05, or the average change in the variational parameters for unary nodes was less than 0.001. The reported results are the predictions based on the best objective function achieved during the optimization. 10,000 samples (S = 10,000) were used for approximating expected log likelihood and its gradients and 10% of these samples were used for the optimal \hat{a} in the control variate calculation. For all the experiments 500 inducing points were used (M = 500).

In experiments with stochastic optimization, similar to the experiments with batch optimization, each set of parameters were optimized separately. In each global iteration, variational parameters for unary nodes were updated for 3000 iterations and variational parameters for pairwise nodes were updated for 1000 iterations (hyper-parameters were not optimized in the stochastic optimization experiments, and they were fixed to 1). 4,000 samples were used for estimating expected log likelihood and its gradients (S = 4000). Similar to the batch optimization case, we used 500 inducing points (M = 500). The step-size for updating the means of the inducing points was set to 1e-4, and the step-size for updating the covariances of the inducing points were set to 1e-5.

E.2 Performance profiles

Figure 1 shows the performance of our algorithm as a function of time. We see that the test likelihood decreases very regularly in all the folds and so does overall the error rate, albeit with more variability. The bulk of the optimization, both with respect to the test likelihood and with respect to the error rate, occurs during the first 120 minutes. This suggests that the kind of approach described in this paper might be particularly suited for cases in which speed of convergence is a priority.

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