A Unifying Framework for Sparse Gaussian Process Approximation using Power Expectation Propagation

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May 24, 2016

Abstract

Pseudo-point based sparse approximation methods sidestep the computational and analytical intractability in Gaussian process models at the cost of accuracy, reducing the complexity from cubic to linear in the number of data points. We propose a new sparse posterior approximation framework using Power Expectation Propagation (Power EP), unifying various existing methods into one single computational and algorithmic viewpoint. This allows us to bring a new posterior approximation perspective to methods that are currently understood to perform prior approximation. Crucially, we demonstrate that the proposed approach outperforms current sparse methods on regression, classification and state space modelling by leveraging the interpolation between Power EP’s special cases, variational inference and EP.

1 Introduction

Gaussian Processes (GPs) are powerful nonparametric distributions over continuous functions that are routinely deployed in probabilistic modelling for applications ranging from regression and classification [1], representation learning [2], and state space modelling [3]. GPs have many elegant theoretical properties, but their use is greatly hindered by analytic and computational intractabilities. A large research effort has been directed at this fundamental problem resulting in the development of a plethora of sparse approximation methods that can sidestep these intractabilities [4–19].

This paper develops a general sparse approximate inference framework based upon Power Expectation Propagation (PEP) [20] that unifies many of these approximations, extends them significantly, and provides improvements in practical settings. In this way, the paper provides a complementary perspective to the seminal review of Quiñonero-Candela and Rasmussen [4], viewing sparse approximations through the lens of approximate inference, rather than approximate generative models.

The paper begins by reviewing several frameworks for sparse approximation focusing on the GP regression and classification setting (section 2). It then lays out the new unifying framework and the relationship to existing techniques (section 3). The extension to state space models follows (section 4). A thorough experimental evaluation is presented in section 5.
2  Pseudo-point approximations for GP regression and classification

This section provides a concise introduction to GP regression and classification and then reviews several pseudo-point based sparse approximation schemes for these models. We consider a supervised learning setting in which the training set comprises \( N \) \( D \)-dimensional input and scalar output pairs \( \{x_n, y_n\}_{n=1}^{N} \) and the goal is to produce probabilistic predictions for the outputs corresponding to novel inputs. A non-linear function, \( f(x) \), can be used to parameterise the probabilistic mapping between inputs and outputs, \( p(y_n|f(x_n), \theta) \). Typical choices are Gaussian \( p(y_n|f(x_n), \theta) = \mathcal{N}(y_n; f(x_n), \sigma_y^2) \) for the regression setting \( (y_n \in \mathbb{R}) \) and Bernoulli \( p(y_n|f(x_n), \theta) = B(y_n; \Phi(f(x_n))) \) with a sigmoidal link function \( \Phi(f) \) for the binary classification setting \( (y_n \in \{0, 1\}) \). Whilst it is possible to specify the non-linear function \( f \) via an explicit parametric form, a more flexible and elegant approach employs a GP prior over the functions directly, \( p(f|\theta) = \mathcal{G}P(0, k_0(\cdot, \cdot)) \), here assumed to have a zero mean-function and a covariance function \( k_0(x, x') \). This class of probabilistic models has a joint distribution \( p(f, y|\theta) = p(f|\theta) \prod_{n=1}^{N} p(y_n|f(x_n), \theta) \) where we have collected the observations into the vector \( y \) and suppressed the inputs on the left hand side to lighten the notation.

This model class contains two potential sources of intractability. First, the possibly non-linear likelihood function can introduce analytic intractabilities that require approximation. Second, the GP prior entails an \( \mathcal{O}(N^3) \) complexity that is computationally intractable for many practical problems. These two types of intractability can handled by combining standard approximate inference methods with pseudo-point approximations that summarise the full Gaussian process via \( M \) pseudo data-points leading to an \( \mathcal{O}(NM^2) \) cost. The main approaches of this sort can be characterised in terms of two parallel frameworks that are described in the following sections.

2.1 Sparse GP approximation via approximate generative models

The first framework begins by constructing a new generative model that is similar to the original, so that inference in the new model might be expected to produce similar results, but which has a special structure that supports efficient computation. Typically this approach involves approximating the Gaussian process prior as it is the origin of the cubic cost \([4]\).

The seminal review by Quiñonero-Candela and Rasmussen \([4]\) reinterprets a family of approximations in terms of this unifying framework. The GP prior is approximated by identifying a small set of \( M \leq N \) pseudo-points \( u \), here assumed to be disjoint from the training function values \( f \) so that \( f = \{u, f, f \neq u\} \). The GP prior \( p(f|\theta) = p(u|\theta)p(f|u, \theta)p(f \neq u|f, u, \theta) \) is then approximated using a new process \( p(f|\theta) \approx q(f|\theta) = p(u|\theta)q(f|u, \theta)p(f \neq u|f, u, \theta) \). Here, computational savings are obtained by simplifying the dependencies between the pseudo-points and the data function values \( q(f|u, \theta) = \mathcal{N}(f; K_{f,u}K_{u,u}^{-1}u, D_{f,f}) \) where \( D_{f,f} = K_{f,f} - Q_{f,f} \) and \( Q_{f,f} = K_{f,u}K_{u,u}^{-1}K_{u,f} \) and using the pseudo-data as a bottleneck between the data function values and test function values \( p(f \neq u|f, u, \theta) \approx p(f \neq u|f, u, \theta) \). We compactly summarise previous work as special cases of the choice \( q(f|u, \theta) = \prod_{b=1}^{B} \mathcal{N}(f_b; K_{f_b,u}K_{u,u}^{-1}u, \alpha D_{f_b,f_b}) \) where \( b \) indexes \( B \) disjoint blocks of data-function values: the Deterministic Training Conditional (DTC) approximation uses \( \alpha \rightarrow 0 \); the Fully Independent Training Conditional (FITC) approximation uses \( \alpha = 1 \) and \( B = N \); the Partially Independent Training Conditional (PITC) approximation uses \( \alpha = 1 \) \([4,7]\). It is possible to extend these methods using the inter-domain
approach that places the pseudo-data in a different domain from the data, defined by a linear integral transform (see [17] for FITC). The expressions above still hold, but the covariance matrices involving pseudo-data are modified.

The approximate generative model framework has attractive properties. When point-wise likelihoods are used, the new resulting modified generative models, \( q(f|\theta) \Pi_{n=1}^{N} p(y_n|f(x_n), \theta) \), have a training and test computational complexity of \( O(NM^2) \) (for testing, \( N \) becomes the number of test data points, assuming dependencies between the test-points are not computed). Moreover, the pseudo-data input locations can be optimised by maximising the new model’s marginal likelihood [5]. When \( M = N \) and the pseudo-data and observed-data inputs coincide, then FITC and PITC are exact which appears reassuring. However, the framework is philosophically challenging as the elegant separation of model and (approximate) inference has been lost. Are we allowed, for example, to add new pseudo-data as more data are acquired and the complexity of the underlying function is revealed? This seems sensible, but effectively changes the modelling assumptions as more data are seen. Similarly, if the pseudo-input locations are optimised, the principled non-parametric model has suddenly acquired \( MD \) parameters and with them all of the concomitant issues of parametric models including overfitting and optimisation difficulties. Finally, for analytically intractable likelihood functions an additional approximate inference step is required anyway, begging the question of why computational and analytic intractabilities are not handled together at inference time.

### 2.2 Sparse GP approximation via approximate inference: VFE

The approximate generative model framework for constructing sparse approximations is philosophically troubling. In addition, learning pseudo-point input locations via optimisation of the model likelihood can perform poorly e.g. for DTC it is prone to overfitting even for \( M \ll N \) [8]. This motivates a more direct approach that commits to the true generative model and performs all of the necessary approximation at inference time.

Perhaps the most well known approach in this vein is Titsias’s beautiful sparse variational free energy (VFE) method [8]. The original presentation of this work employs finite variable sets and an augmentation trick that arguably obscures its full elegance. Here instead we follow [16] and lower bound the marginal likelihood using a distribution \( q(f) \) over the entire infinite dimensional function,

\[
\log p(y|\theta) = \log \int p(y, f|\theta) df \geq \int q(f) \log \frac{p(y, f|\theta)}{q(f)} df = \mathbb{E}_{q(f)} \left[ \log \frac{p(y, f|\theta)}{q(f)} \right] = \mathcal{F}(q, \theta).
\]

The VFE bound can be written as the difference between the model log-marginal likelihood and the KL-divergence between the variational distribution and the true posterior \( \mathcal{F}(q, \theta) = \log p(y|\theta) - \text{KL}(q(f)||p(f|y, \theta)) \). The bound is therefore saturated when \( q(f) = p(f|y, \theta) \), but this is intractable. Instead, pseudo-data are made explicit, \( f = \{u, f \neq u \} \), and an approximate posterior distribution used of the following form \( q(f) = q(u, f \neq u) = p(f \neq u|u, \theta)q(u) \). Under this approximation, the set of variables \( f \neq u \) do not experience the data directly, but rather only through the pseudo-data, as can be seen by comparison to the true posterior \( p(f|y, \theta) = p(f \neq u|y, u, \theta)p(u|y, \theta) \). Importantly, the form of the approximate posterior gives rise to a bound with \( O(NM^2) \) complexity,

\[
\mathcal{F}(q, \theta) = \mathbb{E}_{q(f)} \left[ \log \frac{p(y, f|\theta)p(f \neq u|u, \theta)p(u)}{p(f \neq u|u, \theta)q(u)} \right] = \sum_{n} \mathbb{E}_{q(f)} \left[ \log p(y_n|f_n, \theta) \right] - \text{KL}(q(u)||p(u|\theta)).
\]
For regression, the calculus of variations can be used to find the optimal approximate posterior distribution over pseudo-data, which is identical to that recovered using the DTC approximate generative model [8] (in fact DTC was originally derived using a related KL argument [9,11]). The VFE approach can be extended to non-linear models including classification [14], latent variable models [21] and state space models [18,19] by restricting \( q(u) \) to be Gaussian. Additional approximation is sometimes required to compute any remaining intractable non-linear integrals, but these are often low-dimensional. The VFE approach can also be extended to employ inter-domain variables [16,22].

A key concept underpinning the VFE framework is that the pseudo-input locations are purely parameters of the approximate posterior (‘variational parameters’). Optimisation of these parameters is automatically protected from overfitting since it is equivalent to minimising the KL-divergence between the approximate and true posterior. Indeed, although the DTC posterior is recovered in the regression setting, the free energy is not equal to the log-marginal likelihood of the DTC generative model, containing additional terms that substantially improve the quality of the optimised pseudo-point input locations. The fact that the form of the DTC approximation can be recovered from a direct approximate inference approach and that this new perspective leads to superior pseudo-input optimisation, raises the question; can this also be done for FITC and PITC?

2.3 Sparse GP approximation via approximate inference: EP

Expectation Propagation (EP) is a deterministic inference method [23] that is known to outperform VFE methods in GP classification when unsparsified fully-factored approximations \( q(f) = \prod_n q_n(f_n) \) are used [24]. Motivated by this observation, EP has been combined with the approximate generative modelling approach to handle non-linear likelihoods [12,15]. This begs the question: can the sparsification and the non-linear approximation be handled in a single EP inference stage, as for VFE? Astonishingly Csató and Opper not only developed such a method in 2002 [10], predating much of the work mentioned above, they showed that it is equivalent to applying the FITC approximation and running EP if further approximation is required. In our view, this is a central result, but it appears to have been largely overlooked by the field. Snelson was made aware of it when writing his thesis [6], briefly acknowledging Csató and Opper’s contribution. Qi, Abdel-Gawad and Minka [13] extended Csató and Opper’s work to utilise inter-domain pseudo-data and recognised that the EP energy function at convergence is equal to the FITC log-marginal likelihood approximation. We are unaware of other work in this vein.

It is hard to know why these important results are not more widely known. A contributing factor is that the exposition in these papers is largely at Marr’s algorithmic level [25], and does not focus on the computational level making them challenging to understand. One of the main contributions of this paper is to provide a clear computational exposition. In addition, we will show that a generalisation of EP called Power EP can subsume the EP and VFE approaches (and therefore FITC and DTC) into a single unified framework. PITC emerges too. We consider (Gaussian) regression and probit classification as canonical models on which to test the new framework and end by extending the results to GP state-space-models where there is less prior work. The new contributions and their relation to previous work is summarised in fig. 1.
In this section, we provide a new unifying view of sparse approximation using Power Expectation Propagation (PEP or Power EP) [20]. We review Power EP, describe how to apply it for sparse GP regression and classification, and then discuss its relationship to existing methods.

### 3.1 Power EP

Power EP approximates the unnormalised posterior distribution (the joint distribution) returning a tractable normalised posterior, here a GP \( q(f|\theta) = \mathcal{GP}(m_f, V_{ff}) \), and a marginal likelihood estimate,

\[
p^*(f|y, \theta) = p(f|y, \theta)p(y|\theta) \approx q(f|\theta) Z_{PEP}(\theta) = q^*(f|\theta).
\]  (1)

The * denotes unnormalised densities. The PEP approximation’s form mirrors the joint distribution,

\[
p^*(f|y, \theta) = p(f|y, \theta)p(y|\theta) = p(f) \prod_n p(y_n|f, \theta) \approx p(f|\theta) \prod_n t_n(u) = q^*(f|\theta).
\]  (2)

Here, the approximation retains the exact prior, but each likelihood term in the exact posterior, \( p(y_n|f_n) \), is approximated by a simple factor \( t_n(u) \) that is assumed Gaussian. To remind the reader the GP prior can be decomposed \( p(f|\theta) = p(f|\theta, f, u)p(f|u, \theta)p(u|\theta) \). So, the approximate posterior above can be thought of as the (exact) GP posterior resulting from a surrogate regression problem in which each likelihood involves \( M \) function values \( u \). PEP iteratively refines the approximate factors or surrogate likelihoods so that the GP posterior of the surrogate regression task best approximates the posterior of the original regression/classification problem using the following steps:

1. **Deletion**: compute the cavity distribution by removing a fraction of one approximate factor, \( q_{\alpha}^{\text{un}}(f) \propto q^*(f)/t_n^\alpha(u) \).
2. **Projection:** first, compute the tilted distribution by incorporating a corresponding fraction of the true likelihood into the cavity, \( \tilde{p}(f) = q^n(f)p^\alpha(y_n|f_n) \). Second, project the tilted distribution onto the approximate posterior using the KL divergence for un-normalised densities, \( q^*(f) \leftarrow \arg\min_{q^*(f)\in Q} KL(\tilde{p}(f)||q^*(f)) \). Here \( Q \) is the set of allowed \( q^*(f) \) defined by eq. (2).

3. **Update:** compute a new fraction of the approximate factor by dividing the new approximate posterior by the cavity, \( t_n^{\alpha,\text{new}}(u) = q^*(f)/q^{\alpha}(f) \), and incorporate this fraction back in to obtain the updated factor, \( t_n(u) = t_n^{1-\alpha}(u)t_n^{\alpha,\text{new}}(u) \).

The above steps are iteratively repeated for each factor that needs to be approximated. When \( \alpha = 1 \), PEP is called EP and as \( \alpha \to 0 \) the PEP solution is the minimum of a variational free energy. We will now show that these cases of PEP recover FITC and Titsias’s VFE solution respectively.

### 3.1.1 General results for Gaussian Process Power EP

This section describes the PEP steps in finer detail showing the complexity is \( O(NM^2) \) and laying the ground work for the equivalence relationships. The supplementary material includes a full derivation.

We start by defining the approximate factors to be in natural parameter form, making it simple to combine and delete them, \( t_n(u) = \mathcal{N}(u;z_n,T_{1,n},T_{2,n}) = z_n \exp(u^T T_{1,n} - \frac{1}{2}u^TT_{2,n}u) \).

We consider full rank \( T_{2,n} \), but will show the optimal form is rank 1. The parameterisation means the approximate posterior over the pseudo-outputs has natural parameters \( T_{1,u} = \sum_n T_{1,n} \) and \( T_{2,u} = K_{uu}^{-1} + \sum_n T_{2,n} \) inducing an approximate GP posterior with mean and covariance function,

\[
m_{\ell} = K_{fu}K_{uu}^{-1}T_{2,u}^{-1}T_{1,u}; \quad V_{\ell\ell'} = K_{\ell\ell'} - Q_{\ell\ell'} + K_{fu}K_{uu}^{-1}T_{2,u}^{-1}K_{uu}^{-1}K_{u\ell'}. \tag{3}
\]

**Deletion:** The cavity for datapoint \( n \), \( q^{\alpha}(f) \propto q^*(f)/t_n^{\alpha}(u) \), has a similar form to the posterior, but the natural parameters are modified by the deletion step, \( T_{1,u}^{\alpha,n} = T_{1,u} - \alpha T_{1,n} \) and \( T_{2,u}^{\alpha,n} = T_{2,u} - \alpha T_{2,n} \) yielding a new mean and covariance function

\[
m_{\ell}^{\alpha,n} = K_{fu}K_{uu}^{-1}T_{2,u}^{\alpha,n}^{-1}T_{1,n}^{\alpha,n}; \quad V_{\ell\ell'}^{\alpha,n} = K_{\ell\ell'} - Q_{\ell\ell'} + K_{fu}K_{uu}^{-1}T_{2,u}^{\alpha,n}^{-1}K_{uu}^{-1}K_{u\ell'}. \tag{4}
\]

**Projection:** The central step in PEP is the projection. Obtaining the new approximate unnormalised posterior \( q^*(f) \) by minimising \( KL(\tilde{p}(f)||q^*(f)) \) would naïvely appear intractable. Fortunately,

**Remark 1.** Because of the structure of the approximate posterior, \( q(f) = p(f_n|u)q(u) \), the objective, \( KL(\tilde{p}(f)||q^*(f)) \) is minimised when \( \mathbb{E}_{\tilde{p}(f)}[\phi(u)] = \mathbb{E}_{q^*(f)}[\phi(u)] \), where \( \phi(u) \) are the sufficient statistics, i.e. when the moments at the pseudo-inputs are matched.

This is the central result from which computational savings are derived. Furthermore, this moment matching condition would appear to necessitate computation of a set of integrals to find the zeroth, first and second moments. However, the technique known as ‘differentiation under the integral sign’ provides a useful shortcut that only requires one integral to compute the
log-normaliser of the tilted distribution, \( \log \tilde{Z}_n = \log \mathbb{E}_{q_\beta^n(f)}[p^\beta(y_n|f_n)] \), before differentiating w.r.t. the cavity mean to give

\[
\mathbf{m}_n = \mathbf{m}_n^{\beta^n} + \mathbf{V}_n^{\beta^n} \frac{d \log \tilde{Z}_n}{dm_n^{\beta^n}}; \quad \mathbf{V}_n = \mathbf{V}_n^{\beta^n} + \mathbf{V}_n^{\beta^n} \frac{d^2 \log \tilde{Z}_n}{d(m_n^{\beta^n})^2} \mathbf{V}_n^{\beta^n}. \tag{5}
\]

**Update:** Having computed the new approximate posterior, the approximate factor \( t_{n, \text{new}}(\mathbf{u}) = q^\beta(f)/q^{\beta^n}(f) \) can be straightforwardly obtained, resulting in,

\[
\mathbf{T}_{1,n, \text{new}} = \mathbf{V}_n^{-1} \mathbf{m}_n - (\mathbf{V}_n^{\beta^n})^{-1} \mathbf{m}_n^{\beta^n}, \quad \mathbf{T}_{2,n, \text{new}} = \mathbf{V}_n^{-1} - (\mathbf{V}_n^{\beta^n})^{-1}, \quad z_n = \tilde{Z}_n e^{\mathcal{G}(q^{\beta^n}(\mathbf{u})) - \mathcal{G}(q^\beta(\mathbf{u}))},
\]

where we have defined the log-normaliser \( \mathcal{G}(\mathcal{N}(\mathbf{u}; z, \mathbf{T}_1, \mathbf{T}_2)) = \log \int \mathcal{N}(\mathbf{u}; z, \mathbf{T}_1, \mathbf{T}_2) d\mathbf{u} \). Remarkably, these results and eqs. \([5]\) reveals that \( \mathbf{T}_{2,n, \text{new}} \) is a rank-1 matrix. As a result, the minimal and simplest way to parameterise the approximate factor is \( t_n(\mathbf{u}) = z_n \mathcal{N}(\mathbf{K}_{ff}^{-1} \mathbf{u}; g_n, v_n) \), where \( g_n \) and \( v_n \) are scalars, resulting in a significant memory saving and \( \mathcal{O}(NM^2) \) cost.

In addition to providing the approximate posterior after convergence, PEP also provides an approximate log-marginal likelihood for model selection and hyper-parameter optimisation,

\[
\log \mathcal{Z}_{\text{PEP}}(\theta) = \log \int p(f|\theta) \prod_n t_n(\mathbf{u}) df = \mathcal{G}(q^\beta(\mathbf{u})) - \mathcal{G}(p^\beta(\mathbf{u})) + \sum_n \log z_n. \tag{6}
\]

Armed with these general results, we now consider the implications for Gaussian Process regression.

### 3.2 Gaussian Regression case

When the model contains Gaussian likelihood functions, closed-form expressions for the PEP approximate factors at convergence can be obtained and hence the approximate posterior:

\[
t_n(\mathbf{u}) = \mathcal{N}(\mathbf{K}_{ff}^{-1} \mathbf{u}; g_n, v_n), \quad q(\mathbf{u}) = \mathcal{N}(\mathbf{u}; \mathbf{K}_{uu} \mathbf{K}_{ff}^{-1} \mathbf{y}, \mathbf{K}_{uu} - \mathbf{K}_{uf} \mathbf{K}_{ff}^{-1} \mathbf{K}_{uf})
\]

where \( \mathbf{K}_{ff} = \mathbf{Q}_{ff} + \text{adiag}(\mathbf{D}_{ff}) + \sigma_y^2 \mathbf{I} \) and \( \mathbf{D}_{ff} = \mathbf{K}_{ff} - \mathbf{Q}_{ff} \) as defined in section \([2]\). These analytic expressions can be rigorously proven to be the stable fixed point of the PEP procedure using eq. \([55]\). Briefly, assuming the factors take the form above, the natural parameters of the cavity \( q^{\beta^n}(\mathbf{u}) \) become,

\[
\mathbf{T}_{1,u}^{\beta^n} = \mathbf{T}_{1,u} - \alpha \gamma_n y_n \mathbf{K}_{ff}^{-1} \mathbf{K}_{uu}, \quad \mathbf{T}_{2,u}^{\beta^n} = \mathbf{T}_{2,u} - \alpha \gamma_n \mathbf{K}_{uu}^{-1} \mathbf{K}_{ff}^{-1} \mathbf{K}_{uu}, \tag{7}
\]

where \( \gamma_n^{-1} = \alpha D_{ff} + \sigma_y^2 \). The subtracted quantities in the equations above are exactly the contribution the likelihood factor makes to the cavity distribution (see eq. \([35]\)) so \( \int q^{\beta^n}(f)p^\beta(y_n|f_n) df_n = q^{\beta^n}(u) \int p(f_n|u)p^\beta(y_n|f_n) df_n \propto q(u) \). Therefore, the posterior approximation remains unchanged after an update and the form for the factors above is the fixed point. Moreover, the approximate log-marginal likelihood is also analytically tractable,

\[
\log \mathcal{Z}_{\text{PEP}} = -\frac{N}{2} \log(2\pi) - \frac{1}{2} \log |\mathbf{K}_{ff}| - \frac{1}{2} \mathbf{y}^\top \mathbf{K}_{ff}^{-1} \mathbf{y} + \frac{1}{2\alpha} \sum_n \log \left(1 + \alpha D_{ff} / \sigma_y^2\right).
\]

We now look at special cases and the correspondence to the methods discussed in section \([2]\).
Remark 2. When $\alpha = 1$ [EP], the PEP posterior becomes the FITC posterior and the PEP approximate marginal likelihood becomes the FITC marginal likelihood. In other words, the FITC approximation for GP regression is, surprisingly, sparse posterior approximation using EP.

Remark 3. As $\alpha \to 0$ the approximate posterior and approximate marginal likelihood are identical to that of the VFE approach in [8]. This result uses the limit: $\lim_{x \to 0} x^{-1} \log(1 + x) = 1$.

3.3 Extensions: structured, inter-domain and multi-power PEP approximations

The framework can be generalised to handle structured approximations (retaining more dependencies), versions of PEP that use different powers $\alpha$ for each factor (e.g. VFE for some data points and EP for others) and inter-domain pseudo data (adding flexibility). Taking inspiration from PITC, we partition the data into $B$ disjoint blocks (see section 2.1) and define a new domain via a linear transform $g(x) = \int dx'W(x, x')f(x')$ now containing the pseudo data $g = \{g_{\neq u}, u\}$. Choices for $W(x, x')$ include Gaussians or wavelets. The approximation becomes $p(f, g|\theta) \prod_b p(y_b|f, \theta) \approx p(f, g|\theta) \prod_b t_b(u) = q^*(f|\theta)$. PEP is then performed using private powers $\alpha_b$ for each data block. Analytic solutions are again available (covariance matrices now incorporate the inter-domain transform)

$$t_b(u) = N(K_{f,u}K_{uu}^{-1}u; y_b, \alpha_bD_{f,b} + \sigma_y^2I), \quad q(u) = N(u; K_{uu}K_{ff}^{-1}y, K_{uu} - K_{uf}K_{ff}^{-1}K_{fu})$$

where $K_{ff} = Q_{ff} + \text{blkdiag}(\{\alpha_bD_{f,b}\})_b + \sigma_y^2I$ and blkdiag builds a block-diagonal matrix from its inputs. The approximate log-marginal likelihood can also be obtained in closed-form,

$$\log Z_{\text{PEP}} = -\frac{N}{2} \log(2\pi) - \frac{1}{2} \log |K_{ff}| - \frac{1}{2} \sum_{b} \frac{1 - \alpha_b}{2\alpha_b} \log \left(1 + \alpha_bD_{f,b}/\sigma_y^2 \right).$$

Remark 4. When $\alpha_b = 1$ and $W(x, x') = \delta(x - x')$ the structured PEP posterior becomes the PITC posterior and the PEP approximate marginal likelihood becomes the PITC marginal likelihood. Additionally, when $B = N$ we recover FITC as discussed in section 3.2.

Remark 5. When $\alpha_b = 1$ and $B = N$ we recover the inter-domain EP/FITC approach in [13,17].

Remark 6. When $\alpha_b \to 0$ and $W(x, x') = \delta(x - x')$ the structured PEP posterior and approximate marginal likelihood becomes identical to the VFE approach [8].

See fig. [1] for more relationships.

3.4 Classification

For classification, the non-Gaussian likelihood prevents an analytic solution. As such, the iterative PEP procedure is required to obtain the approximate posterior. The projection step requires computation of the log normaliser of the tilted distribution, $\log Z_n = \log E_q^{\gamma = \gamma_f}[p^\alpha(y_n|f)] = \log E_q^{\gamma = \gamma_f}[\Phi^\alpha(y_n|f_n)]$. For general $\alpha$, this quantity is not available in
closed form\footnote{except when \( \alpha = 1 \) and \( \Phi(x) \) is the probit inverse link function, \( \Phi(x) = \int_{-\infty}^{x} N(a; 0, 1) \, da \).}. However, it is a one-dimensional Gaussian integral and can be approximated using Gauss-Hermite quadrature, resulting in an approximate update for the posterior mean and covariance. The approximate log-marginal likelihood can also be obtained and used for hyperparameter optimisation. As \( \alpha \to 0 \), it becomes the variational free-energy used in \cite{14} which employs quadrature for the same purpose. Since the proposed PEP approach is general, recently proposed techniques to scale EP to larger datasets, such as updates using minibatches of data or stochastic optimisation of the energy \cite{15}, can be employed.

4 Gaussian process state-space model

The PEP framework can be generalised to models with latent variables such as the GP latent variable model \cite{2} or the GP state space model (GPSSM) \cite{3}. Here we focus on the GPSSM for brevity. The GPSSM contains continuous valued latent variables \( x \) that evolve according to nonlinear dynamics with Gaussian innovations noise and observations \( y \) that are Gaussian conditioned on the latents,

\[
p(x_t|f, x_{t-1}) = \mathcal{N}(x_t; f(x_{t-1}), \sigma^2_x I), \quad p(y_t|x_t) = \mathcal{N}(y_t; Cx_t, R_y).
\]

The exact and intractable posterior over the latent function \( f \) and the latent variables \( x \) is

\[
p(x, f|y) \propto p(x_0)p(f_{\neq u}|u)p(u) \prod_t p(x_t|f, x_{t-1}) \prod_t p(y_t|x_t). \]

We posit the following approximate posterior, \( q(x, f) \propto p(x_0)p(f_{\neq u}|u) \prod_t \phi_t(x_t, x_{t-1}, u) \prod_t p(y_t|x_t) \) and we use a factored approximation \( \phi_t(x_t, x_{t-1}, u) = \lambda_t(x_{t-1}) \beta_t(x_t) \gamma_t(u) \). The Power EP procedure updates \( \phi_t(x_t, x_{t-1}, u) \) using the steps described in section 3. One crucial difference is the use of a Gaussian projection nested in the computation of the log normaliser of the tilted distribution, \( \log \tilde{Z}_t \) (see supplementary material). In spite of this Gaussian projection, as \( \alpha \to 0 \), we recover the variational treatment as described in \cite{19} with an additional factorised assumption over \( x_{1:T} \), \( q(x_{1:T}) = \prod_t q(x_t) \).

5 Experiments

Full details of the datasets, results, and extra experiments are included in the supplementary material.

5.1 Regression on synthetic datasets

In the first experiment, we investigate the performance of the proposed Power-EP method on toy regression datasets. We vary \( \alpha \) (from 0 VFE to 1 EP/FITC) and the number of pseudo-points (from 5 to 500). We use thirty datasets, each comprising 1000 datapoints that were drawn from a GP with an ARD squared exponential kernel. A 50:50 train/test split was used. The hyperparameters and pseudo-inputs were optimised using L-BFGS with a maximum of 2000 function evaluations. The performances are compared using two metrics: standardised mean squared error (SMSE) and standardised mean log loss (SMLL) as described in \cite{1}. The approximate negative log-marginal likelihood (NLML) for each experiment is also computed. The mean performance using PEP with different \( \alpha \) values and full GP regression is shown
The results demonstrate that as $M$ increases, the SMLL and SMSE of the sparse methods approach that of full GP. Power EP with $\alpha = 0.8$ or $\alpha = 1$ (EP) overestimates the log-marginal likelihood, even for a modest number of pseudo-points. Importantly, however, an intermediate value of $\alpha$ around 0.8 seems to be best for prediction (on average), outperforming both EP and VFE.

![Figure 2: The performance of various $\alpha$ values averaged over 30 trials. See text for more details](image)

### 5.2 Regression on real-world datasets

The experiment above was replicated on 8 UCI regression datasets, each with 20 train/test splits. $\alpha$ was varied between 0 and 1, and $M$ was varied between 5 and 200. We show in fig. 3 the rank of the performance of various $\alpha$ values, averaged over all datasets and their splits, and over all settings of $M$. This figure is generated using the comparison scheme provided in [26], and shows statistical differences in the performance of different $\alpha$s. More precisely, if the gap between the average ranks of any two values of $\alpha$ is above the critical distance (shown on the bottom right), the performances are statistically significantly different. Methods that are not significantly different from each other are linked by a solid line. The rank results demonstrate that neither VFE nor EP is the best performing method on either metric. Indeed, VFE is the worst method for SMLL and EP the worst for SMSE. Intermediate values such as $\alpha = 0.6$ provide more accurate predictive means and better calibrated predictive uncertainty.

![Figure 3: The rank of various $\alpha$ values across all regression datasets, their splits and all settings of $M$, the lower the better. Intermediate $\alpha$ values (not EP or VFE) are best on average.](image)

### 5.3 Binary classification

We also evaluated the PEP method on 6 UCI classification datasets, each has 20 train/test splits. We adopt the experimental protocol used in [15], including: (i) not waiting for PEP.
to converge before making hyperparameter updates, (ii) using minibatches of data points for each PEP sweep. The Adam optimiser was used with default hyperparameters to handle the noisy gradients produced by these approximations [27]. We average the test performances over the splits and \( M = 10, 50, 100 \) and report the result in fig. 4. The rank results, again, show that intermediate \( \alpha \) values perform best on average and that VFE tends to perform poorly on the test log-likelihood metric whilst EP performs poorly on the error metric. In general, VFE will be poor when the likelihood factors are step-like.

![Figure 4: The rank of various \( \alpha \) values across all regression datasets, their splits and various numbers of pseudo-points.](image)

![Figure 5: Learnt transition function and its uncertainty using EP and VI vs. ground truth [black]. Noisy previous/current hidden states are shown as black cross.](image)

### 5.4 Learning Gaussian Process dynamical systems

Finally, we evaluate the PEP approach for the GPSSM, using a one-dimensional nonlinear system governed by 
\[
p(x_t | x_{t-1}) = \mathcal{N}(x_t; f(x_t), 1) \quad \text{and} \quad p(y_t | x_t) = \mathcal{N}(y_t; x_t, 1)
\]
where the transition function is 
\[
f(x_t) = \begin{cases} 
    x_t + 1 & \text{if } x_t < 4 \\
    -4x_t + 21 & \text{if } x_t > 4
\end{cases}
\]
Figure 5 shows the transition function and associated uncertainty learnt using factored EP (\( \alpha = 1 \)) and two different VFE approximations (\( \alpha \to 0 \)): factored \( q(x_1:T) = \prod_t q(x_t) \) and McHutchon’s Markov approximation \( q(x_1:T) = \prod_t q(x_t | x_{t-1}) \) [18,19]. While EP accurately captures the underlying dynamic, factored VFE prefers a simple and inaccurate transition function. This failure mode of VFE methods for time series is well-documented [28] and is due to the bias introduced by the KL divergence term, which means the variational algorithm will tend to learn simpler functions since then the true posterior over \( x_1:T \) is more Gaussian and less coupled. The Markov VFE approach fixes this issue by introducing dependencies in the approximate posterior over \( x \), effectively removing this bias, but introducing greater computational cost.

### 6 Conclusion

This paper provided a new unifying framework for GP pseudo-data approximations based on Power EP that subsumes many previous approaches including FITC, PÎTC, DTC, Titsias’s VFE method, Qi et al’s EP method, and inter-domain variants. It provided a clean computational perspective on the seminal work of Csató and Opper that related FITC to EP, before extending their analysis significantly to include a closed form PEP marginal likelihood approximation for
regression, connections to PITC, and further results on classification and GPSSMs. The new framework was used to devise new algorithms that outperformed the state-of-the-art on GP regression, GP classification and GPSSMs.

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Appendices

A  Some relevant linear algebra and function expansion identities

In this section, we include some identities that will be used throughout the following sections. The Woodbury matrix identity or Woodbury formula is:

\[(A + UCV)^{-1} = A^{-1} - A^{-1}U(C^{-1} + VA^{-1}U)^{-1}VA^{-1}.\] (8)

In general, \(C\) need not be invertible, we can use the Binomial inverse theorem,

\[(A + UCV)^{-1} = A^{-1} - A^{-1}U(C + CVA^{-1}UC)^{-1}CVA^{-1}.\] (9)

When \(C\) is an identity matrix and \(U\) and \(V\) are vectors, the Woodbury identity can be shortened and become the Sherman-Morrison formula,

\[(A + uv^{\top})^{-1} = A^{-1} - A^{-1}uv^{\top}A^{-1}.\] (10)

Another useful identity is the matrix determinant lemma,

\[\det(A + uv^{\top}) = (1 + v^{\top}A^{-1}u)\det(A).\] (11)

The above theorem can be extend for matrices \(U\) and \(V\),

\[\det(A + UV^{\top}) = \det(I + V^{\top}A^{-1}U)\det(A).\] (12)

We also make use of the following Maclaurin series,

\[\exp(x) = 1 + x + \frac{x^2}{2!} + \frac{x^3}{3!} + \cdots\] (13)

and \(\log(1 + x) = x - \frac{x^2}{2} + \frac{x^3}{3} + \cdots\). (14)

B  KL minimisation and moment matching

The difficult step of Power-EP is the projection step, that is how to find the posterior approximation \(q(f)\) that minimises the KL divergence, \(\text{KL}(\tilde{\pi}(f)||q(f))\), where \(\tilde{\pi}(f)\) is the tilted distribution. We have chosen the form of the approximate posterior

\[q(f) = p(f \neq u|\mathbf{u})q(\mathbf{u}) = p(f \neq u|\mathbf{u})\frac{\exp(\theta_{\mathbf{u}}^{\top}\phi(\mathbf{u}))}{\mathcal{Z}(\theta_{\mathbf{u}})},\] (15)

where \(\mathcal{Z}(\theta_{\mathbf{u}}) = \int \exp(\theta_{\mathbf{u}}^{\top}\phi(\mathbf{u}))d\mathbf{u}\) to ensure normalisation. We can then write the KL minimisation objective as follows,

\[
\mathcal{F}_{\text{KL}} = \text{KL}(\tilde{\pi}(f)||q(f))
\] (16)
\begin{align*}
\mathbb{E}[\hat{\mathcal{F}}_{KL}] &= \int \bar{p}(f) \log \frac{\bar{p}(f)}{q(f)} \, df \\
&= \langle \bar{p}(f) \rangle_{\bar{p}(f)} - \langle p(f \neq u | u) \rangle_{\bar{p}(f)} - \theta_u^T \langle \phi(u) \rangle_{\bar{p}(f)} + \log Z(\theta_u). 
\end{align*}

Since \(p(f \neq u | u)\) is the prior conditional distribution, the only free parameter that controls our posterior approximation is \(\theta_u\). As such, to find \(\theta_u\) that minimises \(\mathcal{F}_{KL}\), we find the gradient of \(\mathcal{F}_{KL}\) w.r.t \(\theta_u\) and set it to zero,

\[0 = \frac{d\mathcal{F}_{KL}}{d\theta_u} = -\langle \phi(u) \rangle_{\bar{p}(f)} + \frac{d \log Z(\theta_u)}{d\theta_u},\]

therefore, \(\langle \phi(u) \rangle_{\bar{p}(f)} = \langle \phi(u) \rangle_{q(u)}\). That is, though we are trying to perform the KL minimisation between two Gaussian processes, due to the special form of the posterior approximation, it is sufficient to only match the moments at the inducing points \(u^2\).

### C Shortcuts to the moment matching equations

The most crucial step in Power-EP is the moment matching step as discussed above. This step can be done analytically for the Gaussian case, as the mean and covariance of the approximate posterior can be linked to the cavity distribution as follows,

\[m_u = m_{u|f} + V_{uf} \frac{d \log Z_{\text{tilted}, n}}{dm_{f|n}},\]

\[V_u = V_{u|f} + V_{uf} \frac{d^2 \log Z_{\text{tilted}, n}}{dm_{f|n}^2} V_{f|u},\]

where \(Z_{\text{tilted}, n}\) is the normaliser of the tilted distribution,

\[Z_{\text{tilted}, n} = \int q^n(f)p(y_n | f) \, df\]

\[= \int q^n(f)p(y_n | f_n) \, df\]

\[= \int q^n(f_n)p(y_n | f_n) \, df_n.\]

In words, \(Z_{\text{tilted}, n}\) only depends on the marginal distribution of the cavity process, \(q^n(f_n)\), simplifying the moment matching equations above,

\[m_u = m_{u|f} + V_{uf|f} \frac{d \log Z_{\text{tilted}, n}}{dm_{f|n}},\]

\[V_u = V_{u|f|f} + V_{uf|f} \frac{d^2 \log Z_{\text{tilted}, n}}{dm_{f|n}^2} V_{f|f},\]

\footnote{We can show that this condition gives the minimum of \(\mathcal{F}_{KL}\) by computing the second derivative.}
We initially consider full rank. We start by defining the approximate factors to be in natural parameter form as this makes it
simple to combine and delete them, \( t_n(u) = \mathcal{N}(u; z_n, T_{1,n}, T_{2,n}) = z_n \exp(u' T_{1,n} - \frac{1}{2} u' T_{2,n} u) \). We
initially consider full rank \( T_{2,n} \), but will show that the optimal form is rank 1.

The next goal is to relate these parameters to the approximate GP posterior. The approximate posterior over the pseudo-outputs
has natural parameters \( T_{1,u} = \sum_n T_{1,n} \) and \( T_{2,u} = K_{uu}^{-1} + \sum_n T_{2,n} \). This induces an approximate GP posterior with mean and
covariance function,

\[
\begin{align*}
    m_f &= K_{fu} K_{uu}^{-1} T_{2,u}^{-1} T_{1,u} = K_{fu} \gamma \\
    V_{ff'} &= K_{ff'} - Q_{ff'} + K_{fu} K_{uu}^{-1} T_{2,u}^{-1} K_{uu}^{-1} K_{uf'} = K_{ff'} - K_{fu} \beta K_{uf'}.
\end{align*}
\]

where \( \gamma \) and \( \beta \) are likelihood-dependent terms we wish to store and update using PEP; \( \gamma \) and \( \beta \) fully specify the approximate posterior.

**Deletion step:** The cavity for datapoint \( n \), \( q^n(f) \propto q^n(f)/t^n_n(u) \), has a similar form to
the posterior, but the natural parameters are modified by the deletion, \( T_{1,u} = T_{1,u} - \alpha T_{1,n} \)
and \( T_{2,u} = T_{2,u} - \alpha T_{2,n} \), yielding a new mean and covariance function

\[
    m_f^n = K_{fu} K_{uu}^{-1} T_{2,u}^{-1} T_{1,u} = K_{fu} \gamma^n
\]

\[
    V_{ff'}^n = K_{ff'} - Q_{ff'} + K_{fu} K_{uu}^{-1} T_{2,u}^{-1} K_{uu}^{-1} K_{uf'} = K_{ff'} - K_{fu} \beta K_{uf'}.
\]
At convergence, we have
\[ \log \tilde{q}_n = \text{log } G_{u'2,u}^{-1} K_{uu}^{-1} K_{u'u'} = K_{uu} - K_{uu} \beta^n K_{u'u'}. \] (35)

**Projection step:** The central step in Power EP is the projection step. Obtaining the new approximate unnormalised posterior \( q^*(f) \) such that \( KL(\tilde{p}(f)||q^*(f)) \) is minimised would naively appear intractable. Fortunately, as shown in the previous section, because of the structure of the approximate posterior, \( q(f) = p(f\not\in u|u)q(u) \), the objective, \( KL(\tilde{p}(f)||q^*(f)) \) is minimised when \( E_{\tilde{p}(f)}[\phi(u)] = E_{q(u)}[\phi(u)] \), where \( \phi(u) \) are the sufficient statistics, i.e. when the moments at the pseudo-inputs are matched. This is the central result from which computational savings are derived. Furthermore, this moment matching condition would appear to necessitate computation of a set of integrals to find the zeroth, first and second moments. Using results from the previous section simplifies and provides the following shortcuts,

\[ m_u = m_u^n + \nabla_{u^n} \frac{d}{dm_{u^n}} \log Z_n \] (36)
\[ V_u = V_u^n + \nabla_{u^n} \frac{d^2}{d(m_{u^n})^2} \log Z_n \] (37)

where \( \log Z_n = \log E_{q_n^{\alpha}(f)}[p^\alpha(y_n|f_n)] \) is the log-normaliser of the tilted distribution.

**Update step:** Having computed the new approximate posterior, the fractional approximate factor \( t_{n,new}(u) = q^*(f)/q^n(f) \) can be straightforwardly obtained, resulting in,

\[ T_{1,n,new} = V_u^{-1} m_u - V_u^{n-1} m_u \] (38)
\[ T_{2,n,new} = V_u^{-1} - V_u^{n-1} \] (39)
\[ z_n^\alpha = \tilde{Z}_n \exp(\mathcal{G}_{q^\alpha(u)} - \mathcal{G}_{q^\alpha(u)}), \] (40)

where \( \mathcal{G}_{N(u;z,T_1,T_2)} = \int N(u;z,T_1,T_2)du \). Let \( d_1 = \frac{d}{dm_n^\alpha} \log \tilde{Z}_n \) and \( d_2 = \frac{d^2}{d(m_{u^n})^2} \log \tilde{Z}_n \). Using eq. (8) and eq. (37), we have,

\[ V_u^{n-1} - V_u^n = -V_u^{n-1} V_{u^n} \left[ d_2 - V_u^{n-1} V_{u^n} \right]^{-1} V_{u^n} V_u^{n-1} \] (41)

Let \( v_n = \alpha (-d_2^{-1} V_{u^n} V_u^{n-1} V_{u^n}) \), and \( w_n = V_u^{n-1} V_{u^n} \). Combining eq. (41) and eq. (39) gives

\[ T_{2,n,new} = w_n v_n^{-1} \] (42)

At convergence, we have \( t_n(u) = t_{n,new}(u) \), hence \( T_{2,n} = w_n v_n^{-1} w_n^T \). In words, \( T_{2,n} \) is optimally a rank-1 matrix. Note that,

\[ w_n = V_u^{n-1} V_{u^n} \] (43)
\[ = (K_{uu} - K_{uu} \beta^n K_{uu})^{-1} (K_{u^n} - K_{uu} \beta^n K_{u^n}) \] (44)
\[ = K_{uu}^{-1} (I - K_{u^n} \beta^n)^{-1} (I - K_{uu} \beta^n) K_{u^n} \] (45)
\[ = K_{uu}^{-1} K_{u^n}. \] (46)
Using eq. (36) an eq. (42) gives,

\[
V_u^{-1}m_u = (V_u^{-1} + w_n\alpha v_n^{-1}w_n^T)(m_u^{\backslash n} + V_{uf_n}^{-1}d_1)
\]

\[
= V_u^{-1}m_u^{\backslash n} + w_n\alpha v_n^{-1}w_n^Tm_u^{\backslash n} + V_u^{-1}V_{uf_n}^{-1}d_1 + w_n\alpha v_n^{-1}w_n^TV_{uf_n}^{-1}d_1
\]

(47)

Substituting this result into eq. (38),

\[
T_{1,n,new} = V_u^{-1}m_u - V_u^{-1}m_u^{\backslash n}
\]

(49)

\[
= w_n\alpha v_n^{-1}w_n^Tm_u^{\backslash n} + V_u^{-1}V_{uf_n}^{-1}d_1 + w_n\alpha v_n^{-1}w_n^TV_{uf_n}^{-1}d_1
\]

(50)

Let \(T_{1,n,new} = w_n\alpha v_n^{-1}g_n\), we obtain,

\[
g_n = -\frac{d_1}{d_2} + K_{t_n}u \gamma^{\backslash n}.
\]

(52)

At convergence, \(T_{1,n} = w_n\alpha v_n^{-1}g_n\). Re-writing the form of the approximate factor using \(T_{1,n}\) and \(T_{2,n}\) at convergence,

\[
t_{n}(u) = \tilde{N}(u; z_n, T_{1,n}, T_{2,n})
\]

(53)

\[
= z_n\exp(u^T T_{1,n} - \frac{1}{2} u^T T_{2,n} u)
\]

(54)

\[
= z_n\exp(u^T w_n v_n^{-1} g_n - \frac{1}{2} u^T w_n v_n^{-1} w_n^T u)
\]

(55)

As a result, the minimal and simplest way to parameterise the approximate factor is \(t_{n}(u) = \tilde{z}_n\tilde{N}(w_n^T u; g_n, v_n) = \tilde{z}_n\tilde{N}(K_{t_n}u K_{uu}^{-1} u; g_n, v_n)\), where \(g_n\) and \(v_n\) are scalars, resulting in a significant memory saving compared to the parameterisation using \(T_{1,n}\) and \(T_{2,n}\).

**D.2 Projection**

We now recall the update equations in the projection step (eqns. 36 and 37):

\[
m_u = m_u^{\backslash n} + V_{uf_n}^{-1}d_1,
\]

(56)

\[
V_u = V_u^{\backslash n} + V_{uf_n}^{-1}d_2V_{uf_n}^{\backslash n}
\]

(57)

Note that:

\[
m_u = K_{uu} \gamma,
\]

(58)

\[
V_{uu} = K_{uu} - K_{uu} \beta K_{uu},
\]

(59)

and

\[
m_u^{\backslash n} = K_{uu} \gamma^{\backslash n},
\]

(60)

\[
V_{uu}^{\backslash n} = K_{uu} - K_{uu} \beta^{\backslash n} K_{uu}.
\]

(61)
Using these results, we can convert the update for the mean and covariance, \( \mathbf{m}_u \) and \( \mathbf{V}_u \), into an update for \( \gamma \) and \( \beta \),

\[
\gamma = \mathbf{K}^{-1}_{uu}\mathbf{m}_u = \mathbf{K}^{-1}_{uu}(\mathbf{m}_u^n + \mathbf{V}_u^n d_1) = \gamma^n + \mathbf{K}^{-1}_{uu}\mathbf{V}_u^n d_1, \quad \text{and} \\
\beta = \mathbf{K}^{-1}_{uu}(\mathbf{K}_{uu} - \mathbf{V}_u)\mathbf{K}^{-1}_{uu} = \mathbf{K}^{-1}_{uu}(\mathbf{V}_u^n - \mathbf{V}_u^n d_2 \mathbf{V}_u^n)\mathbf{K}^{-1}_{uu}
\]

and

\[
\gamma^n = \gamma^n + \mathbf{K}^{-1}_{uu}\mathbf{V}_u^n d_2 \mathbf{V}_u^n \mathbf{K}^{-1}_{uu} \\
\beta^n = \beta^n - \mathbf{K}^{-1}_{uu}\mathbf{V}_u^n d_2 \mathbf{V}_u^n \mathbf{K}^{-1}_{uu}.
\]

D.3 Deletion step

Finally, we present how deletion might be accomplished. One direct approach to this step is to divide out the cavity from the cavity, that is,

\[
\begin{align*}
q^n(f) &\propto p(f_n|f) = p(f_n|f) \frac{p(f|u)q(u)}{t_n^\alpha(u)} = p(f|u)q^n(u).
\end{align*}
\]

Instead, we use an alternative using the KL minimisation as used in [13], by realising that doing this will result in an identical outcome as the direct approach since the factor and distributions are Gaussian. Furthermore, we can re-use results from the projection and inclusion steps, by simply swapping the quantities and negating the site approximation variance. In particular, we present projection and deletion side-by-side, to facilitate the comparison,

Projection: \[ q(f) \approx q^n(f)p(y_n|f_n) \]
Deletion: \[ q^n(f) \propto q(f)\frac{1}{t_n^\alpha(u)} \]

The projection step minimizes the KL between the LHS and RHS while moment matching, to get \( q(f) \). We would like to do the same for the deletion step to find \( q^n(f) \), and thus reuse the same moment matching results for \( \gamma \) and \( \beta \) with some modifications.

Our task will be to reuse Equations 64 and 67, the moment matching equations in \( \gamma \) and \( \beta \). We have two differences to account for. Firstly, we need to change any uses of the parameters of the cavity distribution to the parameters of the approximate posterior, \( \mathbf{V}_{uf_n} \) to \( \mathbf{V}_{uf_n}, \gamma^n \) to \( \gamma \) and \( \beta^n \) to \( \beta \). This is the equivalent of re-deriving the entire projection operation, while swapping the symbols (and quantities) for the cavity and the full distribution. Secondly, the derivatives \( d_1 \) and \( d_2 \) are different here, as

\[
\log \tilde{Z}_n = \log \int q(f)\frac{1}{t_n^\alpha(u)}df
\]

Now, we note

\[
\frac{1}{t_n(u)} \propto \frac{1}{\mathcal{N}^\alpha(w_n u; g_n, v_n)}
\]
\[ \alpha \frac{1}{\exp \left( -\frac{\alpha}{2} v_n^{-1} (w_n^T u - g_n)^2 \right)} \]  
\[ = \exp \left( \frac{1}{2} \alpha v_n^{-1} (w_n^T u - g_n)^2 \right) \]  
\[ \sim N (w_n^T u; g_n, -v_n/\alpha) \]  
\[ N (w_n^T u; g_n, -v_n/\alpha) \]  

Then we obtain the derivatives of \( \log \tilde{Z}_n \)

\[ \delta_2 = \frac{d^2 \log \tilde{Z}_n}{dm_{t_n}^2} = -\left( K_{f_n, u} K_{u, u}^{-1} K_{u, f_n} - K_{f_n, u} \beta K_{u, f_n} - v_n / \alpha \right)^{-1} \]  
\[ \delta_1 = \frac{d \log \tilde{Z}_n}{dm_{t_n}} = (K_{f_n, u} \gamma - g_n) \delta_2 \]  

Putting the above results together, we obtain,

\[ \gamma^n = \gamma + K_{u u}^{-1} V_{u n} \delta_1, \quad \text{and} \]  
\[ \beta^n = \beta - K_{u u}^{-1} V_{u n} \delta_2 V_{f_n u} K_{u u}^{-1} \]  

D.4 Summary of the PEP procedure

We summarise here the key steps and equations that we have obtained, that are used in the implementation:

1. Initialise the parameters: \( \{ g_n = 0 \}_{n=1}^N, \{ v_n = \infty \}_{n=1}^N, \gamma = 0_{M \times 1} \) and \( \beta = 0_{M \times M} \)

2. Loop through all datapoint until convergence:

   (a) Deletion step: find \( \gamma^n \) and \( \beta^n \)

   \[ \gamma^n = \gamma + K_{u u}^{-1} V_{u n} \delta_1, \quad \text{and} \]  
   \[ \beta^n = \beta - K_{u u}^{-1} V_{u n} \delta_2 V_{f_n u} K_{u u}^{-1} \]  

   (b) Projection step: find \( \gamma \) and \( \beta \)

   \[ \gamma = \gamma^n + K_{u u}^{-1} V_{u n} \delta_1, \]  
   \[ \beta = \beta^n - K_{u u}^{-1} V_{u n} \delta_2 V_{f_n u} K_{u u}^{-1} \]  

   (c) Update step: find \( g_{n, \text{new}} \) and \( v_{n, \text{new}} \)

   \[ g_{n, \text{new}} = -\frac{d_1}{d_2} + K_{f_n, u} \gamma^n, \]  
   \[ v_{n, \text{new}} = -d_2^{-1} - V_{f_n u} V_{u}^{n-1} V_{u n}^{n} \]  

and parameters for the full factor,

\[ v_n \left( v_n^{-1} + (1 - \alpha) v_n^{-1} \right)^{-1} \]  
\[ g_n \left( g_n v_n^{-1} + (1 - \alpha) g_n v_n^{-1} \right) \]
E Power-EP energy for sparse GP regression and classification

The Power-EP procedure gives an approximate marginal likelihood, which is the negative Power-EP energy, as follows,

\[ F = \phi_{\text{post}} - \phi_{\text{prior}} + \frac{1}{\alpha} \sum_n \log \mathcal{Z}_{\text{tilted},n} + \phi_{\text{cav},n} - \phi_{\text{post}} \]  

(88)

where \( \phi_{\text{post}} \) is the log normaliser of the approximate posterior, that is,

\[ \phi_{\text{post}} = \log \int p(f_{\neq \mathbf{u}}|\mathbf{u}) \exp(\theta^\top \phi(\mathbf{u})) df_{\neq \mathbf{u}} d\mathbf{u} \]  

(89)

\[ = \frac{M}{2} \log(2\pi) + \frac{1}{2} \log |\mathbf{V}| + \frac{1}{2} \mathbf{m}^\top \mathbf{V}^{-1} \mathbf{m}, \]  

(90)

\[ \phi_{\text{prior}} = \frac{M}{2} \log(2\pi) + \frac{1}{2} \log |\mathbf{K}_{\mathbf{uu}}|. \]  

(93)

where \( \mathbf{m} \) and \( \mathbf{V} \) are the mean and covariance of the posterior distribution over \( \mathbf{u} \), respectively.

Similarly,

\[ \phi_{\text{cav},n} = \frac{M}{2} \log(2\pi) + \frac{1}{2} \log |\mathbf{V}_{\text{cav},n}| + \frac{1}{2} \mathbf{m}_{\text{cav},n}^\top \mathbf{V}_{\text{cav},n}^{-1} \mathbf{m}_{\text{cav},n}, \]  

(92)

and \( \phi_{\text{prior}} = \frac{M}{2} \log(2\pi) + \frac{1}{2} \log |\mathbf{K}_{\mathbf{uu}}|. \)  

(93)

Finally, \( \log \mathcal{Z}_{\text{tilted},n} \) is the log normalising constant of the tilted distribution,

\[ \log \mathcal{Z}_{\text{tilted}} = \log \int q_{\text{cav}}(f)p^\alpha(\mathbf{y}_n|f)df \]  

(94)

\[ = \log \int p(f_{\neq \mathbf{u}}|\mathbf{u})q_{\text{cav}}(\mathbf{u})p^\alpha(\mathbf{y}_n|f)df_{\neq \mathbf{u}} d\mathbf{u} \]  

(95)

\[ = \log \int p(f_n|\mathbf{u})q_{\text{cav}}(\mathbf{u})p^\alpha(\mathbf{y}_n|f_n)df_n d\mathbf{u} \]  

(96)

Next, we can write down the form of the natural parameters of the approximate posterior and the cavity distribution, based on the approximate factor’s parameters, as follows,

\[ \mathbf{V}^{-1} = \mathbf{K}_{\mathbf{uu}}^{-1} + \sum_i \mathbf{w}_i \tau_i \tilde{y}_i \mathbf{w}_i^\top \]  

(97)

\[ \mathbf{V}^{-1} \mathbf{m} = \sum_i \mathbf{w}_i \tau_i \tilde{y}_i \]  

(98)

\[ \mathbf{V}_{\text{cav},n}^{-1} = \mathbf{V}^{-1} - \alpha \mathbf{w}_n \tau_n \mathbf{w}_n^\top \]  

(99)

\[ \mathbf{V}_{\text{cav},n}^{-1} \mathbf{m}_{\text{cav},n} = \mathbf{V}^{-1} - \alpha \mathbf{w}_n \tau_n \tilde{g}_n \]  

(100)

Note that \( \tau_i := u_i^{-1} \). Using eq. (10) and eq. (99) gives,

\[ \mathbf{V}_{\text{cav},n} = \mathbf{V} + \frac{\mathbf{Vw}_n \alpha \tau_n \mathbf{w}_n^\top \mathbf{V}}{1 - \mathbf{w}_n \alpha \tau_n \mathbf{Vw}_n}. \]  

(101)

Using eq. (11) and eq. (99) gives,

\[ \log \det(\mathbf{V}_{\text{cav},n}) = \log \det(\mathbf{V}) - \log(1 - \mathbf{w}_n \alpha \tau_n \mathbf{Vw}_n). \]  

(102)
We have shown in the previous section that the fixed point solution of the Power-EP iterations

$$\phi_{\text{cav},n} = \frac{M}{2} \log(2\pi) + \frac{1}{2} \log \det(V) + \frac{1}{2} m^T V^{-1} m$$

when

$$Q = \frac{1}{2} g_n \alpha \tau_n w_n V_{\text{cav},n} w_n \alpha \tau_n g_n - \frac{1}{2} m^T w_n \alpha \tau_n V w_n$$

Substituting eq. (101) and eq. (102) back to eq. (92) results in,

$$\phi_{\text{cav},n} = \frac{M}{2} \log(2\pi) + \frac{1}{2} \log \det(V) + \frac{1}{2} m^T V^{-1} m$$

We now plug the above result back into the approximate marginal likelihood, yielding,

$$\mathcal{F} = \frac{1}{2} \log |V| + \frac{1}{2} m^T V^{-1} m - \frac{1}{2} \log |K_{uu}| + \frac{1}{\alpha} \sum_n \log Z_{\text{tilted},n}$$

$$+ \sum_n \left[ -\frac{1}{2\alpha} \log(1 - w_n^T \alpha \tau_n V w_n) + \frac{1}{2} m^T w_n \alpha \tau_n V w_n \right]$$

$$+ \frac{1}{2} g_n \alpha \tau_n w_n^T V_{\text{cav},n} w_n \alpha \tau_n g_n - \frac{1}{2} m^T w_n \alpha \tau_n V w_n$$

$$= \frac{1}{2} \log |V| + \frac{1}{2} m^T V^{-1} m - \frac{1}{2} \log |K_{uu}| + \sum_n \left[ -\frac{1}{2} \log(1 - w_n^T \alpha \tau_n V w_n) + \frac{1}{2} m^T w_n \alpha \tau_n V w_n \right]$$

$$+ \frac{1}{2} g_n \alpha \tau_n w_n^T V_{\text{cav},n} w_n \alpha \tau_n g_n - \frac{1}{2} m^T w_n \alpha \tau_n V w_n$$

$$= -\frac{N}{2} \log(2\pi) - \frac{1}{2} \log |D + Q_{ff}| - \frac{1}{2} y^T (D + Q_{ff})^{-1} y - \frac{1}{2} \sum_n \log \left( \frac{d_n}{\sigma^2_y} \right)$$

where

$$Q_{ff} = K_{fu} K_{uu}^{-1} K_{uf}$$

and $D$ is a diagonal matrix, $D_{nn} = d_n$.

E.1 Regression

We have shown in the previous section that the fixed point solution of the Power-EP iterations can be obtained analytically for the regression case, $g_n = y_n$ and $\tau^{-1} = d_n = \alpha(K_{fn} - K_{fu} K_{uu}^{-1} K_{uf}) + \sigma^2_y$. Crucially, we can obtain a closed form expression for $\log Z_{\text{tilted},n}$,

$$\log Z_{\text{tilted},n} = \frac{\alpha}{2} \log(2\pi \sigma^2_y) + \frac{\alpha}{2} \log(\sigma^2_y) - \frac{1}{2} \log(\alpha v_n + \sigma^2_y) - \frac{1}{2} \frac{(y_n - \mu_n)^2}{\alpha v_n + \sigma^2_y}$$

where $\mu_n = w_n^T m_{\text{cav}} = w_n^T V_{\text{cav}} (V^{-1} m - w_n \alpha \tau_n y_n)$ and $v_n = \frac{d_n - \sigma^2_y}{\alpha} + w_n^T V_{\text{cav}} w_n$. We can therefore simplify the approximate marginal likelihood $F$ further,

$$F = -\frac{N}{2} \log(2\pi) - \frac{1}{2} \log |D + Q_{ff}| - \frac{1}{2} \log(\alpha v_n + \sigma^2_y) - \frac{1}{2} \frac{(y_n - \mu_n)^2}{\alpha v_n + \sigma^2_y}$$

where $Q_{ff} = K_{fu} K_{uu}^{-1} K_{uf}$ and $D$ is a diagonal matrix, $D_{nn} = d_n$.

When $\alpha = 1$, the approximate marginal likelihood takes the same form as the FITC marginal likelihood,

$$F = -\frac{N}{2} \log(2\pi) - \frac{1}{2} \log |D + Q_{ff}| - \frac{1}{2} y^T (D + Q_{ff})^{-1} y$$

where $D_{nn} = d_n = K_{fn} - K_{fu} K_{uu}^{-1} K_{uf} + \sigma^2_y$.

When $\alpha$ tends to 0, we have,

$$\lim_{\alpha \to 0} \frac{1 - \alpha}{2\alpha} \sum_n \log \left( \frac{d_n}{\sigma^2_y} \right) = \frac{1}{2} \sum_n \lim_{\alpha \to 0} \frac{\log(1 + \frac{\alpha y_n}{\sigma^2_y})}{\alpha} = \frac{\sum_n h_n}{2\sigma^2_y},$$

22
where \( h_n = K_{f_n f_n} - K_{f_n u} K_{u u}^{-1} K_{u f_n} \). Therefore,

\[
\mathcal{F} = -\frac{N}{2} \log(2\pi) - \frac{1}{2} \log |\sigma_y^2 I + Q_\alpha| - \frac{1}{2} y^T (\sigma_y^2 I + Q_\alpha)^{-1} y - \frac{\sum_n h_n}{2\sigma_y^2},
\] (109)

which is the variational lower bound of Titsias [8].

### E.2 Classification

In contrast to the regression case, the approximate marginal likelihood for classification cannot be simplified due to the non-Gaussian likelihood. Specifically, \( \log Z_{\text{tilted, } n} \) is not analytically tractable, except when \( \alpha = 1 \) and the classification link function is the Gaussian cdf. However, this quantity can be evaluated numerically, using sampling or Gauss-Hermite quadrature, since it only involves a one-dimensional integral.

We now consider the case when \( \alpha \) tends to 0 and verify that in such case the approximate marginal likelihood becomes the variational lower bound. We first find the limits of individual terms in eq. (104):

\[
\lim_{\alpha \to 0} -\frac{1}{2\alpha} \log(1 - w_n^T \alpha \tau_n V w_n) = \frac{1}{2} w_n^T \tau_n V w_n,
\] (110)

\[
\frac{1}{2} \left[ \frac{m^T w_n \tau_n w_n^T m}{1 - w_n^T \alpha \tau_n V w_n} \right]_{\alpha=0} = \frac{1}{2} m^T w_n \tau_n w_n^T m,
\] (111)

\[
\frac{1}{2} g_n \tau_n w_n^T V_{cav, n} \alpha \tau_n g_n \bigg|_{\alpha=0} = 0
\] (112)

\[
-g_n \tau_n w_n^T V_{cav, n} V^{-1} m \bigg|_{\alpha=0} = -g_n \tau_n w_n^T m.
\] (113)

We turn our attention to \( \log Z_{\text{tilted, } n} \). First, we expand \( p^\alpha(y_n | f_n) \) using eq. (13):

\[
p^\alpha(y_n | f_n) = \exp(\alpha \log p(y_n | f_n))
\] (114)

\[
= 1 + \alpha \log p(y_n | f_n) + \xi(\alpha^2).
\] (115)

Substituting this result back into \( \log Z_{\text{tilted}} / \alpha \) gives,

\[
\frac{1}{\alpha} \log Z_{\text{tilted}} = \frac{1}{\alpha} \log \int p(f_n | u) q_{cav}(u) p^\alpha(y_n | f_n) df_n du.
\] (116)

\[
= \frac{1}{\alpha} \log \int p(f_n | u) q_{cav}(u) [1 + \alpha \log p(y_n | f_n) + \xi(\alpha^2)] df_n du
\] (117)

\[
= \frac{1}{\alpha} \log \left[ 1 + \alpha \int p(f_n | u) q_{cav}(u) \log p(y_n | f_n) df_n du + \alpha^2 \xi(1) \right]
\] (118)

\[
= \frac{1}{\alpha} \left[ \alpha \int p(f_n | u) q_{cav}(u) \log p(y_n | f_n) df_n du + \alpha^2 \xi(1) \right]
\] (119)

\[
= \int p(f_n | u) q_{cav}(u) \log p(y_n | f_n) df_n du + \alpha \xi(1).
\] (120)

Therefore,

\[
\lim_{\alpha \to 0} \frac{1}{\alpha} \log Z_{\text{tilted}} = \int p(f_n | u) q(u) \log p(y_n | f_n) df_n du.
\] (121)
Putting these results into eq. (104), we obtain,

\[
\mathcal{F} = \frac{1}{2} \log |V| + \frac{1}{2} m^T V^{-1} m - \frac{1}{2} \log |K_{uu}|
\]

\[+ \sum_n \frac{1}{2} w_n^T \tau_n V w_n + \frac{1}{2} m^T \tau_n w_n^T m - g_n \tau_n w_n^T m + \int p(f_n|u)q(u) \log p(y_n|f_n) df_n du\]

\[= \frac{1}{2} \log |V| + \frac{1}{2} m^T V^{-1} m - \frac{1}{2} \log |K_{uu}| + \frac{1}{2} m^T (V^{-1} - K_{uu}^{-1}) m - m^T V^{-1} m
\]

\[+ \sum_n \frac{1}{2} w_n^T \tau_n V w_n + \int p(f_n|u)q(u) \log p(y_n|f_n) df_n du\]

\[= \frac{1}{2} \log |V| - \frac{1}{2} m^T K_{uu}^{-1} m - \frac{1}{2} \log |K_{uu}| + \sum_n \frac{1}{2} w_n^T \tau_n V w_n + \sum_n \int p(f_n|u)q(u) \log p(y_n|f_n) df_n du.\]  \hspace{1cm} (122)

We now write down the evidence lower bound of the global variational approach of Titsias [8], as applied to the classification case [14],

\[
\mathcal{F}_{VFE} = -\text{KL}(q(u)||p(u)) + \sum_n \int p(f_n|u)q(u) \log p(y_n|f_n) df_n du
\]  \hspace{1cm} (123)

where

\[
-\text{KL}(q(u)||p(u)) = -\frac{1}{2} \text{trace}(K_{uu}^{-1} V) - \frac{1}{2} m^T K_{uu}^{-1} m + \frac{M}{2} - \frac{1}{2} \log |K_{uu}| + \frac{1}{2} \log |V|
\]

\[= -\frac{1}{2} \text{trace}(V^{-1} - \sum_n w_n \tau_n w_n^T) - \frac{1}{2} m^T K_{uu}^{-1} m + \frac{M}{2} - \frac{1}{2} \log |K_{uu}| + \frac{1}{2} \log |V|
\]

\[= \frac{1}{2} \text{trace}(\sum_n w_n \tau_n w_n^T V) - \frac{1}{2} m^T K_{uu}^{-1} m - \frac{1}{2} \log |K_{uu}| + \frac{1}{2} \log |V|. \]  \hspace{1cm} (124)

Therefore, \(\mathcal{F}_{VFE}\) is identical to the limit of the approximate marginal likelihood provided by power-EP as shown in eq. (122).

**F Power-EP for the Gaussian process state space model**

We recap here the description of the model and include the full details of the inference procedure. The GPSSM can be compactly represented as follows in the case where the dynamical noise is assumed Gaussian,

\[
p(x_t|f, x_{t-1}) = \mathcal{N}(x_t; f(x_{t-1}), \sigma_x^2),
\]

\[
p(y_t|x_t) = \mathcal{N}(y_t; Cx_t, R_y),
\]

where \(x\) and \(y\) are the latent variables and the measurements respectively. The exact and intractable posterior over the latent function \(f\) and the hidden states \(x\) is as follows,

\[
p(x, f) \propto p(x_0)p(f) \prod_t p(x_t|f, x_{t-1}) \prod_t p(y_t|x_t)
\]
We posit the following approximate posterior, which allows us to employ Power-EP to perform inference,

\[ q(x, f) \propto p(x_0)p(f \neq u|u) \prod_t \lambda_t(x_{t-1}) \beta_t(x_t) \gamma_t(u) \prod_t p(y_t|x_t), \]

where \( \lambda_t, \beta_t \) and \( \gamma_t \) are approximate factors, and \( u \) are the inducing points. The inducing points \( u \) are used in this context to facilitate analytically tractable message passing, and, if \( |u| < T \), to sidestep the cubic cost of the GP. Note that we did not have separate approximate factors for the emission factors, since the correct factors are assumed Gaussian, the approximation becomes exact here.

### F.1 The Power-EP procedure

We next discuss the detail of the Power-EP procedure, i.e. how to iteratively update \( \lambda_t, \beta_t \) and \( \gamma_t \).

1. **Deletion step:** compute the cavity distribution

\[ q^{\backslash i}(x, f) \propto q(x, f)/(\lambda_i(x_{i-1}) \beta_i(x_i) \gamma_i(u))^\alpha \]

2. **Projection step:**

\[ q(x, f) \leftarrow \arg\min_{q(x, f)} \text{KL}(\tilde{p}(x, f)||q(x, f)) \]

where \( \tilde{p}(x, f) = q^{\backslash i}(x, f)p^\alpha(x_i|f, x_{i-1}) \)

3. **Update step:**

\[ \lambda_{i, new}(x_{i-1}) \beta_{i, new}(x_i) \gamma_{i, new}(u) \propto q(x, f)/q^{\backslash i}(x, f), \]

\[ \lambda_i(x_{i-1}) = \lambda_{i, old}(x_{i-1}) \lambda_{i, new}(x_{i-1}), \]

similarly for \( \beta_i(x_i) \) and \( \gamma_i(u) \).

When the factors are in the exponential family, the deletion and update steps above are simple as they only involve adding or subtracting (fractions of) corresponding natural parameters. The projection step is made tractable by a Gaussian projection which is nested in the computation of the log normaliser of the tilted distribution, \( \log Z_{\text{tilted}, x, i} \), where,

\[ \log Z_{\text{tilted}} = \int p^\alpha(x_i|f, x_{i-1})p(f \neq u|u)q^{\backslash i}(u)q^{\backslash^i}(x_{i-1})q^{\backslash^i}(x_i)df dx_{i-1} dx_i \]

The computation of \( \log Z_{\text{tilted}, x, i} \) is crucial for the moment matching step of Power-EP, since the first and second moments can be computed from \( \log Z_{\text{tilted}, x, i} \) as discussed in section C. The first integral over \( f \) in the equation above is tractable since it only involves a marginal conditional distribution, \( p(f_i|u) \), and the cavity \( q^{\backslash^i}(u) \). Following [29][31], we approximate the second integral w.r.t. \( x_{i-1} \) by a Gaussian distribution over \( x_i \) with the following mean and variance,

\[ \bar{m}_i = E_1 A \quad (125) \]
\[
\tilde{u}_i = \frac{\sigma_x^2}{\alpha} + w_i - \tilde{m}_i^2
\]  

(126)

where \( w_i = E_0 + \text{tr} (\mathbf{B} \mathbf{E}_2) \), \( \mathbf{E}_0 = E_{q(t_0|x_{t-1})} [\mathbf{K}_{f_1}] \), \( \mathbf{E}_1 = E_{q(t_1|x_{t-1})} [\mathbf{K}_{f_1}] \), \( \mathbf{E}_2 = E_{q(t_2|x_{t-1})} [\mathbf{K}_{f_1}] \), \( \mathbf{A} = \mathbf{K}_{u,u}^{-1} \mathbf{m}_u \) and \( \mathbf{B} = \mathbf{K}_{u,u}^{-1} (\mathbf{V}_u^T + \mathbf{m}_u^T \mathbf{m}_u) \mathbf{K}_{u,u}^{-1} - \mathbf{K}_{u,u}^{-1} \). The equations above require the expectations of the kernel matrix under a Gaussian distribution over the inputs, which are analytically tractable for widely used kernels such as exponentiated quadratic, linear or a more general class of spectral mixture kernels [21]. The third integral w.r.t \( x_i \) is now straightforward as it is the normaliser of a convolution of two Gaussian distributions. In spite of this Gaussian projection, as \( \alpha \to 0 \), we recover McHutchon’s variational treatment with an additional factorised assumption over \( x_{1:T} \), \( q(x_{1:T}) = \prod_{t} q(x_t) \) [19]. We will show this equivalence in the next section.

F.2 The approximate marginal likelihood

Similar to the regression and classification case, we can obtain an approximate marginal likelihood as follows,

\[
\mathcal{F} = \phi_{\text{post}} + \phi_{\text{post},x_0} - \phi_{\text{prior}} - \phi_{\text{prior},x_0} + \left[ \frac{1}{\alpha} \sum_t \log Z_{\text{tilted},x,t} + \phi_{\text{cav},x,t} - \phi_{\text{post}} \right]
\]

(127)

\[
+ \left[ \frac{1}{\alpha} \sum_t \log Z_{\text{tilted},y,t} + \phi_{\text{cav},y,t} - \phi_{\text{post}} \right].
\]

The above expression is not analytically tractable due to the difficult term \( \log Z_{\text{tilted},x,t} \); however, this can be approximated using the Gaussian projection discussed in the previous section. For simplicity, we will consider an one dimensional hidden variable case. Letting \( q(t|x_t) = \mathcal{N}(x_t; m_t, v_t) \) and using eqns. eqs. (126) and (127) we have,

\[
2 \log Z_{\text{tilted},x,t} \approx \log \left( \frac{2\pi \sigma_x^2}{\alpha} \right) - \log(2\pi) - \log \left( \frac{\sigma_x^2}{\alpha} + w_t - \tilde{m}_t^2 + v_t \right) - \frac{(m_t - \tilde{m}_t)^2}{\frac{\sigma_x^2}{\alpha} + w_t - \tilde{m}_t^2 + v_t}
\]

(128)

\[
= - \log(1 + \frac{\alpha(w_t - \tilde{m}_t^2 + v_t)}{\sigma_x^2}) - \alpha \log(2\pi \sigma_x^2) - \frac{\alpha(m_t - \tilde{m}_t)^2}{\sigma_x^2 + \alpha(w_t - \tilde{m}_t^2 + v_t)}
\]

(129)

We divide the above by \( \alpha \) and obtain its limits as \( \alpha \to 0 \),

\[
\lim_{\alpha \to 0} \frac{1}{\alpha} \log Z_{\text{approx},x,t} = -\frac{1}{2} \log(2\pi \sigma_x^2) - \frac{1}{2} \left( \frac{m_t - \tilde{m}_t^2 + v_t}{\sigma_x^2} - \frac{(m_t - \tilde{m}_t)^2}{\sigma_x^2} \right)
\]

(130)

\[
= -\frac{1}{2} \log(2\pi \sigma_x^2) - \frac{1}{2} \left( \frac{m_t^2 - 2m_t \tilde{m}_t + v_t}{\sigma_x^2} \right)
\]

(131)

Despite that we have used the Gaussian approximation, the limit above is exactly the expected log likelihood, \( \mathcal{F}_t = \langle \log p(x_t|f_t, x_{t-1}) \rangle_{q(f_t)q(x_t)q(x_{t-1})} \), as appeared in the variational lower bound,

\[
\mathcal{F}_t = \left\langle -\frac{1}{2} \log(2\pi \sigma_x^2) - \frac{1}{2} \left( \frac{x_t - f(x_{t-1})}{\sigma_x^2} \right)^2 \right\rangle_{q(f_t)q(x_t)q(x_{t-1})}
\]

(132)
\begin{align*}
&= -\frac{1}{2} \log(2\pi\sigma^2_x) - \frac{1}{2} \left( \langle x_t^2 \rangle_{q(x_t)} - 2 \langle x_t \rangle_{q(x_t)} \langle f(x_{t-1}) \rangle_{q(f)} q(x_{t-1}) \right) \frac{1}{\sigma_x^2} \\
&= -\frac{1}{2} \log(2\pi\sigma^2_x) - \frac{1}{2} \frac{m_t^2 - 2m_t \tilde{m}_t + w_t + v_t}{\sigma_x^2}. \quad (133)
\end{align*}

\section{Extra experimental results}

\subsection{Comparison between EP and VFE on a 1D example}

We considered a simple 1D regression task that has only two datapoints and the underlying function is generated from a Gaussian process. We fixed the hyperparameters and the pseudo-inputs, and compared the predictions made by sparse approximation techniques and exact inference. We plot the predictions at test points as well as the contours the exact and approximate posteriors at training points, with 1, 3, 5, 6, 8 inducing points in figs. 6, 7, 8, 9, 10 respectively. The exact and approximate marginal likelihoods (MLs) provided by VFE and EP are also included in the plots. The results demonstrate that, for fixed hyperparameters and pseudo-points, VFE tends to give more accurate estimates for the mean and more confident predictions, while EP is more conservative by providing larger uncertainty. This results in a more compact posterior as training points for VFE compared to EP. The variational lower bound is always smaller than the approximate ML provided by EP, and is \textit{loose}, i.e. much smaller than the true ML. EP, despite giving more correct estimates to the true ML, can \textit{overestimate} this value [see fig. 6].

\begin{figure}[h]
\centering
\includegraphics[width=\textwidth]{figure6}
\caption{Predictions at test points [left] and posteriors at training points [right] given by exact inference and approximate inference using VFE and EP with 1 pseudo-point. Training points are shown in black and the pseudo-points are in colour. The exact and approximate log marginal likelihoods, and the symmetric KL divergences between the posteriors are included in the title.}
\end{figure}
\[ L_{\text{full}} = -3.16, F_{\text{VFE}} = -9.29, F_{\text{EP}} = -3.17 \]

Figure 7: Predictions at test points [left] and posteriors at training points [right] given by exact inference and approximate inference using VFE and EP with 3 pseudo-points.

\[ sKL_{\text{VFE}} = 6.493, sKL_{\text{EP}} = 10.020 \]

\[ L_{\text{full}} = -3.16, F_{\text{VFE}} = -11.19, F_{\text{EP}} = -3.16 \]

\[ sKL_{\text{VFE}} = 10.216, sKL_{\text{EP}} = 15.102 \]

Figure 8: Predictions at test points [left] and posteriors at training points [right] given by exact inference and approximate inference using VFE and EP with 5 pseudo-points.
Figure 9: Predictions at test points [left] and posteriors at training points [right] given by exact inference and approximate inference using VFE and EP with 6 pseudo-points.

\[
\mathcal{L}_{\text{full}} = -3.16, \mathcal{F}_{\text{VFE}} = -6.21, \mathcal{F}_{\text{EP}} = -3.15
\]

\[
s_{\text{KL}}_{\text{VFE}} = 5.263, s_{\text{KL}}_{\text{EP}} = 7.518
\]

Figure 10: Predictions at test points [left] and posteriors at training points [right] given by exact inference and approximate inference using VFE and EP with 8 pseudo-points.

\[
\mathcal{L}_{\text{full}} = -3.16, \mathcal{F}_{\text{VFE}} = -3.17, \mathcal{F}_{\text{EP}} = -3.16
\]

\[
s_{\text{KL}}_{\text{VFE}} = 4.905, s_{\text{KL}}_{\text{EP}} = 4.895
\]
G.2 Comparison between various $\alpha$ values on a toy regression problem

Figure 11: Results on a toy regression problem: Standardised mean log-loss on the test set for various values of $\alpha$ and various number of pseudo-points $M$. Each trace is for one split, bold line is the mean. The rightmost figure shows the mean for various $\alpha$, and the results using GP regression.
Figure 12: Results on a toy regression problem: Standardised mean squared error on the test set for various values of $\alpha$ and various number of pseudo-points $M$. Each trace is for one split, bold line is the mean. The rightmost figure shows the mean for various $\alpha$, and the results using GP regression.
Figure 13: Results on a toy regression problem: The negative log marginal likelihood of the training set after training for various values of $\alpha$ and various number of pseudo-points $M$. Each trace is for one split, bold line is the mean. The rightmost figure shows the mean for various $\alpha$, and the results using GP regression. Power EP with $\alpha$ close to 1.
Figure 14: Results on real-world regression problems: Negative training log-marginal likelihood for different datasets, various values of $\alpha$ and various number of pseudo-points $M$. Each trace is for one split, bold line is the mean. The rightmost figures show the mean for various $\alpha$ for comparison. Lower is better [however, lower could mean overestimation].
Figure 15: Results on real-world regression problems: Negative training log-marginal likelihood for different datasets, various values of $\alpha$ and various number of pseudo-points $M$, averaged over 20 splits. Lower is better [however, lower could mean overestimation].
Figure 16: Results on real-world regression problems: Standardised mean squared error on the test set for different datasets, various values of $\alpha$ and various number of pseudo-points $M$. Each trace is for one split, bold line is the mean. The rightmost figures show the mean for various $\alpha$ for comparison. Lower is better.
Figure 17: Results on real-world regression problems: Standardised mean squared error on the test set for different datasets, various values of $\alpha$ and various number of pseudo-points $M$, averaged over 20 splits. Lower is better.
Figure 18: Results on real-world regression problems: Standardised mean log loss on the test set for different datasets, various values of $\alpha$ and various number of pseudo-points $M$. Each trace is for one split, bold line is the mean. The rightmost figures show the mean for various $\alpha$ for comparison. Lower is better.
Figure 19: Results on real-world regression problems: Standardised mean log loss on the test set for different datasets, various values of $\alpha$ and various number of pseudo-points $M$, averaged over 20 splits. Lower is better.
G.4 Binary classification on even/odd MNIST digits

Figure 20: The test error and log-likelihood of the MNIST binary classification task (M=100).

Figure 21: The test error and log-likelihood of the MNIST binary classification task (M=200).